Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 05:36 AM EDT

PDB ID	:	2OGJ
Title	:	Crystal structure of a dihydroorotase
Authors	:	Sugadev, R.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-01-05
Resolution	:	2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

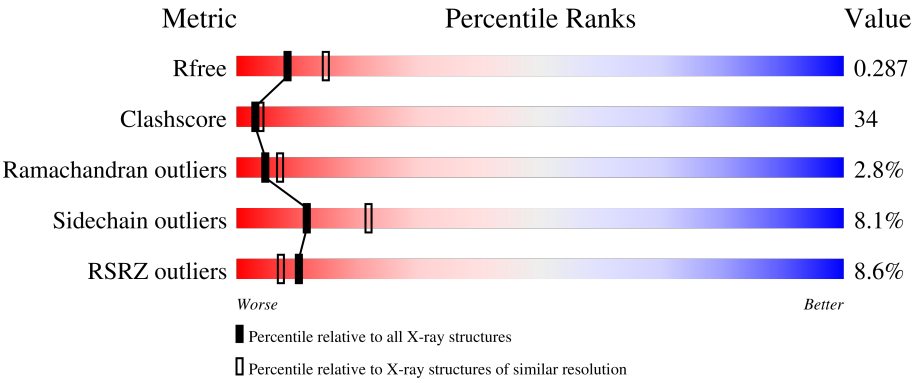
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	417	2% 57% 28% 6% 9%
1	B	417	2% 52% 31% 5% • 12%
1	C	417	13% 34% 36% 6% 24%
1	D	417	9% 46% 37% • 13%
1	E	417	6% 49% 34% 6% 11%

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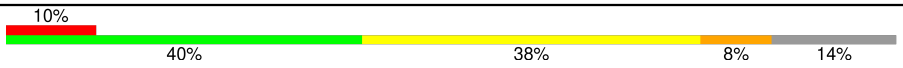
Mol	Chain	Length	Quality of chain
1	F	417	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	KCX	A	175	-	-	X	-
1	KCX	B	175	-	-	X	-
1	KCX	D	175	-	-	X	-
1	KCX	E	175	-	-	X	-
1	KCX	F	175	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16585 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydroorotase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	Se	0	0	0
			2876	1814	503	547	5	7			
1	B	369	Total	C	N	O	S	Se	0	0	0
			2809	1773	488	536	5	7			
1	C	317	Total	C	N	O	S	Se	0	0	0
			2433	1550	419	453	5	6			
1	D	364	Total	C	N	O	S	Se	0	0	0
			2782	1760	484	526	5	7			
1	E	372	Total	C	N	O	S	Se	0	0	0
			2822	1781	492	537	5	7			
1	F	359	Total	C	N	O	S	Se	0	0	0
			2728	1728	469	519	5	7			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q8UAV1
A	2	SER	-	expression tag	UNP Q8UAV1
A	3	LEU	-	expression tag	UNP Q8UAV1
A	410	GLU	-	expression tag	UNP Q8UAV1
A	411	GLY	-	expression tag	UNP Q8UAV1
A	412	HIS	-	expression tag	UNP Q8UAV1
A	413	HIS	-	expression tag	UNP Q8UAV1
A	414	HIS	-	expression tag	UNP Q8UAV1
A	415	HIS	-	expression tag	UNP Q8UAV1
A	416	HIS	-	expression tag	UNP Q8UAV1
A	417	HIS	-	expression tag	UNP Q8UAV1
B	1	MSE	-	expression tag	UNP Q8UAV1
B	2	SER	-	expression tag	UNP Q8UAV1
B	3	LEU	-	expression tag	UNP Q8UAV1
B	410	GLU	-	expression tag	UNP Q8UAV1
B	411	GLY	-	expression tag	UNP Q8UAV1
B	412	HIS	-	expression tag	UNP Q8UAV1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	413	HIS	-	expression tag	UNP Q8UAV1
B	414	HIS	-	expression tag	UNP Q8UAV1
B	415	HIS	-	expression tag	UNP Q8UAV1
B	416	HIS	-	expression tag	UNP Q8UAV1
B	417	HIS	-	expression tag	UNP Q8UAV1
C	1	MSE	-	expression tag	UNP Q8UAV1
C	2	SER	-	expression tag	UNP Q8UAV1
C	3	LEU	-	expression tag	UNP Q8UAV1
C	410	GLU	-	expression tag	UNP Q8UAV1
C	411	GLY	-	expression tag	UNP Q8UAV1
C	412	HIS	-	expression tag	UNP Q8UAV1
C	413	HIS	-	expression tag	UNP Q8UAV1
C	414	HIS	-	expression tag	UNP Q8UAV1
C	415	HIS	-	expression tag	UNP Q8UAV1
C	416	HIS	-	expression tag	UNP Q8UAV1
C	417	HIS	-	expression tag	UNP Q8UAV1
D	1	MSE	-	expression tag	UNP Q8UAV1
D	2	SER	-	expression tag	UNP Q8UAV1
D	3	LEU	-	expression tag	UNP Q8UAV1
D	410	GLU	-	expression tag	UNP Q8UAV1
D	411	GLY	-	expression tag	UNP Q8UAV1
D	412	HIS	-	expression tag	UNP Q8UAV1
D	413	HIS	-	expression tag	UNP Q8UAV1
D	414	HIS	-	expression tag	UNP Q8UAV1
D	415	HIS	-	expression tag	UNP Q8UAV1
D	416	HIS	-	expression tag	UNP Q8UAV1
D	417	HIS	-	expression tag	UNP Q8UAV1
E	1	MSE	-	expression tag	UNP Q8UAV1
E	2	SER	-	expression tag	UNP Q8UAV1
E	3	LEU	-	expression tag	UNP Q8UAV1
E	410	GLU	-	expression tag	UNP Q8UAV1
E	411	GLY	-	expression tag	UNP Q8UAV1
E	412	HIS	-	expression tag	UNP Q8UAV1
E	413	HIS	-	expression tag	UNP Q8UAV1
E	414	HIS	-	expression tag	UNP Q8UAV1
E	415	HIS	-	expression tag	UNP Q8UAV1
E	416	HIS	-	expression tag	UNP Q8UAV1
E	417	HIS	-	expression tag	UNP Q8UAV1
F	1	MSE	-	expression tag	UNP Q8UAV1
F	2	SER	-	expression tag	UNP Q8UAV1
F	3	LEU	-	expression tag	UNP Q8UAV1
F	410	GLU	-	expression tag	UNP Q8UAV1

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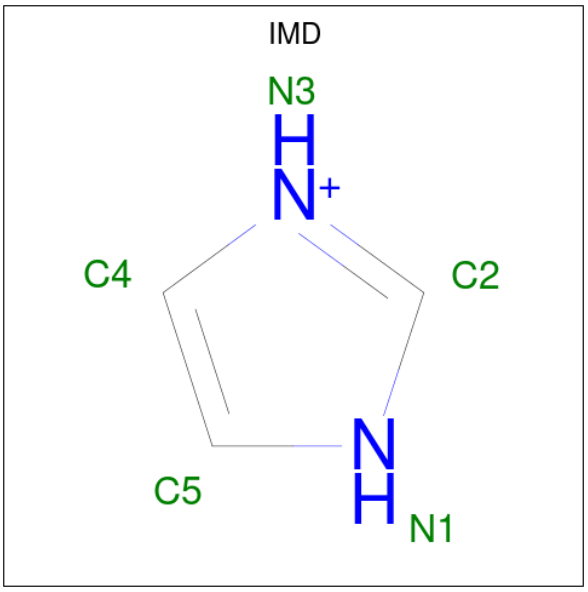
Chain	Residue	Modelled	Actual	Comment	Reference
F	411	GLY	-	expression tag	UNP Q8UAV1
F	412	HIS	-	expression tag	UNP Q8UAV1
F	413	HIS	-	expression tag	UNP Q8UAV1
F	414	HIS	-	expression tag	UNP Q8UAV1
F	415	HIS	-	expression tag	UNP Q8UAV1
F	416	HIS	-	expression tag	UNP Q8UAV1
F	417	HIS	-	expression tag	UNP Q8UAV1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

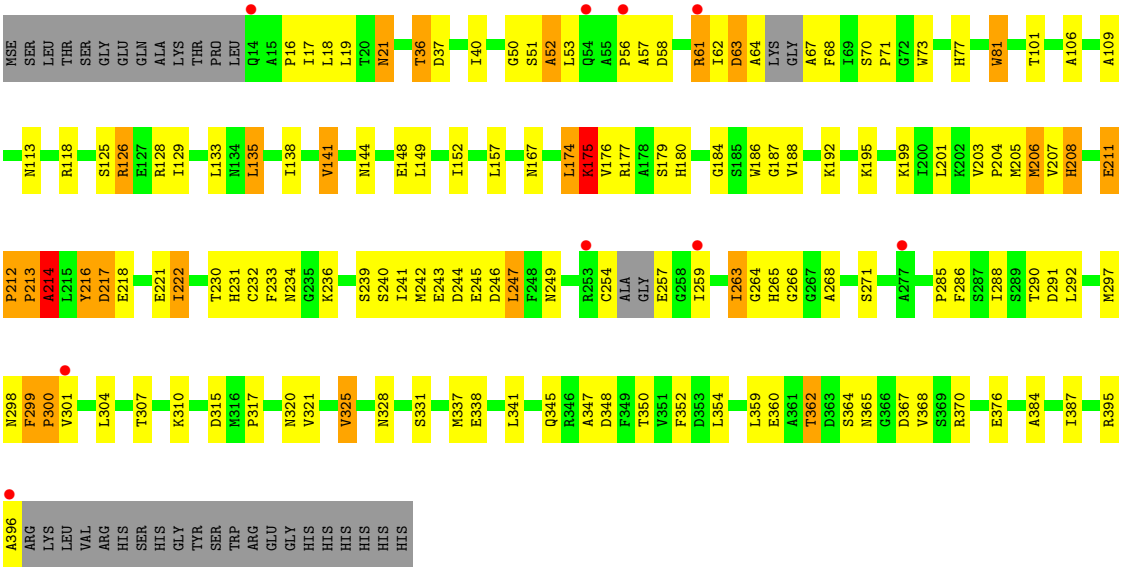
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0
4	B	26	Total O 26 26	0	0
4	C	10	Total O 10 10	0	0
4	D	13	Total O 13 13	0	0
4	E	21	Total O 21 21	0	0
4	F	16	Total O 16 16	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

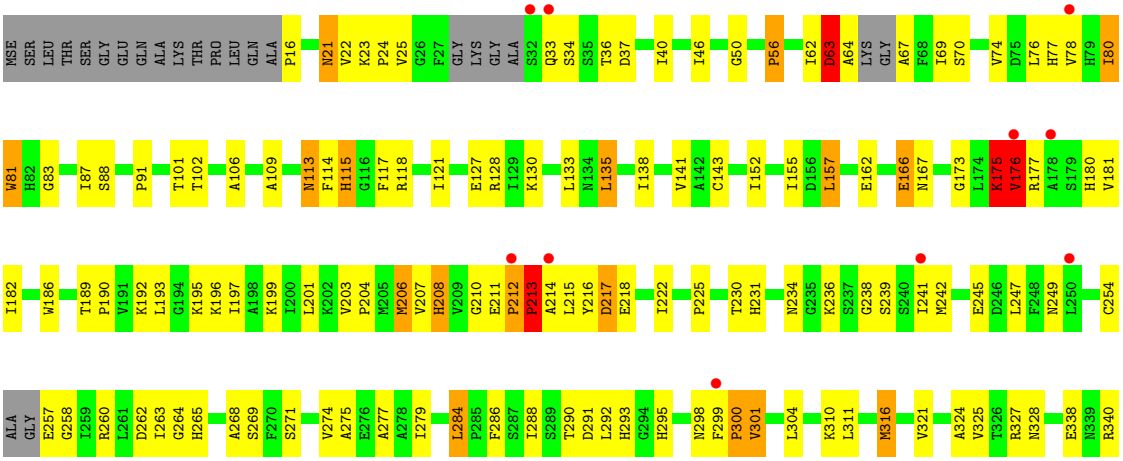
• Molecule 1: Dihydroorotase

Chain A:



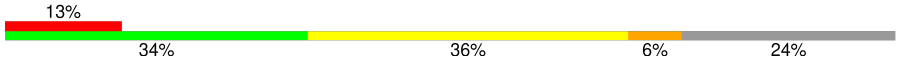
• Molecule 1: Dihydroorotase

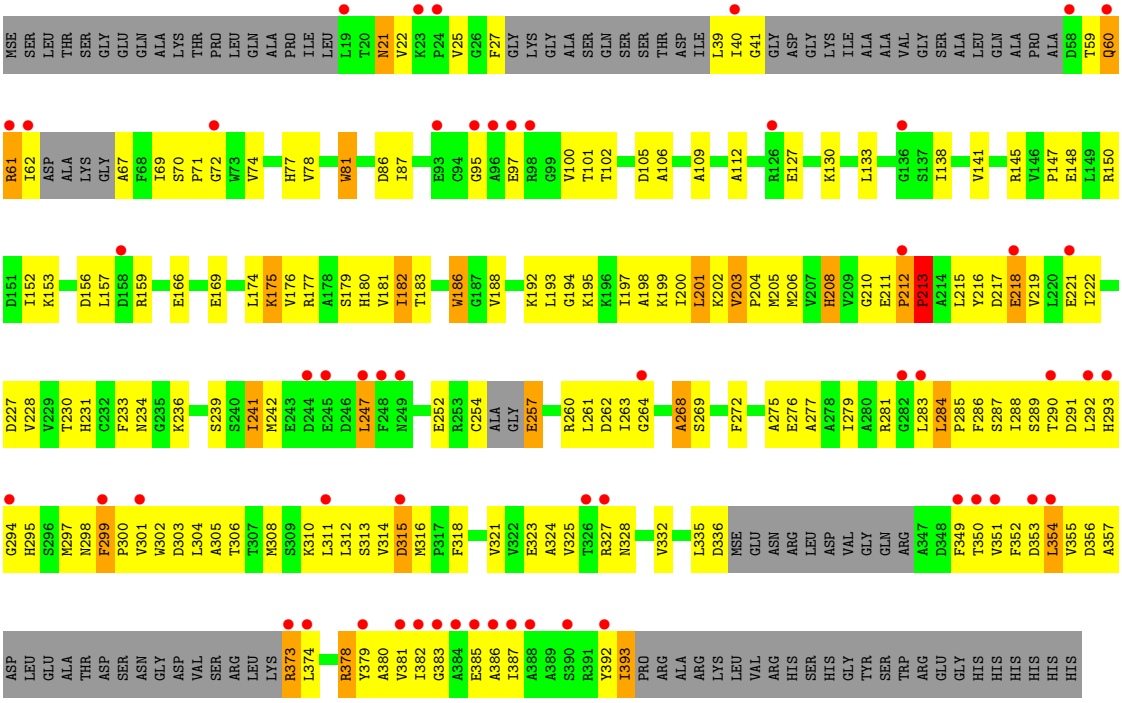
Chain B:



• Molecule 1: Dihydroorotase

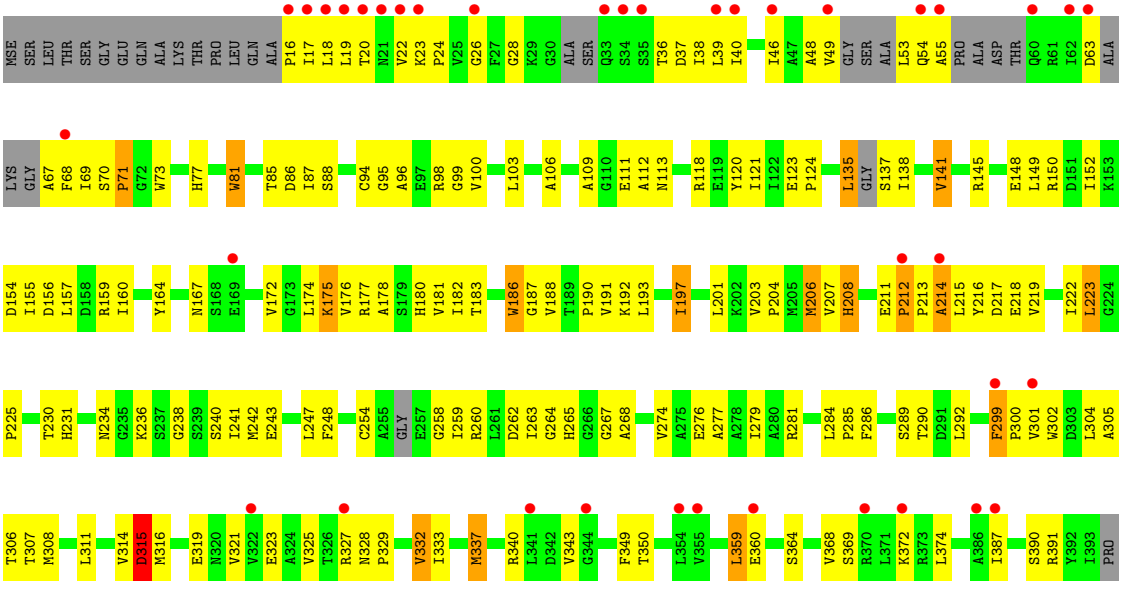
Chain C:





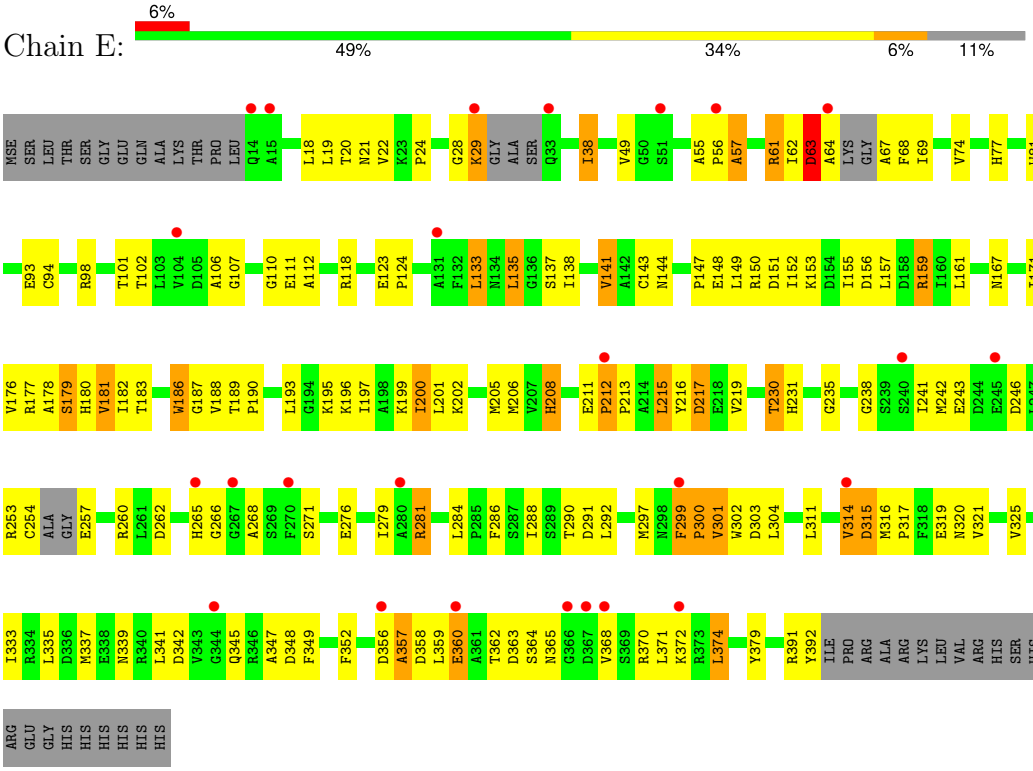
• Molecule 1: Dihydroorotase

Chain D:



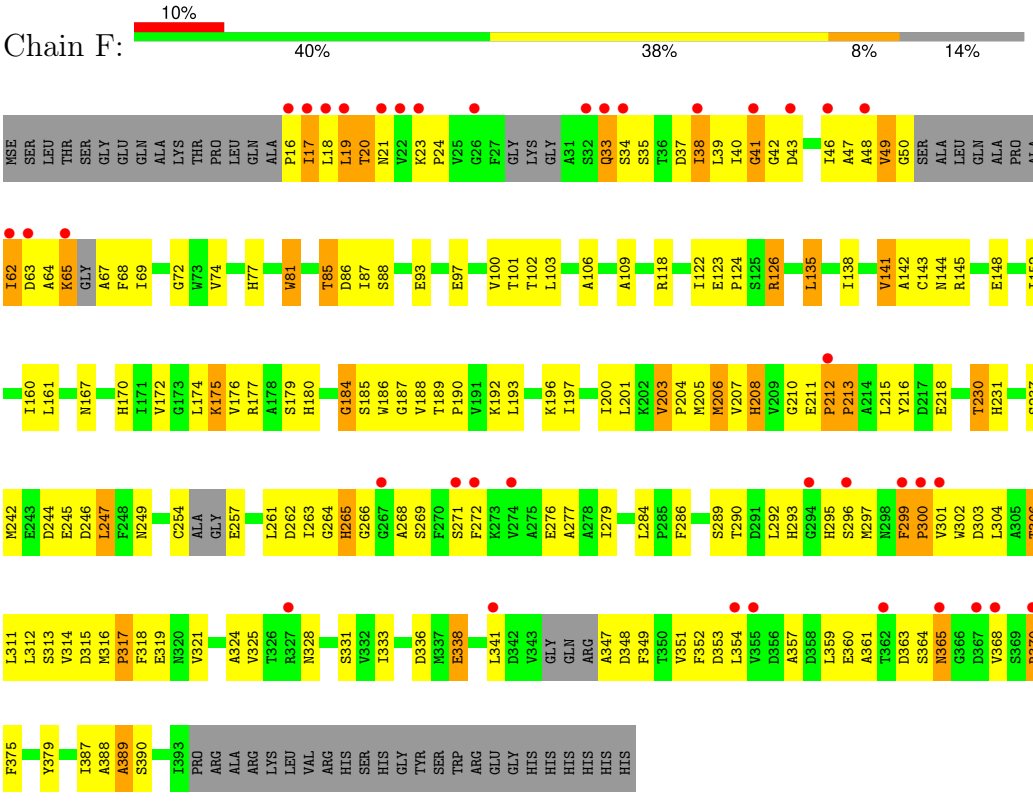
• Molecule 1: Dihydroorotase

Chain E:



• Molecule 1: Dihydroorotase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.65Å 139.20Å 206.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 2.62 39.76 – 2.62	Depositor EDS
% Data completeness (in resolution range)	92.3 (39.76-2.62) 96.1 (39.76-2.62)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.256 , 0.302 0.243 , 0.287	Depositor DCC
R_{free} test set	4173 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16585	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IMD, KCX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	3/2910 (0.1%)	0.75	1/3932 (0.0%)
1	B	0.54	3/2841 (0.1%)	0.74	1/3837 (0.0%)
1	C	0.46	1/2461 (0.0%)	0.67	0/3322
1	D	0.50	2/2810 (0.1%)	0.72	0/3787
1	E	0.53	3/2854 (0.1%)	0.85	3/3856 (0.1%)
1	F	0.48	1/2757 (0.0%)	0.71	0/3721
All	All	0.51	13/16633 (0.1%)	0.74	5/22455 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	E	0	2
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	ASP	C-N	-8.42	1.14	1.34
1	D	206	MSE	SE-CE	-6.25	1.58	1.95
1	B	176	VAL	C-N	6.10	1.48	1.34
1	B	316	MSE	SE-CE	-6.02	1.59	1.95
1	F	206	MSE	SE-CE	-5.84	1.60	1.95
1	B	206	MSE	SE-CE	-5.67	1.62	1.95
1	E	337	MSE	CG-SE	-5.29	1.77	1.95
1	D	337	MSE	CG-SE	-5.28	1.77	1.95
1	A	337	MSE	CG-SE	-5.22	1.77	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	297	MSE	CG-SE	-5.22	1.77	1.95
1	A	297	MSE	CG-SE	-5.15	1.77	1.95
1	C	206	MSE	CG-SE	-5.08	1.78	1.95
1	A	206	MSE	SE-CE	-5.06	1.65	1.95

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	63	ASP	O-C-N	-22.60	86.54	122.70
1	E	63	ASP	CA-C-N	16.26	152.97	117.20
1	E	63	ASP	C-N-CA	9.45	145.32	121.70
1	B	115	HIS	N-CA-C	-5.38	96.48	111.00
1	A	214	ALA	N-CA-C	-5.15	97.10	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	KCX	Mainchain
1	B	175	KCX	Mainchain
1	B	176	VAL	Mainchain
1	E	173	GLY	Mainchain
1	E	63	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2876	0	2862	156	0
1	B	2809	0	2788	185	0
1	C	2433	0	2411	215	0
1	D	2782	0	2771	181	3
1	E	2822	0	2796	168	3
1	F	2728	0	2704	249	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	C	5	0	4	0	0
3	D	5	0	4	0	0
4	A	27	0	0	2	0
4	B	26	0	0	1	0
4	C	10	0	0	1	0
4	D	13	0	0	0	0
4	E	21	0	0	1	0
4	F	16	0	0	0	0
All	All	16585	0	16340	1111	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (1111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ALA:CB	1:E:67:ALA:HB2	1.57	1.32
1:A:317:PRO:HG2	1:A:320:ASN:HD22	1.00	1.17
1:F:17:ILE:CG2	1:F:40:ILE:HB	1.76	1.16
1:B:288:ILE:HD11	1:B:316:MSE:HE1	1.29	1.13
1:E:64:ALA:HB1	1:E:67:ALA:HB2	1.19	1.11
1:F:77:HIS:HD1	1:F:230:THR:HG21	1.15	1.11
1:B:263:ILE:HD11	1:B:288:ILE:HG23	1.27	1.07
1:F:17:ILE:HG23	1:F:40:ILE:CB	1.83	1.07
1:B:80:ILE:HG22	1:B:81:TRP:H	1.12	1.07
1:A:317:PRO:HG2	1:A:320:ASN:ND2	1.69	1.06
1:E:77:HIS:HD1	1:E:230:THR:HG21	1.16	1.06
1:D:242:MSE:HE1	1:D:281:ARG:HH21	1.17	1.04
1:C:261:LEU:HD23	1:C:283:LEU:HD11	1.39	1.03
1:D:180:HIS:HB3	1:D:213:PRO:HB2	1.38	1.02
1:F:312:LEU:HD23	1:F:373:ARG:CZ	1.90	1.02
1:A:317:PRO:CG	1:A:320:ASN:HD22	1.71	1.02
1:B:77:HIS:HD1	1:B:230:THR:HG21	1.24	1.02
1:F:17:ILE:HD12	1:F:40:ILE:HG12	1.36	1.01
1:E:38:ILE:HG22	1:E:49:VAL:HG22	1.43	1.01
1:A:298:ASN:HD21	1:A:396:ALA:HB3	1.28	0.99
1:F:271:SER:HA	1:F:365:ASN:HD21	1.27	0.99
1:F:203:VAL:HG22	1:F:204:PRO:HD2	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:LEU:HD23	1:E:38:ILE:HD11	1.42	0.98
1:E:268:ALA:HA	1:E:364:SER:HB2	1.44	0.97
1:F:365:ASN:H	1:F:365:ASN:ND2	1.60	0.97
1:C:141:VAL:HG11	1:D:141:VAL:HG11	1.46	0.97
1:F:49:VAL:HG13	1:F:50:GLY:H	1.27	0.96
1:B:242:MSE:HE2	1:B:277:ALA:HB1	1.44	0.96
1:A:61:ARG:HH11	1:A:61:ARG:HB2	1.27	0.96
1:D:36:THR:HG22	1:D:37:ASP:H	1.24	0.96
1:C:180:HIS:HB3	1:C:213:PRO:HG2	1.49	0.95
1:E:64:ALA:CB	1:E:67:ALA:CB	2.43	0.95
1:A:19:LEU:HG	1:A:61:ARG:HH12	1.29	0.95
1:A:118:ARG:HH11	1:A:167:ASN:HD21	1.14	0.95
1:D:160:ILE:HG21	1:D:197:ILE:HD11	1.46	0.95
1:D:118:ARG:NH1	1:D:167:ASN:HD21	1.66	0.93
1:B:180:HIS:CD2	1:B:213:PRO:HG2	2.04	0.93
1:F:309:SER:HA	1:F:373:ARG:HH21	1.31	0.93
1:F:118:ARG:HH11	1:F:167:ASN:HD21	1.17	0.91
1:D:118:ARG:HH11	1:D:167:ASN:ND2	1.67	0.91
1:C:203:VAL:HG22	1:C:204:PRO:HD2	1.49	0.91
1:E:62:ILE:HG12	1:E:63:ASP:H	1.36	0.91
1:D:118:ARG:HH11	1:D:167:ASN:HD21	1.17	0.90
1:F:312:LEU:HD23	1:F:373:ARG:NE	1.88	0.89
1:F:77:HIS:ND1	1:F:230:THR:HG21	1.88	0.89
1:C:279:ILE:HD11	1:C:316:MSE:HB2	1.54	0.88
1:C:261:LEU:CD2	1:C:283:LEU:HD11	2.02	0.88
1:C:236:LYS:HE3	1:C:268:ALA:HB1	1.55	0.88
1:C:21:ASN:OD1	1:C:21:ASN:O	1.91	0.87
1:B:80:ILE:HG22	1:B:81:TRP:N	1.89	0.87
1:B:180:HIS:HD2	1:B:213:PRO:HG2	1.40	0.87
1:E:118:ARG:HH11	1:E:167:ASN:HD21	1.21	0.87
1:C:242:MSE:HE2	1:C:277:ALA:HB1	1.58	0.86
1:C:316:MSE:HE3	1:C:321:VAL:HG22	1.58	0.86
1:F:365:ASN:H	1:F:365:ASN:HD22	0.92	0.86
1:D:22:VAL:HG21	1:D:69:ILE:HB	1.57	0.86
1:D:279:ILE:HD12	1:D:314:VAL:HG12	1.57	0.86
1:F:373:ARG:HB2	1:F:373:ARG:HH11	1.38	0.85
1:B:62:ILE:HG12	1:B:63:ASP:N	1.89	0.85
1:F:61:ARG:O	1:F:62:ILE:HG13	1.77	0.84
1:F:370:ARG:H	1:F:370:ARG:NE	1.75	0.84
1:E:106:ALA:HB1	1:E:206:MSE:HE1	1.60	0.84
1:A:101:THR:HG21	1:A:348:ASP:OD2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ALA:HB3	1:E:67:ALA:HB2	1.56	0.83
1:A:17:ILE:HG21	1:A:61:ARG:NH2	1.94	0.83
1:D:242:MSE:HE1	1:D:281:ARG:NH2	1.92	0.83
1:F:85:THR:HG22	1:F:88:SER:H	1.43	0.83
1:F:17:ILE:HG23	1:F:40:ILE:HB	0.90	0.83
1:A:17:ILE:HD11	1:A:384:ALA:O	1.78	0.83
1:B:290:THR:HG21	1:B:304:LEU:HA	1.59	0.82
1:B:193:LEU:HD21	1:C:213:PRO:HA	1.61	0.82
1:D:203:VAL:HG22	1:D:204:PRO:HD2	1.62	0.82
1:C:71:PRO:HG3	1:C:327:ARG:HH12	1.43	0.82
1:E:358:ASP:HB2	1:E:370:ARG:HD3	1.59	0.82
1:B:62:ILE:HG12	1:B:63:ASP:H	1.44	0.82
1:F:17:ILE:HD12	1:F:40:ILE:CG1	2.09	0.82
1:C:150:ARG:HH11	1:D:150:ARG:HH21	1.24	0.81
1:A:203:VAL:HG22	1:A:204:PRO:HD2	1.63	0.81
1:F:46:ILE:HD12	1:F:46:ILE:H	1.44	0.81
1:F:180:HIS:HB3	1:F:213:PRO:HB2	1.62	0.81
1:F:172:VAL:HG21	1:F:333:ILE:HG22	1.63	0.81
1:F:39:LEU:HB3	1:F:48:ALA:HB3	1.62	0.81
1:D:39:LEU:HB3	1:D:48:ALA:HB3	1.62	0.80
1:C:218:GLU:O	1:C:221:GLU:HG2	1.80	0.80
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.44	0.80
1:B:77:HIS:ND1	1:B:230:THR:HG21	1.95	0.80
1:B:101:THR:HG21	1:B:348:ASP:OD2	1.81	0.80
1:C:180:HIS:CD2	1:C:213:PRO:HG2	2.16	0.80
1:D:174:LEU:HD11	1:D:197:ILE:HG12	1.62	0.80
1:F:18:LEU:HD13	1:F:39:LEU:HD12	1.64	0.80
1:A:174:LEU:C	1:A:175:KCX:CA	2.50	0.80
1:A:19:LEU:HD11	1:A:61:ARG:HH22	1.47	0.79
1:D:18:LEU:HB2	1:D:39:LEU:HD13	1.62	0.79
1:F:40:ILE:HD13	1:F:46:ILE:HG23	1.64	0.79
1:C:311:LEU:HB3	1:C:316:MSE:HE2	1.64	0.79
1:D:48:ALA:HB1	1:D:53:LEU:HD12	1.65	0.79
1:C:150:ARG:NH1	1:D:150:ARG:HE	1.81	0.78
1:D:254:CYS:HB3	1:D:259:ILE:HD12	1.66	0.78
1:C:72:GLY:HA2	1:C:350:THR:OG1	1.84	0.78
1:B:257:GLU:HG3	1:B:257:GLU:O	1.82	0.77
1:A:317:PRO:CG	1:A:320:ASN:ND2	2.38	0.77
1:B:316:MSE:HE3	1:B:321:VAL:HG22	1.64	0.77
1:F:65:LYS:HE2	1:F:351:VAL:HG11	1.65	0.77
1:F:74:VAL:HG22	1:F:102:THR:HB	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:HB3	1:B:316:MSE:HE2	1.66	0.77
1:E:94:CYS:HA	1:E:98:ARG:HG3	1.65	0.77
1:F:299:PHE:HB3	1:F:300:PRO:HD3	1.67	0.77
1:D:22:VAL:CG2	1:D:69:ILE:HB	2.15	0.77
1:C:201:LEU:O	1:C:202:LYS:HG2	1.83	0.77
1:E:77:HIS:ND1	1:E:230:THR:HG21	1.98	0.77
1:C:188:VAL:HG12	1:C:218:GLU:OE1	1.85	0.77
1:F:365:ASN:HD22	1:F:365:ASN:N	1.75	0.76
1:D:137:SER:HB2	1:D:154:ASP:O	1.85	0.76
1:F:241:ILE:HA	1:F:247:LEU:HD13	1.65	0.76
1:F:373:ARG:HH11	1:F:373:ARG:CB	1.98	0.76
1:F:86:ASP:OD2	1:F:142:ALA:HA	1.86	0.76
1:C:70:SER:HB2	1:C:71:PRO:HD2	1.66	0.76
1:A:241:ILE:HG13	1:A:242:MSE:HE2	1.68	0.75
1:F:106:ALA:HB1	1:F:206:MSE:HE1	1.68	0.75
1:B:189:THR:HB	1:B:190:PRO:HD3	1.68	0.75
1:E:180:HIS:ND1	1:E:213:PRO:HG2	2.01	0.75
1:A:179:SER:HB3	1:A:211:GLU:OE1	1.85	0.75
1:F:97:GLU:HA	1:F:389:ALA:HB3	1.67	0.75
1:B:230:THR:HG23	1:B:262:ASP:OD2	1.86	0.75
1:C:218:GLU:OE2	1:C:219:VAL:HG23	1.87	0.75
1:E:180:HIS:HB3	1:E:213:PRO:HB2	1.68	0.75
1:F:279:ILE:HD11	1:F:315:ASP:HB3	1.68	0.75
1:A:395:ARG:HG3	1:A:395:ARG:NH1	2.01	0.74
1:A:16:PRO:HG2	1:A:58:ASP:HB3	1.70	0.74
1:C:180:HIS:HB3	1:C:213:PRO:CG	2.16	0.74
1:A:118:ARG:NH1	1:A:167:ASN:HD21	1.86	0.74
1:B:180:HIS:HB3	1:B:213:PRO:HB2	1.70	0.74
1:B:203:VAL:CG2	1:B:204:PRO:HD2	2.16	0.74
1:E:22:VAL:O	1:E:24:PRO:HD3	1.88	0.74
1:F:93:GLU:HB3	1:F:297:MSE:HE1	1.70	0.74
1:C:21:ASN:O	1:C:21:ASN:CG	2.25	0.74
1:C:156:ASP:CG	1:C:159:ARG:HG3	2.08	0.74
1:D:316:MSE:HE2	1:D:321:VAL:HA	1.70	0.74
1:E:106:ALA:CB	1:E:206:MSE:HE1	2.18	0.74
1:B:33:GLN:HG2	1:B:34:SER:H	1.51	0.73
1:C:180:HIS:CB	1:C:213:PRO:HG2	2.18	0.73
1:E:61:ARG:HB2	1:E:61:ARG:NH1	2.02	0.73
1:F:17:ILE:C	1:F:17:ILE:HD13	2.09	0.73
1:A:180:HIS:HB3	1:A:213:PRO:HB2	1.70	0.73
1:C:242:MSE:HE2	1:C:277:ALA:CB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:ALA:HB1	1:D:206:MSE:HE1	1.70	0.73
1:F:148:GLU:OE1	1:F:177:ARG:HD3	1.88	0.73
1:A:62:ILE:HG12	1:A:63:ASP:N	2.04	0.73
1:A:81:TRP:CD1	1:A:109:ALA:HB2	2.23	0.73
1:E:290:THR:HG23	1:E:292:LEU:H	1.54	0.73
1:F:180:HIS:ND1	1:F:213:PRO:HG2	2.03	0.73
1:B:288:ILE:HD11	1:B:316:MSE:CE	2.15	0.72
1:F:175:KCX:HD3	1:F:206:MSE:HE2	1.70	0.72
1:A:175:KCX:HD3	1:A:206:MSE:HE2	1.71	0.72
1:A:290:THR:HB	1:A:301:VAL:HG11	1.71	0.72
1:A:241:ILE:HA	1:A:247:LEU:HD13	1.72	0.72
1:C:288:ILE:HD11	1:C:316:MSE:CE	2.18	0.72
1:D:276:GLU:HA	1:D:314:VAL:HG13	1.70	0.72
1:C:212:PRO:O	1:C:215:LEU:HD12	1.90	0.72
1:E:357:ALA:HB3	1:E:374:LEU:HD21	1.70	0.72
1:F:180:HIS:HB3	1:F:213:PRO:CB	2.19	0.72
1:B:203:VAL:HG23	1:B:204:PRO:HD2	1.72	0.71
1:F:361:ALA:HB3	1:F:371:LEU:HD11	1.72	0.71
1:A:61:ARG:HB2	1:A:61:ARG:NH1	2.05	0.71
1:A:40:ILE:HD12	1:A:347:ALA:HB2	1.72	0.71
1:C:288:ILE:HD11	1:C:316:MSE:HE1	1.72	0.71
1:D:230:THR:HG22	1:D:262:ASP:OD2	1.89	0.71
1:C:290:THR:HG21	1:C:304:LEU:HA	1.72	0.71
1:D:148:GLU:OE1	1:D:177:ARG:HD3	1.91	0.71
1:D:95:GLY:HA2	1:D:100:VAL:HB	1.73	0.71
1:B:80:ILE:HG23	1:B:91:PRO:HD3	1.73	0.70
1:B:316:MSE:CE	1:B:321:VAL:HG22	2.20	0.70
1:E:303:ASP:OD1	1:E:391:ARG:HB2	1.91	0.70
1:F:309:SER:CA	1:F:373:ARG:HH21	2.02	0.70
1:C:288:ILE:HG12	1:C:311:LEU:HD13	1.73	0.70
1:C:95:GLY:HA2	1:C:100:VAL:HB	1.72	0.70
1:D:85:THR:HG22	1:D:88:SER:H	1.57	0.70
1:D:279:ILE:HD12	1:D:314:VAL:CG1	2.22	0.70
1:F:16:PRO:HB2	1:F:61:ARG:NE	2.06	0.70
1:E:181:VAL:HG13	1:E:211:GLU:OE1	1.91	0.70
1:B:106:ALA:HB1	1:B:206:MSE:HE1	1.74	0.69
1:E:64:ALA:HB3	1:E:67:ALA:CB	2.19	0.69
1:F:123:GLU:HB2	1:F:124:PRO:HD3	1.75	0.69
1:C:279:ILE:CD1	1:C:316:MSE:HB2	2.23	0.69
1:D:368:VAL:HG12	1:D:369:SER:H	1.56	0.69
1:F:302:TRP:HB2	1:F:306:THR:HG21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:O	1:C:292:LEU:N	2.25	0.69
1:F:271:SER:HA	1:F:365:ASN:ND2	2.05	0.69
1:B:138:ILE:O	1:B:141:VAL:HG23	1.93	0.69
1:E:230:THR:HG23	1:E:262:ASP:OD2	1.93	0.68
1:E:62:ILE:HG12	1:E:63:ASP:N	2.08	0.68
1:A:61:ARG:HH11	1:A:61:ARG:CB	2.03	0.68
1:B:77:HIS:NE2	1:B:175:KCX:OQ2	2.25	0.68
1:B:268:ALA:HA	1:B:364:SER:HB2	1.75	0.68
1:F:118:ARG:NH1	1:F:167:ASN:HD21	1.91	0.68
1:F:284:LEU:HD12	1:F:316:MSE:HG3	1.76	0.68
1:E:138:ILE:O	1:E:141:VAL:HG22	1.94	0.68
1:C:311:LEU:O	1:C:316:MSE:HB3	1.92	0.68
1:C:353:ASP:HB3	1:C:378:ARG:HH12	1.57	0.68
1:E:118:ARG:O	1:E:123:GLU:HG3	1.94	0.68
1:C:215:LEU:O	1:C:218:GLU:HG3	1.94	0.68
1:C:195:LYS:HE2	1:C:227:ASP:OD1	1.93	0.68
1:B:64:ALA:O	1:B:67:ALA:N	2.27	0.68
1:D:46:ILE:HD11	1:D:349:PHE:HZ	1.58	0.68
1:F:265:HIS:HD2	1:F:266:GLY:O	1.77	0.68
1:F:359:LEU:HD23	1:F:360:GLU:N	2.08	0.68
1:C:215:LEU:HB2	1:C:218:GLU:HG3	1.74	0.68
1:D:368:VAL:HG12	1:D:369:SER:N	2.09	0.68
1:F:373:ARG:NE	1:F:373:ARG:O	2.27	0.68
1:A:106:ALA:HB1	1:A:206:MSE:HE1	1.75	0.67
1:E:61:ARG:HB2	1:E:61:ARG:CZ	2.24	0.67
1:D:323:GLU:HG3	1:D:327:ARG:HH11	1.60	0.67
1:F:308:MSE:HE3	1:F:325:VAL:HG11	1.77	0.67
1:D:180:HIS:HD2	1:D:213:PRO:HD2	1.58	0.67
1:C:157:LEU:HD22	1:E:212:PRO:HG3	1.76	0.67
1:B:118:ARG:HH11	1:B:167:ASN:HD21	1.43	0.67
1:F:49:VAL:HG13	1:F:50:GLY:N	2.05	0.67
1:F:328:ASN:O	1:F:331:SER:HB3	1.95	0.67
1:B:284:LEU:N	1:B:284:LEU:HD23	2.10	0.66
1:B:325:VAL:HG12	1:B:325:VAL:O	1.94	0.66
1:D:36:THR:HG22	1:D:37:ASP:N	2.05	0.66
1:A:118:ARG:HH11	1:A:167:ASN:ND2	1.90	0.66
1:C:101:THR:CG2	1:C:382:ILE:HD11	2.25	0.66
1:E:28:GLY:O	1:E:29:LYS:HB2	1.95	0.66
1:F:370:ARG:H	1:F:370:ARG:HE	1.43	0.66
1:B:23:LYS:HZ3	1:B:34:SER:HA	1.59	0.66
1:D:48:ALA:HB1	1:D:53:LEU:CD1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:HIS:HB3	1:E:213:PRO:CB	2.26	0.66
1:F:24:PRO:HD2	1:F:33:GLN:HG2	1.77	0.66
1:F:308:MSE:HE3	1:F:325:VAL:HG21	1.78	0.66
1:A:211:GLU:CD	1:A:211:GLU:H	1.96	0.65
1:A:290:THR:O	1:A:292:LEU:N	2.26	0.65
1:C:215:LEU:CB	1:C:218:GLU:HG3	2.26	0.65
1:C:287:SER:HA	1:C:324:ALA:HB1	1.76	0.65
1:E:235:GLY:HA3	1:E:365:ASN:HD21	1.61	0.65
1:E:359:LEU:HD22	1:E:391:ARG:HH22	1.61	0.65
1:B:157:LEU:CD2	1:B:197:ILE:HG12	2.27	0.65
1:B:360:GLU:OE2	1:B:370:ARG:HG2	1.94	0.65
1:D:203:VAL:CG2	1:D:204:PRO:HD2	2.27	0.65
1:F:336:ASP:HB2	1:F:338:GLU:OE1	1.96	0.65
1:B:230:THR:HG22	1:B:264:GLY:HA3	1.79	0.65
1:F:38:ILE:HD11	1:F:40:ILE:HG12	1.79	0.65
1:F:308:MSE:CE	1:F:325:VAL:HG21	2.27	0.65
1:D:77:HIS:HD1	1:D:230:THR:HG21	1.60	0.65
1:B:80:ILE:CG2	1:B:91:PRO:HD3	2.27	0.65
1:C:71:PRO:HG3	1:C:327:ARG:NH1	2.10	0.65
1:D:325:VAL:HG12	1:D:325:VAL:O	1.96	0.65
1:E:253:ARG:O	1:E:257:GLU:HG3	1.96	0.65
1:D:94:CYS:O	1:D:103:LEU:HD21	1.96	0.64
1:F:179:SER:HB3	1:F:211:GLU:OE1	1.97	0.64
1:A:77:HIS:NE2	1:A:175:KCX:OQ2	2.30	0.64
1:B:180:HIS:HD2	1:B:213:PRO:CG	2.08	0.64
1:D:19:LEU:O	1:D:37:ASP:HB2	1.97	0.64
1:C:180:HIS:CG	1:C:213:PRO:HG2	2.32	0.64
1:F:40:ILE:CD1	1:F:46:ILE:HG13	2.28	0.64
1:E:246:ASP:HA	1:E:249:ASN:HD22	1.62	0.64
1:F:175:KCX:HD3	1:F:206:MSE:CE	2.28	0.64
1:A:148:GLU:OE1	1:A:177:ARG:HD3	1.99	0.63
1:B:195:LYS:HD2	1:B:199:LYS:HE3	1.79	0.63
1:E:265:HIS:CD2	1:E:301:VAL:HG22	2.34	0.63
1:E:188:VAL:HG22	1:E:188:VAL:O	1.98	0.63
1:B:290:THR:CG2	1:B:304:LEU:HA	2.28	0.63
1:C:233:PHE:HE2	1:C:285:PRO:HD3	1.62	0.63
1:D:268:ALA:HA	1:D:364:SER:HB3	1.80	0.63
1:B:357:ALA:O	1:B:372:LYS:HA	1.99	0.63
1:F:77:HIS:HD1	1:F:230:THR:CG2	2.03	0.63
1:C:157:LEU:HD13	1:C:197:ILE:HG12	1.81	0.63
1:F:286:PHE:CE1	1:F:328:ASN:HB3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:PRO:HG2	1:F:213:PRO:HD3	1.81	0.63
1:A:174:LEU:CA	1:A:175:KCX:N	2.61	0.62
1:C:299:PHE:HB3	1:C:300:PRO:HD3	1.81	0.62
1:D:18:LEU:HB2	1:D:39:LEU:CD1	2.29	0.62
1:D:242:MSE:HE2	1:D:277:ALA:HB1	1.80	0.62
1:A:157:LEU:HD13	1:F:212:PRO:HG3	1.81	0.62
1:A:299:PHE:HB3	1:A:300:PRO:HD3	1.80	0.62
1:A:106:ALA:O	1:A:175:KCX:HD2	1.99	0.62
1:A:73:TRP:CD1	1:A:350:THR:HG21	2.35	0.62
1:C:97:GLU:HG2	1:C:387:ILE:HG21	1.82	0.62
1:E:241:ILE:HG13	1:E:242:MSE:HE2	1.82	0.62
1:E:288:ILE:HG12	1:E:311:LEU:HD13	1.80	0.62
1:F:100:VAL:HG21	1:F:103:LEU:HD21	1.82	0.62
1:B:290:THR:O	1:B:292:LEU:N	2.32	0.62
1:F:65:LYS:HZ2	1:F:65:LYS:HB2	1.64	0.62
1:A:254:CYS:C	1:A:257:GLU:N	2.53	0.62
1:B:186:TRP:CE3	1:B:190:PRO:HG3	2.33	0.62
1:B:242:MSE:HE2	1:B:277:ALA:CB	2.26	0.62
1:C:272:PHE:O	1:C:276:GLU:HG3	2.00	0.62
1:C:313:SER:HB3	1:C:373:ARG:HH22	1.64	0.62
1:D:20:THR:HA	1:D:37:ASP:HB3	1.81	0.62
1:D:106:ALA:CB	1:D:206:MSE:HE1	2.29	0.62
1:C:180:HIS:HB3	1:C:213:PRO:CB	2.30	0.61
1:B:77:HIS:CE1	1:B:175:KCX:OQ2	2.54	0.61
1:E:325:VAL:HG12	1:E:325:VAL:O	1.99	0.61
1:B:180:HIS:HB3	1:B:213:PRO:CB	2.29	0.61
1:F:16:PRO:HB2	1:F:61:ARG:CZ	2.30	0.61
1:A:64:ALA:O	1:A:67:ALA:HA	1.99	0.61
1:B:37:ASP:HB2	1:B:50:GLY:O	2.01	0.61
1:E:135:LEU:HD22	1:E:155:ILE:HG12	1.82	0.61
1:F:34:SER:O	1:F:35:SER:HB3	2.00	0.61
1:C:210:GLY:O	1:C:239:SER:HB3	2.01	0.61
1:D:359:LEU:HD12	1:D:360:GLU:N	2.15	0.61
1:F:373:ARG:HB2	1:F:373:ARG:NH1	2.14	0.61
1:F:138:ILE:O	1:F:141:VAL:HG22	2.00	0.61
1:F:230:THR:HG23	1:F:262:ASP:OD2	2.00	0.61
1:F:312:LEU:CD2	1:F:373:ARG:CZ	2.74	0.61
1:B:193:LEU:HD21	1:C:213:PRO:CA	2.30	0.60
1:F:39:LEU:CB	1:F:48:ALA:HB3	2.28	0.60
1:B:177:ARG:NH2	1:B:182:ILE:HG12	2.16	0.60
1:C:138:ILE:HG12	4:C:3748:HOH:O	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ARG:NH1	1:D:150:ARG:HH21	1.98	0.60
1:D:16:PRO:C	1:D:17:ILE:HD12	2.20	0.60
1:D:175:KCX:HD3	1:D:206:MSE:CE	2.30	0.60
1:E:177:ARG:O	1:E:178:ALA:HB3	2.02	0.60
1:D:208:HIS:C	1:D:208:HIS:CD2	2.74	0.60
1:F:373:ARG:CZ	1:F:373:ARG:O	2.49	0.60
1:F:351:VAL:HB	1:F:379:TYR:H	1.65	0.60
1:A:217:ASP:O	1:A:221:GLU:HG2	2.01	0.60
1:E:317:PRO:HB2	1:E:320:ASN:HD22	1.66	0.60
1:E:359:LEU:HD12	1:E:360:GLU:OE1	2.01	0.60
1:E:372:LYS:O	1:E:372:LYS:HD3	2.01	0.60
1:F:317:PRO:O	1:F:321:VAL:HG23	2.01	0.60
1:F:365:ASN:ND2	1:F:365:ASN:N	2.37	0.60
1:A:138:ILE:O	1:A:141:VAL:HG22	2.02	0.60
1:C:179:SER:HB2	1:C:182:ILE:CD1	2.32	0.60
1:C:293:HIS:HD2	1:C:295:HIS:H	1.50	0.60
1:E:175:KCX:HD3	1:E:206:MSE:CE	2.31	0.60
1:B:211:GLU:C	1:B:213:PRO:HD2	2.21	0.59
1:C:215:LEU:CA	1:C:218:GLU:HG3	2.32	0.59
1:B:106:ALA:O	1:B:175:KCX:HE3	2.02	0.59
1:C:242:MSE:CE	1:C:277:ALA:HB1	2.31	0.59
1:E:339:ASN:O	1:E:345:GLN:HG3	2.03	0.59
1:F:363:ASP:CG	1:F:365:ASN:ND2	2.55	0.59
1:B:155:ILE:HD12	1:B:193:LEU:HD13	1.84	0.59
1:F:106:ALA:O	1:F:175:KCX:HD2	2.02	0.59
1:F:268:ALA:HA	1:F:364:SER:HB3	1.84	0.59
1:B:23:LYS:HE2	1:B:34:SER:HA	1.84	0.59
1:D:188:VAL:HG11	1:D:218:GLU:HB3	1.84	0.59
1:F:254:CYS:C	1:F:257:GLU:N	2.56	0.59
1:F:373:ARG:HH11	1:F:373:ARG:CG	2.15	0.59
1:B:46:ILE:HD11	1:B:349:PHE:HZ	1.66	0.59
1:D:213:PRO:HG2	1:F:152:ILE:HD11	1.84	0.59
1:D:323:GLU:HG3	1:D:327:ARG:NH1	2.16	0.59
1:E:135:LEU:HD12	1:E:176:VAL:HG22	1.84	0.59
1:F:38:ILE:HD11	1:F:40:ILE:CD1	2.33	0.59
1:F:135:LEU:HD22	1:F:155:ILE:HG12	1.84	0.59
1:F:309:SER:HA	1:F:373:ARG:NH2	2.11	0.59
1:B:62:ILE:CG1	1:B:63:ASP:H	2.14	0.59
1:F:341:LEU:HD23	1:F:341:LEU:H	1.68	0.59
1:A:212:PRO:O	1:A:214:ALA:N	2.36	0.59
1:C:212:PRO:HG2	1:C:213:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:THR:OG1	1:F:292:LEU:HG	2.01	0.59
1:A:19:LEU:HG	1:A:61:ARG:NH1	2.11	0.58
1:A:362:THR:HB	1:A:368:VAL:HG22	1.84	0.58
1:B:359:LEU:HD12	1:B:359:LEU:O	2.02	0.58
1:D:314:VAL:O	1:D:315:ASP:HB2	2.01	0.58
1:E:159:ARG:HH11	1:E:159:ARG:HG2	1.68	0.58
1:E:28:GLY:O	1:E:29:LYS:CB	2.51	0.58
1:E:123:GLU:HB2	1:E:124:PRO:HD3	1.85	0.58
1:E:175:KCX:HD3	1:E:206:MSE:HE3	1.85	0.58
1:B:157:LEU:HD22	1:B:197:ILE:HG12	1.85	0.58
1:B:279:ILE:HD13	1:B:284:LEU:HA	1.86	0.58
1:C:203:VAL:CG2	1:C:204:PRO:HD2	2.30	0.58
1:C:312:LEU:HD13	1:C:312:LEU:O	2.04	0.58
1:A:157:LEU:CD1	1:F:212:PRO:HG3	2.33	0.58
1:B:175:KCX:HD3	1:B:206:MSE:HE2	1.85	0.58
1:F:16:PRO:HB2	1:F:61:ARG:CD	2.34	0.58
1:F:68:PHE:HB2	1:F:352:PHE:O	2.03	0.58
1:F:106:ALA:CB	1:F:206:MSE:HE1	2.33	0.58
1:F:371:LEU:N	1:F:371:LEU:HD12	2.19	0.58
1:C:233:PHE:CD2	1:C:263:ILE:HD11	2.38	0.58
1:D:160:ILE:CG2	1:D:197:ILE:HD11	2.26	0.58
1:D:234:ASN:HD22	1:D:236:LYS:H	1.50	0.58
1:A:175:KCX:OQ1	1:A:208:HIS:HB2	2.03	0.58
1:C:311:LEU:HB3	1:C:316:MSE:CE	2.33	0.58
1:F:20:THR:HA	1:F:37:ASP:HB3	1.85	0.58
1:F:97:GLU:HA	1:F:389:ALA:CB	2.33	0.58
1:B:80:ILE:HG21	1:B:121:ILE:CG2	2.34	0.58
1:C:351:VAL:HG23	1:C:378:ARG:HB2	1.86	0.58
1:D:123:GLU:HB2	1:D:124:PRO:HD3	1.85	0.58
1:D:372:LYS:O	1:D:372:LYS:HD3	2.04	0.57
1:D:284:LEU:HD22	1:D:316:MSE:HG3	1.85	0.57
1:A:77:HIS:CE1	1:A:175:KCX:OQ2	2.57	0.57
1:E:29:LYS:HA	1:E:29:LYS:NZ	2.20	0.57
1:E:85:THR:HA	1:E:141:VAL:HA	1.86	0.57
1:E:195:LYS:HE3	1:E:199:LYS:HE3	1.85	0.57
1:A:126:ARG:HG3	1:A:126:ARG:HH11	1.69	0.57
1:A:359:LEU:O	1:A:370:ARG:HA	2.04	0.57
1:D:106:ALA:O	1:D:175:KCX:HD2	2.05	0.57
1:C:241:ILE:HD13	1:C:242:MSE:HG2	1.87	0.57
1:F:17:ILE:HD11	1:F:19:LEU:CD1	2.33	0.57
1:C:241:ILE:HA	1:C:247:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:304:LEU:O	1:F:308:MSE:HG3	2.04	0.57
1:C:188:VAL:HG12	1:C:218:GLU:CD	2.24	0.57
1:F:86:ASP:OD1	1:F:87:ILE:N	2.38	0.57
1:B:21:ASN:OD1	1:B:21:ASN:N	2.38	0.57
1:D:213:PRO:HG2	1:F:152:ILE:CD1	2.35	0.57
1:E:148:GLU:OE1	1:E:177:ARG:HD3	2.05	0.57
1:B:106:ALA:CB	1:B:206:MSE:HE1	2.35	0.56
1:C:194:GLY:HA3	1:C:205:MSE:HE1	1.86	0.56
1:F:189:THR:HB	1:F:190:PRO:CD	2.35	0.56
1:A:144:ASN:OD1	1:A:177:ARG:NH2	2.38	0.56
1:C:314:VAL:HG23	1:C:315:ASP:H	1.70	0.56
1:C:354:LEU:CD2	1:C:373:ARG:HB2	2.36	0.56
1:A:126:ARG:HH11	1:A:126:ARG:CG	2.19	0.56
1:E:179:SER:HB3	1:E:211:GLU:OE1	2.05	0.56
1:A:240:SER:HB3	1:A:243:GLU:HG2	1.86	0.56
1:C:199:LYS:C	1:C:201:LEU:H	2.09	0.56
1:C:354:LEU:HD22	1:C:373:ARG:HB2	1.86	0.56
1:F:21:ASN:HB2	1:F:65:LYS:H	1.71	0.56
1:A:304:LEU:HD21	1:A:325:VAL:HG22	1.85	0.56
1:B:263:ILE:HG12	1:B:288:ILE:HA	1.87	0.56
1:A:106:ALA:CB	1:A:206:MSE:HE1	2.36	0.56
1:E:276:GLU:HA	1:E:314:VAL:CG2	2.35	0.56
1:B:33:GLN:HG2	1:B:34:SER:N	2.20	0.56
1:B:368:VAL:HG12	1:B:369:SER:N	2.21	0.56
1:D:175:KCX:HD3	1:D:206:MSE:HE2	1.87	0.56
1:E:201:LEU:O	1:E:202:LYS:HB2	2.04	0.56
1:E:211:GLU:O	1:E:213:PRO:HD2	2.06	0.56
1:C:182:ILE:HD12	1:C:182:ILE:N	2.21	0.56
1:C:208:HIS:C	1:C:208:HIS:CD2	2.78	0.56
1:F:118:ARG:HH11	1:F:167:ASN:ND2	1.96	0.56
1:F:310:LYS:O	1:F:313:SER:HB3	2.05	0.56
1:A:62:ILE:C	1:A:63:ASP:OD1	2.44	0.55
1:D:49:VAL:C	1:D:53:LEU:HD21	2.27	0.55
1:D:118:ARG:HD3	1:D:167:ASN:HD22	1.70	0.55
1:F:39:LEU:HB3	1:F:48:ALA:CB	2.33	0.55
1:F:211:GLU:CD	1:F:211:GLU:H	2.08	0.55
1:B:23:LYS:NZ	1:B:34:SER:HA	2.21	0.55
1:C:211:GLU:C	1:C:213:PRO:HD2	2.27	0.55
1:D:135:LEU:HB3	1:D:149:LEU:HD21	1.89	0.55
1:E:215:LEU:O	1:E:219:VAL:HG23	2.05	0.55
1:A:57:ALA:HA	4:A:446:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:HD21	1:D:325:VAL:HG13	1.87	0.55
1:C:182:ILE:HD12	1:C:182:ILE:H	1.72	0.55
1:D:46:ILE:HD11	1:D:349:PHE:CZ	2.40	0.55
1:E:61:ARG:CZ	1:E:61:ARG:CB	2.82	0.55
1:A:192:LYS:NZ	1:A:222:ILE:HD13	2.22	0.55
1:A:234:ASN:HD22	1:A:236:LYS:H	1.52	0.55
1:B:254:CYS:C	1:B:257:GLU:N	2.60	0.55
1:A:62:ILE:HG12	1:A:63:ASP:H	1.71	0.55
1:A:338:GLU:OE2	1:A:338:GLU:HA	2.07	0.55
1:B:23:LYS:CE	1:B:34:SER:HA	2.37	0.55
1:B:152:ILE:HG12	1:C:213:PRO:CG	2.37	0.55
1:C:208:HIS:HD2	1:C:208:HIS:O	1.90	0.55
1:E:68:PHE:HB2	1:E:352:PHE:O	2.07	0.55
1:E:178:ALA:HA	1:E:183:THR:CG2	2.37	0.55
1:F:64:ALA:O	1:F:65:LYS:HG3	2.06	0.55
1:A:175:KCX:HD3	1:A:206:MSE:CE	2.37	0.55
1:B:62:ILE:CG1	1:B:63:ASP:N	2.63	0.55
1:D:208:HIS:HD2	1:D:208:HIS:O	1.90	0.55
1:D:268:ALA:CA	1:D:364:SER:HB3	2.36	0.55
1:E:61:ARG:HD3	1:E:379:TYR:CZ	2.42	0.55
1:E:211:GLU:C	1:E:213:PRO:HD2	2.28	0.55
1:D:121:ILE:N	1:D:121:ILE:HD12	2.22	0.55
1:B:234:ASN:ND2	1:B:236:LYS:H	2.06	0.54
1:D:181:VAL:HG12	1:D:182:ILE:HD13	1.89	0.54
1:F:19:LEU:HD23	1:F:63:ASP:OD1	2.06	0.54
1:D:302:TRP:CE3	1:D:306:THR:HG21	2.42	0.54
1:E:276:GLU:HA	1:E:314:VAL:HG23	1.88	0.54
1:E:304:LEU:HD21	1:E:325:VAL:HG13	1.88	0.54
1:F:16:PRO:HB2	1:F:61:ARG:HD2	1.88	0.54
1:F:39:LEU:HD23	1:F:40:ILE:N	2.22	0.54
1:B:279:ILE:CD1	1:B:284:LEU:HA	2.37	0.54
1:C:318:PHE:CE1	1:C:354:LEU:HD12	2.42	0.54
1:C:152:ILE:HD11	1:E:213:PRO:HG3	1.89	0.54
1:C:393:ILE:HD12	1:C:393:ILE:H	1.72	0.54
1:D:192:LYS:HG2	1:D:222:ILE:HD13	1.89	0.54
1:C:264:GLY:O	1:C:269:SER:HB2	2.08	0.54
1:C:356:ASP:O	1:C:357:ALA:HB2	2.06	0.54
1:C:387:ILE:HD12	1:C:387:ILE:N	2.21	0.54
1:F:318:PHE:CD1	1:F:354:LEU:HD11	2.42	0.54
1:A:254:CYS:O	1:A:257:GLU:N	2.41	0.54
1:B:176:VAL:O	1:B:176:VAL:CG2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:VAL:O	1:D:223:LEU:HD22	2.07	0.54
1:F:263:ILE:HG13	1:F:311:LEU:HD11	1.90	0.54
1:A:21:ASN:N	1:A:21:ASN:OD1	2.41	0.54
1:C:211:GLU:CD	1:C:211:GLU:H	2.11	0.54
1:A:203:VAL:CG2	1:A:204:PRO:HD2	2.35	0.54
1:B:271:SER:HA	1:B:363:ASP:OD1	2.08	0.54
1:B:327:ARG:NH2	1:B:338:GLU:OE2	2.40	0.54
1:D:387:ILE:N	1:D:387:ILE:HD12	2.23	0.54
1:F:242:MSE:HE2	1:F:277:ALA:HB1	1.88	0.54
1:C:215:LEU:O	1:C:218:GLU:CG	2.56	0.53
1:F:188:VAL:HG11	1:F:218:GLU:HB3	1.89	0.53
1:B:80:ILE:HG21	1:B:121:ILE:HG21	1.90	0.53
1:C:380:ALA:O	1:C:386:ALA:HA	2.08	0.53
1:A:265:HIS:O	1:A:291:ASP:N	2.39	0.53
1:A:298:ASN:ND2	1:A:396:ALA:HB3	2.12	0.53
1:B:196:LYS:O	1:B:196:LYS:HD3	2.09	0.53
1:B:311:LEU:HB3	1:B:316:MSE:CE	2.38	0.53
1:C:153:LYS:NZ	1:C:153:LYS:HB3	2.22	0.53
1:E:314:VAL:HG13	1:E:315:ASP:H	1.72	0.53
1:F:40:ILE:HD12	1:F:46:ILE:HG13	1.91	0.53
1:E:29:LYS:HA	1:E:29:LYS:HZ2	1.74	0.53
1:E:133:LEU:O	1:E:175:KCX:N	2.41	0.53
1:F:388:ALA:O	1:F:389:ALA:HB2	2.09	0.53
1:C:62:ILE:HD12	1:C:62:ILE:N	2.24	0.53
1:D:374:LEU:HD22	1:D:391:ARG:NH1	2.24	0.53
1:A:208:HIS:C	1:A:208:HIS:CD2	2.82	0.53
1:B:211:GLU:O	1:B:213:PRO:HD2	2.08	0.53
1:C:25:VAL:HG23	1:C:70:SER:HB3	1.89	0.53
1:C:299:PHE:HB3	1:C:300:PRO:CD	2.39	0.53
1:D:172:VAL:HG21	1:D:333:ILE:HG22	1.90	0.53
1:D:314:VAL:CG1	1:D:314:VAL:O	2.56	0.53
1:A:40:ILE:HD12	1:A:347:ALA:CB	2.37	0.53
1:B:245:GLU:O	1:B:249:ASN:ND2	2.42	0.53
1:C:78:VAL:O	1:C:105:ASP:HA	2.09	0.53
1:C:174:LEU:HD12	1:C:198:ALA:HB2	1.91	0.53
1:E:106:ALA:HB1	1:E:206:MSE:CE	2.35	0.53
1:F:38:ILE:HD11	1:F:40:ILE:CG1	2.39	0.53
1:F:161:LEU:HD23	1:F:201:LEU:HD13	1.90	0.53
1:C:241:ILE:HG12	1:C:241:ILE:O	2.09	0.53
1:D:203:VAL:HG22	1:D:204:PRO:CD	2.35	0.53
1:E:61:ARG:HD3	1:E:379:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:ILE:HG12	1:E:284:LEU:HD23	1.91	0.53
1:B:265:HIS:CE1	1:B:310:LYS:NZ	2.77	0.53
1:B:325:VAL:O	1:B:325:VAL:CG1	2.57	0.53
1:C:69:ILE:HD11	1:C:349:PHE:CD2	2.43	0.53
1:C:201:LEU:O	1:C:202:LYS:CG	2.54	0.53
1:C:261:LEU:HD22	1:C:283:LEU:HD21	1.90	0.53
1:E:101:THR:HG21	1:E:348:ASP:OD2	2.09	0.53
1:E:151:ASP:OD1	1:E:153:LYS:HB2	2.09	0.53
1:A:180:HIS:HD2	1:A:213:PRO:HD2	1.74	0.52
1:B:230:THR:HA	1:B:262:ASP:O	2.09	0.52
1:C:22:VAL:HA	1:C:67:ALA:O	2.08	0.52
1:C:176:VAL:HG21	1:C:205:MSE:HE2	1.90	0.52
1:D:73:TRP:CE3	1:D:308:MSE:HE1	2.44	0.52
1:D:290:THR:OG1	1:D:292:LEU:HB2	2.09	0.52
1:F:176:VAL:CG1	1:F:207:VAL:HG22	2.39	0.52
1:C:69:ILE:HB	1:C:351:VAL:HG12	1.91	0.52
1:C:176:VAL:CG2	1:C:205:MSE:HE2	2.39	0.52
1:D:212:PRO:HG3	1:D:238:GLY:HA3	1.91	0.52
1:E:208:HIS:C	1:E:208:HIS:CD2	2.83	0.52
1:F:77:HIS:HB3	1:F:289:SER:HB2	1.90	0.52
1:F:161:LEU:HD21	1:F:200:ILE:HD11	1.90	0.52
1:C:77:HIS:HB3	1:C:289:SER:OG	2.10	0.52
1:C:279:ILE:HD12	1:C:285:PRO:HD2	1.90	0.52
1:E:290:THR:CG2	1:E:292:LEU:HB2	2.40	0.52
1:D:20:THR:HA	1:D:37:ASP:CB	2.39	0.52
1:F:23:LYS:HG3	1:F:33:GLN:OE1	2.10	0.52
1:A:188:VAL:HG11	1:A:218:GLU:HB3	1.91	0.52
1:B:203:VAL:HG22	1:B:204:PRO:HD2	1.89	0.52
1:E:254:CYS:O	1:E:257:GLU:N	2.43	0.52
1:F:41:GLY:O	1:F:43:ASP:N	2.41	0.52
1:F:180:HIS:CG	1:F:213:PRO:HG2	2.43	0.52
1:E:64:ALA:CB	1:E:67:ALA:CA	2.88	0.52
1:F:49:VAL:CG1	1:F:50:GLY:H	2.06	0.52
1:B:268:ALA:CA	1:B:364:SER:HB2	2.39	0.52
1:B:372:LYS:HB2	1:B:372:LYS:NZ	2.25	0.52
1:A:19:LEU:CD1	1:A:61:ARG:HH22	2.20	0.52
1:A:213:PRO:HG3	1:D:193:LEU:HD22	1.91	0.52
1:D:54:GLN:O	1:D:55:ALA:HB2	2.10	0.52
1:E:74:VAL:HG22	1:E:102:THR:HB	1.90	0.52
1:E:235:GLY:CA	1:E:365:ASN:HD21	2.23	0.52
1:A:152:ILE:HG12	1:F:184:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:THR:HB	1:B:301:VAL:HG21	1.91	0.52
1:B:293:HIS:HD2	1:B:295:HIS:H	1.58	0.52
1:C:308:MSE:HE3	1:C:325:VAL:HG21	1.91	0.52
1:D:17:ILE:HB	1:D:40:ILE:HD11	1.92	0.52
1:E:106:ALA:O	1:E:175:KCX:HD2	2.10	0.52
1:E:314:VAL:HG22	1:E:315:ASP:N	2.25	0.52
1:E:254:CYS:C	1:E:257:GLU:N	2.63	0.51
1:F:338:GLU:H	1:F:338:GLU:CD	2.14	0.51
1:A:360:GLU:HG2	1:A:370:ARG:HB3	1.91	0.51
1:D:73:TRP:CD2	1:D:350:THR:HG21	2.45	0.51
1:F:46:ILE:HD12	1:F:46:ILE:N	2.22	0.51
1:F:106:ALA:O	1:F:175:KCX:CD	2.58	0.51
1:A:213:PRO:HG3	1:D:193:LEU:CD2	2.41	0.51
1:B:81:TRP:HA	1:B:81:TRP:CE3	2.44	0.51
1:A:395:ARG:HH11	1:A:395:ARG:CG	2.19	0.51
1:B:46:ILE:HD11	1:B:349:PHE:CZ	2.44	0.51
1:B:16:PRO:HA	1:B:40:ILE:O	2.11	0.51
1:D:73:TRP:CZ3	1:D:308:MSE:HE1	2.46	0.51
1:D:120:TYR:C	1:D:121:ILE:HD12	2.31	0.51
1:F:61:ARG:O	1:F:61:ARG:HG3	2.10	0.51
1:F:230:THR:HG22	1:F:264:GLY:HA3	1.92	0.51
1:B:242:MSE:CE	1:B:277:ALA:HB1	2.31	0.51
1:D:316:MSE:CE	1:D:321:VAL:HA	2.39	0.51
1:F:97:GLU:O	1:F:389:ALA:HB1	2.11	0.51
1:C:313:SER:HB3	1:C:373:ARG:NH2	2.25	0.51
1:A:106:ALA:HB1	1:A:206:MSE:CE	2.40	0.51
1:A:195:LYS:HG2	1:A:222:ILE:HD11	1.93	0.51
1:F:312:LEU:HD23	1:F:373:ARG:CD	2.41	0.51
1:A:174:LEU:C	1:A:175:KCX:HA	2.31	0.51
1:C:106:ALA:O	1:C:175:KCX:HD2	2.10	0.51
1:F:16:PRO:O	1:F:61:ARG:HD2	2.10	0.51
1:F:208:HIS:C	1:F:208:HIS:CD2	2.83	0.51
1:A:268:ALA:HA	1:A:364:SER:HB3	1.91	0.51
1:C:180:HIS:HD2	1:C:213:PRO:HG2	1.73	0.51
1:C:183:THR:O	1:C:186:TRP:HD1	1.94	0.51
1:F:19:LEU:HD23	1:F:63:ASP:OD2	2.09	0.51
1:F:67:ALA:N	1:F:353:ASP:HB3	2.26	0.51
1:B:230:THR:HG22	1:B:264:GLY:CA	2.41	0.50
1:C:87:ILE:HG13	1:C:293:HIS:HB2	1.93	0.50
1:A:36:THR:HG22	1:A:37:ASP:H	1.76	0.50
1:A:77:HIS:O	1:A:290:THR:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ILE:O	1:B:81:TRP:CB	2.57	0.50
1:C:40:ILE:HG22	1:C:41:GLY:H	1.75	0.50
1:E:181:VAL:HG22	1:E:182:ILE:HG13	1.93	0.50
1:F:18:LEU:HD13	1:F:39:LEU:CD1	2.40	0.50
1:D:314:VAL:O	1:D:315:ASP:CB	2.59	0.50
1:F:176:VAL:HG13	1:F:207:VAL:HG22	1.93	0.50
1:A:387:ILE:HD12	1:A:387:ILE:N	2.26	0.50
1:B:127:GLU:CD	1:B:127:GLU:H	2.15	0.50
1:B:192:LYS:CD	1:B:222:ILE:HD12	2.41	0.50
1:C:254:CYS:C	1:C:257:GLU:N	2.65	0.50
1:C:301:VAL:O	1:C:301:VAL:HG22	2.10	0.50
1:D:180:HIS:CD2	1:D:213:PRO:HD2	2.43	0.50
1:E:98:ARG:NH1	1:E:392:TYR:HA	2.26	0.50
1:E:172:VAL:HG21	1:E:333:ILE:HG22	1.93	0.50
1:F:271:SER:CA	1:F:365:ASN:HD21	2.10	0.50
1:A:175:KCX:HZ	1:A:206:MSE:HE3	1.76	0.50
1:B:80:ILE:O	1:B:88:SER:OG	2.20	0.50
1:C:156:ASP:OD1	1:C:159:ARG:HG3	2.12	0.50
1:E:147:PRO:HB2	1:E:150:ARG:HG3	1.94	0.50
1:A:234:ASN:ND2	1:A:236:LYS:H	2.09	0.50
1:B:135:LEU:HD22	1:B:155:ILE:HG23	1.92	0.50
1:C:145:ARG:NH1	1:D:159:ARG:HD2	2.27	0.50
1:D:316:MSE:HE2	1:D:321:VAL:HG22	1.94	0.50
1:E:330:ALA:HB1	1:E:335:LEU:HB3	1.93	0.50
1:D:207:VAL:HG11	1:D:219:VAL:CG1	2.42	0.50
1:E:62:ILE:C	1:E:63:ASP:OD1	2.50	0.50
1:E:107:GLY:HA3	1:E:175:KCX:HD2	1.93	0.50
1:F:257:GLU:O	1:F:257:GLU:HG3	2.11	0.50
1:F:387:ILE:HD12	1:F:387:ILE:N	2.26	0.50
1:B:212:PRO:HB2	1:E:193:LEU:CD1	2.42	0.50
1:D:135:LEU:HD22	1:D:155:ILE:HG23	1.93	0.50
1:E:193:LEU:O	1:E:197:ILE:HG13	2.12	0.50
1:C:71:PRO:CG	1:C:327:ARG:HH12	2.20	0.50
1:C:86:ASP:HB3	1:D:112:ALA:O	2.12	0.50
1:C:262:ASP:OD2	1:C:289:SER:HB2	2.11	0.49
1:C:325:VAL:O	1:C:325:VAL:HG12	2.11	0.49
1:F:41:GLY:C	1:F:43:ASP:H	2.15	0.49
1:F:69:ILE:HD11	1:F:349:PHE:HB3	1.93	0.49
1:E:112:ALA:O	1:F:86:ASP:HB3	2.12	0.49
1:E:133:LEU:HG	1:E:171:ILE:HD13	1.94	0.49
1:F:156:ASP:O	1:F:160:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:HIS:C	1:B:208:HIS:CD2	2.86	0.49
1:B:215:LEU:HD21	1:E:193:LEU:HD22	1.93	0.49
1:B:234:ASN:HD22	1:B:236:LYS:H	1.60	0.49
1:D:36:THR:CG2	1:D:37:ASP:H	2.02	0.49
1:E:106:ALA:O	1:E:175:KCX:HE3	2.13	0.49
1:A:263:ILE:HG22	1:A:264:GLY:N	2.27	0.49
1:B:22:VAL:O	1:B:24:PRO:HD3	2.13	0.49
1:E:177:ARG:O	1:E:208:HIS:O	2.31	0.49
1:B:176:VAL:O	1:B:176:VAL:HG23	2.11	0.49
1:D:258:GLY:O	1:D:260:ARG:HD3	2.12	0.49
1:A:288:ILE:HD12	1:A:321:VAL:HG13	1.94	0.49
1:B:195:LYS:CD	1:B:199:LYS:HE3	2.41	0.49
1:C:228:VAL:HG22	1:C:260:ARG:HB2	1.94	0.49
1:C:318:PHE:HE1	1:C:354:LEU:HD12	1.78	0.49
1:D:211:GLU:H	1:D:211:GLU:CD	2.16	0.49
1:E:106:ALA:O	1:E:175:KCX:CD	2.60	0.49
1:E:302:TRP:HB3	1:E:392:TYR:HB3	1.94	0.49
1:A:50:GLY:N	1:A:53:LEU:HD21	2.28	0.49
1:C:159:ARG:NH2	1:D:145:ARG:HD3	2.27	0.49
1:D:368:VAL:CG1	1:D:369:SER:H	2.24	0.49
1:B:175:KCX:HD3	1:B:206:MSE:CE	2.43	0.49
1:E:118:ARG:NH1	1:E:167:ASN:HD21	2.00	0.49
1:F:373:ARG:NH2	1:F:375:PHE:CD1	2.81	0.49
1:B:114:PHE:O	1:B:117:PHE:HB3	2.12	0.48
1:C:21:ASN:OD1	1:C:21:ASN:C	2.51	0.48
1:D:157:LEU:C	1:D:157:LEU:HD23	2.34	0.48
1:D:211:GLU:HA	1:D:212:PRO:HD2	1.52	0.48
1:C:81:TRP:CD1	1:C:109:ALA:HB2	2.47	0.48
1:C:381:VAL:HA	1:C:385:GLU:O	2.13	0.48
1:F:18:LEU:O	1:F:62:ILE:HA	2.12	0.48
1:A:230:THR:O	1:A:231:HIS:HB2	2.14	0.48
1:D:85:THR:CG2	1:D:87:ILE:HG22	2.43	0.48
1:A:19:LEU:CG	1:A:61:ARG:HH12	2.15	0.48
1:A:245:GLU:O	1:A:249:ASN:ND2	2.47	0.48
1:C:335:LEU:HG	1:C:336:ASP:N	2.28	0.48
1:E:325:VAL:O	1:E:325:VAL:CG1	2.61	0.48
1:E:356:ASP:O	1:E:357:ALA:HB2	2.12	0.48
1:F:240:SER:C	1:F:242:MSE:H	2.17	0.48
1:B:106:ALA:HB1	1:B:206:MSE:CE	2.41	0.48
1:B:217:ASP:OD2	1:B:217:ASP:N	2.45	0.48
1:C:261:LEU:CD2	1:C:283:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ILE:HD12	1:D:193:LEU:HD23	1.93	0.48
1:F:306:THR:O	1:F:310:LYS:HG3	2.13	0.48
1:B:101:THR:HB	4:B:514:HOH:O	2.14	0.48
1:C:208:HIS:CD2	1:C:208:HIS:O	2.66	0.48
1:C:327:ARG:NE	1:C:327:ARG:HA	2.29	0.48
1:D:22:VAL:HG23	1:D:67:ALA:O	2.13	0.48
1:D:23:LYS:HD2	1:D:68:PHE:CE2	2.49	0.48
1:A:213:PRO:O	1:A:214:ALA:CB	2.62	0.48
1:A:263:ILE:HG22	1:A:265:HIS:H	1.79	0.48
1:B:74:VAL:HG22	1:B:102:THR:HB	1.94	0.48
1:E:196:LYS:O	1:E:200:ILE:HG22	2.14	0.48
1:E:316:MSE:HE2	1:E:321:VAL:HA	1.94	0.48
1:E:347:ALA:HB1	1:E:349:PHE:CE1	2.49	0.48
1:A:290:THR:O	1:A:290:THR:OG1	2.29	0.48
1:D:360:GLU:H	1:D:360:GLU:CD	2.17	0.48
1:E:195:LYS:CE	1:E:199:LYS:HE3	2.43	0.48
1:F:38:ILE:O	1:F:38:ILE:HD13	2.14	0.48
1:F:65:LYS:HZ2	1:F:65:LYS:CB	2.26	0.48
1:A:259:ILE:HD12	1:A:259:ILE:N	2.29	0.48
1:C:284:LEU:HD13	1:C:284:LEU:H	1.79	0.48
1:D:49:VAL:O	1:D:53:LEU:HD21	2.14	0.48
1:E:98:ARG:HH12	1:E:392:TYR:HA	1.79	0.48
1:E:357:ALA:O	1:E:371:LEU:O	2.32	0.48
1:F:174:LEU:HD21	1:F:197:ILE:HG22	1.96	0.48
1:F:231:HIS:HB3	1:F:269:SER:HB3	1.95	0.48
1:F:271:SER:HB2	1:F:365:ASN:CG	2.33	0.48
1:F:360:GLU:HG3	1:F:368:VAL:CG1	2.43	0.48
1:A:113:ASN:HB2	1:B:83:GLY:O	2.14	0.48
1:A:268:ALA:CA	1:A:364:SER:HB3	2.44	0.48
1:B:152:ILE:CD1	1:C:213:PRO:HG3	2.44	0.48
1:C:252:GLU:OE1	1:C:283:LEU:HB2	2.13	0.48
1:C:260:ARG:HD2	1:C:286:PHE:CD1	2.49	0.48
1:D:178:ALA:HB1	1:D:214:ALA:HB1	1.95	0.48
1:D:208:HIS:CD2	1:D:208:HIS:O	2.67	0.48
1:D:325:VAL:O	1:D:325:VAL:CG1	2.60	0.48
1:F:311:LEU:HA	1:F:314:VAL:HG22	1.96	0.48
1:C:106:ALA:O	1:C:175:KCX:CD	2.61	0.47
1:C:152:ILE:CD1	1:E:213:PRO:HG3	2.43	0.47
1:D:183:THR:O	1:D:186:TRP:HD1	1.96	0.47
1:E:89:ILE:HB	1:E:93:GLU:OE1	2.14	0.47
1:F:309:SER:CB	1:F:373:ARG:HH21	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:CD2	1:A:301:VAL:HG22	2.48	0.47
1:F:106:ALA:O	1:F:175:KCX:HE3	2.14	0.47
1:F:370:ARG:H	1:F:370:ARG:CD	2.27	0.47
1:A:133:LEU:O	1:A:175:KCX:N	2.47	0.47
1:B:25:VAL:HG23	1:B:70:SER:HB3	1.95	0.47
1:F:361:ALA:HB3	1:F:371:LEU:CD1	2.43	0.47
1:B:80:ILE:O	1:B:88:SER:CB	2.62	0.47
1:B:157:LEU:HD22	1:B:197:ILE:CD1	2.44	0.47
1:B:181:VAL:HG12	1:B:211:GLU:OE1	2.14	0.47
1:C:150:ARG:HH11	1:D:150:ARG:NH2	2.03	0.47
1:D:368:VAL:CG1	1:D:369:SER:N	2.77	0.47
1:E:178:ALA:HA	1:E:183:THR:HG21	1.96	0.47
1:F:271:SER:CB	1:F:365:ASN:ND2	2.78	0.47
1:A:233:PHE:HE2	1:A:285:PRO:HD3	1.78	0.47
1:B:324:ALA:HA	1:B:328:ASN:HD22	1.79	0.47
1:C:106:ALA:O	1:C:175:KCX:HE3	2.14	0.47
1:C:150:ARG:NH1	1:D:150:ARG:NE	2.57	0.47
1:C:263:ILE:HG13	1:C:311:LEU:HD11	1.96	0.47
1:D:180:HIS:HD2	1:D:213:PRO:CD	2.25	0.47
1:E:156:ASP:CG	1:E:159:ARG:HG3	2.34	0.47
1:B:114:PHE:C	1:B:115:HIS:O	2.47	0.47
1:C:197:ILE:O	1:C:201:LEU:HB2	2.15	0.47
1:D:138:ILE:O	1:D:141:VAL:HG22	2.14	0.47
1:D:299:PHE:HB3	1:D:300:PRO:CD	2.45	0.47
1:A:152:ILE:HG13	1:F:185:SER:OG	2.14	0.47
1:A:180:HIS:CD2	1:A:211:GLU:HB2	2.50	0.47
1:B:218:GLU:O	1:B:222:ILE:HG12	2.15	0.47
1:C:234:ASN:HA	1:C:269:SER:O	2.15	0.47
1:F:19:LEU:HD23	1:F:63:ASP:CG	2.35	0.47
1:F:126:ARG:NH2	1:F:387:ILE:HG12	2.30	0.47
1:F:373:ARG:HD3	1:F:373:ARG:H	1.78	0.47
1:B:175:KCX:HZ	1:B:206:MSE:HE3	1.80	0.47
1:D:374:LEU:HD12	1:D:374:LEU:O	2.14	0.47
1:E:110:GLY:HA2	1:E:133:LEU:HD22	1.97	0.47
1:E:112:ALA:HB3	1:E:137:SER:O	2.15	0.47
1:F:299:PHE:O	1:F:300:PRO:C	2.51	0.47
1:A:63:ASP:N	1:A:63:ASP:OD1	2.46	0.47
1:B:180:HIS:HD2	1:B:213:PRO:CD	2.28	0.47
1:C:288:ILE:HD11	1:C:316:MSE:HE3	1.94	0.47
1:F:20:THR:O	1:F:64:ALA:HA	2.15	0.47
1:F:100:VAL:HG21	1:F:103:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:VAL:HG12	1:B:356:ASP:N	2.29	0.47
1:C:211:GLU:O	1:C:213:PRO:HD2	2.14	0.47
1:C:254:CYS:O	1:C:257:GLU:N	2.48	0.47
1:F:174:LEU:HD21	1:F:197:ILE:CG2	2.45	0.47
1:C:260:ARG:HD2	1:C:286:PHE:CE1	2.50	0.46
1:D:242:MSE:HG2	1:D:274:VAL:HG13	1.95	0.46
1:D:329:PRO:O	1:D:332:VAL:HG13	2.14	0.46
1:E:38:ILE:HG22	1:E:49:VAL:CG2	2.29	0.46
1:A:328:ASN:O	1:A:331:SER:OG	2.30	0.46
1:C:215:LEU:HB2	1:C:218:GLU:CG	2.43	0.46
1:C:233:PHE:CZ	1:C:283:LEU:HD12	2.50	0.46
1:C:374:LEU:N	1:C:374:LEU:HD23	2.29	0.46
1:A:135:LEU:HB2	1:A:176:VAL:HG22	1.97	0.46
1:B:215:LEU:HB2	1:B:218:GLU:HG3	1.97	0.46
1:D:86:ASP:OD1	1:D:87:ILE:N	2.48	0.46
1:D:180:HIS:HB3	1:D:213:PRO:CB	2.28	0.46
1:D:207:VAL:HG11	1:D:219:VAL:HG13	1.96	0.46
1:F:363:ASP:CG	1:F:365:ASN:HD21	2.19	0.46
1:A:68:PHE:HB2	1:A:352:PHE:O	2.15	0.46
1:B:293:HIS:HD2	1:B:295:HIS:N	2.14	0.46
1:E:299:PHE:HB3	1:E:300:PRO:HD3	1.97	0.46
1:F:205:MSE:HE3	1:F:207:VAL:CG2	2.46	0.46
1:F:210:GLY:O	1:F:239:SER:HB3	2.15	0.46
1:F:373:ARG:NH2	1:F:375:PHE:HD1	2.13	0.46
1:A:317:PRO:HG3	1:A:320:ASN:ND2	2.26	0.46
1:D:290:THR:HB	1:D:301:VAL:HG21	1.95	0.46
1:E:189:THR:N	1:E:190:PRO:HD2	2.31	0.46
1:F:17:ILE:HD11	1:F:19:LEU:HD12	1.97	0.46
1:F:175:KCX:HZ	1:F:206:MSE:HE3	1.79	0.46
1:B:152:ILE:HG12	1:C:213:PRO:HG3	1.96	0.46
1:E:248:PHE:CE2	1:E:281:ARG:NH1	2.84	0.46
1:F:324:ALA:HA	1:F:328:ASN:HD22	1.81	0.46
1:A:16:PRO:O	1:A:58:ASP:HB2	2.16	0.46
1:B:192:LYS:HD2	1:B:222:ILE:HD12	1.98	0.46
1:B:212:PRO:HD3	1:B:238:GLY:HA3	1.97	0.46
1:C:101:THR:HB	1:C:382:ILE:HD11	1.98	0.46
1:C:203:VAL:HG22	1:C:204:PRO:CD	2.35	0.46
1:F:271:SER:CA	1:F:365:ASN:ND2	2.75	0.46
1:B:173:GLY:HA2	1:B:203:VAL:HG22	1.98	0.46
1:B:368:VAL:CG1	1:B:369:SER:N	2.78	0.46
1:D:17:ILE:O	1:D:40:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:CE1	1:A:310:LYS:NZ	2.84	0.46
1:B:176:VAL:HG22	1:B:207:VAL:HG22	1.97	0.46
1:F:123:GLU:CB	1:F:124:PRO:HD3	2.42	0.46
1:F:143:CYS:O	1:F:144:ASN:HB2	2.16	0.46
1:A:288:ILE:CG2	1:A:307:THR:HG22	2.46	0.46
1:C:97:GLU:HG2	1:C:387:ILE:CG2	2.45	0.46
1:D:81:TRP:CD1	1:D:109:ALA:HB2	2.51	0.46
1:B:33:GLN:CG	1:B:34:SER:H	2.27	0.45
1:B:225:PRO:HA	1:B:258:GLY:O	2.16	0.45
1:C:323:GLU:HG2	1:C:328:ASN:ND2	2.31	0.45
1:D:106:ALA:O	1:D:175:KCX:CD	2.65	0.45
1:E:56:PRO:O	1:E:57:ALA:C	2.54	0.45
1:E:271:SER:HB2	1:E:365:ASN:HD22	1.80	0.45
1:A:17:ILE:HG22	1:A:18:LEU:N	2.32	0.45
1:B:77:HIS:CE1	1:B:175:KCX:CX	2.99	0.45
1:F:72:GLY:HA3	1:F:101:THR:CG2	2.46	0.45
1:B:80:ILE:CG2	1:B:121:ILE:HG21	2.47	0.45
1:C:61:ARG:HD3	1:C:61:ARG:N	2.30	0.45
1:D:188:VAL:HA	1:D:191:VAL:HG23	1.98	0.45
1:F:373:ARG:HH22	1:F:375:PHE:HD1	1.62	0.45
1:C:59:THR:OG1	1:C:60:GLN:N	2.48	0.45
1:D:304:LEU:HG	1:D:308:MSE:HE2	1.98	0.45
1:F:65:LYS:HB2	1:F:65:LYS:NZ	2.30	0.45
1:F:254:CYS:O	1:F:257:GLU:N	2.50	0.45
1:F:308:MSE:HE3	1:F:325:VAL:CG1	2.46	0.45
1:F:373:ARG:CZ	1:F:373:ARG:C	2.85	0.45
1:A:106:ALA:C	1:A:175:KCX:HD2	2.36	0.45
1:A:152:ILE:HG21	1:F:213:PRO:HB3	1.98	0.45
1:B:23:LYS:NZ	1:B:33:GLN:O	2.48	0.45
1:C:67:ALA:N	1:C:353:ASP:HB2	2.31	0.45
1:C:181:VAL:HG23	1:C:211:GLU:OE1	2.16	0.45
1:C:297:MSE:O	1:C:302:TRP:HA	2.16	0.45
1:F:303:ASP:OD2	1:F:306:THR:HG22	2.16	0.45
1:C:283:LEU:C	1:C:283:LEU:HD13	2.37	0.45
1:D:94:CYS:HB3	1:D:292:LEU:HD23	1.98	0.45
1:D:98:ARG:HD3	1:D:390:SER:O	2.17	0.45
1:D:118:ARG:NH1	1:D:167:ASN:ND2	2.37	0.45
1:F:38:ILE:HD13	1:F:38:ILE:C	2.37	0.45
1:F:49:VAL:HG22	1:F:50:GLY:N	2.31	0.45
1:F:189:THR:O	1:F:192:LYS:HB2	2.16	0.45
1:D:241:ILE:O	1:D:248:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ALA:HA	1:D:308:MSE:HE3	1.98	0.45
1:E:18:LEU:HD12	1:E:55:ALA:CB	2.47	0.45
1:A:218:GLU:O	1:A:222:ILE:HG22	2.16	0.45
1:B:300:PRO:HG2	1:B:301:VAL:H	1.81	0.45
1:C:228:VAL:HG21	1:C:332:VAL:HG11	1.98	0.45
1:C:316:MSE:HG2	1:C:321:VAL:HG23	1.99	0.45
1:E:250:LEU:HD22	1:E:250:LEU:O	2.17	0.45
1:F:87:ILE:HG13	1:F:293:HIS:HB2	1.97	0.45
1:F:126:ARG:NH1	1:F:126:ARG:HG3	2.31	0.45
1:F:126:ARG:HH22	1:F:387:ILE:HG12	1.82	0.45
1:C:145:ARG:HH12	1:D:111:GLU:CD	2.19	0.45
1:C:230:THR:O	1:C:231:HIS:HB2	2.16	0.45
1:F:286:PHE:CZ	1:F:328:ASN:HB3	2.52	0.45
1:A:195:LYS:O	1:A:199:LYS:HG3	2.16	0.44
1:F:46:ILE:HG22	1:F:47:ALA:N	2.31	0.44
1:A:125:SER:HB2	1:A:129:ILE:HD12	1.99	0.44
1:A:152:ILE:HG21	1:F:213:PRO:CG	2.47	0.44
1:C:74:VAL:HG23	1:C:102:THR:HG22	2.00	0.44
1:E:217:ASP:OD2	1:E:217:ASP:N	2.48	0.44
1:E:235:GLY:HA3	1:E:365:ASN:ND2	2.30	0.44
1:C:217:ASP:OD1	1:C:247:LEU:HG	2.18	0.44
1:E:177:ARG:O	1:E:208:HIS:HD2	2.01	0.44
1:F:318:PHE:CE1	1:F:354:LEU:HD11	2.52	0.44
1:B:63:ASP:HB2	1:B:64:ALA:H	1.62	0.44
1:E:69:ILE:O	1:E:69:ILE:HG23	2.17	0.44
1:F:38:ILE:HD11	1:F:40:ILE:HD11	1.98	0.44
1:A:17:ILE:CD1	1:A:384:ALA:O	2.59	0.44
1:A:211:GLU:CD	1:A:211:GLU:N	2.68	0.44
1:C:100:VAL:HG22	1:C:304:LEU:HD23	1.99	0.44
1:F:161:LEU:CD2	1:F:201:LEU:HD13	2.47	0.44
1:F:271:SER:HB2	1:F:365:ASN:ND2	2.33	0.44
1:A:157:LEU:HD21	1:F:237:SER:HB3	1.99	0.44
1:A:290:THR:OG1	1:A:292:LEU:HB2	2.17	0.44
1:B:173:GLY:HA2	1:B:203:VAL:CG2	2.47	0.44
1:B:260:ARG:HB3	1:B:286:PHE:CD2	2.53	0.44
1:C:40:ILE:N	1:C:40:ILE:HD12	2.33	0.44
1:D:123:GLU:CB	1:D:124:PRO:HD3	2.47	0.44
1:F:284:LEU:CD1	1:F:316:MSE:HG3	2.47	0.44
1:A:213:PRO:HG2	1:D:152:ILE:CG2	2.46	0.44
1:B:242:MSE:HG2	1:B:274:VAL:HG13	1.98	0.44
1:C:212:PRO:O	1:C:213:PRO:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:PHE:CE2	1:D:328:ASN:HB3	2.53	0.44
1:E:339:ASN:HB3	1:E:342:ASP:OD1	2.17	0.44
1:F:373:ARG:CB	1:F:373:ARG:NH1	2.75	0.44
1:A:241:ILE:HA	1:A:247:LEU:CD1	2.43	0.44
1:A:266:GLY:HA3	1:A:291:ASP:HB3	1.98	0.44
1:B:64:ALA:C	1:B:67:ALA:N	2.71	0.44
1:B:260:ARG:HD2	1:B:286:PHE:CG	2.53	0.44
1:C:61:ARG:HH12	1:C:386:ALA:HB1	1.83	0.44
1:C:263:ILE:HG22	1:C:263:ILE:O	2.17	0.44
1:C:306:THR:O	1:C:310:LYS:HG3	2.18	0.44
1:B:290:THR:HG21	1:B:304:LEU:CA	2.41	0.44
1:C:351:VAL:CG2	1:C:379:TYR:HB2	2.48	0.44
1:D:106:ALA:O	1:D:175:KCX:HE3	2.18	0.44
1:E:211:GLU:HA	1:E:212:PRO:HD2	1.62	0.44
1:E:328:ASN:HB2	1:E:329:PRO:CD	2.47	0.44
1:B:133:LEU:O	1:B:175:KCX:N	2.51	0.43
1:E:143:CYS:O	1:E:144:ASN:HB2	2.18	0.43
1:F:244:ASP:O	1:F:247:LEU:N	2.49	0.43
1:A:244:ASP:OD1	1:A:246:ASP:HB2	2.18	0.43
1:D:118:ARG:HD3	1:D:167:ASN:ND2	2.31	0.43
1:F:65:LYS:CE	1:F:351:VAL:HG11	2.42	0.43
1:B:113:ASN:HD22	1:B:113:ASN:H	1.66	0.43
1:E:159:ARG:HH21	1:F:145:ARG:HD3	1.82	0.43
1:F:122:ILE:HG21	1:F:170:HIS:CE1	2.53	0.43
1:A:16:PRO:HG2	1:A:58:ASP:CB	2.44	0.43
1:A:70:SER:HB2	1:A:71:PRO:HD2	1.98	0.43
1:A:370:ARG:HH11	1:A:370:ARG:HB2	1.83	0.43
1:D:240:SER:HB3	1:D:243:GLU:HG2	1.99	0.43
1:E:362:THR:OG1	1:E:368:VAL:HG22	2.19	0.43
1:F:46:ILE:HG22	1:F:47:ALA:H	1.83	0.43
1:B:212:PRO:HG2	1:B:213:PRO:HD3	2.00	0.43
1:B:241:ILE:HA	1:B:247:LEU:HD23	2.00	0.43
1:C:275:ALA:O	1:C:279:ILE:HG22	2.18	0.43
1:F:17:ILE:HD13	1:F:17:ILE:O	2.19	0.43
1:B:348:ASP:HA	1:B:381:VAL:O	2.18	0.43
1:E:156:ASP:OD1	1:E:159:ARG:HG3	2.18	0.43
1:F:180:HIS:HB3	1:F:213:PRO:CG	2.49	0.43
1:F:357:ALA:O	1:F:372:LYS:HA	2.18	0.43
1:A:271:SER:HB2	1:A:365:ASN:ND2	2.33	0.43
1:B:275:ALA:O	1:B:279:ILE:HG12	2.18	0.43
1:C:152:ILE:HG12	1:E:213:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:KCX:OQ1	1:C:208:HIS:ND1	2.51	0.43
1:D:213:PRO:HG3	1:F:193:LEU:HD11	2.01	0.43
1:D:267:GLY:HA2	1:D:300:PRO:HG3	2.00	0.43
1:D:164:TYR:CD2	1:D:201:LEU:HD22	2.54	0.43
1:A:62:ILE:CG1	1:A:63:ASP:N	2.78	0.43
1:A:216:TYR:HD2	1:A:239:SER:O	2.01	0.43
1:A:257:GLU:O	1:A:257:GLU:HG3	2.17	0.43
1:B:290:THR:HG23	1:B:304:LEU:CD1	2.48	0.43
1:E:238:GLY:N	1:E:243:GLU:OE2	2.52	0.43
1:F:363:ASP:C	1:F:363:ASP:OD2	2.57	0.43
1:F:373:ARG:O	1:F:373:ARG:CD	2.67	0.43
1:C:39:LEU:O	1:C:39:LEU:HD12	2.19	0.43
1:C:101:THR:HG21	1:C:382:ILE:HD11	2.01	0.43
1:E:200:ILE:O	1:E:200:ILE:HG13	2.19	0.43
1:F:85:THR:CG2	1:F:88:SER:H	2.23	0.43
1:F:211:GLU:C	1:F:213:PRO:HD2	2.39	0.43
1:A:304:LEU:HD21	1:A:325:VAL:CG2	2.49	0.42
1:B:203:VAL:HG22	1:B:204:PRO:CD	2.48	0.42
1:C:218:GLU:OE1	1:C:218:GLU:C	2.57	0.42
1:C:316:MSE:CE	1:C:321:VAL:HG22	2.39	0.42
1:D:37:ASP:N	1:D:37:ASP:OD2	2.52	0.42
1:D:175:KCX:HZ	1:D:206:MSE:HE3	1.84	0.42
1:F:299:PHE:CB	1:F:300:PRO:HD3	2.43	0.42
1:A:77:HIS:CE1	1:A:175:KCX:CX	3.02	0.42
1:B:70:SER:O	1:B:349:PHE:HB3	2.19	0.42
1:B:135:LEU:HD21	1:B:197:ILE:HD12	2.00	0.42
1:C:152:ILE:HG12	1:E:213:PRO:CG	2.49	0.42
1:C:241:ILE:CD1	1:C:242:MSE:HG2	2.49	0.42
1:D:18:LEU:HD13	1:D:39:LEU:HB2	2.00	0.42
1:D:172:VAL:HG11	1:D:333:ILE:HB	2.01	0.42
1:E:178:ALA:HA	1:E:183:THR:HG23	2.01	0.42
1:A:290:THR:C	1:A:292:LEU:N	2.72	0.42
1:B:152:ILE:HG21	1:C:180:HIS:HB2	2.01	0.42
1:C:351:VAL:O	1:C:378:ARG:HB2	2.19	0.42
1:E:183:THR:O	1:E:186:TRP:HD1	2.02	0.42
1:A:149:LEU:CD1	1:A:176:VAL:HG13	2.50	0.42
1:A:205:MSE:HE2	1:A:207:VAL:HG22	2.02	0.42
1:A:232:CYS:SG	1:A:263:ILE:HD12	2.60	0.42
1:C:127:GLU:CD	1:C:127:GLU:H	2.22	0.42
1:D:217:ASP:OD1	1:D:247:LEU:HB2	2.19	0.42
1:E:363:ASP:OD2	1:E:363:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:THR:CB	1:F:292:LEU:HG	2.49	0.42
1:F:308:MSE:HE3	1:F:325:VAL:CG2	2.46	0.42
1:F:371:LEU:HD12	1:F:371:LEU:H	1.83	0.42
1:B:265:HIS:CE1	1:B:310:LYS:HZ3	2.37	0.42
1:C:211:GLU:HA	1:C:212:PRO:HD2	1.75	0.42
1:C:215:LEU:C	1:C:218:GLU:HG3	2.40	0.42
1:F:17:ILE:HD13	1:F:18:LEU:N	2.33	0.42
1:F:97:GLU:O	1:F:389:ALA:CB	2.67	0.42
1:A:241:ILE:HG22	1:A:247:LEU:HD13	2.01	0.42
1:B:387:ILE:HD12	1:B:387:ILE:H	1.85	0.42
1:D:46:ILE:O	1:D:343:VAL:HA	2.20	0.42
1:D:230:THR:HG22	1:D:262:ASP:HB3	2.00	0.42
1:A:126:ARG:CG	1:A:126:ARG:NH1	2.83	0.42
1:A:290:THR:CG2	1:A:304:LEU:HA	2.49	0.42
1:B:87:ILE:HD13	1:B:143:CYS:SG	2.59	0.42
1:B:263:ILE:HD11	1:B:288:ILE:CG2	2.20	0.42
1:C:61:ARG:HH12	1:C:386:ALA:CB	2.33	0.42
1:C:141:VAL:HG11	1:D:141:VAL:CG1	2.32	0.42
1:C:180:HIS:HD2	1:C:213:PRO:CG	2.31	0.42
1:C:192:LYS:HG2	1:C:222:ILE:HD12	2.01	0.42
1:C:293:HIS:CD2	1:C:295:HIS:H	2.33	0.42
1:E:177:ARG:HB3	1:E:182:ILE:CD1	2.49	0.42
1:E:208:HIS:ND1	1:E:231:HIS:CD2	2.87	0.42
1:E:265:HIS:HD2	1:E:266:GLY:O	2.03	0.42
1:F:293:HIS:CE1	1:F:296:SER:H	2.38	0.42
1:A:50:GLY:CA	1:A:53:LEU:HD21	2.50	0.42
1:B:201:LEU:HB2	1:B:203:VAL:HG12	2.01	0.42
1:B:213:PRO:HB3	1:E:152:ILE:HG21	2.01	0.42
1:B:260:ARG:HD2	1:B:286:PHE:CD2	2.55	0.42
1:C:112:ALA:O	1:D:86:ASP:HB3	2.19	0.42
1:C:306:THR:HG22	1:C:310:LYS:HE3	2.00	0.42
1:E:195:LYS:NZ	1:E:199:LYS:HE3	2.34	0.42
1:E:211:GLU:CD	1:E:211:GLU:H	2.23	0.42
1:E:268:ALA:CA	1:E:364:SER:HB2	2.31	0.42
1:D:135:LEU:O	1:D:137:SER:N	2.53	0.42
1:F:126:ARG:HG3	1:F:126:ARG:HH11	1.85	0.42
1:A:216:TYR:CD2	1:A:239:SER:O	2.73	0.42
1:A:286:PHE:CE2	1:A:328:ASN:HB3	2.55	0.42
1:B:162:GLU:O	1:B:166:GLU:HG3	2.20	0.42
1:C:233:PHE:HD2	1:C:263:ILE:HD11	1.83	0.42
1:D:70:SER:HB2	1:D:71:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:LEU:HD23	1:E:133:LEU:HA	1.92	0.42
1:E:135:LEU:CD2	1:E:155:ILE:HG23	2.50	0.42
1:E:288:ILE:HG12	1:E:311:LEU:CD1	2.49	0.42
1:F:293:HIS:HE1	1:F:295:HIS:HB2	1.84	0.42
1:F:302:TRP:CZ3	1:F:359:LEU:HD21	2.54	0.42
1:A:174:LEU:HD21	1:A:201:LEU:HD12	2.02	0.41
1:A:233:PHE:CD2	1:A:263:ILE:HD11	2.55	0.41
1:B:36:THR:HG23	1:B:37:ASP:N	2.35	0.41
1:B:80:ILE:CG2	1:B:81:TRP:N	2.63	0.41
1:B:81:TRP:CD1	1:B:109:ALA:HB2	2.55	0.41
1:B:203:VAL:CG2	1:B:204:PRO:CD	2.93	0.41
1:B:225:PRO:HB3	1:B:258:GLY:HA3	2.02	0.41
1:C:147:PRO:HB2	1:C:150:ARG:HG2	2.02	0.41
1:D:106:ALA:C	1:D:175:KCX:HD2	2.39	0.41
1:E:290:THR:HG23	1:E:292:LEU:N	2.30	0.41
1:E:341:LEU:HD23	1:E:341:LEU:HA	1.90	0.41
1:F:379:TYR:CE2	1:F:388:ALA:HB2	2.55	0.41
1:B:212:PRO:O	1:B:214:ALA:N	2.53	0.41
1:D:111:GLU:OE2	1:D:137:SER:OG	2.38	0.41
1:D:231:HIS:ND1	1:D:264:GLY:O	2.52	0.41
1:E:111:GLU:HG3	4:E:805:HOH:O	2.18	0.41
1:F:20:THR:HA	1:F:37:ASP:CB	2.49	0.41
1:F:77:HIS:CE1	1:F:230:THR:HG21	2.54	0.41
1:B:192:LYS:HD3	1:B:222:ILE:HD12	2.01	0.41
1:B:359:LEU:HD12	1:B:359:LEU:C	2.40	0.41
1:C:27:PHE:CE1	1:C:70:SER:HA	2.55	0.41
1:D:262:ASP:OD2	1:D:289:SER:OG	2.34	0.41
1:F:196:LYS:O	1:F:200:ILE:HG23	2.20	0.41
1:A:211:GLU:HA	1:A:212:PRO:HD2	1.65	0.41
1:A:213:PRO:HG2	1:D:152:ILE:HG21	2.01	0.41
1:B:69:ILE:HD12	1:B:351:VAL:HG22	2.01	0.41
1:B:128:ARG:CG	1:B:130:LYS:HE2	2.50	0.41
1:C:234:ASN:ND2	1:C:239:SER:OG	2.52	0.41
1:B:157:LEU:HD22	1:B:197:ILE:CG1	2.50	0.41
1:B:387:ILE:HD12	1:B:387:ILE:N	2.35	0.41
1:C:133:LEU:O	1:C:174:LEU:HA	2.21	0.41
1:E:157:LEU:HD12	1:E:161:LEU:HG	2.02	0.41
1:E:271:SER:HB2	1:E:365:ASN:ND2	2.35	0.41
1:F:312:LEU:HD23	1:F:373:ARG:NH1	2.30	0.41
1:F:370:ARG:O	1:F:370:ARG:HG2	2.19	0.41
1:A:180:HIS:O	1:A:184:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLU:OE1	1:C:219:VAL:N	2.54	0.41
1:F:370:ARG:NE	1:F:370:ARG:N	2.57	0.41
1:B:372:LYS:HB2	1:B:372:LYS:HZ2	1.85	0.41
1:C:61:ARG:NH1	1:C:386:ALA:HB1	2.36	0.41
1:C:202:LYS:O	1:C:202:LYS:HG3	2.21	0.41
1:D:23:LYS:HA	1:D:24:PRO:HD3	1.90	0.41
1:D:152:ILE:H	1:D:152:ILE:HG13	1.65	0.41
1:D:156:ASP:OD1	1:D:159:ARG:NH1	2.40	0.41
1:D:299:PHE:CB	1:D:300:PRO:CD	2.98	0.41
1:A:157:LEU:HD23	1:A:157:LEU:C	2.41	0.41
1:C:298:ASN:HA	1:C:392:TYR:CE2	2.56	0.41
1:C:352:PHE:CD2	1:C:352:PHE:N	2.89	0.41
1:D:26:GLY:C	1:D:327:ARG:HH22	2.24	0.41
1:A:51:SER:O	1:A:52:ALA:HB2	2.21	0.41
1:A:128:ARG:NH1	4:A:420:HOH:O	2.52	0.41
1:B:210:GLY:O	1:B:239:SER:HB3	2.21	0.41
1:B:211:GLU:HA	1:B:212:PRO:HD2	1.67	0.41
1:D:73:TRP:HB2	1:D:99:GLY:O	2.21	0.41
1:D:337:MSE:O	1:D:340:ARG:HG2	2.21	0.41
1:E:135:LEU:HD12	1:E:176:VAL:CG2	2.50	0.41
1:E:180:HIS:HB3	1:E:213:PRO:CG	2.50	0.41
1:E:208:HIS:CD2	1:E:208:HIS:O	2.74	0.41
1:E:358:ASP:HA	1:E:371:LEU:O	2.21	0.41
1:F:303:ASP:CG	1:F:306:THR:HG22	2.41	0.41
1:B:231:HIS:CE1	1:B:269:SER:HG	2.39	0.41
1:B:265:HIS:CE1	1:B:310:LYS:HZ2	2.39	0.41
1:D:285:PRO:HG2	1:D:316:MSE:SE	2.71	0.41
1:E:64:ALA:HB2	1:E:67:ALA:CA	2.51	0.41
1:F:231:HIS:CB	1:F:269:SER:HB3	2.51	0.41
1:F:272:PHE:CD2	1:F:363:ASP:HB3	2.56	0.41
1:B:186:TRP:CD2	1:B:190:PRO:HG3	2.55	0.40
1:B:196:LYS:HD3	1:B:196:LYS:C	2.42	0.40
1:C:353:ASP:HB3	1:C:378:ARG:NH1	2.32	0.40
1:D:73:TRP:CE2	1:D:350:THR:HG21	2.55	0.40
1:D:149:LEU:CD1	1:D:176:VAL:HG13	2.51	0.40
1:D:372:LYS:HD3	1:D:372:LYS:C	2.41	0.40
1:F:100:VAL:CG2	1:F:103:LEU:HD21	2.49	0.40
1:F:244:ASP:O	1:F:246:ASP:N	2.54	0.40
1:B:340:ARG:HD3	1:B:345:GLN:NE2	2.36	0.40
1:C:325:VAL:O	1:C:325:VAL:CG1	2.68	0.40
1:D:299:PHE:O	1:D:300:PRO:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:HIS:HB3	1:E:213:PRO:HG2	2.02	0.40
1:E:260:ARG:HD2	1:E:286:PHE:CG	2.56	0.40
1:E:311:LEU:O	1:E:314:VAL:HG13	2.21	0.40
1:F:265:HIS:CD2	1:F:266:GLY:O	2.67	0.40
1:F:308:MSE:HG2	1:F:325:VAL:HG11	2.03	0.40
1:C:71:PRO:O	1:C:72:GLY:C	2.60	0.40
1:C:284:LEU:HB2	1:C:285:PRO:HD2	2.02	0.40
1:C:305:ALA:O	1:C:308:MSE:HB2	2.22	0.40
1:C:353:ASP:O	1:C:355:VAL:HG13	2.21	0.40
1:F:347:ALA:HB1	1:F:349:PHE:HE1	1.87	0.40
1:C:40:ILE:HG22	1:C:41:GLY:N	2.35	0.40
1:C:101:THR:CB	1:C:382:ILE:HD11	2.51	0.40
1:C:130:LYS:NZ	1:C:169:GLU:O	2.42	0.40
1:F:81:TRP:CD1	1:F:109:ALA:HB2	2.57	0.40
1:A:148:GLU:OE2	1:A:177:ARG:NH1	2.54	0.40
1:C:215:LEU:O	1:C:218:GLU:CD	2.60	0.40
1:D:187:GLY:O	1:D:190:PRO:HD2	2.22	0.40
1:D:263:ILE:HG22	1:D:265:HIS:N	2.37	0.40
1:D:307:THR:O	1:D:311:LEU:HD23	2.22	0.40
1:D:359:LEU:HD23	1:D:374:LEU:CD2	2.51	0.40
1:E:266:GLY:HA3	1:E:291:ASP:OD2	2.21	0.40
1:F:24:PRO:HD3	1:F:35:SER:HA	2.02	0.40
1:F:106:ALA:C	1:F:175:KCX:HD2	2.41	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:PRO:CB	1:E:29:LYS:CD[1_655]	1.55	0.65
1:D:225:PRO:CB	1:E:29:LYS:CG[1_655]	1.70	0.50
1:D:225:PRO:CB	1:E:29:LYS:CE[1_655]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	372/417 (89%)	330 (89%)	34 (9%)	8 (2%)	6 11
1	B	360/417 (86%)	314 (87%)	38 (11%)	8 (2%)	6 11
1	C	302/417 (72%)	245 (81%)	47 (16%)	10 (3%)	4 5
1	D	349/417 (84%)	308 (88%)	33 (10%)	8 (2%)	6 10
1	E	363/417 (87%)	306 (84%)	47 (13%)	10 (3%)	5 7
1	F	346/417 (83%)	294 (85%)	37 (11%)	15 (4%)	2 3
All	All	2092/2502 (84%)	1797 (86%)	236 (11%)	59 (3%)	5 7

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	212	PRO
1	A	214	ALA
1	D	212	PRO
1	D	214	ALA
1	D	299	PHE
1	E	215	LEU
1	F	49	VAL
1	A	52	ALA
1	A	213	PRO
1	B	56	PRO
1	B	63	ASP
1	B	212	PRO
1	B	291	ASP
1	B	299	PHE
1	B	300	PRO
1	C	200	ILE
1	C	291	ASP
1	C	299	PHE
1	C	315	ASP
1	C	383	GLY
1	D	28	GLY
1	D	96	ALA
1	D	315	ASP
1	E	57	ALA
1	E	63	ASP
1	E	212	PRO

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Mol	Chain	Res	Type
1	E	315	ASP
1	E	357	ALA
1	F	41	GLY
1	F	42	GLY
1	F	245	GLU
1	F	299	PHE
1	F	300	PRO
1	A	299	PHE
1	A	300	PRO
1	D	71	PRO
1	D	215	LEU
1	C	268	ALA
1	C	281	ARG
1	E	187	GLY
1	E	300	PRO
1	F	317	PRO
1	C	294	GLY
1	E	21	ASN
1	E	299	PHE
1	F	62	ILE
1	F	184	GLY
1	F	265	HIS
1	F	389	ALA
1	C	212	PRO
1	C	213	PRO
1	F	212	PRO
1	F	390	SER
1	B	80	ILE
1	A	187	GLY
1	B	213	PRO
1	F	241	ILE
1	F	187	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	306/329 (93%)	281 (92%)	25 (8%)	11 21
1	B	301/329 (92%)	281 (93%)	20 (7%)	16 32
1	C	260/329 (79%)	235 (90%)	25 (10%)	8 15
1	D	298/329 (91%)	283 (95%)	15 (5%)	24 46
1	E	300/329 (91%)	275 (92%)	25 (8%)	11 21
1	F	292/329 (89%)	260 (89%)	32 (11%)	6 10
All	All	1757/1974 (89%)	1615 (92%)	142 (8%)	11 22

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	36	THR
1	A	61	ARG
1	A	63	ASP
1	A	81	TRP
1	A	126	ARG
1	A	135	LEU
1	A	141	VAL
1	A	174	LEU
1	A	186	TRP
1	A	208	HIS
1	A	211	GLU
1	A	216	TYR
1	A	217	ASP
1	A	222	ILE
1	A	247	LEU
1	A	263	ILE
1	A	315	ASP
1	A	325	VAL
1	A	341	LEU
1	A	345	GLN
1	A	354	LEU
1	A	362	THR
1	A	367	ASP
1	A	376	GLU
1	B	21	ASN
1	B	56	PRO
1	B	63	ASP
1	B	76	LEU
1	B	78	VAL

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Mol	Chain	Res	Type
1	B	81	TRP
1	B	113	ASN
1	B	135	LEU
1	B	157	LEU
1	B	166	GLU
1	B	208	HIS
1	B	213	PRO
1	B	216	TYR
1	B	217	ASP
1	B	284	LEU
1	B	298	ASN
1	B	301	VAL
1	B	345	GLN
1	B	349	PHE
1	B	360	GLU
1	C	21	ASN
1	C	60	GLN
1	C	61	ARG
1	C	81	TRP
1	C	148	GLU
1	C	166	GLU
1	C	177	ARG
1	C	182	ILE
1	C	186	TRP
1	C	193	LEU
1	C	201	LEU
1	C	203	VAL
1	C	208	HIS
1	C	213	PRO
1	C	216	TYR
1	C	218	GLU
1	C	241	ILE
1	C	247	LEU
1	C	257	GLU
1	C	284	LEU
1	C	303	ASP
1	C	354	LEU
1	C	373	ARG
1	C	378	ARG
1	C	393	ILE
1	D	38	ILE
1	D	63	ASP

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Mol	Chain	Res	Type
1	D	81	TRP
1	D	113	ASN
1	D	135	LEU
1	D	141	VAL
1	D	186	TRP
1	D	197	ILE
1	D	208	HIS
1	D	216	TYR
1	D	223	LEU
1	D	315	ASP
1	D	319	GLU
1	D	332	VAL
1	D	359	LEU
1	E	20	THR
1	E	29	LYS
1	E	38	ILE
1	E	61	ARG
1	E	81	TRP
1	E	133	LEU
1	E	135	LEU
1	E	141	VAL
1	E	149	LEU
1	E	159	ARG
1	E	179	SER
1	E	181	VAL
1	E	186	TRP
1	E	200	ILE
1	E	205	MSE
1	E	208	HIS
1	E	216	TYR
1	E	217	ASP
1	E	230	THR
1	E	281	ARG
1	E	301	VAL
1	E	314	VAL
1	E	319	GLU
1	E	360	GLU
1	E	374	LEU
1	F	17	ILE
1	F	19	LEU
1	F	20	THR
1	F	33	GLN

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Mol	Chain	Res	Type
1	F	38	ILE
1	F	65	LYS
1	F	81	TRP
1	F	85	THR
1	F	126	ARG
1	F	135	LEU
1	F	141	VAL
1	F	153	LYS
1	F	154	ASP
1	F	186	TRP
1	F	203	VAL
1	F	208	HIS
1	F	213	PRO
1	F	215	LEU
1	F	216	TYR
1	F	230	THR
1	F	247	LEU
1	F	249	ASN
1	F	261	LEU
1	F	276	GLU
1	F	301	VAL
1	F	306	THR
1	F	319	GLU
1	F	338	GLU
1	F	348	ASP
1	F	365	ASN
1	F	370	ARG
1	F	373	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	167	ASN
1	A	180	HIS
1	A	234	ASN
1	A	249	ASN
1	A	265	HIS
1	A	295	HIS
1	A	298	ASN
1	A	320	ASN
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	365	ASN
1	B	113	ASN
1	B	115	HIS
1	B	167	ASN
1	B	180	HIS
1	B	234	ASN
1	B	249	ASN
1	B	265	HIS
1	B	293	HIS
1	B	328	ASN
1	B	345	GLN
1	C	167	ASN
1	C	180	HIS
1	C	234	ASN
1	C	265	HIS
1	C	293	HIS
1	C	295	HIS
1	C	328	ASN
1	D	21	ASN
1	D	33	GLN
1	D	113	ASN
1	D	167	ASN
1	D	180	HIS
1	D	234	ASN
1	D	249	ASN
1	E	60	GLN
1	E	167	ASN
1	E	234	ASN
1	E	249	ASN
1	E	265	HIS
1	E	320	ASN
1	F	21	ASN
1	F	167	ASN
1	F	249	ASN
1	F	265	HIS
1	F	298	ASN
1	F	320	ASN
1	F	328	ASN
1	F	339	ASN
1	F	365	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	F	175	2,1	10,11,12	0.80	0	6,12,14	2.78	2 (33%)
1	KCX	B	175	2,1	10,11,12	0.79	0	6,12,14	2.79	2 (33%)
1	KCX	C	175	2,1	10,11,12	0.79	0	6,12,14	2.78	2 (33%)
1	KCX	A	175	2,1	10,11,12	0.79	0	6,12,14	2.78	2 (33%)
1	KCX	E	175	2,1	10,11,12	0.80	0	6,12,14	2.78	2 (33%)
1	KCX	D	175	2,1	10,11,12	0.79	0	6,12,14	2.76	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	F	175	2,1	-	3/9/10/12	-
1	KCX	B	175	2,1	-	3/9/10/12	-
1	KCX	C	175	2,1	-	3/9/10/12	-
1	KCX	A	175	2,1	-	3/9/10/12	-
1	KCX	E	175	2,1	-	3/9/10/12	-
1	KCX	D	175	2,1	-	3/9/10/12	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	KCX	CE-NZ-CX	-6.26	111.36	121.98
1	C	175	KCX	CE-NZ-CX	-6.25	111.38	121.98
1	E	175	KCX	CE-NZ-CX	-6.25	111.38	121.98
1	F	175	KCX	CE-NZ-CX	-6.24	111.39	121.98
1	A	175	KCX	CE-NZ-CX	-6.24	111.39	121.98
1	D	175	KCX	CE-NZ-CX	-6.21	111.44	121.98
1	F	175	KCX	OQ1-CX-NZ	-2.62	120.94	124.92
1	E	175	KCX	OQ1-CX-NZ	-2.61	120.96	124.92
1	B	175	KCX	OQ1-CX-NZ	-2.60	120.97	124.92
1	C	175	KCX	OQ1-CX-NZ	-2.58	121.01	124.92
1	A	175	KCX	OQ1-CX-NZ	-2.57	121.01	124.92
1	D	175	KCX	OQ1-CX-NZ	-2.53	121.08	124.92

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	175	KCX	OQ1-CX-NZ-CE
1	A	175	KCX	OQ2-CX-NZ-CE
1	B	175	KCX	OQ1-CX-NZ-CE
1	B	175	KCX	OQ2-CX-NZ-CE
1	C	175	KCX	OQ1-CX-NZ-CE
1	C	175	KCX	OQ2-CX-NZ-CE
1	D	175	KCX	OQ1-CX-NZ-CE
1	D	175	KCX	OQ2-CX-NZ-CE
1	E	175	KCX	OQ1-CX-NZ-CE
1	E	175	KCX	OQ2-CX-NZ-CE
1	F	175	KCX	OQ1-CX-NZ-CE
1	F	175	KCX	OQ2-CX-NZ-CE
1	A	175	KCX	CG-CD-CE-NZ
1	C	175	KCX	CG-CD-CE-NZ
1	E	175	KCX	CG-CD-CE-NZ
1	B	175	KCX	CG-CD-CE-NZ
1	D	175	KCX	CG-CD-CE-NZ
1	F	175	KCX	CG-CD-CE-NZ

There are no ring outliers.

6 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	175	KCX	7	0
1	B	175	KCX	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	175	KCX	4	0
1	A	175	KCX	13	0
1	E	175	KCX	7	0
1	D	175	KCX	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IMD	C	3744	2	3,5,5	0.72	0	4,5,5	0.55	0
3	IMD	D	3745	2	3,5,5	0.70	0	4,5,5	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	C	3744	2	-	-	0/1/1/1
3	IMD	D	3745	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:LEU	C	175:KCX	N	1.70
1	E	174:LEU	C	175:KCX	N	1.60
1	E	63:ASP	C	64:ALA	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	371/417 (88%)	0.07	9 (2%) 59 53	32, 50, 72, 89	0
1	B	361/417 (86%)	0.22	10 (2%) 53 47	30, 54, 79, 90	0
1	C	310/417 (74%)	0.95	56 (18%) 1 0	48, 74, 96, 99	0
1	D	356/417 (85%)	0.36	38 (10%) 6 4	39, 60, 89, 99	0
1	E	364/417 (87%)	0.46	26 (7%) 16 11	35, 60, 80, 91	0
1	F	351/417 (84%)	0.59	42 (11%) 4 2	39, 66, 88, 99	0
All	All	2113/2502 (84%)	0.43	181 (8%) 10 7	30, 60, 87, 99	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	373	ARG	10.2
1	F	62	ILE	9.1
1	C	315	ASP	6.8
1	C	61	ARG	6.6
1	C	384	ALA	6.0
1	F	22	VAL	6.0
1	F	34	SER	5.9
1	F	370	ARG	5.7
1	C	373	ARG	5.7
1	C	19	LEU	5.6
1	D	23	LYS	5.6
1	D	17	ILE	5.5
1	F	299	PHE	5.2
1	F	63	ASP	5.2
1	E	14	GLN	5.1
1	F	17	ILE	4.9
1	C	350	THR	4.9
1	C	382	ILE	4.9
1	C	327	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	355	VAL	4.8
1	C	351	VAL	4.6
1	D	370	ARG	4.6
1	C	392	TYR	4.6
1	F	18	LEU	4.5
1	C	62	ILE	4.5
1	D	21	ASN	4.5
1	D	63	ASP	4.5
1	C	218	GLU	4.4
1	E	368	VAL	4.4
1	C	301	VAL	4.3
1	A	396	ALA	4.3
1	E	267	GLY	4.3
1	F	327	ARG	4.2
1	F	341	LEU	4.1
1	F	61	ARG	4.1
1	E	29	LYS	4.1
1	F	367	ASP	4.0
1	C	388	ALA	4.0
1	D	20	THR	4.0
1	D	54	GLN	3.9
1	C	379	TYR	3.9
1	E	367	ASP	3.9
1	C	158	ASP	3.8
1	D	327	ARG	3.8
1	D	22	VAL	3.8
1	A	14	GLN	3.7
1	F	301	VAL	3.7
1	C	383	GLY	3.7
1	F	294	GLY	3.7
1	C	249	ASN	3.7
1	B	299	PHE	3.6
1	F	19	LEU	3.6
1	C	293	HIS	3.6
1	F	65	LYS	3.6
1	F	354	LEU	3.6
1	E	56	PRO	3.5
1	F	32	SER	3.5
1	A	54	GLN	3.5
1	D	322	VAL	3.5
1	B	250	LEU	3.4
1	F	21	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	245	GLU	3.4
1	C	58	ASP	3.4
1	D	33	GLN	3.4
1	D	299	PHE	3.3
1	E	372	LYS	3.2
1	E	356	ASP	3.2
1	C	40	ILE	3.2
1	D	68	PHE	3.1
1	E	299	PHE	3.1
1	F	26	GLY	3.1
1	C	386	ALA	3.1
1	D	169	GLU	3.1
1	F	368	VAL	3.1
1	D	55	ALA	3.1
1	E	51	SER	3.1
1	F	271	SER	3.1
1	C	349	PHE	3.1
1	F	300	PRO	3.1
1	D	35	SER	3.0
1	F	23	LYS	3.0
1	B	33	GLN	3.0
1	D	360	GLU	3.0
1	F	372	LYS	3.0
1	F	296	SER	2.9
1	F	46	ILE	2.9
1	B	241	ILE	2.9
1	E	64	ALA	2.9
1	F	48	ALA	2.9
1	C	387	ILE	2.9
1	F	365	ASN	2.8
1	F	272	PHE	2.8
1	D	34	SER	2.8
1	D	62	ILE	2.8
1	F	362	THR	2.8
1	A	259	ILE	2.8
1	C	381	VAL	2.8
1	C	212	PRO	2.7
1	F	212	PRO	2.7
1	D	301	VAL	2.7
1	D	18	LEU	2.7
1	C	290	THR	2.7
1	B	32	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	61	ARG	2.7
1	D	19	LEU	2.7
1	E	270	PHE	2.7
1	C	60	GLN	2.7
1	E	366	GLY	2.7
1	F	33	GLN	2.7
1	C	326	THR	2.6
1	F	267	GLY	2.6
1	F	374	LEU	2.6
1	D	214	ALA	2.6
1	C	248	PHE	2.6
1	C	23	LYS	2.6
1	C	354	LEU	2.6
1	C	353	ASP	2.6
1	C	299	PHE	2.6
1	D	354	LEU	2.5
1	C	374	LEU	2.5
1	C	390	SER	2.5
1	D	49	VAL	2.5
1	F	38	ILE	2.5
1	E	33	GLN	2.5
1	F	43	ASP	2.5
1	C	311	LEU	2.5
1	E	131	ALA	2.4
1	D	387	ILE	2.4
1	C	282	GLY	2.4
1	E	314	VAL	2.4
1	E	280	ALA	2.4
1	C	136	GLY	2.4
1	D	26	GLY	2.4
1	E	360	GLU	2.4
1	D	40	ILE	2.3
1	B	176	VAL	2.3
1	F	41	GLY	2.3
1	C	126	ARG	2.3
1	A	56	PRO	2.3
1	B	212	PRO	2.3
1	C	95	GLY	2.3
1	C	264	GLY	2.3
1	D	386	ALA	2.3
1	C	244	ASP	2.3
1	E	240	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	60	GLN	2.3
1	E	104	VAL	2.3
1	A	277	ALA	2.3
1	C	96	ALA	2.3
1	A	253	ARG	2.3
1	E	265	HIS	2.2
1	C	283	LEU	2.2
1	C	24	PRO	2.2
1	C	247	LEU	2.2
1	C	294	GLY	2.2
1	D	372	LYS	2.2
1	D	16	PRO	2.2
1	D	39	LEU	2.2
1	D	341	LEU	2.2
1	C	72	GLY	2.2
1	F	16	PRO	2.2
1	B	214	ALA	2.2
1	E	344	GLY	2.2
1	A	301	VAL	2.1
1	E	245	GLU	2.1
1	C	292	LEU	2.1
1	E	174	LEU	2.1
1	B	78	VAL	2.1
1	B	178	ALA	2.1
1	D	355	VAL	2.1
1	C	97	GLU	2.1
1	E	15	ALA	2.1
1	C	98	ARG	2.1
1	C	385	GLU	2.1
1	D	46	ILE	2.1
1	C	93	GLU	2.1
1	D	344	GLY	2.1
1	D	212	PRO	2.0
1	E	212	PRO	2.0
1	F	274	VAL	2.0
1	C	221	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	B	175	12/13	0.81	0.30	48,52,64,65	0
1	KCX	A	175	12/13	0.82	0.30	36,45,70,72	0
1	KCX	E	175	12/13	0.84	0.23	48,57,74,77	0
1	KCX	D	175	12/13	0.85	0.22	47,53,71,72	0
1	KCX	C	175	12/13	0.85	0.26	62,65,76,78	0
1	KCX	F	175	12/13	0.87	0.23	47,52,73,75	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	C	601	1/1	0.77	0.07	87,87,87,87	0
2	ZN	E	801	1/1	0.83	0.10	86,86,86,86	0
2	ZN	D	701	1/1	0.86	0.05	71,71,71,71	0
2	ZN	D	700	1/1	0.88	0.10	60,60,60,60	0
2	ZN	F	901	1/1	0.89	0.05	83,83,83,83	0
2	ZN	F	900	1/1	0.91	0.10	58,58,58,58	0
3	IMD	D	3745	5/5	0.91	0.19	61,61,61,62	0
2	ZN	C	600	1/1	0.94	0.09	65,65,65,65	0
2	ZN	A	419	1/1	0.95	0.06	60,60,60,60	0
2	ZN	B	500	1/1	0.95	0.09	53,53,53,53	0
3	IMD	C	3744	5/5	0.96	0.14	69,69,69,70	0
2	ZN	E	800	1/1	0.96	0.14	59,59,59,59	0
2	ZN	A	418	1/1	0.97	0.07	42,42,42,42	0
2	ZN	B	501	1/1	0.97	0.11	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.