Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 12:33 PM EDT

PDB ID	:	3DPJ / pdb_00003dpj
Title	:	The crystal structure of a TetR transcription regulator from Silicibacter pomeroyi DSS
Authors	:	Tan, K.; Li, H.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-07-08
Resolution	:	1.90 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:

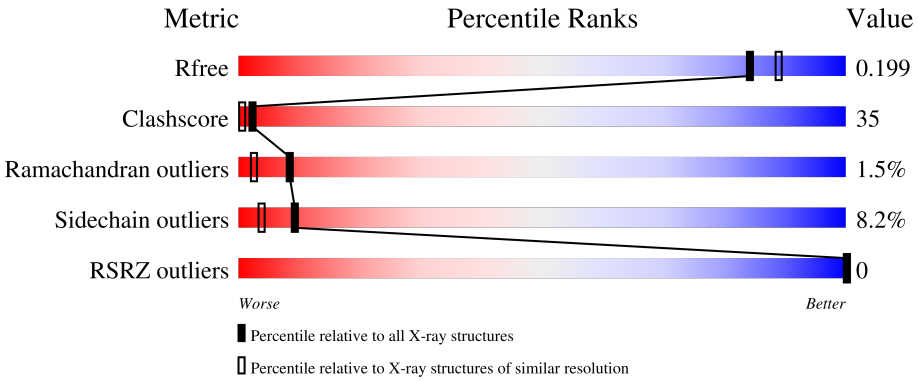
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	194	47% 47% 6%
1	B	194	48% 47%
1	C	194	51% 44% 5%
1	D	194	41% 47% 9%
1	E	194	54% 41% 5%

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Mol	Chain	Length	Quality of chain
1	F	194	47% 43% 6%
1	G	194	53% 42% 5%
1	H	194	48% 43% 6%

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
2	MES	G	192	-	-	X	-
3	EDO	C	195	-	-	X	-
3	EDO	D	195	-	-	X	-
3	EDO	F	195	-	-	X	-
3	EDO	H	198	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12978 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 Transcription regulator, TetR family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	Se	0	0	0
			1514	949	274	281	3	7			
1	B	190	Total	C	N	O	S	Se	0	0	0
			1487	934	269	275	3	6			
1	C	194	Total	C	N	O	S	Se	0	0	0
			1514	949	274	281	3	7			
1	D	190	Total	C	N	O	S	Se	0	0	0
			1487	934	269	275	3	6			
1	E	193	Total	C	N	O	S	Se	0	0	0
			1505	944	273	279	3	6			
1	F	188	Total	C	N	O	S	Se	0	0	0
			1473	925	267	272	3	6			
1	G	193	Total	C	N	O	S	Se	0	0	0
			1505	944	273	279	3	6			
1	H	188	Total	C	N	O	S	Se	0	0	0
			1473	925	267	272	3	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5LS67
A	-1	ASN	-	expression tag	UNP Q5LS67
A	0	ALA	-	expression tag	UNP Q5LS67
B	-2	SER	-	expression tag	UNP Q5LS67
B	-1	ASN	-	expression tag	UNP Q5LS67
B	0	ALA	-	expression tag	UNP Q5LS67
C	-2	SER	-	expression tag	UNP Q5LS67
C	-1	ASN	-	expression tag	UNP Q5LS67
C	0	ALA	-	expression tag	UNP Q5LS67
D	-2	SER	-	expression tag	UNP Q5LS67
D	-1	ASN	-	expression tag	UNP Q5LS67
D	0	ALA	-	expression tag	UNP Q5LS67
E	-2	SER	-	expression tag	UNP Q5LS67

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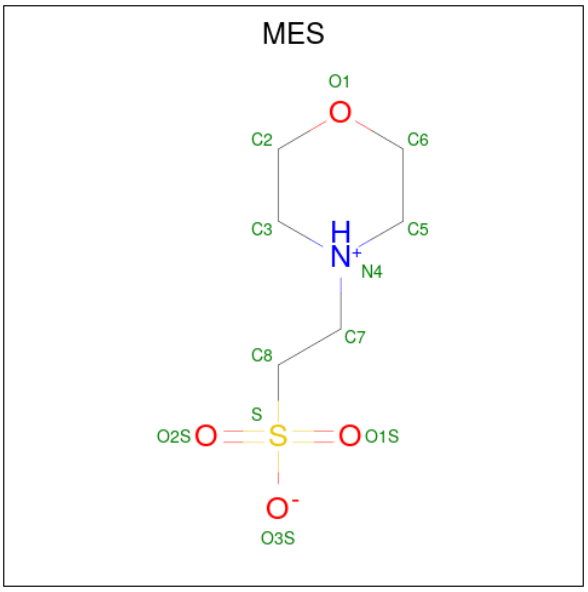
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q5LS67
E	0	ALA	-	expression tag	UNP Q5LS67
F	-2	SER	-	expression tag	UNP Q5LS67
F	-1	ASN	-	expression tag	UNP Q5LS67
F	0	ALA	-	expression tag	UNP Q5LS67
G	-2	SER	-	expression tag	UNP Q5LS67
G	-1	ASN	-	expression tag	UNP Q5LS67
G	0	ALA	-	expression tag	UNP Q5LS67
H	-2	SER	-	expression tag	UNP Q5LS67
H	-1	ASN	-	expression tag	UNP Q5LS67
H	0	ALA	-	expression tag	UNP Q5LS67

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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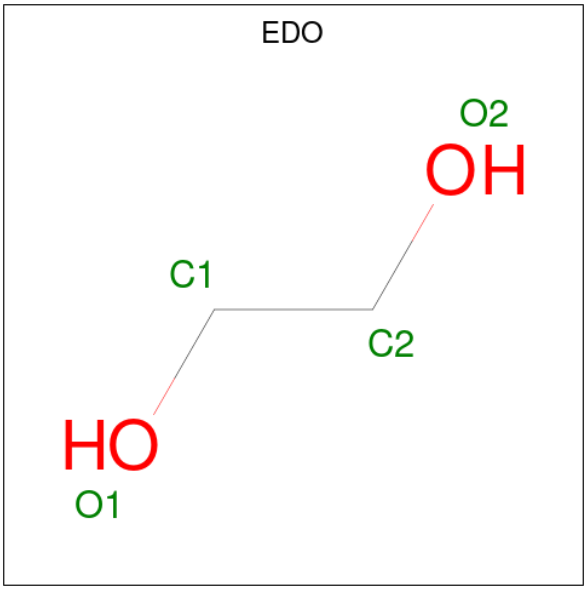
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

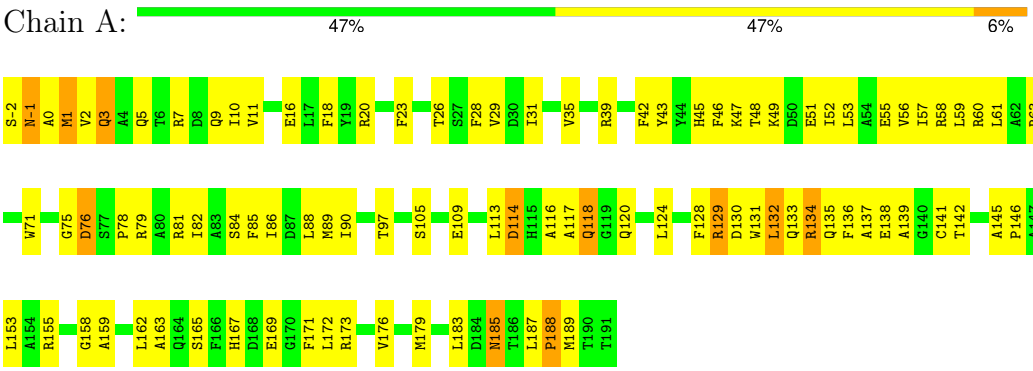
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	100	Total	O	0	0
			100	100		
4	C	95	Total	O	0	0
			95	95		
4	D	107	Total	O	0	0
			107	107		
4	E	95	Total	O	0	0
			95	95		
4	F	107	Total	O	0	0
			107	107		
4	G	94	Total	O	0	0
			94	94		
4	H	105	Total	O	0	0
			105	105		

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.

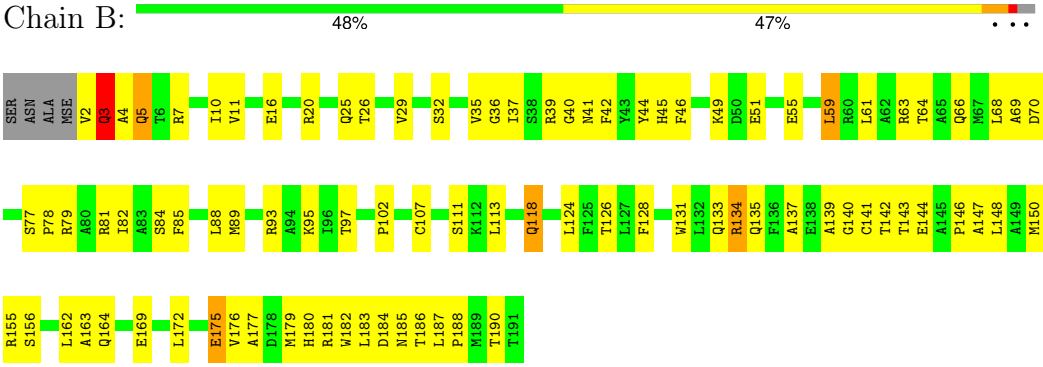
• Molecule 1: Transcription regulator, TetR family

Chain A:



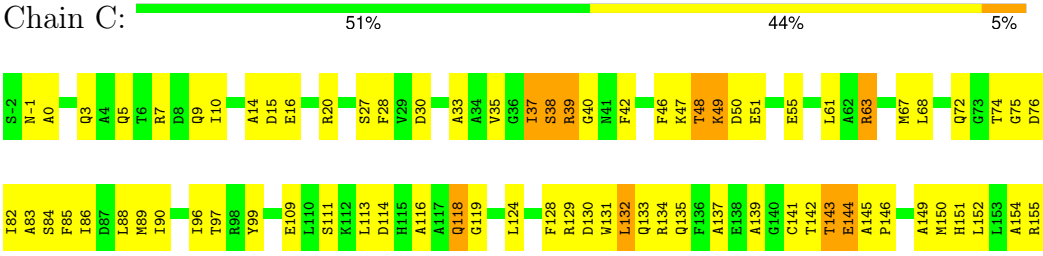
• Molecule 1: Transcription regulator, TetR family

Chain B:



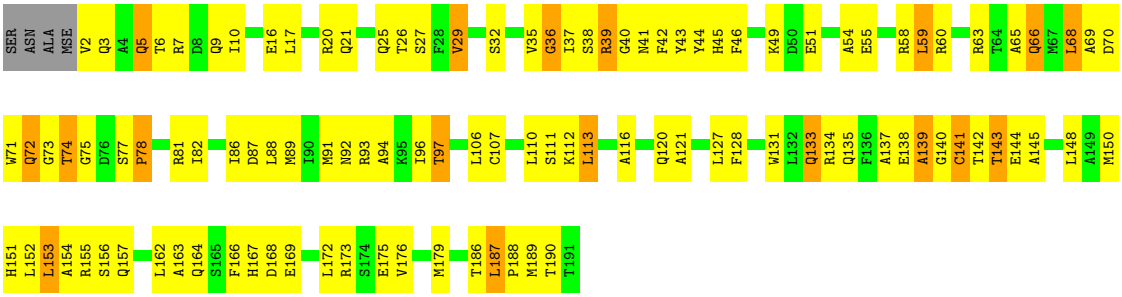
• Molecule 1: Transcription regulator, TetR family

Chain C:



• Molecule 1: Transcription regulator, TetR family

Chain D:

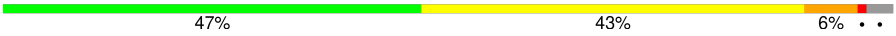


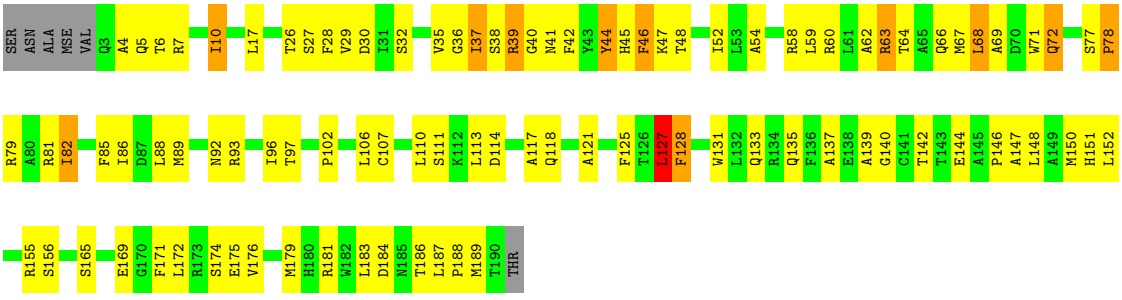
• Molecule 1: Transcription regulator, TetR family

Chain E:

• Molecule 1: Transcription regulator, TetR family

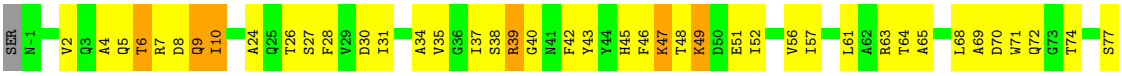
Chain F:

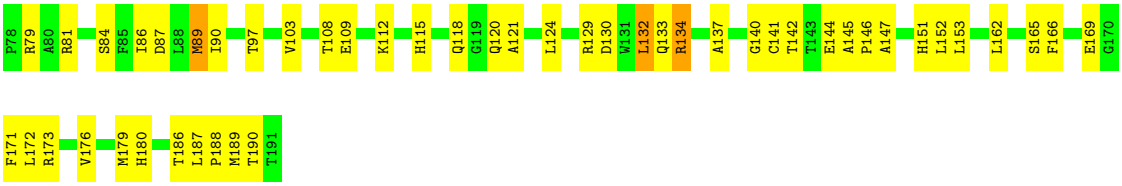




• Molecule 1: Transcription regulator, TetR family

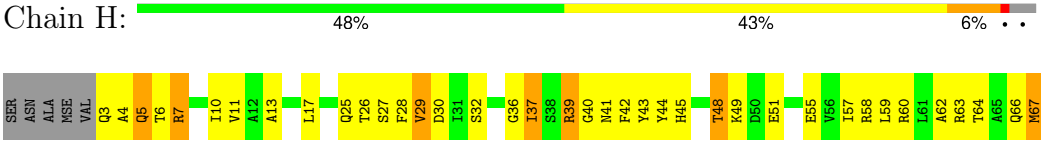
Chain G:





• Molecule 1: Transcription regulator, TetR family

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.52Å 93.07Å 93.40Å 89.35° 71.02° 71.04°	Depositor
Resolution (Å)	41.61 – 1.90 41.61 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (41.61-1.90) 95.8 (41.61-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.243 0.177 , 0.199	Depositor DCC
R_{free} test set	6942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 66.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.469 for h,h-k,h-l 0.457 for -h,-h+l,-h+k 0.458 for -h,-l,-k	Xtriage
Reported twinning fraction	0.502 for h,h-k,h-l	Depositor
Outliers	0 of 138037 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	12978	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 94.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2214e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MES, EDO

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	0.50	0/1536	0.88	0/2065
1	B	0.50	0/1510	0.88	0/2032
1	C	0.51	0/1536	0.81	1/2065 (0.0%)
1	D	0.50	0/1510	0.86	3/2032 (0.1%)
1	E	0.50	0/1527	0.86	1/2054 (0.0%)
1	F	0.50	0/1496	0.85	1/2012 (0.0%)
1	G	0.50	0/1527	0.91	5/2054 (0.2%)
1	H	0.48	0/1496	0.82	0/2012
All	All	0.50	0/12138	0.86	11/16326 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	39	ARG	N-CA-C	-7.17	104.27	112.87
1	C	49	LYS	N-CA-C	-6.59	104.17	111.82
1	G	39	ARG	N-CA-C	-6.24	104.77	112.38
1	F	46	PHE	N-CA-C	6.21	118.86	109.23
1	D	190	THR	N-CA-C	5.93	116.11	108.34
1	G	141	CYS	N-CA-C	-5.58	103.74	110.88
1	G	77	SER	CA-C-N	5.54	125.00	119.24
1	G	77	SER	C-N-CA	5.54	125.00	119.24
1	G	6	THR	N-CA-C	-5.48	106.72	113.41
1	D	187	LEU	CA-C-N	5.36	126.54	119.84
1	D	187	LEU	C-N-CA	5.36	126.54	119.84

There are no chirality outliers.

There are no planarity outliers.

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	1514	0	1485	127	0
1	B	1487	0	1457	107	0
1	C	1514	0	1485	102	0
1	D	1487	0	1457	118	0
1	E	1505	0	1473	79	0
1	F	1473	0	1441	123	0
1	G	1505	0	1473	99	0
1	H	1473	0	1441	116	0
2	A	12	0	12	3	0
2	B	12	0	12	4	0
2	C	12	0	12	5	0
2	D	12	0	12	2	0
2	E	12	0	12	4	0
2	F	12	0	12	5	0
2	G	12	0	12	7	0
2	H	12	0	12	3	0
3	A	4	0	6	2	0
3	B	12	0	18	2	0
3	C	28	0	42	13	0
3	D	20	0	30	7	0
3	E	12	0	18	1	0
3	F	16	0	24	7	0
3	H	28	0	42	14	0
4	A	101	0	0	14	0
4	B	100	0	0	13	0
4	C	95	0	0	17	0
4	D	107	0	0	16	0
4	E	95	0	0	8	0
4	F	107	0	0	8	0
4	G	94	0	0	12	0
4	H	105	0	0	13	0
All	All	12978	0	11988	852	0

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 35.

All (852) 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:D:72:GLN:HA	1:D:81:ARG:HD3	1.19	1.15
1:E:6:THR:HA	1:E:9:GLN:HE21	1.19	1.04
1:B:144:GLU:HG3	1:B:148:LEU:HG	1.36	1.03
1:E:63:ARG:HD3	2:E:192:MES:H81	1.36	1.03
1:B:72:GLN:HA	1:B:81:ARG:HD3	1.41	1.02
1:H:89:MSE:HE1	1:H:156:SER:HB2	1.43	0.97
1:B:11:VAL:HG12	1:B:59:LEU:HD23	1.43	0.97
1:F:88:LEU:HG	3:F:195:EDO:H12	1.45	0.97
1:C:63:ARG:HH12	3:C:194:EDO:H12	1.30	0.95
1:F:72:GLN:HE22	1:F:135:GLN:HE22	1.04	0.93
1:A:78:PRO:HB2	1:A:139:ALA:HB2	1.50	0.92
1:D:72:GLN:CA	1:D:81:ARG:HD3	2.00	0.91
1:D:72:GLN:HA	1:D:81:ARG:CD	2.02	0.90
1:H:89:MSE:CE	1:H:156:SER:HB2	2.00	0.90
1:E:48:THR:OG1	1:E:51:GLU:HG3	1.71	0.90
1:E:48:THR:HG1	1:E:51:GLU:HG3	1.36	0.89
1:B:7:ARG:HB2	1:B:45:HIS:CD2	2.08	0.88
1:D:144:GLU:HG3	1:D:148:LEU:HG	1.55	0.88
1:H:123:GLY:HA3	3:H:196:EDO:H12	1.55	0.86
1:D:46:PHE:HD1	1:D:51:GLU:HB3	1.40	0.86
1:F:133:GLN:NE2	1:F:146:PRO:HG3	1.91	0.86
1:B:49:LYS:HD2	3:B:195:EDO:H22	1.58	0.86
1:E:171:PHE:CE1	1:F:150:MSE:HB3	2.10	0.86
1:F:78:PRO:HB2	1:F:139:ALA:HB2	1.57	0.85
1:D:137:ALA:HA	1:D:142:THR:HA	1.58	0.85
1:A:173:ARG:HH11	3:A:193:EDO:H22	1.40	0.85
1:A:7:ARG:HB2	1:A:45:HIS:CD2	2.12	0.84
1:F:72:GLN:HE22	1:F:135:GLN:NE2	1.74	0.84
1:E:56:VAL:O	1:E:60:ARG:HG3	1.78	0.84
1:E:6:THR:HA	1:E:9:GLN:NE2	1.91	0.84
1:C:10:ILE:HD12	1:C:35:VAL:HG21	1.59	0.83
1:A:152:LEU:HD12	1:A:179:MSE:HE2	1.59	0.83
1:B:77:SER:HB2	1:B:78:PRO:HD2	1.59	0.83
1:F:156:SER:HB3	1:F:179:MSE:HE1	1.58	0.82
1:C:30:ASP:HA	3:C:195:EDO:H12	1.61	0.82
1:H:96:ILE:HD11	3:H:194:EDO:H11	1.61	0.82
1:A:158:GLY:HA3	1:B:154:ALA:O	1.79	0.82
1:H:89:MSE:HE2	4:H:304:HOH:O	1.79	0.82
1:H:102:PRO:HG3	2:H:192:MES:H52	1.62	0.81
1:F:133:GLN:HE21	1:F:146:PRO:HG3	1.44	0.81
1:F:72:GLN:NE2	1:F:81:ARG:HD3	1.96	0.80
2:C:192:MES:H82	4:C:291:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:MSE:HE1	1:H:156:SER:CB	2.12	0.79
1:G:121:ALA:O	1:G:124:LEU:HB2	1.83	0.79
1:G:189:MSE:HG2	1:G:190:THR:H	1.47	0.79
1:H:25:GLN:HG2	4:H:300:HOH:O	1.84	0.78
1:A:90:ILE:HG12	1:A:176:VAL:HG11	1.65	0.77
1:G:63:ARG:HD3	2:G:192:MES:H81	1.63	0.77
1:E:-1:ASN:HB3	1:E:2:VAL:HG13	1.67	0.77
1:G:145:ALA:HB3	1:G:146:PRO:HD3	1.67	0.77
2:A:192:MES:H82	4:A:252:HOH:O	1.85	0.76
1:D:92:ASN:HD22	3:D:195:EDO:H22	1.49	0.76
1:G:63:ARG:HB2	2:G:192:MES:H72	1.68	0.76
1:C:129:ARG:HG3	1:C:150:MSE:HG2	1.68	0.76
1:G:48:THR:OG1	1:G:51:GLU:HG3	1.85	0.75
1:D:93:ARG:O	1:D:97:THR:HG23	1.85	0.75
1:C:109:GLU:O	1:C:113:LEU:HG	1.85	0.75
1:F:152:LEU:HD12	1:F:179:MSE:HE2	1.68	0.75
1:G:171:PHE:CE1	1:H:150:MSE:HB3	2.20	0.75
1:B:16:GLU:HG3	1:B:20:ARG:HE	1.51	0.75
1:C:10:ILE:HD11	1:C:37:ILE:HD11	1.69	0.75
1:F:152:LEU:CD1	1:F:179:MSE:HE2	2.17	0.75
1:A:132:LEU:HD11	1:A:152:LEU:HD23	1.68	0.75
1:D:150:MSE:HG3	3:D:194:EDO:H22	1.69	0.74
1:E:72:GLN:HE22	1:E:135:GLN:HE22	1.33	0.74
1:H:78:PRO:HG2	1:H:79:ARG:H	1.52	0.74
1:C:50:ASP:HB3	3:C:198:EDO:H21	1.67	0.74
1:D:46:PHE:CD1	1:D:51:GLU:HB3	2.22	0.74
3:H:194:EDO:H21	4:H:251:HOH:O	1.86	0.74
1:G:10:ILE:HG13	1:G:35:VAL:HG21	1.69	0.74
1:A:173:ARG:NH1	3:A:193:EDO:H22	2.02	0.73
1:H:7:ARG:HB2	1:H:45:HIS:HD2	1.54	0.73
1:G:186:THR:O	1:G:188:PRO:HD3	1.89	0.73
1:A:155:ARG:HB2	1:A:179:MSE:HE3	1.72	0.72
1:F:96:ILE:HD11	3:F:195:EDO:H22	1.72	0.72
1:C:186:THR:O	1:C:188:PRO:HD3	1.90	0.71
1:D:63:ARG:HD2	4:D:225:HOH:O	1.89	0.71
1:F:171:PHE:HB2	3:F:196:EDO:H11	1.72	0.71
1:F:60:ARG:HG2	2:F:192:MES:O3S	1.89	0.71
1:F:68:LEU:HG	1:F:131:TRP:CD2	2.25	0.71
1:F:60:ARG:HA	1:F:63:ARG:HG3	1.72	0.71
1:C:61:LEU:HD23	1:C:124:LEU:HD23	1.73	0.71
1:H:77:SER:HB3	1:H:78:PRO:HD2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:GLU:HG3	1:H:148:LEU:HG	1.72	0.71
1:C:85:PHE:CE2	1:C:152:LEU:HG	2.25	0.70
1:E:72:GLN:NE2	1:E:81:ARG:HD2	2.05	0.70
1:A:155:ARG:CB	1:A:179:MSE:HE3	2.21	0.70
1:A:68:LEU:HD22	1:A:131:TRP:CG	2.26	0.70
1:F:77:SER:HB2	1:F:78:PRO:HD2	1.73	0.70
1:A:78:PRO:CB	1:A:139:ALA:HB2	2.22	0.70
1:A:153:LEU:HG	1:B:162:LEU:HD11	1.74	0.70
1:B:69:ALA:HA	4:B:272:HOH:O	1.91	0.70
1:G:115:HIS:O	1:G:118:GLN:HB2	1.91	0.70
1:C:90:ILE:HG12	1:C:176:VAL:HG11	1.73	0.69
1:D:69:ALA:O	1:D:72:GLN:HB3	1.93	0.69
1:D:49:LYS:HD2	3:D:193:EDO:H22	1.74	0.69
1:G:86:ILE:HG23	1:G:179:MSE:HE2	1.74	0.69
1:A:47:LYS:HD2	4:A:275:HOH:O	1.93	0.68
1:F:72:GLN:NE2	1:F:135:GLN:HE22	1.85	0.68
1:E:86:ILE:HG22	1:E:176:VAL:HG13	1.75	0.68
1:A:48:THR:OG1	1:A:51:GLU:HG3	1.94	0.68
1:F:175:GLU:HA	1:F:175:GLU:OE2	1.91	0.68
1:G:7:ARG:HB2	1:G:45:HIS:HD2	1.59	0.68
1:G:65:ALA:HA	1:G:68:LEU:HB2	1.75	0.68
1:A:7:ARG:HB2	1:A:45:HIS:HD2	1.57	0.67
1:B:77:SER:HB2	1:B:78:PRO:CD	2.24	0.67
1:D:120:GLN:HB2	4:D:287:HOH:O	1.95	0.67
1:D:176:VAL:HA	1:D:179:MSE:HE3	1.75	0.67
1:F:10:ILE:HD13	1:F:46:PHE:HD2	1.60	0.67
1:H:4:ALA:HB2	4:H:287:HOH:O	1.94	0.67
1:F:60:ARG:NH1	1:F:106:LEU:HD22	2.10	0.67
1:C:143:THR:HG22	4:C:240:HOH:O	1.94	0.67
1:F:64:THR:HG22	1:F:127:LEU:HD13	1.76	0.67
1:E:165:SER:HA	1:F:118:GLN:HE22	1.60	0.67
1:F:39:ARG:HB2	1:G:189:MSE:HG3	1.76	0.66
1:G:6:THR:O	1:G:10:ILE:HD12	1.95	0.66
1:A:109:GLU:O	1:A:113:LEU:HG	1.96	0.66
1:F:183:LEU:HG	1:F:183:LEU:O	1.95	0.66
1:H:37:ILE:HG22	1:H:41:ASN:ND2	2.10	0.66
1:F:64:THR:CG2	1:F:127:LEU:HD13	2.27	0.65
2:A:192:MES:H61	4:A:213:HOH:O	1.96	0.65
1:E:55:GLU:OE2	1:E:58:ARG:HD2	1.96	0.65
1:F:144:GLU:HG3	1:F:148:LEU:HG	1.78	0.65
1:F:155:ARG:CB	1:F:179:MSE:HE3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:GLN:HA	1:E:8:ASP:OD2	1.97	0.65
1:A:47:LYS:HE2	1:A:51:GLU:OE1	1.97	0.65
1:A:56:VAL:O	1:A:60:ARG:HG3	1.97	0.65
1:C:151:HIS:O	1:C:155:ARG:HG2	1.97	0.65
1:E:78:PRO:HD3	1:E:81:ARG:HH21	1.61	0.65
1:A:152:LEU:CD1	1:A:179:MSE:HE2	2.27	0.65
1:G:69:ALA:HA	4:G:211:HOH:O	1.96	0.65
1:D:96:ILE:HD11	3:D:195:EDO:H11	1.79	0.64
1:D:44:TYR:HD1	1:D:45:HIS:CE1	2.15	0.64
1:D:89:MSE:SE	1:D:156:SER:HB2	2.48	0.64
1:F:137:ALA:HA	1:F:142:THR:HA	1.79	0.64
1:F:144:GLU:OE2	1:F:147:ALA:HB3	1.97	0.64
2:H:192:MES:H51	4:H:301:HOH:O	1.96	0.64
1:D:66:GLN:HG3	1:D:70:ASP:OD1	1.96	0.64
1:G:137:ALA:HA	1:G:142:THR:HA	1.80	0.64
1:H:55:GLU:HG2	1:H:58:ARG:NH1	2.12	0.64
1:H:97:THR:HG21	4:H:214:HOH:O	1.97	0.64
1:A:61:LEU:HD23	1:A:124:LEU:HD23	1.79	0.64
1:B:3:GLN:HB2	1:B:44:TYR:HE1	1.62	0.64
1:A:152:LEU:HD12	1:A:179:MSE:CE	2.26	0.64
1:F:140:GLY:HA3	1:F:188:PRO:HG2	1.80	0.64
1:H:28:PHE:H	3:H:193:EDO:H11	1.60	0.64
1:H:63:ARG:O	1:H:67:MSE:HB3	1.97	0.64
1:C:47:LYS:HE3	1:C:51:GLU:OE1	1.99	0.63
1:D:72:GLN:HG3	1:D:81:ARG:NH1	2.12	0.63
1:H:109:GLU:HB2	3:H:198:EDO:H22	1.80	0.63
1:C:48:THR:HB	1:C:50:ASP:H	1.64	0.63
4:C:230:HOH:O	1:D:112:LYS:HE2	1.99	0.63
1:D:25:GLN:HG2	4:D:267:HOH:O	1.99	0.63
1:F:117:ALA:HB2	4:F:230:HOH:O	1.98	0.63
1:A:183:LEU:HD11	1:A:187:LEU:HD11	1.81	0.63
1:G:132:LEU:HG	1:G:152:LEU:HD23	1.79	0.63
1:H:68:LEU:HG	1:H:131:TRP:CD2	2.33	0.63
1:C:89:MSE:HE1	1:C:179:MSE:HE1	1.80	0.63
1:B:25:GLN:HG2	4:B:232:HOH:O	1.97	0.63
1:G:103:VAL:HA	4:G:204:HOH:O	1.99	0.63
1:A:155:ARG:HG3	4:A:228:HOH:O	1.99	0.62
1:C:171:PHE:CE1	1:D:150:MSE:HB3	2.34	0.62
3:C:199:EDO:H21	4:C:280:HOH:O	1.99	0.62
1:F:186:THR:HA	4:F:234:HOH:O	1.98	0.62
1:G:137:ALA:HA	1:G:142:THR:CA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLN:OE1	1:B:81:ARG:HD2	1.99	0.62
1:D:97:THR:HG21	1:D:169:GLU:HA	1.81	0.62
1:A:82:ILE:O	1:A:85:PHE:HB3	2.00	0.62
1:A:171:PHE:CE1	1:B:150:MSE:HG3	2.35	0.62
1:C:86:ILE:HG22	1:C:176:VAL:HG13	1.82	0.62
1:C:158:GLY:HA3	1:D:154:ALA:O	1.99	0.62
1:D:172:LEU:O	1:D:176:VAL:HG23	1.99	0.62
1:G:5:GLN:HA	1:G:8:ASP:HB2	1.80	0.62
1:H:64:THR:O	1:H:68:LEU:HB2	2.00	0.61
2:G:192:MES:O3S	2:G:192:MES:H62	2.00	0.61
1:E:63:ARG:CD	2:E:192:MES:H81	2.22	0.61
1:A:131:TRP:O	1:A:135:GLN:HG2	2.00	0.61
1:D:72:GLN:HG3	1:D:81:ARG:HH11	1.65	0.61
1:H:71:TRP:O	1:H:81:ARG:HG2	2.00	0.61
1:G:133:GLN:HG3	1:G:146:PRO:HG3	1.83	0.61
1:D:27:SER:OG	1:D:29:VAL:HG13	2.00	0.61
1:E:60:ARG:HG2	2:E:192:MES:H52	1.83	0.61
1:A:81:ARG:O	1:A:84:SER:HB2	2.00	0.61
1:D:143:THR:HG22	4:D:217:HOH:O	2.00	0.61
1:H:27:SER:O	1:H:30:ASP:HB2	2.01	0.61
1:H:144:GLU:OE2	1:H:144:GLU:O	2.18	0.61
1:G:169:GLU:HG3	4:G:217:HOH:O	1.99	0.60
1:A:31:ILE:O	1:A:35:VAL:HG23	2.01	0.60
1:E:186:THR:O	1:E:188:PRO:HD3	2.02	0.60
1:A:29:VAL:HG23	4:A:269:HOH:O	2.01	0.60
1:A:-1:ASN:O	1:A:3:GLN:HG2	2.02	0.60
1:B:3:GLN:HG3	4:B:284:HOH:O	2.02	0.60
1:C:7:ARG:NH2	1:C:46:PHE:CZ	2.70	0.60
1:E:28:PHE:CE1	1:E:49:LYS:HG2	2.35	0.60
1:C:63:ARG:NH1	3:C:194:EDO:H12	2.09	0.60
1:B:39:ARG:HG3	1:B:40:GLY:N	2.16	0.60
1:A:-1:ASN:HA	1:A:2:VAL:HG12	1.83	0.60
1:H:123:GLY:CA	3:H:196:EDO:H12	2.30	0.60
1:B:141:CYS:SG	1:B:144:GLU:HB3	2.41	0.59
1:D:66:GLN:O	1:D:70:ASP:N	2.34	0.59
1:A:85:PHE:CE2	1:A:152:LEU:HG	2.37	0.59
1:A:137:ALA:CB	1:A:142:THR:HA	2.32	0.59
1:C:119:GLY:O	3:C:193:EDO:H12	2.03	0.59
1:D:46:PHE:HD1	1:D:51:GLU:CB	2.14	0.59
1:F:77:SER:HB2	1:F:78:PRO:CD	2.30	0.59
1:G:130:ASP:O	1:G:133:GLN:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:MSE:CE	1:C:179:MSE:HE1	2.31	0.59
1:F:37:ILE:HG22	1:F:41:ASN:ND2	2.18	0.59
1:A:133:GLN:HG3	1:A:146:PRO:HD3	1.84	0.59
1:B:93:ARG:O	1:B:97:THR:HG23	2.03	0.59
1:B:184:ASP:C	1:B:186:THR:H	2.11	0.59
1:D:7:ARG:HB2	1:D:45:HIS:CD2	2.37	0.59
1:A:11:VAL:HG12	1:A:59:LEU:HD22	1.84	0.59
2:D:192:MES:H62	4:D:249:HOH:O	2.02	0.59
1:G:189:MSE:HG2	1:G:190:THR:N	2.18	0.59
1:H:66:GLN:O	1:H:69:ALA:HB3	2.03	0.58
1:H:175:GLU:OE2	1:H:175:GLU:HA	2.02	0.58
1:A:187:LEU:O	1:D:38:SER:HB2	2.04	0.58
1:A:79:ARG:HD3	4:A:196:HOH:O	2.02	0.58
1:D:92:ASN:HD22	3:D:195:EDO:C2	2.16	0.58
1:F:92:ASN:HB2	3:F:195:EDO:H11	1.85	0.58
1:E:28:PHE:CD2	1:E:42:PHE:HE1	2.20	0.58
1:E:72:GLN:HE22	1:E:135:GLN:NE2	2.02	0.58
1:H:144:GLU:OE2	1:H:147:ALA:HB3	2.04	0.58
1:A:10:ILE:HD12	1:A:35:VAL:HG11	1.86	0.58
1:A:133:GLN:HG3	1:A:146:PRO:CD	2.33	0.58
1:B:141:CYS:HB2	4:B:231:HOH:O	2.02	0.58
1:G:89:MSE:HE2	1:G:172:LEU:HD11	1.85	0.58
1:A:188:PRO:HA	1:D:38:SER:HA	1.86	0.57
1:A:57:ILE:HD12	1:A:120:GLN:OE1	2.03	0.57
1:F:64:THR:HG23	1:F:128:PHE:CE2	2.39	0.57
1:H:177:ALA:HB2	4:H:294:HOH:O	2.03	0.57
1:B:46:PHE:CZ	1:B:55:GLU:HG3	2.40	0.57
1:F:68:LEU:HG	1:F:131:TRP:CG	2.39	0.57
1:E:133:GLN:O	1:E:145:ALA:HB1	2.05	0.57
1:F:78:PRO:HB2	1:F:139:ALA:CB	2.31	0.57
1:F:181:ARG:HH11	1:F:181:ARG:HB3	1.70	0.57
1:D:32:SER:HB3	1:D:42:PHE:CD2	2.40	0.57
1:D:60:ARG:NH1	1:D:106:LEU:HD22	2.19	0.57
1:E:72:GLN:NE2	1:E:135:GLN:HE22	2.03	0.56
1:H:5:GLN:H	1:H:5:GLN:NE2	2.02	0.56
1:F:54:ALA:O	1:F:58:ARG:HG3	2.05	0.56
1:B:68:LEU:HB3	1:B:131:TRP:CD1	2.40	0.56
1:C:47:LYS:HD3	4:C:287:HOH:O	2.05	0.56
1:E:121:ALA:O	1:E:124:LEU:HB2	2.05	0.56
1:F:68:LEU:HD12	1:F:71:TRP:CE3	2.41	0.56
1:D:141:CYS:HB3	4:D:247:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ALA:HA	4:E:279:HOH:O	2.05	0.56
1:G:47:LYS:HB2	1:G:47:LYS:HZ2	1.70	0.56
1:A:132:LEU:HB3	1:A:149:ALA:CB	2.35	0.56
1:B:70:ASP:O	1:B:74:THR:HG23	2.06	0.56
1:G:43:TYR:HA	1:G:46:PHE:O	2.06	0.56
1:A:155:ARG:NH1	4:A:228:HOH:O	2.39	0.56
1:F:102:PRO:HG3	2:F:192:MES:H32	1.88	0.56
1:H:86:ILE:HG22	1:H:176:VAL:HG13	1.86	0.56
1:B:2:VAL:CG2	1:B:5:GLN:HE22	2.19	0.56
1:E:132:LEU:HG	1:E:152:LEU:HD23	1.88	0.56
1:C:28:PHE:CE1	1:C:49:LYS:HG2	2.41	0.55
1:F:184:ASP:C	1:F:186:THR:H	2.14	0.55
1:C:155:ARG:HB3	1:C:179:MSE:SE	2.56	0.55
1:G:79:ARG:HB3	4:G:267:HOH:O	2.07	0.55
1:H:109:GLU:CG	3:H:198:EDO:H22	2.36	0.55
1:A:68:LEU:O	1:A:71:TRP:HB2	2.05	0.55
1:A:134:ARG:HD2	1:A:134:ARG:C	2.32	0.55
1:F:60:ARG:HH11	1:F:106:LEU:HD22	1.69	0.55
1:E:2:VAL:HG23	4:E:241:HOH:O	2.06	0.55
1:G:137:ALA:HA	1:G:142:THR:N	2.22	0.55
1:B:102:PRO:HG2	4:B:239:HOH:O	2.05	0.55
1:B:2:VAL:HB	1:B:4:ALA:HB3	1.89	0.55
1:B:176:VAL:HA	1:B:179:MSE:HE3	1.88	0.55
1:B:11:VAL:CG1	1:B:59:LEU:HD23	2.27	0.55
1:E:38:SER:C	1:E:40:GLY:N	2.64	0.55
1:G:35:VAL:HG12	1:G:37:ILE:HG23	1.89	0.55
1:B:177:ALA:HB2	4:B:288:HOH:O	2.07	0.54
1:E:87:ASP:OD1	1:E:180:HIS:NE2	2.33	0.54
1:B:181:ARG:HH12	3:B:194:EDO:H22	1.72	0.54
1:C:132:LEU:HB3	1:C:149:ALA:CB	2.38	0.54
1:A:28:PHE:HD2	1:A:42:PHE:CE1	2.25	0.54
1:C:30:ASP:CA	3:C:195:EDO:H12	2.37	0.54
1:F:78:PRO:HG2	1:F:79:ARG:H	1.73	0.54
1:F:79:ARG:CD	1:F:187:LEU:HD12	2.36	0.54
1:G:165:SER:HA	1:H:118:GLN:HE22	1.71	0.54
1:H:109:GLU:CB	3:H:198:EDO:H22	2.36	0.54
1:C:81:ARG:CZ	4:C:284:HOH:O	2.55	0.54
1:G:87:ASP:OD1	1:G:180:HIS:NE2	2.35	0.54
1:A:132:LEU:HB3	1:A:149:ALA:HB1	1.90	0.54
1:D:10:ILE:HD11	1:D:46:PHE:CD2	2.41	0.54
1:F:38:SER:HA	1:G:188:PRO:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:PRO:HD3	1:C:81:ARG:HH21	1.73	0.54
1:D:7:ARG:NH1	1:D:45:HIS:HB3	2.23	0.54
1:E:6:THR:O	1:E:10:ILE:HD12	2.07	0.54
1:E:90:ILE:HG12	1:E:176:VAL:HG11	1.90	0.54
1:C:75:GLY:HA3	1:C:81:ARG:HD3	1.90	0.54
1:A:116:ALA:C	1:A:118:GLN:H	2.16	0.54
1:B:113:LEU:HD21	4:B:230:HOH:O	2.07	0.54
4:E:217:HOH:O	1:F:118:GLN:HG2	2.08	0.54
1:F:66:GLN:O	1:F:69:ALA:HB3	2.08	0.54
1:H:78:PRO:CG	1:H:79:ARG:H	2.20	0.54
1:E:37:ILE:HD12	1:E:41:ASN:HB3	1.89	0.54
1:A:28:PHE:CD2	1:A:42:PHE:HE1	2.26	0.53
1:C:163:ALA:O	1:C:167:HIS:HA	2.08	0.53
1:D:6:THR:O	1:D:9:GLN:HB3	2.08	0.53
1:B:68:LEU:HD23	1:B:131:TRP:HB2	1.89	0.53
1:C:81:ARG:O	1:C:84:SER:HB2	2.09	0.53
1:D:60:ARG:NH1	4:D:206:HOH:O	2.38	0.53
1:F:68:LEU:HD22	1:F:127:LEU:HD22	1.90	0.53
1:A:63:ARG:HD3	2:A:192:MES:O3S	2.09	0.53
1:F:155:ARG:HB3	1:F:179:MSE:HE3	1.91	0.53
1:A:39:ARG:HD2	1:A:43:TYR:HE2	1.73	0.53
1:A:113:LEU:O	1:A:114:ASP:C	2.52	0.53
1:B:111:SER:HB2	1:B:118:GLN:HE22	1.74	0.53
1:D:54:ALA:O	1:D:58:ARG:HG3	2.08	0.53
1:H:78:PRO:CB	1:H:139:ALA:HA	2.39	0.53
1:C:16:GLU:HG3	1:C:20:ARG:HE	1.73	0.53
1:C:131:TRP:CD1	4:C:278:HOH:O	2.62	0.53
1:E:145:ALA:HB3	1:E:146:PRO:HD3	1.91	0.53
1:F:38:SER:HB2	1:G:187:LEU:O	2.09	0.53
1:D:68:LEU:HD12	1:D:71:TRP:CZ3	2.44	0.53
1:B:78:PRO:HB2	1:B:139:ALA:HB2	1.91	0.52
1:B:131:TRP:O	1:B:135:GLN:HG2	2.08	0.52
1:D:16:GLU:OE2	1:D:20:ARG:NE	2.36	0.52
1:A:89:MSE:HE3	1:A:172:LEU:HD11	1.90	0.52
1:B:46:PHE:HZ	1:B:55:GLU:HG3	1.73	0.52
1:G:133:GLN:O	1:G:145:ALA:HB1	2.10	0.52
1:E:97:THR:OG1	1:E:169:GLU:HG3	2.10	0.52
1:F:155:ARG:HB2	1:F:179:MSE:HE3	1.91	0.52
1:H:37:ILE:HB	1:H:41:ASN:HB3	1.91	0.52
1:B:35:VAL:HG23	1:B:37:ILE:HG12	1.91	0.52
1:E:38:SER:C	1:E:40:GLY:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:ILE:O	1:G:56:VAL:HG23	2.09	0.52
1:C:116:ALA:C	1:C:118:GLN:H	2.16	0.52
1:D:74:THR:OG1	1:D:75:GLY:N	2.42	0.52
1:D:77:SER:HB2	1:D:78:PRO:CD	2.40	0.52
1:F:39:ARG:CB	1:G:189:MSE:HB2	2.40	0.52
1:G:112:LYS:NZ	1:H:99:TYR:O	2.33	0.52
1:H:68:LEU:HG	1:H:131:TRP:CG	2.45	0.52
1:H:71:TRP:CH2	1:H:88:LEU:HD22	2.45	0.52
1:A:167:HIS:HE1	1:B:118:GLN:HE21	1.57	0.52
1:B:144:GLU:OE2	1:B:147:ALA:HB3	2.10	0.52
1:C:33:ALA:HB3	3:C:195:EDO:H21	1.92	0.52
1:E:78:PRO:O	1:E:82:ILE:HG13	2.09	0.52
1:D:144:GLU:CG	1:D:148:LEU:HG	2.33	0.52
1:E:28:PHE:HD2	1:E:42:PHE:HE1	1.57	0.52
1:B:2:VAL:C	1:B:4:ALA:N	2.68	0.52
1:D:73:GLY:O	1:D:74:THR:C	2.52	0.52
1:A:68:LEU:HD22	1:A:131:TRP:CB	2.39	0.51
1:F:71:TRP:CH2	1:F:85:PHE:HA	2.44	0.51
1:A:16:GLU:HG3	1:A:20:ARG:HE	1.75	0.51
1:A:81:ARG:HB3	1:A:131:TRP:CH2	2.45	0.51
1:A:155:ARG:HB3	1:A:179:MSE:HE3	1.91	0.51
1:A:183:LEU:CD1	1:A:187:LEU:HD11	2.39	0.51
1:C:76:ASP:C	4:C:284:HOH:O	2.53	0.51
1:C:162:LEU:HB2	1:C:171:PHE:CE2	2.45	0.51
1:F:59:LEU:O	1:F:63:ARG:HG2	2.09	0.51
1:H:32:SER:HB3	1:H:42:PHE:CD2	2.45	0.51
1:H:184:ASP:C	1:H:186:THR:H	2.17	0.51
1:A:134:ARG:HD2	1:A:134:ARG:O	2.11	0.51
1:B:79:ARG:HD2	1:B:187:LEU:HD12	1.92	0.51
1:B:89:MSE:SE	1:B:156:SER:HB2	2.60	0.51
1:A:0:ALA:C	1:A:1:MSE:HG2	2.35	0.51
1:A:158:GLY:C	1:B:154:ALA:HB1	2.35	0.51
1:D:91:MSE:HG3	4:D:264:HOH:O	2.10	0.51
1:D:134:ARG:NH2	4:D:303:HOH:O	2.42	0.51
1:H:29:VAL:O	1:H:30:ASP:C	2.53	0.51
1:A:46:PHE:CZ	1:A:55:GLU:HG3	2.46	0.51
1:C:5:GLN:O	1:C:9:GLN:HG3	2.11	0.51
1:E:5:GLN:HB3	4:E:275:HOH:O	2.09	0.51
1:H:93:ARG:HD2	1:H:169:GLU:CD	2.36	0.51
1:B:71:TRP:CH2	1:B:85:PHE:HA	2.46	0.51
1:G:27:SER:O	1:G:31:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:GLU:HG3	1:H:148:LEU:CG	2.40	0.51
1:H:186:THR:HA	4:H:286:HOH:O	2.10	0.51
1:B:37:ILE:HG22	1:B:41:ASN:ND2	2.26	0.51
1:D:144:GLU:OE2	1:D:144:GLU:O	2.28	0.51
1:F:102:PRO:HB3	2:F:192:MES:H31	1.92	0.51
1:H:78:PRO:HB2	1:H:139:ALA:HB2	1.93	0.51
1:A:128:PHE:O	1:A:130:ASP:N	2.44	0.51
1:C:0:ALA:O	1:C:3:GLN:HG3	2.11	0.51
1:G:46:PHE:C	1:G:47:LYS:HG3	2.36	0.51
1:G:97:THR:OG1	1:G:169:GLU:HG2	2.11	0.51
1:B:111:SER:HB2	1:B:118:GLN:NE2	2.26	0.51
3:C:197:EDO:H21	4:C:248:HOH:O	2.10	0.51
1:D:46:PHE:CZ	1:D:55:GLU:HG3	2.46	0.51
1:F:10:ILE:CD1	1:F:46:PHE:HD2	2.23	0.51
2:B:192:MES:H62	4:B:270:HOH:O	2.10	0.50
1:C:38:SER:C	1:C:40:GLY:H	2.17	0.50
1:D:44:TYR:CD1	1:D:45:HIS:CE1	2.99	0.50
1:F:89:MSE:SE	1:F:156:SER:HB2	2.62	0.50
1:G:63:ARG:HD3	2:G:192:MES:C8	2.37	0.50
1:H:29:VAL:HA	1:H:32:SER:OG	2.11	0.50
1:H:143:THR:HG22	4:H:221:HOH:O	2.10	0.50
1:A:132:LEU:O	1:A:136:PHE:HD2	1.95	0.50
1:B:63:ARG:CD	4:B:212:HOH:O	2.59	0.50
1:B:143:THR:HG22	4:B:244:HOH:O	2.09	0.50
1:C:61:LEU:HD23	1:C:124:LEU:CD2	2.41	0.50
1:F:67:MSE:HE1	4:F:254:HOH:O	2.11	0.50
1:B:81:ARG:HA	1:B:84:SER:OG	2.11	0.50
1:F:171:PHE:CZ	1:F:175:GLU:HG2	2.46	0.50
1:G:90:ILE:HD12	1:G:173:ARG:HG2	1.92	0.50
1:H:11:VAL:HG12	1:H:59:LEU:CD2	2.42	0.50
1:H:123:GLY:HA3	3:H:196:EDO:C1	2.35	0.50
1:A:132:LEU:HD11	1:A:152:LEU:CD2	2.41	0.50
2:B:192:MES:H71	4:B:208:HOH:O	2.12	0.50
1:E:71:TRP:CD2	1:E:84:SER:HB3	2.47	0.50
1:F:36:GLY:O	1:F:37:ILE:HG23	2.12	0.50
1:B:85:PHE:O	1:B:88:LEU:HB3	2.12	0.50
1:D:163:ALA:HB2	1:D:172:LEU:HD13	1.94	0.50
2:C:192:MES:H21	4:C:214:HOH:O	2.11	0.49
1:D:78:PRO:HB2	1:D:139:ALA:HB2	1.94	0.49
1:F:92:ASN:HD22	3:F:195:EDO:C1	2.25	0.49
1:H:36:GLY:O	1:H:37:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:ARG:HG3	1:H:40:GLY:N	2.27	0.49
1:C:10:ILE:HD11	1:C:37:ILE:CD1	2.38	0.49
1:E:86:ILE:HD13	1:E:179:MSE:HB3	1.94	0.49
1:F:39:ARG:HG3	1:F:40:GLY:N	2.26	0.49
1:G:27:SER:O	1:G:30:ASP:HB2	2.12	0.49
1:E:35:VAL:HG12	1:E:37:ILE:HG23	1.94	0.49
1:H:5:GLN:H	1:H:5:GLN:CD	2.21	0.49
1:H:68:LEU:HD12	1:H:71:TRP:CE3	2.48	0.49
1:B:72:GLN:HA	1:B:81:ARG:CD	2.28	0.49
1:B:72:GLN:CA	1:B:81:ARG:HD3	2.28	0.49
1:B:175:GLU:OE2	1:B:175:GLU:HA	2.11	0.49
1:F:88:LEU:CG	3:F:195:EDO:H12	2.30	0.49
1:G:26:THR:O	1:G:49:LYS:HE3	2.12	0.49
1:A:116:ALA:O	1:A:118:GLN:N	2.45	0.49
1:A:52:ILE:O	1:A:56:VAL:HG23	2.12	0.49
1:A:165:SER:OG	1:B:107:CYS:HB3	2.13	0.49
1:C:90:ILE:HD12	1:C:173:ARG:HG2	1.94	0.49
1:E:189:MSE:HG2	1:E:190:THR:H	1.78	0.49
1:F:62:ALA:C	1:F:64:THR:H	2.21	0.49
1:G:57:ILE:HD12	1:G:120:GLN:OE1	2.12	0.49
1:C:7:ARG:NH2	1:C:46:PHE:HZ	2.11	0.49
1:D:72:GLN:HE22	1:D:135:GLN:NE2	2.11	0.49
1:F:64:THR:O	1:F:68:LEU:HB2	2.13	0.49
1:A:136:PHE:CD1	1:A:148:LEU:HD13	2.48	0.48
1:D:107:CYS:O	1:D:111:SER:HB2	2.12	0.48
1:F:60:ARG:NH1	4:F:204:HOH:O	2.46	0.48
1:F:156:SER:CB	1:F:179:MSE:HE1	2.39	0.48
1:G:28:PHE:CE1	1:G:49:LYS:HG2	2.48	0.48
1:G:153:LEU:HB3	1:H:162:LEU:HD11	1.95	0.48
1:B:97:THR:HG21	1:B:169:GLU:HA	1.95	0.48
1:C:46:PHE:HZ	1:C:55:GLU:HG3	1.78	0.48
1:C:83:ALA:HB1	1:C:180:HIS:HE1	1.77	0.48
1:F:82:ILE:HG22	1:F:135:GLN:HB3	1.95	0.48
1:G:90:ILE:HD11	1:G:173:ARG:HA	1.94	0.48
1:D:5:GLN:NE2	1:D:5:GLN:H	2.11	0.48
1:D:37:ILE:HG22	1:D:41:ASN:ND2	2.27	0.48
1:D:94:ALA:HB3	4:D:212:HOH:O	2.13	0.48
1:C:63:ARG:CD	2:C:192:MES:O1S	2.61	0.48
1:F:68:LEU:HG	1:F:131:TRP:CE2	2.48	0.48
1:H:77:SER:HB2	1:H:80:ALA:H	1.79	0.48
1:C:131:TRP:O	1:C:135:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HB3	1:C:149:ALA:HB1	1.96	0.48
1:D:39:ARG:HD3	1:D:43:TYR:HE2	1.79	0.48
1:E:189:MSE:HG2	1:E:190:THR:N	2.29	0.48
1:A:26:THR:O	1:A:49:LYS:HE3	2.14	0.48
1:A:63:ARG:O	1:A:66:GLN:HB3	2.14	0.48
1:C:48:THR:OG1	1:C:51:GLU:HG3	2.14	0.48
1:C:85:PHE:HE2	1:C:152:LEU:HG	1.73	0.48
1:G:34:ALA:HB2	4:G:248:HOH:O	2.14	0.48
1:E:28:PHE:HD2	1:E:42:PHE:CE1	2.32	0.48
1:G:2:VAL:HG22	1:G:2:VAL:O	2.12	0.48
1:D:152:LEU:O	1:D:155:ARG:HB2	2.14	0.48
1:E:32:SER:O	1:E:36:GLY:N	2.46	0.48
1:F:44:TYR:C	1:F:44:TYR:CD2	2.92	0.48
1:F:127:LEU:O	1:F:128:PHE:C	2.55	0.48
1:G:7:ARG:HB2	1:G:45:HIS:CD2	2.44	0.48
1:G:57:ILE:HB	1:G:120:GLN:NE2	2.28	0.48
1:D:68:LEU:HG	1:D:131:TRP:CG	2.50	0.47
1:B:2:VAL:HG21	1:B:5:GLN:HE22	1.79	0.47
1:G:165:SER:HA	1:H:118:GLN:NE2	2.29	0.47
1:H:127:LEU:O	1:H:128:PHE:C	2.54	0.47
1:A:23:PHE:CD1	1:A:53:LEU:HD13	2.49	0.47
1:A:78:PRO:O	1:A:79:ARG:C	2.56	0.47
1:B:46:PHE:CD1	1:B:51:GLU:HB3	2.50	0.47
1:B:46:PHE:HD1	1:B:51:GLU:HB3	1.78	0.47
1:C:137:ALA:CB	1:C:142:THR:HA	2.45	0.47
2:C:192:MES:H52	2:C:192:MES:H81	1.55	0.47
1:E:43:TYR:HA	1:E:46:PHE:O	2.14	0.47
1:A:145:ALA:HB3	1:A:146:PRO:HD3	1.96	0.47
1:B:61:LEU:HD23	1:B:124:LEU:HD23	1.96	0.47
1:B:163:ALA:CB	1:B:172:LEU:HD13	2.44	0.47
1:H:57:ILE:HG21	1:H:120:GLN:HG2	1.97	0.47
1:H:88:LEU:HG	3:H:194:EDO:H12	1.96	0.47
1:A:86:ILE:HG22	1:A:176:VAL:HG13	1.97	0.47
1:A:137:ALA:HA	1:A:142:THR:N	2.30	0.47
1:B:126:THR:HG21	1:E:143:THR:HA	1.95	0.47
1:C:46:PHE:CZ	1:C:55:GLU:HG3	2.49	0.47
1:C:47:LYS:HD2	3:C:197:EDO:O1	2.14	0.47
1:D:72:GLN:O	1:D:81:ARG:NH1	2.48	0.47
1:F:7:ARG:NH1	1:F:45:HIS:O	2.47	0.47
1:G:86:ILE:HG22	1:G:176:VAL:HG13	1.97	0.47
1:G:108:THR:HB	4:G:199:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:GLU:HB2	3:H:198:EDO:H11	1.97	0.47
1:G:133:GLN:HG3	1:G:146:PRO:CG	2.45	0.47
1:H:32:SER:HB2	1:H:37:ILE:HG13	1.96	0.47
1:A:81:ARG:HB3	1:A:131:TRP:HH2	1.79	0.47
1:A:97:THR:O	1:A:167:HIS:CD2	2.68	0.47
1:A:132:LEU:CD1	1:A:152:LEU:HD23	2.43	0.47
1:B:44:TYR:CD1	1:B:45:HIS:CE1	3.02	0.47
1:G:6:THR:HA	1:G:9:GLN:HE21	1.80	0.47
1:H:144:GLU:HG3	1:H:148:LEU:CD1	2.44	0.47
1:H:151:HIS:O	1:H:154:ALA:HB3	2.13	0.47
1:B:78:PRO:HG3	1:B:139:ALA:HA	1.97	0.47
1:A:28:PHE:CD2	1:A:42:PHE:CE1	3.02	0.47
1:A:90:ILE:HD11	1:A:173:ARG:HA	1.97	0.47
1:E:38:SER:HB2	1:E:40:GLY:H	1.80	0.47
1:A:89:MSE:HE3	1:A:172:LEU:CD1	2.44	0.46
1:A:89:MSE:HE1	1:A:159:ALA:CB	2.44	0.46
1:C:141:CYS:SG	4:C:281:HOH:O	2.58	0.46
1:E:52:ILE:O	1:E:56:VAL:HG23	2.15	0.46
1:A:82:ILE:HD13	1:A:136:PHE:CZ	2.50	0.46
1:A:162:LEU:HD11	1:B:153:LEU:HB3	1.97	0.46
1:D:7:ARG:HD2	1:D:45:HIS:HD2	1.79	0.46
1:F:189:MSE:HE2	1:F:189:MSE:HB3	1.82	0.46
1:B:68:LEU:HG	1:B:131:TRP:CG	2.51	0.46
1:C:116:ALA:C	1:C:118:GLN:N	2.74	0.46
1:D:63:ARG:CD	4:D:225:HOH:O	2.58	0.46
1:E:78:PRO:HB3	1:E:135:GLN:O	2.15	0.46
1:H:3:GLN:CD	1:H:44:TYR:HE1	2.23	0.46
1:B:152:LEU:O	1:B:155:ARG:HB2	2.16	0.46
1:E:5:GLN:O	1:E:9:GLN:HG3	2.15	0.46
1:H:64:THR:CG2	1:H:128:PHE:CE2	2.99	0.46
1:A:39:ARG:HD2	1:A:43:TYR:CE2	2.49	0.46
1:B:64:THR:HG21	1:B:128:PHE:CE2	2.51	0.46
1:E:23:PHE:CE1	1:E:53:LEU:HD22	2.51	0.46
1:E:75:GLY:HA3	1:E:81:ARG:HG2	1.98	0.46
2:E:192:MES:H32	2:E:192:MES:H82	1.48	0.46
1:G:70:ASP:O	1:G:74:THR:HB	2.14	0.46
1:G:90:ILE:CD1	1:G:173:ARG:HG2	2.45	0.46
1:H:110:LEU:HD12	1:H:121:ALA:CB	2.46	0.46
1:C:-1:ASN:O	1:C:3:GLN:HB3	2.16	0.46
1:F:32:SER:HB2	1:F:37:ILE:HG13	1.98	0.46
1:G:162:LEU:HD22	1:G:166:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ALA:HB2	1:D:162:LEU:HD12	1.97	0.46
1:F:7:ARG:HB2	1:F:45:HIS:HD2	1.80	0.46
1:H:39:ARG:O	1:H:43:TYR:HD2	1.99	0.46
1:H:60:ARG:HD3	2:H:192:MES:O3S	2.16	0.46
1:H:78:PRO:HB2	1:H:139:ALA:HA	1.96	0.46
1:B:63:ARG:HD2	4:B:212:HOH:O	2.15	0.46
1:B:82:ILE:HG13	1:B:135:GLN:HB3	1.98	0.46
1:C:38:SER:C	1:C:40:GLY:N	2.72	0.46
1:D:153:LEU:O	1:D:157:GLN:HG2	2.16	0.46
1:C:137:ALA:HA	1:C:142:THR:N	2.31	0.46
1:G:64:THR:HG22	1:G:68:LEU:HD12	1.98	0.46
1:G:137:ALA:CA	1:G:142:THR:HA	2.46	0.46
1:B:184:ASP:C	1:B:186:THR:N	2.75	0.45
1:D:68:LEU:HD11	1:D:128:PHE:CD1	2.51	0.45
1:D:69:ALA:O	1:D:72:GLN:CB	2.63	0.45
1:B:64:THR:CG2	1:B:128:PHE:CE2	2.99	0.45
1:B:95:LYS:HD2	4:B:253:HOH:O	2.15	0.45
1:G:57:ILE:O	1:G:61:LEU:HG	2.17	0.45
1:G:134:ARG:O	1:G:134:ARG:HG2	2.15	0.45
1:C:68:LEU:HB2	4:C:275:HOH:O	2.15	0.45
1:F:93:ARG:O	1:F:97:THR:HG23	2.16	0.45
2:G:192:MES:H52	4:G:198:HOH:O	2.16	0.45
1:A:2:VAL:HG22	1:A:2:VAL:O	2.15	0.45
1:A:76:ASP:OD1	1:A:76:ASP:N	2.46	0.45
1:C:111:SER:OG	1:D:164:GLN:NE2	2.50	0.45
1:C:128:PHE:O	1:C:132:LEU:HB2	2.16	0.45
1:F:72:GLN:HE21	1:F:72:GLN:HA	1.81	0.45
1:F:155:ARG:NH2	1:F:179:MSE:HG3	2.31	0.45
1:G:133:GLN:HG3	1:G:146:PRO:CD	2.47	0.45
1:H:39:ARG:HD3	1:H:43:TYR:CE2	2.51	0.45
1:A:82:ILE:HD13	1:A:136:PHE:CE1	2.52	0.45
1:B:3:GLN:H	1:B:3:GLN:HG2	1.60	0.45
1:B:7:ARG:NH1	1:B:45:HIS:HB3	2.32	0.45
1:D:140:GLY:O	1:D:142:THR:N	2.48	0.45
1:F:4:ALA:HB1	1:F:5:GLN:OE1	2.15	0.45
1:A:153:LEU:CG	1:B:162:LEU:HD11	2.44	0.45
1:C:33:ALA:CB	3:C:195:EDO:H21	2.47	0.45
1:D:68:LEU:HD12	1:D:71:TRP:CE3	2.52	0.45
1:E:88:LEU:HD12	1:E:91:MSE:HE2	1.98	0.45
1:E:90:ILE:HD12	1:E:173:ARG:HG2	1.99	0.45
1:E:155:ARG:CZ	1:F:151:HIS:HE1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ALA:HB1	1:C:180:HIS:CE1	2.52	0.45
1:D:26:THR:O	1:D:49:LYS:HE3	2.17	0.45
1:G:89:MSE:HE2	1:G:89:MSE:HB3	1.92	0.45
1:D:68:LEU:HG	1:D:131:TRP:CD2	2.52	0.45
1:F:86:ILE:HG22	1:F:176:VAL:HG13	1.98	0.45
1:G:24:ALA:HA	4:G:253:HOH:O	2.16	0.45
1:B:81:ARG:HB3	1:B:131:TRP:CH2	2.52	0.45
1:D:82:ILE:CG1	1:D:135:GLN:HB3	2.47	0.45
1:F:44:TYR:C	1:F:44:TYR:HD2	2.24	0.45
1:H:5:GLN:CD	1:H:5:GLN:N	2.75	0.45
1:H:11:VAL:HG12	1:H:59:LEU:HD22	1.98	0.45
1:H:166:PHE:O	1:H:167:HIS:C	2.60	0.45
1:A:5:GLN:O	1:A:9:GLN:HG3	2.16	0.45
1:A:59:LEU:HD13	4:A:260:HOH:O	2.16	0.45
1:B:36:GLY:O	1:B:37:ILE:HG23	2.17	0.45
1:F:110:LEU:HD12	1:F:121:ALA:CB	2.47	0.45
1:F:140:GLY:HA3	1:F:188:PRO:CG	2.46	0.45
1:G:112:LYS:HD3	1:G:112:LYS:HA	1.83	0.45
1:H:67:MSE:C	1:H:69:ALA:H	2.25	0.45
1:H:110:LEU:HD12	1:H:121:ALA:HB2	1.99	0.45
1:C:97:THR:O	1:C:167:HIS:CD2	2.70	0.44
1:D:59:LEU:HD11	1:D:63:ARG:NE	2.32	0.44
1:D:166:PHE:O	1:D:167:HIS:C	2.59	0.44
1:E:23:PHE:CE1	1:E:53:LEU:HB2	2.52	0.44
1:E:176:VAL:HA	1:E:179:MSE:HE3	1.99	0.44
1:A:46:PHE:HZ	1:A:55:GLU:HG3	1.82	0.44
1:A:116:ALA:C	1:A:118:GLN:N	2.75	0.44
1:A:128:PHE:C	1:A:130:ASP:H	2.25	0.44
1:C:128:PHE:C	1:C:130:ASP:N	2.75	0.44
1:C:90:ILE:CD1	1:C:173:ARG:HG2	2.48	0.44
1:D:166:PHE:HB3	1:D:168:ASP:HB2	2.00	0.44
1:F:64:THR:CG2	1:F:128:PHE:CE2	3.00	0.44
1:G:47:LYS:HB2	1:G:47:LYS:NZ	2.29	0.44
2:G:192:MES:H51	2:G:192:MES:H82	1.76	0.44
1:H:72:GLN:HA	1:H:81:ARG:HE	1.82	0.44
1:B:97:THR:O	1:B:164:GLN:HA	2.17	0.44
1:D:37:ILE:HD12	1:D:42:PHE:HA	1.99	0.44
1:G:4:ALA:O	1:G:8:ASP:CG	2.60	0.44
1:G:63:ARG:CB	2:G:192:MES:H72	2.43	0.44
1:H:69:ALA:HA	4:H:204:HOH:O	2.17	0.44
1:H:78:PRO:HB2	1:H:139:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LEU:O	1:B:183:LEU:HG	2.18	0.44
4:E:217:HOH:O	1:F:111:SER:HA	2.17	0.44
1:F:39:ARG:NH1	1:G:189:MSE:HE3	2.33	0.44
1:B:59:LEU:C	1:B:59:LEU:HD12	2.42	0.44
1:C:162:LEU:HB2	1:C:171:PHE:HE2	1.83	0.44
1:D:40:GLY:O	1:D:44:TYR:HB2	2.17	0.44
1:D:112:LYS:HE2	1:D:112:LYS:HB2	1.80	0.44
1:F:102:PRO:HG3	2:F:192:MES:C3	2.48	0.44
1:A:185:ASN:N	1:A:185:ASN:HD22	2.15	0.44
1:B:176:VAL:O	1:B:180:HIS:CD2	2.71	0.44
1:C:28:PHE:HD2	1:C:42:PHE:CE1	2.36	0.44
1:C:82:ILE:O	1:C:85:PHE:HB3	2.18	0.44
1:D:92:ASN:ND2	3:D:195:EDO:H22	2.27	0.44
1:F:77:SER:CB	1:F:78:PRO:CD	2.96	0.44
1:H:127:LEU:O	1:H:129:ARG:N	2.51	0.44
1:C:155:ARG:NH2	1:D:151:HIS:HE1	2.16	0.44
1:F:6:THR:HB	4:F:282:HOH:O	2.18	0.44
1:G:129:ARG:CD	4:G:215:HOH:O	2.66	0.44
1:E:1:MSE:O	1:E:4:ALA:HB3	2.18	0.44
1:F:181:ARG:NH1	1:F:181:ARG:CB	2.81	0.44
1:H:98:ARG:HD3	4:H:248:HOH:O	2.17	0.44
1:A:89:MSE:HE2	1:A:176:VAL:HG23	2.00	0.43
1:A:128:PHE:C	1:A:130:ASP:N	2.75	0.43
1:B:63:ARG:HD3	2:B:192:MES:O3S	2.18	0.43
1:C:63:ARG:HD3	2:C:192:MES:O1S	2.18	0.43
1:C:165:SER:OG	1:D:107:CYS:HB3	2.17	0.43
1:G:87:ASP:CG	1:G:180:HIS:HE2	2.24	0.43
1:H:78:PRO:HG2	1:H:79:ARG:N	2.26	0.43
1:H:78:PRO:HB2	1:H:139:ALA:CA	2.48	0.43
1:A:71:TRP:CZ2	1:A:88:LEU:HD22	2.53	0.43
1:D:110:LEU:HD12	1:D:121:ALA:HB2	1.99	0.43
1:D:113:LEU:HD21	4:D:231:HOH:O	2.18	0.43
1:E:124:LEU:HD13	4:E:208:HOH:O	2.18	0.43
1:G:162:LEU:O	1:G:166:PHE:HD2	2.02	0.43
1:A:68:LEU:HD22	1:A:131:TRP:HB3	2.00	0.43
1:A:128:PHE:O	1:A:132:LEU:HB2	2.18	0.43
1:A:162:LEU:HB2	1:A:171:PHE:CE2	2.54	0.43
1:C:72:GLN:HE22	1:C:135:GLN:NE2	2.16	0.43
1:F:71:TRP:CH2	1:F:88:LEU:HD22	2.53	0.43
1:A:132:LEU:HD21	1:A:152:LEU:HD23	1.99	0.43
1:D:43:TYR:C	1:D:45:HIS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:TYR:C	1:H:44:TYR:CD2	2.96	0.43
1:D:144:GLU:HG3	1:D:144:GLU:O	2.17	0.43
1:F:35:VAL:HG23	1:F:36:GLY:N	2.33	0.43
1:H:64:THR:HG21	1:H:128:PHE:CE2	2.53	0.43
1:B:26:THR:O	1:B:49:LYS:NZ	2.52	0.43
1:C:27:SER:O	1:C:30:ASP:HB2	2.19	0.43
1:D:59:LEU:O	1:D:63:ARG:HG3	2.19	0.43
1:D:186:THR:HA	4:D:277:HOH:O	2.18	0.43
1:G:90:ILE:HG12	1:G:176:VAL:HG21	2.01	0.43
1:H:123:GLY:HA2	1:H:126:THR:HB	2.01	0.43
1:A:155:ARG:CZ	1:B:151:HIS:HE1	2.31	0.43
1:C:89:MSE:HA	1:C:96:ILE:HD12	2.00	0.43
1:D:39:ARG:HD3	1:D:43:TYR:CE2	2.54	0.43
1:D:65:ALA:C	4:D:294:HOH:O	2.61	0.43
1:E:89:MSE:HA	1:E:96:ILE:CD1	2.49	0.43
1:G:81:ARG:NE	4:G:222:HOH:O	2.51	0.43
1:H:7:ARG:O	1:H:10:ILE:HG23	2.19	0.43
1:H:109:GLU:HG3	3:H:198:EDO:H22	1.99	0.43
1:E:166:PHE:CZ	1:F:125:PHE:HB3	2.54	0.43
1:F:181:ARG:O	1:F:184:ASP:HB2	2.18	0.43
3:F:193:EDO:H11	4:F:215:HOH:O	2.19	0.43
1:D:144:GLU:CG	1:D:144:GLU:O	2.66	0.43
1:A:-2:SER:C	1:A:-1:ASN:HD22	2.27	0.43
1:C:77:SER:N	4:C:284:HOH:O	2.51	0.43
1:C:167:HIS:CE1	1:D:111:SER:OG	2.72	0.43
1:F:60:ARG:HD3	4:F:201:HOH:O	2.18	0.43
1:F:156:SER:N	1:F:179:MSE:HE3	2.34	0.43
1:G:79:ARG:CB	4:G:267:HOH:O	2.65	0.43
1:A:134:ARG:HD3	1:A:138:GLU:CD	2.44	0.42
1:A:158:GLY:CA	1:B:154:ALA:O	2.61	0.42
1:B:151:HIS:HD2	1:B:182:TRP:CZ2	2.37	0.42
1:F:152:LEU:O	1:F:155:ARG:HB2	2.18	0.42
1:H:29:VAL:HG22	3:H:197:EDO:H22	2.01	0.42
1:A:58:ARG:NH1	4:A:217:HOH:O	2.52	0.42
1:E:23:PHE:HE1	1:E:53:LEU:HB2	1.83	0.42
1:E:141:CYS:SG	1:E:188:PRO:HD2	2.58	0.42
1:G:71:TRP:O	1:G:81:ARG:HG2	2.19	0.42
1:G:72:GLN:HA	1:G:81:ARG:HD3	2.00	0.42
1:G:144:GLU:OE2	1:G:147:ALA:HB3	2.18	0.42
1:H:134:ARG:O	1:H:138:GLU:HG3	2.20	0.42
1:A:18:PHE:CD2	1:A:56:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:VAL:C	1:B:4:ALA:H	2.27	0.42
1:B:37:ILE:HB	1:B:41:ASN:HB3	2.01	0.42
1:C:78:PRO:HB2	1:C:139:ALA:HB2	2.00	0.42
1:D:68:LEU:O	1:D:131:TRP:CZ2	2.72	0.42
1:D:89:MSE:HE1	1:D:179:MSE:HE1	2.02	0.42
1:E:28:PHE:CD2	1:E:42:PHE:CE1	3.05	0.42
1:F:113:LEU:O	1:F:114:ASP:CB	2.67	0.42
1:H:49:LYS:CD	4:H:241:HOH:O	2.66	0.42
1:A:82:ILE:HG13	1:A:135:GLN:HB3	2.02	0.42
1:B:32:SER:HB3	1:B:42:PHE:CD2	2.54	0.42
1:C:133:GLN:HG3	1:C:146:PRO:N	2.34	0.42
1:D:36:GLY:O	1:D:37:ILE:HG23	2.20	0.42
1:E:179:MSE:O	1:E:182:TRP:HB3	2.19	0.42
1:F:110:LEU:HD12	1:F:121:ALA:HB2	2.01	0.42
1:G:90:ILE:HG12	1:G:176:VAL:HG11	2.01	0.42
1:B:2:VAL:O	1:B:4:ALA:N	2.48	0.42
1:D:175:GLU:OE2	1:D:175:GLU:HA	2.18	0.42
1:E:174:SER:HA	3:E:194:EDO:H11	2.01	0.42
1:F:144:GLU:OE2	1:F:144:GLU:O	2.37	0.42
1:G:97:THR:HG21	1:G:169:GLU:HG2	2.01	0.42
1:A:75:GLY:HA3	1:A:81:ARG:HD3	2.01	0.42
1:A:131:TRP:CD1	4:A:271:HOH:O	2.71	0.42
1:B:69:ALA:O	1:B:72:GLN:CB	2.67	0.42
1:C:14:ALA:O	1:C:15:ASP:C	2.63	0.42
1:C:48:THR:HB	1:C:50:ASP:N	2.33	0.42
1:C:89:MSE:HA	1:C:96:ILE:CD1	2.50	0.42
1:C:167:HIS:HE1	1:D:111:SER:OG	2.03	0.42
1:D:74:THR:O	1:D:75:GLY:C	2.62	0.42
1:E:48:THR:HG1	1:E:51:GLU:CG	2.18	0.42
1:F:39:ARG:HB2	1:G:189:MSE:CG	2.47	0.42
1:H:7:ARG:HB2	1:H:45:HIS:CD2	2.44	0.42
1:H:62:ALA:C	1:H:64:THR:N	2.76	0.42
1:H:71:TRP:CZ2	1:H:88:LEU:HD22	2.55	0.42
1:D:17:LEU:O	1:D:21:GLN:HB2	2.18	0.42
1:D:86:ILE:HG22	1:D:176:VAL:HG13	2.01	0.42
1:E:57:ILE:HG21	1:E:120:GLN:HG2	2.00	0.42
1:E:78:PRO:HB2	1:E:139:ALA:HB2	2.02	0.42
1:E:90:ILE:CG1	1:E:176:VAL:HG11	2.49	0.42
1:F:62:ALA:C	1:F:64:THR:N	2.76	0.42
1:F:81:ARG:HB2	1:F:135:GLN:OE1	2.19	0.42
1:F:107:CYS:O	1:F:111:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:ALA:C	1:H:64:THR:H	2.28	0.42
1:B:42:PHE:C	1:B:44:TYR:H	2.28	0.42
1:C:67:MSE:O	1:C:68:LEU:C	2.63	0.42
1:F:10:ILE:HD13	1:F:46:PHE:CD2	2.47	0.42
1:F:27:SER:OG	1:F:29:VAL:HG12	2.20	0.42
1:F:78:PRO:CG	1:F:79:ARG:H	2.33	0.42
1:G:28:PHE:CD2	1:G:42:PHE:HE1	2.38	0.42
1:B:72:GLN:NE2	1:B:134:ARG:NH1	2.68	0.42
1:C:39:ARG:NH1	4:C:270:HOH:O	2.52	0.42
1:E:72:GLN:HA	1:E:81:ARG:HD3	2.01	0.42
1:F:32:SER:HB3	1:F:42:PHE:CD2	2.55	0.42
1:F:72:GLN:HE21	1:F:72:GLN:CA	2.31	0.42
1:F:93:ARG:HD2	1:F:169:GLU:OE2	2.20	0.42
1:H:44:TYR:C	1:H:44:TYR:HD2	2.28	0.42
1:A:105:SER:HB3	4:A:212:HOH:O	2.19	0.42
1:C:143:THR:HB	4:C:218:HOH:O	2.19	0.42
1:G:38:SER:C	1:G:40:GLY:N	2.77	0.42
1:A:10:ILE:CD1	1:A:35:VAL:HG11	2.50	0.41
1:A:47:LYS:HG2	4:A:277:HOH:O	2.18	0.41
1:A:183:LEU:O	1:A:187:LEU:HG	2.20	0.41
1:B:35:VAL:CG2	1:B:37:ILE:HG12	2.50	0.41
1:D:10:ILE:HD11	1:D:46:PHE:CE2	2.55	0.41
1:D:72:GLN:CG	1:D:81:ARG:HH11	2.31	0.41
1:E:129:ARG:HD3	1:E:150:MSE:SE	2.70	0.41
1:F:113:LEU:O	1:F:114:ASP:HB3	2.20	0.41
1:G:6:THR:HA	1:G:9:GLN:NE2	2.35	0.41
1:H:98:ARG:CD	4:H:248:HOH:O	2.67	0.41
1:H:178:ASP:OD1	1:H:181:ARG:NH2	2.51	0.41
1:A:90:ILE:HD12	1:A:173:ARG:HG2	2.02	0.41
1:A:129:ARG:CD	4:A:224:HOH:O	2.68	0.41
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.84	0.41
1:C:20:ARG:HA	1:C:99:TYR:CD1	2.55	0.41
1:C:145:ALA:HB3	1:C:146:PRO:HD3	2.02	0.41
1:F:28:PHE:CE1	1:F:52:ILE:HD12	2.55	0.41
1:A:135:GLN:OE1	1:A:135:GLN:HA	2.19	0.41
1:A:137:ALA:HA	1:A:141:CYS:C	2.45	0.41
1:B:81:ARG:O	1:B:84:SER:HB2	2.19	0.41
1:D:49:LYS:CD	3:D:193:EDO:H22	2.47	0.41
1:D:144:GLU:HB3	4:D:247:HOH:O	2.19	0.41
1:F:97:THR:HG21	1:F:169:GLU:HA	2.02	0.41
1:A:90:ILE:HD13	1:A:90:ILE:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLN:HG3	1:B:146:PRO:HA	2.03	0.41
1:C:81:ARG:NE	4:C:284:HOH:O	2.54	0.41
1:E:122:ASN:HB3	4:E:199:HOH:O	2.21	0.41
1:F:131:TRP:O	1:F:135:GLN:HG2	2.20	0.41
1:C:137:ALA:C	1:C:139:ALA:N	2.77	0.41
1:D:173:ARG:NH1	4:D:302:HOH:O	2.53	0.41
1:G:146:PRO:HB3	4:G:254:HOH:O	2.20	0.41
1:H:39:ARG:HD3	1:H:43:TYR:CD2	2.56	0.41
1:B:71:TRP:CD1	1:B:84:SER:HB3	2.55	0.41
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.21	0.41
1:F:17:LEU:HB3	1:F:26:THR:HG21	2.02	0.41
1:H:68:LEU:CD2	1:H:127:LEU:HD22	2.51	0.41
1:B:7:ARG:HH11	1:B:45:HIS:HB3	1.84	0.41
1:B:79:ARG:HG3	1:B:187:LEU:CD1	2.51	0.41
1:B:137:ALA:HA	1:B:142:THR:HA	2.02	0.41
1:C:146:PRO:HB2	4:C:236:HOH:O	2.19	0.41
1:F:7:ARG:O	1:F:10:ILE:HG23	2.21	0.41
1:G:165:SER:OG	1:H:107:CYS:HB3	2.21	0.41
1:H:68:LEU:HD22	1:H:127:LEU:HD22	2.02	0.41
1:A:118:GLN:HG2	4:A:239:HOH:O	2.20	0.41
1:D:97:THR:O	1:D:164:GLN:HA	2.20	0.41
1:E:89:MSE:HE1	1:E:179:MSE:SE	2.70	0.41
1:H:13:ALA:O	1:H:17:LEU:HD12	2.21	0.41
1:B:7:ARG:HB2	1:B:45:HIS:HD2	1.74	0.41
1:C:132:LEU:HD12	1:C:132:LEU:HA	1.75	0.41
1:D:39:ARG:O	1:D:43:TYR:CD2	2.74	0.41
1:D:78:PRO:HB3	1:D:138:GLU:O	2.20	0.41
1:F:82:ILE:HD11	1:F:183:LEU:CD1	2.51	0.41
1:H:29:VAL:HA	1:H:32:SER:HG	1.86	0.41
1:H:48:THR:O	1:H:51:GLU:HB2	2.21	0.41
1:B:143:THR:OG1	1:E:126:THR:HG21	2.19	0.41
1:C:50:ASP:CB	3:C:198:EDO:H21	2.43	0.41
3:C:195:EDO:H11	3:C:199:EDO:O2	2.20	0.41
1:E:19:TYR:HB2	1:E:60:ARG:HH22	1.86	0.41
1:F:172:LEU:HD12	1:F:172:LEU:HA	1.81	0.41
1:G:89:MSE:CE	1:G:172:LEU:HD11	2.51	0.41
1:G:137:ALA:O	1:G:140:GLY:N	2.45	0.41
1:H:69:ALA:C	1:H:71:TRP:N	2.79	0.41
1:A:137:ALA:C	1:A:139:ALA:N	2.76	0.40
1:B:151:HIS:CD2	1:B:182:TRP:CZ2	3.08	0.40
1:C:74:THR:HG22	1:C:74:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LEU:HD12	1:C:88:LEU:HA	1.89	0.40
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.69	0.40
1:D:89:MSE:CE	1:D:179:MSE:HE1	2.51	0.40
1:G:69:ALA:C	1:G:71:TRP:N	2.78	0.40
1:G:132:LEU:HD12	1:G:132:LEU:HA	1.82	0.40
1:H:93:ARG:HD2	1:H:169:GLU:OE2	2.21	0.40
1:C:155:ARG:NH2	1:D:151:HIS:CE1	2.89	0.40
1:D:127:LEU:O	1:D:128:PHE:C	2.64	0.40
1:E:91:MSE:HE1	4:E:256:HOH:O	2.21	0.40
1:F:29:VAL:HG13	1:F:30:ASP:H	1.86	0.40
1:H:82:ILE:HG13	1:H:135:GLN:HB3	2.02	0.40
1:A:129:ARG:O	1:A:129:ARG:HG2	2.22	0.40
1:B:68:LEU:HG	1:B:131:TRP:CD2	2.56	0.40
1:C:144:GLU:H	1:C:144:GLU:HG2	1.75	0.40
1:D:7:ARG:O	1:D:10:ILE:HG12	2.21	0.40
2:F:192:MES:H51	4:F:257:HOH:O	2.20	0.40
1:G:109:GLU:CB	3:H:198:EDO:H11	2.51	0.40
1:H:57:ILE:CG2	1:H:120:GLN:HG2	2.51	0.40
1:H:71:TRP:HH2	1:H:88:LEU:HD22	1.85	0.40
1:A:163:ALA:O	1:A:167:HIS:N	2.54	0.40
1:D:71:TRP:CZ2	1:D:88:LEU:HD22	2.56	0.40
1:D:133:GLN:HG2	1:D:145:ALA:HB1	2.02	0.40
2:D:192:MES:H31	2:D:192:MES:H81	1.63	0.40
1:E:122:ASN:O	1:E:126:THR:HG23	2.21	0.40
1:H:172:LEU:HD12	1:H:172:LEU:HA	1.84	0.40
2:B:192:MES:H32	2:B:192:MES:H81	1.54	0.40
1:G:71:TRP:CD2	1:G:84:SER:HB3	2.57	0.40
1:G:151:HIS:HE1	1:H:155:ARG:CZ	2.35	0.40
1:H:17:LEU:HB3	1:H:26:THR:HG21	2.04	0.40
1:H:64:THR:HG23	1:H:128:PHE:CZ	2.56	0.40
1:H:189:MSE:HE2	1:H:189:MSE:HB3	1.79	0.40

There are no symmetry-related clashes.

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	192/194 (99%)	178 (93%)	9 (5%)	5 (3%)	4 1
1	B	188/194 (97%)	170 (90%)	14 (7%)	4 (2%)	5 1
1	C	192/194 (99%)	172 (90%)	19 (10%)	1 (0%)	25 17
1	D	188/194 (97%)	151 (80%)	30 (16%)	7 (4%)	2 0
1	E	191/194 (98%)	179 (94%)	11 (6%)	1 (0%)	25 17
1	F	186/194 (96%)	169 (91%)	14 (8%)	3 (2%)	8 2
1	G	191/194 (98%)	175 (92%)	16 (8%)	0	100 100
1	H	186/194 (96%)	166 (89%)	18 (10%)	2 (1%)	12 4
All	All	1514/1552 (98%)	1360 (90%)	131 (9%)	23 (2%)	8 2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	THR
1	F	127	LEU
1	A	117	ALA
1	A	118	GLN
1	A	129	ARG
1	B	188	PRO
1	D	36	GLY
1	E	0	ALA
1	H	127	LEU
1	D	78	PRO
1	D	141	CYS
1	F	78	PRO
1	B	3	GLN
1	B	185	ASN
1	C	118	GLN
1	D	139	ALA
1	D	188	PRO
1	H	139	ALA
1	A	114	ASP
1	D	116	ALA
1	A	188	PRO
1	F	128	PHE
1	B	140	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	154/147 (105%)	145 (94%)	9 (6%)	17 9
1	B	151/147 (103%)	141 (93%)	10 (7%)	14 7
1	C	154/147 (105%)	140 (91%)	14 (9%)	7 3
1	D	151/147 (103%)	133 (88%)	18 (12%)	4 1
1	E	152/147 (103%)	137 (90%)	15 (10%)	6 2
1	F	149/147 (101%)	136 (91%)	13 (9%)	8 3
1	G	152/147 (103%)	144 (95%)	8 (5%)	19 11
1	H	149/147 (101%)	137 (92%)	12 (8%)	9 4
All	All	1212/1176 (103%)	1113 (92%)	99 (8%)	9 4

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	1	MSE
1	A	3	GLN
1	A	76	ASP
1	A	132	LEU
1	A	134	ARG
1	A	169	GLU
1	A	185	ASN
1	A	189	MSE
1	B	3	GLN
1	B	5	GLN
1	B	10	ILE
1	B	29	VAL
1	B	59	LEU
1	B	66	GLN
1	B	118	GLN
1	B	134	ARG
1	B	175	GLU
1	B	190	THR

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Mol	Chain	Res	Type
1	C	37	ILE
1	C	38	SER
1	C	39	ARG
1	C	48	THR
1	C	63	ARG
1	C	114	ASP
1	C	132	LEU
1	C	134	ARG
1	C	143	THR
1	C	144	GLU
1	C	161	THR
1	C	169	GLU
1	C	185	ASN
1	C	190	THR
1	D	2	VAL
1	D	3	GLN
1	D	5	GLN
1	D	29	VAL
1	D	35	VAL
1	D	39	ARG
1	D	59	LEU
1	D	66	GLN
1	D	68	LEU
1	D	72	GLN
1	D	87	ASP
1	D	97	THR
1	D	113	LEU
1	D	133	GLN
1	D	143	THR
1	D	153	LEU
1	D	187	LEU
1	D	189	MSE
1	E	2	VAL
1	E	38	SER
1	E	39	ARG
1	E	41	ASN
1	E	47	LYS
1	E	77	SER
1	E	118	GLN
1	E	122	ASN
1	E	132	LEU
1	E	134	ARG

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Mol	Chain	Res	Type
1	E	162	LEU
1	E	174	SER
1	E	185	ASN
1	E	189	MSE
1	E	190	THR
1	F	10	ILE
1	F	37	ILE
1	F	39	ARG
1	F	44	TYR
1	F	47	LYS
1	F	48	THR
1	F	63	ARG
1	F	68	LEU
1	F	72	GLN
1	F	82	ILE
1	F	127	LEU
1	F	165	SER
1	F	174	SER
1	G	9	GLN
1	G	10	ILE
1	G	39	ARG
1	G	47	LYS
1	G	49	LYS
1	G	89	MSE
1	G	132	LEU
1	G	134	ARG
1	H	5	GLN
1	H	6	THR
1	H	7	ARG
1	H	29	VAL
1	H	37	ILE
1	H	39	ARG
1	H	48	THR
1	H	67	MSE
1	H	68	LEU
1	H	72	GLN
1	H	97	THR
1	H	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	5	GLN
1	A	9	GLN
1	A	41	ASN
1	A	66	GLN
1	A	72	GLN
1	A	151	HIS
1	A	167	HIS
1	A	180	HIS
1	A	185	ASN
1	B	5	GLN
1	B	45	HIS
1	B	66	GLN
1	B	118	GLN
1	B	133	GLN
1	B	151	HIS
1	B	157	GLN
1	B	185	ASN
1	C	5	GLN
1	C	9	GLN
1	C	21	GLN
1	C	45	HIS
1	C	72	GLN
1	C	92	ASN
1	C	118	GLN
1	C	135	GLN
1	C	151	HIS
1	C	167	HIS
1	C	185	ASN
1	D	3	GLN
1	D	5	GLN
1	D	9	GLN
1	D	25	GLN
1	D	45	HIS
1	D	66	GLN
1	D	72	GLN
1	D	92	ASN
1	D	118	GLN
1	D	133	GLN
1	D	135	GLN
1	D	167	HIS
1	D	185	ASN
1	E	5	GLN

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Mol	Chain	Res	Type
1	E	9	GLN
1	E	45	HIS
1	E	92	ASN
1	E	122	ASN
1	E	133	GLN
1	E	135	GLN
1	E	167	HIS
1	F	3	GLN
1	F	9	GLN
1	F	25	GLN
1	F	66	GLN
1	F	72	GLN
1	F	92	ASN
1	F	118	GLN
1	F	122	ASN
1	F	133	GLN
1	F	157	GLN
1	G	5	GLN
1	G	9	GLN
1	G	45	HIS
1	G	122	ASN
1	G	133	GLN
1	G	135	GLN
1	G	151	HIS
1	H	3	GLN
1	H	5	GLN
1	H	9	GLN
1	H	66	GLN
1	H	92	ASN
1	H	118	GLN
1	H	122	ASN
1	H	157	GLN
1	H	167	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

38 ligands 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	$\#\|Z\| > 2$
3	EDO	E	193	-	3,3,3	0.54	0	2,2,2	0.21	0
3	EDO	D	195	-	3,3,3	0.66	0	2,2,2	0.02	0
3	EDO	H	195	-	3,3,3	0.50	0	2,2,2	0.10	0
3	EDO	B	193	-	3,3,3	0.42	0	2,2,2	0.54	0
2	MES	F	192	-	12,12,12	2.14	1 (8%)	15,16,16	2.52	7 (46%)
3	EDO	E	195	-	3,3,3	0.44	0	2,2,2	0.33	0
2	MES	G	192	-	12,12,12	2.21	1 (8%)	15,16,16	2.82	8 (53%)
2	MES	A	192	-	12,12,12	2.20	1 (8%)	15,16,16	2.41	6 (40%)
3	EDO	C	199	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	C	195	-	3,3,3	0.54	0	2,2,2	0.19	0
3	EDO	D	193	-	3,3,3	0.44	0	2,2,2	0.33	0
3	EDO	C	197	-	3,3,3	0.42	0	2,2,2	0.47	0
3	EDO	H	199	-	3,3,3	0.40	0	2,2,2	0.55	0
3	EDO	H	193	-	3,3,3	0.53	0	2,2,2	0.17	0
3	EDO	D	197	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	H	197	-	3,3,3	0.36	0	2,2,2	0.57	0
3	EDO	C	193	-	3,3,3	0.52	0	2,2,2	0.21	0
3	EDO	F	195	-	3,3,3	0.42	0	2,2,2	0.37	0
3	EDO	E	194	-	3,3,3	0.60	0	2,2,2	0.10	0
3	EDO	F	193	-	3,3,3	0.41	0	2,2,2	0.53	0
3	EDO	B	194	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	D	196	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	H	196	-	3,3,3	0.51	0	2,2,2	0.19	0
3	EDO	C	194	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	A	193	-	3,3,3	0.47	0	2,2,2	0.33	0
2	MES	E	192	-	12,12,12	2.27	1 (8%)	15,16,16	2.35	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MES	B	192	-	12,12,12	2.03	1 (8%)	15,16,16	2.51	7 (46%)
3	EDO	C	198	-	3,3,3	0.43	0	2,2,2	0.44	0
3	EDO	D	194	-	3,3,3	0.54	0	2,2,2	0.20	0
3	EDO	H	194	-	3,3,3	0.54	0	2,2,2	0.17	0
3	EDO	B	195	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	C	196	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	H	198	-	3,3,3	0.54	0	2,2,2	0.43	0
3	EDO	F	194	-	3,3,3	0.31	0	2,2,2	0.79	0
2	MES	H	192	-	12,12,12	2.50	1 (8%)	15,16,16	2.73	8 (53%)
2	MES	C	192	-	12,12,12	2.12	1 (8%)	15,16,16	2.30	5 (33%)
3	EDO	F	196	-	3,3,3	0.48	0	2,2,2	0.29	0
2	MES	D	192	-	12,12,12	1.86	1 (8%)	15,16,16	2.54	7 (46%)

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	EDO	E	193	-	-	1/1/1/1	-
3	EDO	D	195	-	-	1/1/1/1	-
3	EDO	H	195	-	-	0/1/1/1	-
3	EDO	B	193	-	-	0/1/1/1	-
2	MES	F	192	-	-	1/6/14/14	0/1/1/1
3	EDO	E	195	-	-	0/1/1/1	-
2	MES	G	192	-	-	4/6/14/14	0/1/1/1
2	MES	A	192	-	-	5/6/14/14	0/1/1/1
3	EDO	C	199	-	-	0/1/1/1	-
3	EDO	C	195	-	-	0/1/1/1	-
3	EDO	D	193	-	-	1/1/1/1	-
3	EDO	C	197	-	-	1/1/1/1	-
3	EDO	H	199	-	-	1/1/1/1	-
3	EDO	H	193	-	-	1/1/1/1	-
3	EDO	D	197	-	-	0/1/1/1	-
3	EDO	H	197	-	-	1/1/1/1	-
3	EDO	C	193	-	-	0/1/1/1	-
3	EDO	F	195	-	-	1/1/1/1	-
3	EDO	E	194	-	-	0/1/1/1	-
3	EDO	F	193	-	-	1/1/1/1	-
3	EDO	B	194	-	-	1/1/1/1	-
3	EDO	D	196	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	196	-	-	0/1/1/1	-
3	EDO	C	194	-	-	0/1/1/1	-
3	EDO	A	193	-	-	1/1/1/1	-
2	MES	E	192	-	-	4/6/14/14	0/1/1/1
2	MES	B	192	-	-	5/6/14/14	0/1/1/1
3	EDO	C	198	-	-	1/1/1/1	-
3	EDO	D	194	-	-	0/1/1/1	-
3	EDO	H	194	-	-	0/1/1/1	-
3	EDO	B	195	-	-	0/1/1/1	-
3	EDO	C	196	-	-	1/1/1/1	-
3	EDO	H	198	-	-	1/1/1/1	-
3	EDO	F	194	-	-	0/1/1/1	-
2	MES	H	192	-	-	5/6/14/14	0/1/1/1
2	MES	C	192	-	-	6/6/14/14	0/1/1/1
3	EDO	F	196	-	-	1/1/1/1	-
2	MES	D	192	-	-	5/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	192	MES	C8-S	-8.27	1.66	1.77
2	E	192	MES	C8-S	-7.51	1.67	1.77
2	G	192	MES	C8-S	-7.35	1.67	1.77
2	A	192	MES	C8-S	-7.23	1.67	1.77
2	F	192	MES	C8-S	-6.99	1.67	1.77
2	C	192	MES	C8-S	-6.98	1.67	1.77
2	B	192	MES	C8-S	-6.44	1.68	1.77
2	D	192	MES	C8-S	-5.98	1.69	1.77

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	192	MES	C5-N4-C3	7.26	124.47	108.84
2	C	192	MES	C5-N4-C3	5.70	121.12	108.84
2	H	192	MES	C5-N4-C3	5.64	120.99	108.84
2	A	192	MES	C5-N4-C3	5.36	120.38	108.84
2	G	192	MES	C5-N4-C3	5.28	120.21	108.84
2	B	192	MES	C5-N4-C3	5.20	120.05	108.84
2	G	192	MES	C6-C5-N4	-4.85	102.75	110.12
2	F	192	MES	C5-N4-C3	4.43	118.38	108.84
2	E	192	MES	C5-N4-C3	4.38	118.27	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	192	MES	C6-C5-N4	-4.26	103.65	110.12
2	B	192	MES	C6-C5-N4	-4.16	103.80	110.12
2	G	192	MES	C2-C3-N4	-4.14	103.82	110.12
2	F	192	MES	C6-C5-N4	-3.81	104.33	110.12
2	B	192	MES	C7-N4-C5	3.79	121.34	111.24
2	F	192	MES	C7-N4-C5	3.67	121.03	111.24
2	G	192	MES	C7-N4-C3	3.66	120.99	111.24
2	E	192	MES	C7-N4-C3	3.65	120.96	111.24
2	A	192	MES	C6-C5-N4	-3.58	104.68	110.12
2	E	192	MES	C7-N4-C5	3.57	120.75	111.24
2	H	192	MES	C8-C7-N4	-3.50	99.13	112.36
2	F	192	MES	C7-N4-C3	3.50	120.56	111.24
2	F	192	MES	O2S-S-C8	3.36	111.80	106.73
2	C	192	MES	C7-N4-C3	3.34	120.14	111.24
2	A	192	MES	C7-N4-C3	3.27	119.94	111.24
2	H	192	MES	C2-C3-N4	-3.24	105.19	110.12
2	A	192	MES	C7-N4-C5	3.17	119.68	111.24
2	C	192	MES	O2S-S-C8	3.13	111.46	106.73
2	H	192	MES	C7-N4-C3	3.12	119.57	111.24
2	H	192	MES	C7-N4-C5	3.08	119.44	111.24
2	H	192	MES	O2S-S-C8	3.07	111.37	106.73
2	F	192	MES	C2-C3-N4	-2.92	105.69	110.12
2	B	192	MES	O3S-S-O2S	-2.85	104.26	111.40
2	G	192	MES	C7-N4-C5	2.84	118.80	111.24
2	B	192	MES	O3S-S-C8	2.82	111.52	106.00
2	G	192	MES	C8-C7-N4	-2.79	101.79	112.36
2	C	192	MES	C7-N4-C5	2.79	118.68	111.24
2	D	192	MES	C2-C3-N4	2.78	114.35	110.12
2	B	192	MES	C7-N4-C3	2.77	118.61	111.24
2	E	192	MES	C2-C3-N4	-2.76	105.93	110.12
2	D	192	MES	O1S-S-C8	2.66	110.74	106.73
2	D	192	MES	C7-N4-C3	2.62	118.21	111.24
2	D	192	MES	O2S-S-C8	2.49	110.49	106.73
2	A	192	MES	O1S-S-C8	2.49	110.49	106.73
2	F	192	MES	O1S-S-C8	2.45	110.43	106.73
2	E	192	MES	O1S-S-C8	2.41	110.37	106.73
2	G	192	MES	O2S-S-C8	2.39	110.34	106.73
2	G	192	MES	O3S-S-C8	2.32	110.53	106.00
2	E	192	MES	C6-O1-C2	2.30	117.32	109.88
2	B	192	MES	C8-C7-N4	-2.28	103.73	112.36
2	D	192	MES	C7-N4-C5	2.28	117.30	111.24
2	E	192	MES	C6-C5-N4	-2.27	106.67	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	192	MES	O3S-S-O1S	-2.26	105.76	111.40
2	C	192	MES	C6-O1-C2	2.22	117.05	109.88
2	H	192	MES	O1S-S-C8	2.20	110.06	106.73
2	A	192	MES	C8-C7-N4	-2.01	104.74	112.36

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	192	MES	C8-C7-N4-C3
2	A	192	MES	N4-C7-C8-S
2	A	192	MES	C7-C8-S-O2S
2	A	192	MES	C7-C8-S-O3S
2	B	192	MES	C8-C7-N4-C3
2	B	192	MES	N4-C7-C8-S
2	C	192	MES	C8-C7-N4-C5
2	C	192	MES	N4-C7-C8-S
2	C	192	MES	C7-C8-S-O1S
2	C	192	MES	C7-C8-S-O2S
2	C	192	MES	C7-C8-S-O3S
2	D	192	MES	C8-C7-N4-C3
2	D	192	MES	N4-C7-C8-S
2	E	192	MES	C8-C7-N4-C3
2	E	192	MES	C7-C8-S-O2S
2	E	192	MES	C7-C8-S-O3S
2	G	192	MES	C8-C7-N4-C3
2	G	192	MES	C7-C8-S-O1S
2	H	192	MES	C7-C8-S-O1S
2	H	192	MES	C7-C8-S-O2S
2	B	192	MES	C7-C8-S-O3S
2	H	192	MES	C7-C8-S-O3S
3	A	193	EDO	O1-C1-C2-O2
3	F	193	EDO	O1-C1-C2-O2
3	F	195	EDO	O1-C1-C2-O2
3	H	198	EDO	O1-C1-C2-O2
2	G	192	MES	C7-C8-S-O3S
3	B	194	EDO	O1-C1-C2-O2
3	C	197	EDO	O1-C1-C2-O2
3	C	198	EDO	O1-C1-C2-O2
3	D	196	EDO	O1-C1-C2-O2
2	F	192	MES	C8-C7-N4-C3
2	H	192	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
3	H	199	EDO	O1-C1-C2-O2
2	D	192	MES	C7-C8-S-O3S
2	A	192	MES	C7-C8-S-O1S
2	B	192	MES	C7-C8-S-O1S
2	B	192	MES	C7-C8-S-O2S
2	D	192	MES	C7-C8-S-O1S
2	D	192	MES	C7-C8-S-O2S
2	E	192	MES	C7-C8-S-O1S
2	G	192	MES	C7-C8-S-O2S
2	H	192	MES	N4-C7-C8-S
3	D	195	EDO	O1-C1-C2-O2
3	H	193	EDO	O1-C1-C2-O2
3	H	197	EDO	O1-C1-C2-O2
3	E	193	EDO	O1-C1-C2-O2
3	C	196	EDO	O1-C1-C2-O2
2	C	192	MES	C8-C7-N4-C3
3	D	193	EDO	O1-C1-C2-O2
3	F	196	EDO	O1-C1-C2-O2

There are no ring outliers.

29 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	195	EDO	4	0
2	F	192	MES	5	0
2	G	192	MES	7	0
2	A	192	MES	3	0
3	C	199	EDO	2	0
3	C	195	EDO	5	0
3	D	193	EDO	2	0
3	C	197	EDO	2	0
3	H	193	EDO	1	0
3	H	197	EDO	1	0
3	C	193	EDO	1	0
3	F	195	EDO	5	0
3	E	194	EDO	1	0
3	F	193	EDO	1	0
3	B	194	EDO	1	0
3	H	196	EDO	3	0
3	C	194	EDO	2	0
3	A	193	EDO	2	0
2	E	192	MES	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	192	MES	4	0
3	C	198	EDO	2	0
3	D	194	EDO	1	0
3	H	194	EDO	3	0
3	B	195	EDO	1	0
3	H	198	EDO	6	0
2	H	192	MES	3	0
2	C	192	MES	5	0
3	F	196	EDO	1	0
2	D	192	MES	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	187/194 (96%)	-1.02	0	100	100	21, 46, 98, 134	0
1	B	184/194 (94%)	-1.19	0	100	100	25, 44, 77, 102	0
1	C	187/194 (96%)	-1.16	0	100	100	24, 42, 87, 128	0
1	D	184/194 (94%)	-1.07	0	100	100	21, 43, 87, 101	0
1	E	186/194 (95%)	-1.20	0	100	100	22, 42, 87, 110	0
1	F	182/194 (93%)	-1.18	0	100	100	26, 44, 87, 152	0
1	G	186/194 (95%)	-1.03	0	100	100	22, 48, 94, 121	0
1	H	182/194 (93%)	-1.03	0	100	100	27, 49, 96, 140	0
All	All	1478/1552 (95%)	-1.11	0	100	100	21, 45, 90, 152	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
3	EDO	E	195	4/4	0.92	0.05	73,74,76,77	0
3	EDO	C	197	4/4	0.96	0.05	75,75,79,82	0
2	MES	G	192	12/12	0.97	0.07	57,69,202,202	0
3	EDO	D	197	4/4	0.97	0.05	54,59,66,70	0
3	EDO	B	193	4/4	0.97	0.06	47,58,64,70	0
3	EDO	H	195	4/4	0.97	0.05	46,50,51,53	0
3	EDO	H	199	4/4	0.97	0.04	49,50,50,53	0
3	EDO	B	194	4/4	0.98	0.05	45,46,46,47	0
3	EDO	C	199	4/4	0.98	0.03	57,58,59,60	0
3	EDO	C	194	4/4	0.98	0.04	56,59,63,68	0
3	EDO	B	195	4/4	0.99	0.02	31,32,43,47	0
3	EDO	C	193	4/4	0.99	0.03	36,41,48,53	0
2	MES	E	192	12/12	0.99	0.05	40,51,194,195	0
3	EDO	C	195	4/4	0.99	0.04	37,39,39,41	0
3	EDO	C	196	4/4	0.99	0.04	45,45,48,48	0
2	MES	F	192	12/12	0.99	0.03	47,50,73,74	0
3	EDO	C	198	4/4	0.99	0.04	55,56,56,58	0
2	MES	B	192	12/12	0.99	0.03	37,43,63,71	0
3	EDO	D	193	4/4	0.99	0.04	31,35,41,42	0
3	EDO	D	194	4/4	0.99	0.04	38,45,55,59	0
3	EDO	D	195	4/4	0.99	0.10	34,35,38,47	0
3	EDO	D	196	4/4	0.99	0.06	60,60,60,61	0
2	MES	H	192	12/12	0.99	0.04	69,72,77,79	0
3	EDO	E	193	4/4	0.99	0.04	39,42,44,45	0
3	EDO	E	194	4/4	0.99	0.06	25,33,36,43	0
3	EDO	A	193	4/4	0.99	0.04	37,40,42,51	0
3	EDO	F	193	4/4	0.99	0.02	24,32,36,42	0
3	EDO	F	194	4/4	0.99	0.07	57,58,59,61	0
3	EDO	F	195	4/4	0.99	0.05	47,48,49,50	0
3	EDO	F	196	4/4	0.99	0.04	36,43,43,47	0
3	EDO	H	193	4/4	0.99	0.04	39,40,40,43	0
3	EDO	H	194	4/4	0.99	0.04	37,39,39,44	0
2	MES	C	192	12/12	0.99	0.03	24,41,62,68	0
3	EDO	H	196	4/4	0.99	0.05	42,47,47,48	0
3	EDO	H	197	4/4	0.99	0.05	53,56,60,63	0
2	MES	D	192	12/12	0.99	0.03	29,41,82,83	0
3	EDO	H	198	4/4	1.00	0.08	33,37,43,45	0
2	MES	A	192	12/12	1.00	0.02	35,45,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.