Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 01:39 PM EST

PDB ID	:	3BYT
Title	:	A complex between a variant of staphylococcal enterotoxin C3 and the variable domain of the murine T cell receptor beta chain 8.2
Authors	:	Cho, S.; Eric, J.S.
Deposited on	:	2008-01-16
Resolution	:	2.30 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:

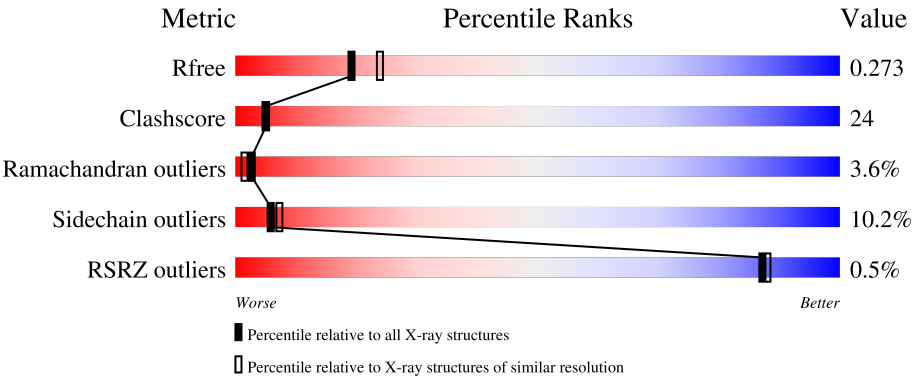
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 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	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	109	48% 40% 10%
1	C	109	47% 36% 16%
1	E	109	39% 50% 12%
1	G	109	2% 48% 40% 10%
2	B	239	47% 38% 10%

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Mol	Chain	Length	Quality of chain
2	D	239	42% 43% 11%
2	F	239	44% 41% 11%
2	H	239	44% 43% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11054 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 T cell receptor beta chain 8.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	C	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	E	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			
1	G	109	Total	C	N	O	S	0	0	0
			828	513	147	165	3			

- Molecule 2 is a protein called Enterotoxin type C-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1900	1205	312	373	10			
2	D	233	Total	C	N	O	S	0	0	0
			1906	1208	313	375	10			
2	F	234	Total	C	N	O	S	0	0	0
			1917	1215	315	377	10			
2	H	230	Total	C	N	O	S	0	0	0
			1873	1186	307	370	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	VAL	SEE REMARK 999	UNP P0A0L5
B	?	-	GLY	SEE REMARK 999	UNP P0A0L5
B	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
B	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
B	103	TRP	-	SEE REMARK 999	UNP P0A0L5
B	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
D	?	-	VAL	SEE REMARK 999	UNP P0A0L5
D	?	-	GLY	SEE REMARK 999	UNP P0A0L5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
D	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
D	103	TRP	-	SEE REMARK 999	UNP P0A0L5
D	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
F	?	-	VAL	SEE REMARK 999	UNP P0A0L5
F	?	-	GLY	SEE REMARK 999	UNP P0A0L5
F	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
F	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
F	103	TRP	-	SEE REMARK 999	UNP P0A0L5
F	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
H	?	-	VAL	SEE REMARK 999	UNP P0A0L5
H	?	-	GLY	SEE REMARK 999	UNP P0A0L5
H	100B	ALA	-	SEE REMARK 999	UNP P0A0L5
H	101	SER	VAL	SEE REMARK 999	UNP P0A0L5
H	103	TRP	-	SEE REMARK 999	UNP P0A0L5
H	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5

- Molecule 3 is water.

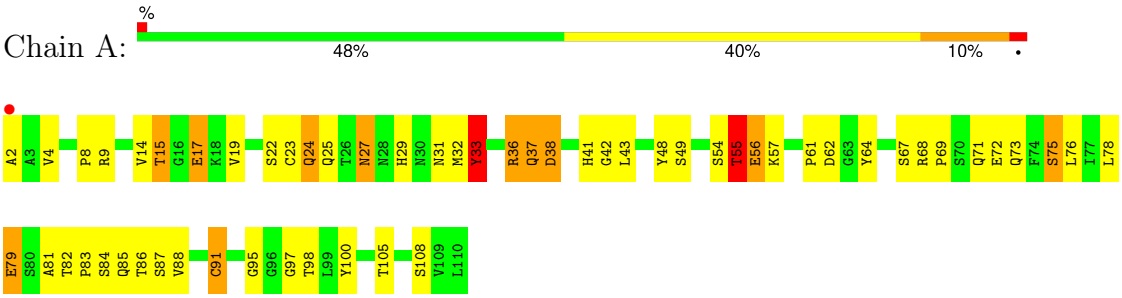
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	21	Total O 21 21	0	0
3	C	14	Total O 14 14	0	0
3	D	27	Total O 27 27	0	0
3	E	12	Total O 12 12	0	0
3	F	23	Total O 23 23	0	0
3	G	10	Total O 10 10	0	0
3	H	28	Total O 28 28	0	0

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.

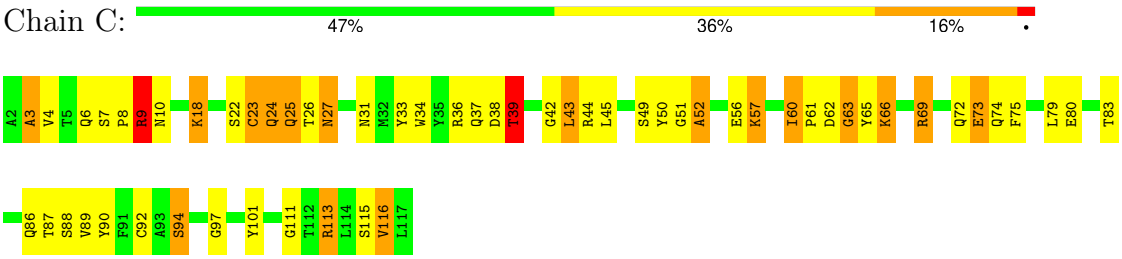
• Molecule 1: T cell receptor beta chain 8.2

Chain A:



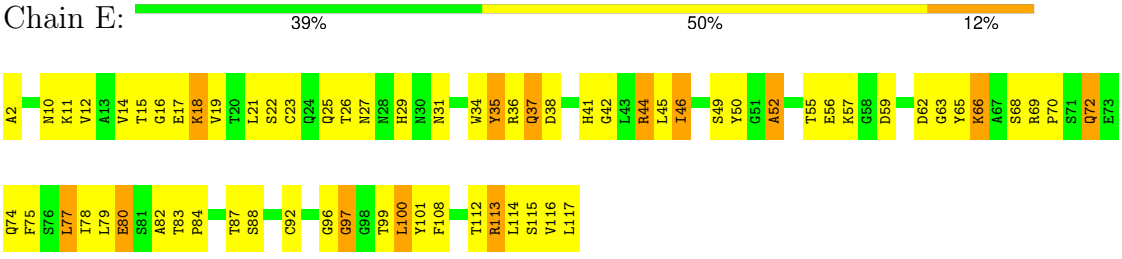
• Molecule 1: T cell receptor beta chain 8.2

Chain C:



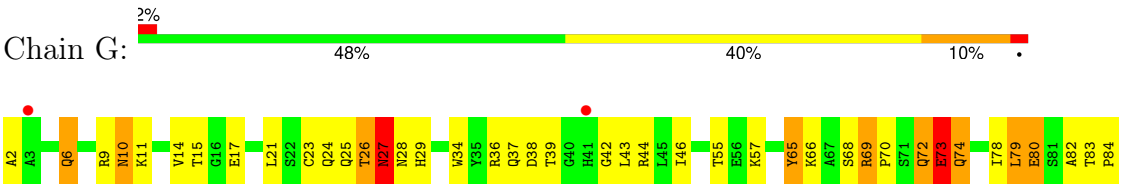
• Molecule 1: T cell receptor beta chain 8.2

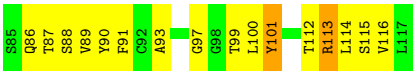
Chain E:



• Molecule 1: T cell receptor beta chain 8.2

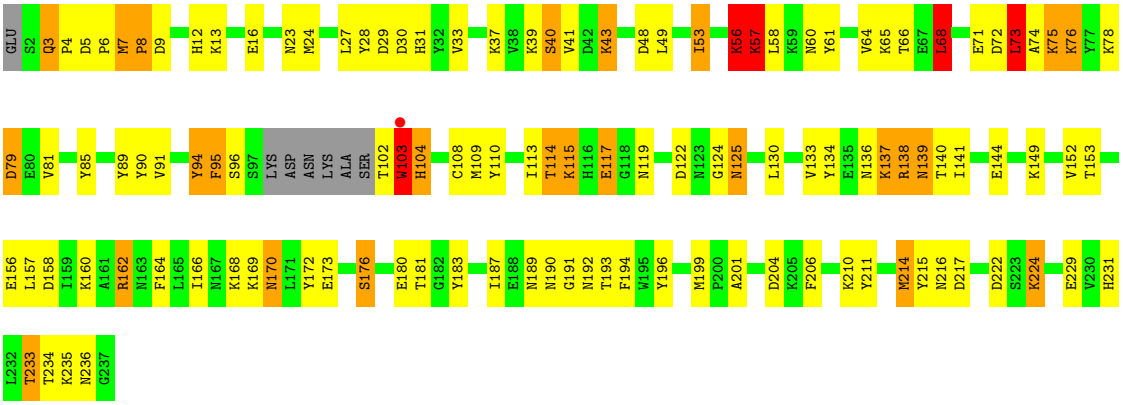
Chain G:





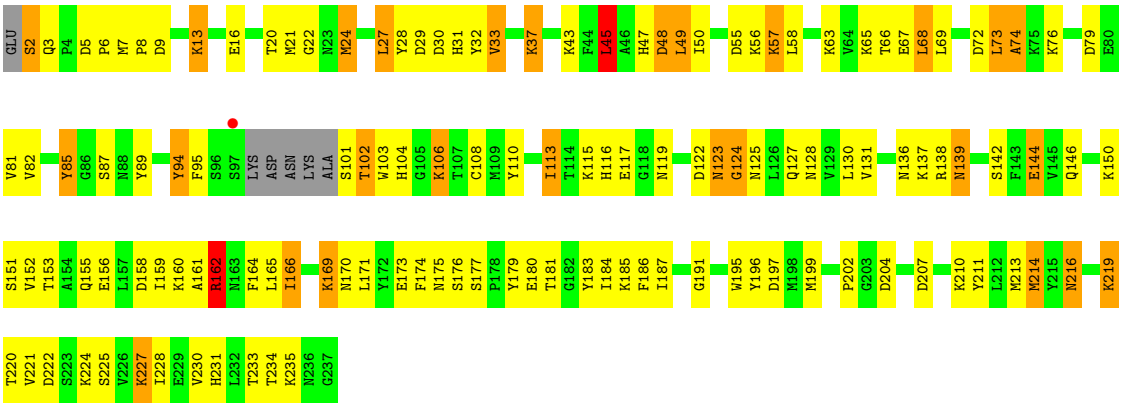
• Molecule 2: Enterotoxin type C-3

Chain B:



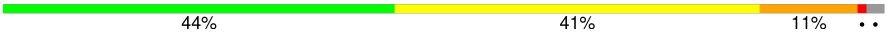
• Molecule 2: Enterotoxin type C-3

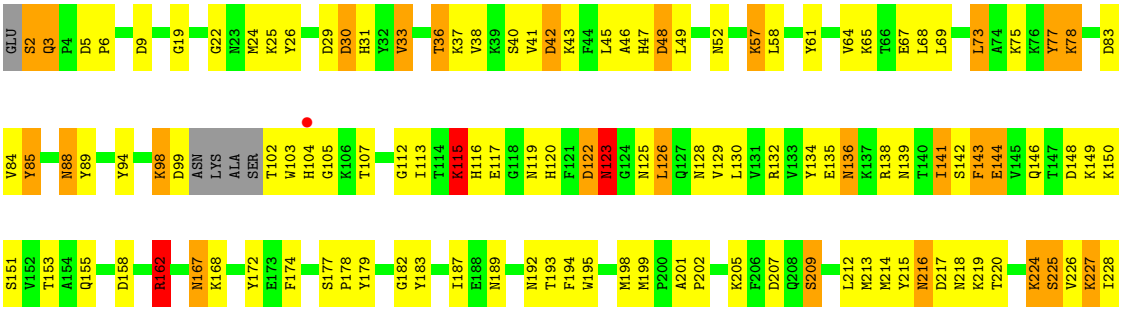
Chain D:



• Molecule 2: Enterotoxin type C-3

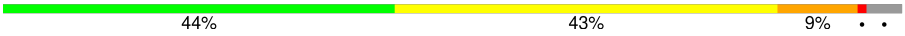
Chain F:

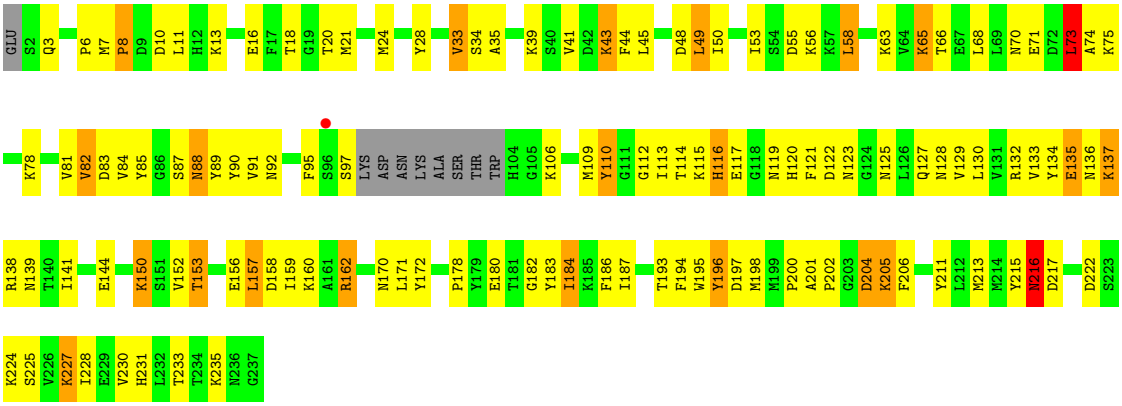




• Molecule 2: Enterotoxin type C-3

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.16Å 70.64Å 98.84Å 74.78° 75.16° 88.26°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (30.00-2.30) 95.2 (30.00-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.278 0.222 , 0.273	Depositor DCC
R_{free} test set	3424 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11054	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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

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	1.93	16/846 (1.9%)	1.56	11/1145 (1.0%)
1	C	1.96	16/846 (1.9%)	1.66	13/1145 (1.1%)
1	E	1.84	13/846 (1.5%)	1.51	15/1145 (1.3%)
1	G	1.76	8/846 (0.9%)	1.41	7/1145 (0.6%)
2	B	1.74	22/1943 (1.1%)	1.37	10/2617 (0.4%)
2	D	1.81	34/1949 (1.7%)	1.48	22/2625 (0.8%)
2	F	1.73	26/1960 (1.3%)	1.41	17/2639 (0.6%)
2	H	1.72	17/1913 (0.9%)	1.38	12/2574 (0.5%)
All	All	1.79	152/11149 (1.4%)	1.45	107/15035 (0.7%)

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	C	0	1

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	80	GLU	CG-CD	13.77	1.72	1.51
1	C	52	ALA	CA-CB	12.30	1.78	1.52
1	A	79	GLU	CG-CD	11.22	1.68	1.51
1	A	55	THR	CB-CG2	9.50	1.83	1.52
2	H	211	TYR	CD2-CE2	-9.36	1.25	1.39
1	G	101	TYR	C-N	8.59	1.53	1.34
1	E	80	GLU	CD-OE1	8.39	1.34	1.25
1	A	91	CYS	CB-SG	-8.35	1.68	1.82
1	C	92	CYS	CB-SG	-8.26	1.68	1.82
1	A	75	SER	CB-OG	-8.04	1.31	1.42
1	A	81	ALA	CA-CB	-7.80	1.36	1.52
2	D	152	VAL	CB-CG2	-7.74	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	SER	CB-OG	7.69	1.52	1.42
2	F	144	GLU	CB-CG	7.41	1.66	1.52
1	G	80	GLU	CD-OE2	7.41	1.33	1.25
1	A	33	TYR	CG-CD2	7.34	1.48	1.39
1	G	17	GLU	CG-CD	7.29	1.62	1.51
2	F	78	LYS	CD-CE	7.25	1.69	1.51
1	E	57	LYS	CD-CE	7.17	1.69	1.51
2	B	215	TYR	CD1-CE1	7.12	1.50	1.39
1	C	63	GLY	C-N	7.09	1.50	1.34
2	D	63	LYS	CE-NZ	7.07	1.66	1.49
2	B	196	TYR	CE2-CZ	-7.00	1.29	1.38
1	E	80	GLU	CD-OE2	6.94	1.33	1.25
1	C	18	LYS	CE-NZ	6.93	1.66	1.49
1	C	39	THR	CB-CG2	6.93	1.75	1.52
1	C	24	GLN	CG-CD	6.86	1.66	1.51
2	F	85	TYR	CD1-CE1	-6.86	1.29	1.39
2	B	61	TYR	CE1-CZ	-6.84	1.29	1.38
2	B	94	TYR	CE1-CZ	6.83	1.47	1.38
2	H	89	TYR	CD1-CE1	-6.83	1.29	1.39
2	B	206	PHE	CE2-CZ	-6.82	1.24	1.37
2	B	172	TYR	CE2-CZ	6.75	1.47	1.38
2	H	43	LYS	CD-CE	6.75	1.68	1.51
2	F	201	ALA	CA-CB	6.70	1.66	1.52
2	D	221	VAL	CB-CG1	-6.68	1.38	1.52
1	E	63	GLY	C-N	6.68	1.49	1.34
2	B	41	VAL	CB-CG2	6.66	1.66	1.52
1	G	65	TYR	CD2-CE2	6.63	1.49	1.39
2	B	117	GLU	CG-CD	6.59	1.61	1.51
2	F	22	GLY	C-O	-6.58	1.13	1.23
2	B	9	ASP	CB-CG	6.53	1.65	1.51
2	F	64	VAL	CB-CG2	-6.52	1.39	1.52
2	D	74	ALA	CA-CB	-6.49	1.38	1.52
2	D	106	LYS	CD-CE	6.44	1.67	1.51
1	G	44	ARG	CZ-NH1	6.43	1.41	1.33
2	D	142	SER	C-O	6.41	1.35	1.23
2	D	27	LEU	CG-CD1	6.36	1.75	1.51
2	D	164	PHE	CE1-CZ	6.36	1.49	1.37
2	F	141	ILE	CB-CG2	6.33	1.72	1.52
2	D	176	SER	CB-OG	6.29	1.50	1.42
2	B	7	MET	CB-CG	6.25	1.71	1.51
2	D	33	VAL	CB-CG2	-6.24	1.39	1.52
1	E	35	TYR	CD1-CE1	-6.23	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	150	LYS	CD-CE	6.17	1.66	1.51
1	C	57	LYS	CE-NZ	6.14	1.64	1.49
1	A	2	ALA	CA-CB	6.14	1.65	1.52
2	D	85	TYR	CE2-CZ	-6.12	1.30	1.38
1	E	57	LYS	CE-NZ	6.09	1.64	1.49
2	D	169	LYS	CE-NZ	6.08	1.64	1.49
2	D	45	LEU	CG-CD1	6.06	1.74	1.51
1	C	25	GLN	CB-CG	-6.03	1.36	1.52
2	D	204	ASP	CB-CG	6.01	1.64	1.51
2	H	135	GLU	CD-OE1	6.01	1.32	1.25
1	A	33	TYR	CD2-CE2	-6.01	1.30	1.39
1	C	23	CYS	CB-SG	6.00	1.92	1.82
2	D	63	LYS	CB-CG	5.99	1.68	1.52
1	A	19	VAL	N-CA	5.99	1.58	1.46
2	H	16	GLU	CB-CG	5.98	1.63	1.52
2	B	115	LYS	CD-CE	5.96	1.66	1.51
1	E	50	TYR	CD1-CE1	-5.96	1.30	1.39
2	H	117	GLU	CD-OE2	5.95	1.32	1.25
1	A	75	SER	C-O	-5.95	1.12	1.23
2	F	227	LYS	CG-CD	5.92	1.72	1.52
2	D	211	TYR	CE2-CZ	-5.89	1.30	1.38
2	D	137	LYS	CD-CE	5.89	1.66	1.51
2	H	33	VAL	CB-CG1	5.87	1.65	1.52
1	G	73	GLU	CB-CG	5.85	1.63	1.52
2	F	78	LYS	CE-NZ	5.83	1.63	1.49
2	B	90	TYR	CD1-CE1	5.82	1.48	1.39
2	D	137	LYS	CE-NZ	5.76	1.63	1.49
2	B	94	TYR	CE2-CZ	5.73	1.46	1.38
2	H	230	VAL	CA-CB	-5.71	1.42	1.54
2	F	77	TYR	CD2-CE2	5.69	1.47	1.39
2	F	94	TYR	CG-CD1	5.69	1.46	1.39
1	E	101	TYR	C-N	5.67	1.47	1.34
1	C	116	VAL	CB-CG1	-5.66	1.41	1.52
2	F	46	ALA	CA-CB	5.66	1.64	1.52
2	B	183	TYR	CB-CG	5.63	1.60	1.51
2	H	63	LYS	CD-CE	5.57	1.65	1.51
2	F	3	GLN	CG-CD	5.56	1.63	1.51
1	E	52	ALA	CA-CB	5.55	1.64	1.52
1	A	64	TYR	CD1-CE1	-5.55	1.31	1.39
2	F	26	TYR	CD1-CE1	-5.54	1.31	1.39
2	D	173	GLU	CD-OE2	-5.53	1.19	1.25
2	B	204	ASP	C-O	-5.51	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	ILE	CA-CB	5.51	1.67	1.54
2	H	196	TYR	CE1-CZ	-5.51	1.31	1.38
2	D	196	TYR	CG-CD2	5.48	1.46	1.39
1	E	100	LEU	C-O	-5.48	1.12	1.23
2	F	115	LYS	CD-CE	5.47	1.65	1.51
2	F	33	VAL	CB-CG2	-5.47	1.41	1.52
1	E	56	GLU	CB-CG	5.46	1.62	1.52
1	A	61	PRO	CG-CD	-5.46	1.32	1.50
2	D	177	SER	CA-CB	-5.46	1.44	1.52
1	G	42	GLY	C-O	5.44	1.32	1.23
2	F	75	LYS	CD-CE	5.44	1.64	1.51
2	D	32	TYR	CD1-CE1	-5.43	1.31	1.39
1	E	10	ASN	CB-CG	5.43	1.63	1.51
2	F	225	SER	CB-OG	-5.42	1.35	1.42
2	D	146	GLN	CB-CG	-5.41	1.38	1.52
1	C	33	TYR	CE2-CZ	-5.37	1.31	1.38
2	D	179	TYR	CE2-CZ	-5.37	1.31	1.38
2	D	94	TYR	CD2-CE2	5.35	1.47	1.39
2	D	235	LYS	N-CA	5.34	1.57	1.46
1	A	57	LYS	CE-NZ	5.34	1.62	1.49
2	F	143	PHE	CE1-CZ	5.32	1.47	1.37
2	B	117	GLU	CD-OE1	5.29	1.31	1.25
2	H	205	LYS	CE-NZ	5.28	1.62	1.49
2	B	210	LYS	CD-CE	5.28	1.64	1.51
2	D	89	TYR	CD1-CE1	-5.28	1.31	1.39
2	D	37	LYS	CB-CG	5.27	1.66	1.52
2	D	87	SER	CB-OG	-5.25	1.35	1.42
1	C	8	PRO	N-CA	5.24	1.56	1.47
2	H	39	LYS	N-CA	5.24	1.56	1.46
2	F	123	ASN	CB-CG	5.22	1.63	1.51
2	F	117	GLU	CB-CG	5.21	1.62	1.52
1	A	64	TYR	CG-CD1	-5.19	1.32	1.39
1	A	64	TYR	CE2-CZ	-5.19	1.31	1.38
1	G	90	TYR	CE2-CZ	-5.19	1.31	1.38
1	C	25	GLN	CD-OE1	-5.17	1.12	1.24
2	H	82	VAL	CB-CG2	-5.17	1.42	1.52
1	A	17	GLU	CB-CG	5.15	1.61	1.52
2	B	57	LYS	CD-CE	5.15	1.64	1.51
2	D	214	MET	N-CA	-5.14	1.36	1.46
2	F	38	VAL	CB-CG1	-5.14	1.42	1.52
2	B	183	TYR	CD2-CE2	-5.13	1.31	1.39
2	D	32	TYR	CG-CD1	5.13	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	94	TYR	CE2-CZ	5.13	1.45	1.38
2	B	156	GLU	CD-OE2	5.11	1.31	1.25
2	H	90	TYR	CD1-CE1	-5.10	1.31	1.39
2	H	180	GLU	CG-CD	5.09	1.59	1.51
1	C	62	ASP	CB-CG	5.09	1.62	1.51
2	D	186	PHE	CB-CG	5.06	1.59	1.51
2	H	227	LYS	CD-CE	5.05	1.63	1.51
2	B	201	ALA	CA-CB	-5.04	1.41	1.52
2	B	94	TYR	CG-CD1	5.03	1.45	1.39
2	F	229	GLU	CD-OE2	-5.03	1.20	1.25
1	C	50	TYR	CD1-CE1	5.03	1.46	1.39
2	F	205	LYS	CB-CG	5.02	1.66	1.52
2	D	124	GLY	C-O	5.02	1.31	1.23
2	F	233	THR	C-O	-5.00	1.13	1.23

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	162	ARG	NE-CZ-NH1	-13.66	113.47	120.30
1	C	63	GLY	O-C-N	-12.84	102.16	122.70
1	C	9	ARG	NE-CZ-NH1	11.95	126.27	120.30
2	D	162	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	C	9	ARG	NE-CZ-NH2	-10.93	114.84	120.30
2	F	24	MET	CG-SD-CE	-10.17	83.92	100.20
2	D	162	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	A	36	ARG	NE-CZ-NH2	-9.03	115.78	120.30
2	F	65	LYS	CD-CE-NZ	-8.84	91.36	111.70
1	A	38	ASP	CB-CG-OD1	-8.66	110.51	118.30
2	D	166	ILE	CG1-CB-CG2	-8.41	92.89	111.40
1	A	78	LEU	CB-CG-CD1	8.09	124.75	111.00
1	A	36	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	38	ASP	CB-CG-OD2	7.78	125.30	118.30
1	E	36	ARG	NE-CZ-NH2	7.76	124.18	120.30
2	D	58	LEU	CB-CG-CD2	-7.72	97.88	111.00
2	F	207	ASP	CB-CG-OD2	-7.66	111.41	118.30
2	D	204	ASP	CB-CG-OD1	7.65	125.19	118.30
2	F	148	ASP	CB-CG-OD2	-7.63	111.44	118.30
2	B	214	MET	CG-SD-CE	-7.61	88.03	100.20
2	B	217	ASP	CB-CG-OD1	7.41	124.97	118.30
1	G	44	ARG	NE-CZ-NH2	-7.35	116.62	120.30
2	H	160	LYS	CD-CE-NZ	7.29	128.48	111.70
1	C	113	ARG	NE-CZ-NH1	7.11	123.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	68	LEU	CA-CB-CG	7.10	131.62	115.30
2	F	5	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	9	ARG	NE-CZ-NH2	7.01	123.80	120.30
2	D	76	LYS	CD-CE-NZ	-7.00	95.61	111.70
2	D	79	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	C	101	TYR	O-C-N	-6.86	111.73	122.70
2	D	55	ASP	CB-CG-OD1	6.84	124.46	118.30
2	F	148	ASP	CB-CG-OD1	6.68	124.31	118.30
1	E	36	ARG	NE-CZ-NH1	-6.68	116.96	120.30
2	D	123	ASN	C-N-CA	-6.67	108.30	122.30
2	F	5	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	G	79	LEU	CB-CG-CD2	-6.63	99.73	111.00
2	H	157	LEU	CB-CG-CD1	-6.56	99.85	111.00
2	H	162	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	E	77	LEU	CB-CG-CD1	6.44	121.95	111.00
1	E	63	GLY	O-C-N	-6.44	112.40	122.70
1	C	57	LYS	CD-CE-NZ	-6.43	96.90	111.70
2	D	137	LYS	CD-CE-NZ	6.38	126.36	111.70
2	D	122	ASP	CB-CG-OD2	6.35	124.02	118.30
1	E	113	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	H	132	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	G	44	ARG	NE-CZ-NH1	-6.25	117.18	120.30
2	D	24	MET	CG-SD-CE	-6.24	90.22	100.20
1	C	101	TYR	CA-C-N	6.22	130.89	117.20
1	C	45	LEU	CB-CG-CD1	6.21	121.55	111.00
2	D	113	ILE	CG1-CB-CG2	-6.15	97.86	111.40
1	E	97	GLY	N-CA-C	-6.11	97.83	113.10
2	D	199	MET	CG-SD-CE	6.09	109.95	100.20
1	G	44	ARG	NH1-CZ-NH2	6.09	126.10	119.40
2	F	113	ILE	CB-CA-C	-6.07	99.46	111.60
1	A	78	LEU	CB-CG-CD2	-5.97	100.85	111.00
1	G	66	LYS	CB-CG-CD	-5.95	96.14	111.60
1	C	69	ARG	NE-CZ-NH1	-5.94	117.33	120.30
2	H	171	LEU	CB-CG-CD1	5.94	121.10	111.00
2	B	169	LYS	CD-CE-NZ	-5.90	98.13	111.70
2	F	75	LYS	CD-CE-NZ	-5.88	98.18	111.70
1	E	79	LEU	CB-CG-CD2	-5.85	101.06	111.00
2	F	36	THR	CA-CB-CG2	-5.81	104.26	112.40
2	H	49	LEU	CB-CG-CD2	-5.77	101.19	111.00
2	H	204	ASP	CB-CG-OD1	-5.75	113.12	118.30
2	B	73	LEU	CA-CB-CG	5.72	128.46	115.30
1	A	15	THR	OG1-CB-CG2	-5.71	96.86	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	108	CYS	CB-CA-C	-5.65	99.10	110.40
2	D	197	ASP	CB-CG-OD2	5.64	123.38	118.30
1	G	57	LYS	CD-CE-NZ	5.64	124.67	111.70
1	A	23	CYS	CA-CB-SG	5.62	124.12	114.00
2	F	207	ASP	CB-CG-OD1	5.62	123.36	118.30
1	G	78	ILE	CG1-CB-CG2	5.61	123.75	111.40
1	E	57	LYS	CD-CE-NZ	5.61	124.59	111.70
2	F	48	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	H	73	LEU	CA-CB-CG	5.57	128.12	115.30
2	H	129	VAL	CG1-CB-CG2	5.55	119.78	110.90
1	E	66	LYS	N-CA-C	-5.51	96.13	111.00
1	A	95	GLY	N-CA-C	-5.49	99.37	113.10
2	H	156	GLU	OE1-CD-OE2	-5.41	116.80	123.30
1	E	77	LEU	CB-CG-CD2	-5.38	101.84	111.00
2	B	103	TRP	CA-CB-CG	5.36	123.89	113.70
1	A	76	LEU	CB-CG-CD1	-5.33	101.94	111.00
2	H	39	LYS	CD-CE-NZ	5.33	123.96	111.70
2	B	79	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	B	9	ASP	CB-CG-OD2	5.31	123.08	118.30
1	E	96	GLY	N-CA-C	-5.31	99.83	113.10
2	F	33	VAL	CG1-CB-CG2	-5.30	102.42	110.90
2	F	228	ILE	N-CA-C	-5.30	96.70	111.00
2	D	165	LEU	CB-CG-CD2	-5.29	102.00	111.00
2	D	32	TYR	CZ-CE2-CD2	-5.26	115.07	119.80
1	C	23	CYS	CA-CB-SG	5.23	123.42	114.00
1	C	75	PHE	CG-CD1-CE1	5.19	126.51	120.80
1	E	55	THR	N-CA-CB	5.17	120.12	110.30
2	B	53	ILE	N-CA-C	-5.17	97.05	111.00
1	C	113	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	E	38	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	F	30	ASP	CB-CG-OD1	5.13	122.92	118.30
1	E	92	CYS	CA-CB-SG	5.10	123.18	114.00
2	F	126	LEU	CB-CG-CD1	-5.08	102.36	111.00
2	H	130	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	C	45	LEU	CB-CG-CD2	-5.07	102.38	111.00
2	D	21	MET	CG-SD-CE	-5.07	92.09	100.20
2	F	162	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	D	49	LEU	CB-CG-CD1	-5.06	102.39	111.00
2	D	48	ASP	CB-CG-OD2	5.06	122.86	118.30
2	D	214	MET	CB-CG-SD	5.02	127.45	112.40
1	E	79	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	63	GLY	Mainchain

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	828	0	788	34	0
1	C	828	0	788	51	0
1	E	828	0	788	56	0
1	G	828	0	788	48	0
2	B	1900	0	1827	89	0
2	D	1906	0	1832	81	1
2	F	1917	0	1844	94	1
2	H	1873	0	1804	88	0
3	A	11	0	0	0	0
3	B	21	0	0	1	0
3	C	14	0	0	0	0
3	D	27	0	0	0	0
3	E	12	0	0	0	0
3	F	23	0	0	0	0
3	G	10	0	0	1	0
3	H	28	0	0	0	0
All	All	11054	0	10459	521	1

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 24.

All (521) 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)
2:D:27:LEU:CD1	2:D:27:LEU:CG	1.75	1.60
1:C:52:ALA:CB	1:C:52:ALA:CA	1.78	1.60
1:C:39:THR:CG2	1:C:39:THR:CB	1.75	1.58
1:A:55:THR:CG2	1:A:55:THR:CB	1.83	1.53
2:F:115:LYS:N	2:F:115:LYS:HE3	1.66	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:HIS:HA	2:F:57:LYS:NZ	1.68	1.08
1:E:87:THR:HG23	1:E:115:SER:HA	1.27	1.07
2:F:115:LYS:HE3	2:F:115:LYS:H	0.92	1.04
1:E:26:THR:HG1	1:G:2:ALA:N	1.56	1.03
1:E:21:LEU:HD22	1:E:112:THR:HG21	1.39	1.02
2:F:115:LYS:H	2:F:115:LYS:CE	1.72	1.02
1:C:26:THR:O	1:C:27:ASN:HB2	1.59	1.00
1:C:87:THR:HG23	1:C:115:SER:HA	1.48	0.96
2:H:11:LEU:HD11	2:H:183:TYR:HD2	1.32	0.92
2:H:88:ASN:H	2:H:88:ASN:HD22	1.18	0.92
2:F:99:ASP:HA	2:F:102:THR:CG2	2.02	0.90
2:D:123:ASN:O	2:D:125:ASN:N	2.07	0.88
2:D:45:LEU:HD12	2:D:48:ASP:OD2	1.75	0.85
1:G:55:THR:HG23	2:H:20:THR:HG21	1.59	0.85
1:C:26:THR:O	1:C:27:ASN:CB	2.22	0.84
1:C:22:SER:HB3	1:C:24:GLN:NE2	1.92	0.84
2:F:88:ASN:H	2:F:88:ASN:HD22	1.24	0.83
2:D:119:ASN:HD21	2:D:151:SER:H	1.25	0.83
1:A:8:PRO:O	1:A:105:THR:HG23	1.78	0.82
1:E:37:GLN:O	1:E:37:GLN:HG3	1.78	0.82
1:G:27:ASN:HB3	3:G:127:HOH:O	1.80	0.81
2:B:102:THR:HG22	2:B:103:TRP:H	1.44	0.81
2:F:31:HIS:HA	2:F:57:LYS:HZ1	1.39	0.81
1:G:36:ARG:HH11	1:G:88:SER:HB2	1.44	0.80
2:H:110:TYR:HE2	2:H:213:MET:HG3	1.47	0.80
2:B:136:ASN:O	2:B:137:LYS:HB2	1.78	0.80
2:D:47:HIS:CD2	2:H:45:LEU:HD11	2.16	0.80
2:H:11:LEU:HD11	2:H:183:TYR:CD2	2.16	0.79
1:C:9:ARG:NH2	1:C:111:GLY:O	2.14	0.79
1:G:69:ARG:HH21	1:G:69:ARG:HG3	1.46	0.79
2:B:76:LYS:HZ3	2:B:115:LYS:HE2	1.45	0.79
2:D:47:HIS:CE1	2:D:67:GLU:HG2	2.19	0.78
2:D:31:HIS:HA	2:D:57:LYS:HE2	1.65	0.77
1:E:87:THR:CG2	1:E:115:SER:HA	2.13	0.77
2:H:110:TYR:CD2	2:H:213:MET:HA	2.19	0.77
2:H:66:THR:HG21	2:H:113:ILE:HD11	1.68	0.76
2:F:213:MET:O	2:F:216:ASN:HB2	1.85	0.76
1:G:69:ARG:HH21	1:G:69:ARG:CG	1.99	0.76
1:C:22:SER:HB3	1:C:24:GLN:HE22	1.49	0.76
2:B:43:LYS:HZ2	2:B:43:LYS:HB2	1.51	0.75
2:B:76:LYS:NZ	2:B:115:LYS:HE2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:LYS:HG3	2:H:115:LYS:O	1.86	0.75
2:H:110:TYR:CE2	2:H:213:MET:HG3	2.22	0.74
1:E:2:ALA:N	1:G:26:THR:HG1	1.84	0.74
2:H:88:ASN:H	2:H:88:ASN:ND2	1.84	0.74
2:B:173:GLU:HB2	2:B:176:SER:O	1.88	0.74
2:B:43:LYS:HE3	2:B:75:LYS:HZ1	1.53	0.74
2:B:33:VAL:O	2:B:85:TYR:HA	1.88	0.74
1:G:73:GLU:O	1:G:74:GLN:HB2	1.88	0.73
1:G:69:ARG:HG3	1:G:69:ARG:NH2	2.00	0.73
2:B:187:ILE:HA	2:B:193:THR:HG22	1.71	0.73
2:H:8:PRO:O	2:H:13:LYS:NZ	2.22	0.73
2:B:13:LYS:HB3	2:B:180:GLU:OE1	1.89	0.73
2:B:233:THR:HG23	2:B:235:LYS:NZ	2.04	0.73
2:B:40:SER:HB3	2:B:78:LYS:O	1.88	0.72
1:G:79:LEU:HD23	1:G:86:GLN:OE1	1.89	0.72
2:D:184:ILE:HG13	2:D:230:VAL:HG22	1.72	0.71
1:E:72:GLN:HE21	1:E:72:GLN:HA	1.54	0.71
2:H:35:ALA:HB2	2:H:53:ILE:HD12	1.71	0.71
2:F:99:ASP:HA	2:F:102:THR:HG22	1.73	0.71
2:F:138:ARG:HG2	2:F:138:ARG:HH11	1.54	0.70
1:A:27:ASN:HD22	1:C:27:ASN:ND2	1.90	0.69
2:D:128:ASN:HD22	2:D:144:GLU:HG2	1.58	0.69
2:F:123:ASN:N	2:F:123:ASN:HD22	1.89	0.69
2:B:43:LYS:HD3	2:B:48:ASP:O	1.92	0.69
2:H:110:TYR:N	2:H:110:TYR:CD1	2.57	0.68
2:H:120:HIS:O	2:H:150:LYS:HE3	1.93	0.68
1:A:27:ASN:HD22	1:C:27:ASN:HD21	1.42	0.68
1:C:69:ARG:HD2	1:C:74:GLN:O	1.94	0.68
2:F:99:ASP:HA	2:F:102:THR:HG23	1.73	0.67
2:B:190:ASN:HD21	2:B:192:ASN:HB2	1.60	0.67
2:F:41:VAL:HG21	2:F:52:ASN:OD1	1.95	0.67
1:G:36:ARG:NH1	1:G:88:SER:HB2	2.10	0.67
2:F:77:TYR:HE2	2:F:115:LYS:HE2	1.60	0.67
2:D:8:PRO:O	2:D:13:LYS:HE3	1.96	0.66
1:G:87:THR:HG23	1:G:114:LEU:O	1.96	0.66
1:E:83:THR:O	1:E:116:VAL:HG11	1.95	0.65
1:A:67:SER:O	1:A:69:PRO:HD3	1.95	0.65
1:C:37:GLN:OE1	1:C:42:GLY:O	2.15	0.65
2:F:89:TYR:HD1	2:F:212:LEU:HD12	1.62	0.65
2:H:35:ALA:CB	2:H:53:ILE:HD12	2.26	0.65
1:C:66:LYS:NZ	1:C:80:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:SER:C	1:E:70:PRO:HD3	2.17	0.65
2:D:27:LEU:CD1	2:D:27:LEU:CD2	2.72	0.65
1:E:25:GLN:HE22	1:E:29:HIS:H	1.45	0.65
2:F:31:HIS:CA	2:F:57:LYS:HZ1	2.08	0.65
2:H:213:MET:O	2:H:216:ASN:HB2	1.96	0.65
2:D:27:LEU:CD1	2:D:27:LEU:CB	2.73	0.65
2:H:83:ASP:HB2	2:H:114:THR:OG1	1.96	0.64
1:E:65:TYR:HA	1:E:78:ILE:O	1.97	0.64
2:B:56:LYS:HB2	2:B:56:LYS:HZ3	1.61	0.64
2:H:222:ASP:OD1	2:H:225:SER:OG	2.12	0.64
2:D:219:LYS:HD3	2:D:220:THR:N	2.13	0.64
2:D:33:VAL:O	2:D:85:TYR:HA	1.97	0.64
2:H:110:TYR:N	2:H:110:TYR:HD1	1.96	0.64
2:B:37:LYS:HZ1	2:B:37:LYS:HB3	1.63	0.64
1:G:72:GLN:HE21	1:G:72:GLN:HA	1.62	0.64
2:F:155:GLN:NE2	2:F:215:TYR:HB3	2.13	0.63
2:F:167:ASN:N	2:F:167:ASN:HD22	1.94	0.63
2:H:18:THR:OG1	2:H:204:ASP:HB3	1.98	0.63
2:B:68:LEU:HD11	2:B:113:ILE:HD12	1.80	0.63
2:B:3:GLN:HG3	2:B:194:PHE:HA	1.80	0.63
2:H:152:VAL:HG11	2:H:157:LEU:HD21	1.81	0.63
2:B:139:ASN:C	2:B:139:ASN:HD22	2.01	0.62
1:A:55:THR:HG22	2:B:23:ASN:OD1	1.99	0.62
1:G:73:GLU:O	1:G:74:GLN:CB	2.47	0.62
1:A:4:VAL:HG21	1:A:100:TYR:O	1.98	0.62
2:D:94:TYR:O	2:D:95:PHE:HB3	1.99	0.61
2:D:213:MET:O	2:D:216:ASN:HB2	2.00	0.61
1:E:68:SER:O	1:E:70:PRO:HD3	2.01	0.61
2:H:137:LYS:HB2	2:H:137:LYS:NZ	2.16	0.61
1:A:22:SER:HB3	1:A:73:GLN:HE22	1.65	0.61
1:C:57:LYS:HB3	1:C:61:PRO:HG3	1.81	0.61
1:E:87:THR:O	1:E:88:SER:HB2	1.99	0.61
1:G:37:GLN:HG2	1:G:38:ASP:N	2.15	0.61
1:A:36:ARG:CG	1:A:36:ARG:O	2.49	0.60
2:D:47:HIS:HE1	2:D:67:GLU:HG2	1.61	0.60
1:E:26:THR:HG21	1:G:2:ALA:HB2	1.83	0.60
2:B:43:LYS:CE	2:B:75:LYS:NZ	2.63	0.60
2:F:40:SER:HB3	2:F:49:LEU:HD22	1.83	0.60
2:D:130:LEU:HB2	2:D:144:GLU:OE2	2.01	0.60
2:F:194:PHE:CE2	2:F:219:LYS:HE3	2.37	0.60
2:F:31:HIS:HA	2:F:57:LYS:HZ2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LYS:NZ	2:D:175:ASN:HD21	2.00	0.59
2:B:43:LYS:HE2	2:B:75:LYS:HZ3	1.67	0.59
2:B:134:TYR:HD2	2:B:137:LYS:O	1.85	0.59
2:B:233:THR:CG2	2:B:235:LYS:NZ	2.65	0.59
2:D:16:GLU:HB3	2:D:202:PRO:HB3	1.84	0.59
2:H:28:TYR:CE1	2:H:162:ARG:NH1	2.70	0.59
2:F:138:ARG:HG2	2:F:138:ARG:NH1	2.16	0.59
1:C:36:ARG:HD3	1:C:60:ILE:HD12	1.85	0.59
2:F:167:ASN:N	2:F:167:ASN:ND2	2.51	0.59
1:C:80:GLU:OE2	1:C:80:GLU:N	2.35	0.58
2:B:136:ASN:HD21	2:B:234:THR:H	1.51	0.58
2:B:130:LEU:HA	2:B:144:GLU:HG2	1.85	0.58
1:E:72:GLN:HE21	1:E:72:GLN:CA	2.15	0.58
2:B:24:MET:HE1	2:B:28:TYR:HE1	1.68	0.58
1:C:66:LYS:HB2	1:C:66:LYS:HZ3	1.67	0.58
2:H:7:MET:HB3	2:H:8:PRO:HD2	1.84	0.58
1:G:21:LEU:HD22	1:G:112:THR:HG21	1.84	0.58
2:H:34:SER:HA	2:H:84:VAL:O	2.04	0.58
2:H:110:TYR:CE2	2:H:213:MET:HA	2.38	0.58
2:F:226:VAL:O	2:F:227:LYS:HE2	2.04	0.58
2:D:117:GLU:HA	2:D:117:GLU:OE1	2.04	0.57
1:E:72:GLN:HA	1:E:72:GLN:NE2	2.18	0.57
2:F:49:LEU:HD21	2:F:78:LYS:HA	1.85	0.57
1:C:36:ARG:HD3	1:C:60:ILE:CD1	2.34	0.57
2:F:130:LEU:HD11	2:F:142:SER:HB3	1.86	0.57
2:D:130:LEU:O	2:D:227:LYS:NZ	2.36	0.57
2:B:24:MET:CE	2:B:28:TYR:HE1	2.17	0.57
2:B:94:TYR:O	2:B:95:PHE:HB3	2.04	0.57
2:D:187:ILE:HB	2:D:227:LYS:HB3	1.85	0.57
1:G:113:ARG:CZ	1:G:113:ARG:HB3	2.34	0.57
2:B:56:LYS:HB2	2:B:56:LYS:NZ	2.20	0.57
2:H:24:MET:HE1	2:H:28:TYR:HE1	1.69	0.57
2:H:184:ILE:HD11	2:H:228:ILE:CG2	2.35	0.57
1:E:25:GLN:NE2	1:E:29:HIS:H	2.02	0.56
2:H:91:VAL:O	2:H:92:ASN:HB2	2.05	0.56
1:A:82:THR:HG22	1:A:85:GLN:HG3	1.87	0.56
1:C:36:ARG:CG	1:C:60:ILE:HD11	2.35	0.56
2:B:43:LYS:HE2	2:B:75:LYS:NZ	2.21	0.56
2:D:136:ASN:ND2	2:D:233:THR:HA	2.19	0.56
2:F:88:ASN:H	2:F:88:ASN:ND2	1.99	0.56
2:H:119:ASN:O	2:H:150:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:GLY:O	1:C:69:ARG:HG2	2.05	0.56
1:E:87:THR:HG23	1:E:114:LEU:O	2.06	0.56
1:C:65:TYR:CZ	1:C:86:GLN:HG2	2.41	0.56
1:C:66:LYS:HG3	2:D:174:PHE:CG	2.40	0.56
1:G:25:GLN:O	1:G:73:GLU:HB3	2.06	0.56
1:E:23:CYS:H	1:E:74:GLN:HE22	1.52	0.56
1:E:14:VAL:HG12	1:E:15:THR:O	2.06	0.56
2:H:121:PHE:CZ	2:H:127:GLN:HB2	2.41	0.56
2:F:3:GLN:NE2	2:F:195:TRP:NE1	2.54	0.56
2:D:95:PHE:CZ	2:D:106:LYS:HB2	2.41	0.56
2:F:183:TYR:CE2	2:F:231:HIS:HB2	2.40	0.56
2:D:73:LEU:O	2:D:73:LEU:HD13	2.06	0.56
2:D:207:ASP:HB3	2:D:210:LYS:HB3	1.87	0.55
2:F:42:ASP:OD2	2:F:43:LYS:N	2.31	0.55
2:H:74:ALA:O	2:H:78:LYS:HB2	2.07	0.55
2:F:129:VAL:HG12	2:F:130:LEU:N	2.21	0.55
2:D:158:ASP:OD1	2:D:162:ARG:HD3	2.06	0.55
1:A:15:THR:HG23	1:A:15:THR:O	2.07	0.55
1:G:99:THR:HG22	1:G:100:LEU:N	2.21	0.55
2:F:189:ASN:HB3	2:F:225:SER:HB2	1.89	0.55
1:A:87:SER:OG	1:A:88:VAL:N	2.40	0.55
1:A:33:TYR:N	1:A:33:TYR:CD1	2.75	0.54
2:F:84:VAL:HA	2:F:112:GLY:O	2.06	0.54
2:F:89:TYR:CZ	2:F:209:SER:HB2	2.43	0.54
2:D:156:GLU:O	2:D:160:LYS:HG3	2.07	0.54
2:B:75:LYS:HE3	2:B:75:LYS:HA	1.90	0.54
2:D:119:ASN:ND2	2:D:150:LYS:HB2	2.23	0.54
2:F:99:ASP:CA	2:F:102:THR:HG22	2.37	0.54
2:F:120:HIS:O	2:F:150:LYS:NZ	2.40	0.54
2:F:129:VAL:HG12	2:F:130:LEU:H	1.72	0.54
2:B:43:LYS:HE3	2:B:75:LYS:NZ	2.20	0.54
2:F:135:GLU:O	2:F:136:ASN:HB2	2.08	0.53
2:B:4:PRO:O	2:B:5:ASP:C	2.46	0.53
1:E:25:GLN:HE22	1:E:29:HIS:N	2.07	0.53
2:H:187:ILE:HG23	2:H:193:THR:HG22	1.91	0.53
2:D:123:ASN:C	2:D:125:ASN:N	2.61	0.53
2:B:89:TYR:CE1	2:B:108:CYS:HB2	2.44	0.53
2:H:158:ASP:OD2	2:H:215:TYR:OH	2.24	0.53
2:B:75:LYS:HE2	2:B:78:LYS:HD2	1.91	0.53
2:B:13:LYS:HD3	2:B:16:GLU:OE1	2.08	0.53
2:D:139:ASN:CG	2:D:139:ASN:O	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:134:TYR:CE2	2:H:139:ASN:HB2	2.44	0.53
2:B:24:MET:CE	2:B:28:TYR:CE1	2.91	0.52
2:H:222:ASP:HB3	2:H:225:SER:OG	2.09	0.52
2:B:181:THR:OG1	2:B:233:THR:HB	2.07	0.52
2:D:50:ILE:HD12	2:D:65:LYS:HB2	1.92	0.52
1:E:66:LYS:HA	2:F:174:PHE:CE2	2.44	0.52
2:F:128:ASN:HD22	2:F:144:GLU:CD	2.13	0.52
2:H:184:ILE:HD11	2:H:228:ILE:HG23	1.92	0.52
1:C:65:TYR:OH	1:C:86:GLN:HG2	2.09	0.52
2:B:39:LYS:HE3	2:B:79:ASP:OD1	2.10	0.52
2:F:123:ASN:HD22	2:F:123:ASN:H	1.54	0.52
2:D:5:ASP:OD2	2:D:185:LYS:NZ	2.42	0.52
2:F:57:LYS:HB3	2:F:58:LEU:HD22	1.91	0.52
2:F:194:PHE:CD2	2:F:219:LYS:HE3	2.44	0.52
1:C:25:GLN:O	1:C:25:GLN:HG3	2.07	0.52
2:F:31:HIS:CE1	2:F:88:ASN:ND2	2.78	0.52
2:B:189:ASN:C	2:B:191:GLY:H	2.12	0.52
1:A:86:THR:HG23	1:A:108:SER:HA	1.92	0.51
2:F:182:GLY:HA2	2:F:231:HIS:O	2.11	0.51
2:H:82:VAL:HB	2:H:114:THR:O	2.09	0.51
2:D:123:ASN:C	2:D:125:ASN:H	2.13	0.51
1:C:36:ARG:HG2	1:C:60:ILE:HD11	1.92	0.51
2:H:28:TYR:CZ	2:H:162:ARG:NH1	2.79	0.51
2:B:53:ILE:HB	2:B:64:VAL:CG2	2.40	0.51
2:B:138:ARG:HG2	2:B:138:ARG:HH11	1.76	0.51
2:F:158:ASP:CG	2:F:162:ARG:HH11	2.13	0.51
1:E:26:THR:HG21	1:G:2:ALA:N	2.25	0.51
2:F:40:SER:CB	2:F:49:LEU:HD22	2.41	0.51
2:H:182:GLY:HA2	2:H:231:HIS:O	2.10	0.51
2:B:136:ASN:O	2:B:137:LYS:CB	2.54	0.51
2:B:166:ILE:O	2:B:170:ASN:HA	2.09	0.51
2:B:12:HIS:HB2	2:B:199:MET:HB2	1.94	0.50
2:B:164:PHE:C	2:B:164:PHE:CD2	2.85	0.50
2:F:130:LEU:HD12	2:F:143:PHE:O	2.12	0.50
1:A:37:GLN:C	1:A:38:ASP:OD1	2.49	0.50
2:B:43:LYS:CE	2:B:75:LYS:HZ1	2.20	0.50
2:B:37:LYS:HB3	2:B:37:LYS:NZ	2.26	0.50
1:E:46:ILE:CG2	1:E:65:TYR:CD2	2.94	0.50
2:F:3:GLN:NE2	2:F:195:TRP:CE2	2.80	0.50
2:B:158:ASP:O	2:B:162:ARG:HG3	2.12	0.50
1:E:23:CYS:HB2	1:E:34:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:PHE:HB3	2:H:48:ASP:OD2	2.11	0.49
2:D:110:TYR:CD1	2:D:110:TYR:N	2.80	0.49
2:F:178:PRO:O	2:F:234:THR:HG22	2.12	0.49
2:H:95:PHE:CZ	2:H:106:LYS:HB2	2.46	0.49
2:B:152:VAL:HG13	2:B:157:LEU:HD11	1.93	0.49
1:E:83:THR:C	1:E:116:VAL:HG11	2.31	0.49
2:F:61:TYR:HA	2:F:105:GLY:CA	2.42	0.49
1:E:34:TRP:O	1:E:46:ILE:HG13	2.12	0.49
2:H:88:ASN:HD22	2:H:88:ASN:N	1.98	0.49
2:H:133:VAL:HB	2:H:141:ILE:HG23	1.94	0.49
1:C:22:SER:CB	1:C:24:GLN:HE22	2.24	0.49
2:B:66:THR:HA	2:B:109:MET:O	2.13	0.49
1:C:3:ALA:HA	1:C:26:THR:OG1	2.12	0.49
1:E:26:THR:OG1	1:G:2:ALA:N	2.34	0.49
2:H:184:ILE:HG23	2:H:184:ILE:O	2.13	0.49
1:E:14:VAL:O	1:E:15:THR:C	2.51	0.49
2:H:135:GLU:O	2:H:138:ARG:HB3	2.12	0.49
1:C:39:THR:CG2	1:C:39:THR:HB	2.17	0.49
2:H:7:MET:O	2:H:8:PRO:C	2.51	0.48
2:H:115:LYS:O	2:H:115:LYS:CG	2.59	0.48
1:A:36:ARG:O	1:A:36:ARG:HG3	2.12	0.48
1:A:48:TYR:CE1	1:A:56:GLU:HB3	2.48	0.48
2:D:29:ASP:O	2:D:30:ASP:C	2.50	0.48
2:D:37:LYS:HZ2	2:D:37:LYS:HB3	1.79	0.48
2:D:101:SER:HA	2:D:103:TRP:CZ3	2.48	0.48
2:B:27:LEU:HA	2:B:31:HIS:HD2	1.78	0.48
2:B:71:GLU:O	2:B:74:ALA:N	2.46	0.48
2:D:48:ASP:C	2:D:48:ASP:OD1	2.51	0.48
2:D:68:LEU:HD23	2:D:74:ALA:HA	1.95	0.48
2:D:48:ASP:O	2:D:49:LEU:HD23	2.13	0.48
2:F:214:MET:C	2:F:216:ASN:H	2.16	0.48
2:D:13:LYS:HB3	2:D:180:GLU:OE2	2.14	0.48
1:G:83:THR:HG22	1:G:86:GLN:NE2	2.29	0.48
2:H:134:TYR:HA	2:H:138:ARG:O	2.13	0.48
1:G:68:SER:O	1:G:70:PRO:HD3	2.14	0.48
1:G:73:GLU:H	1:G:73:GLU:CD	2.16	0.48
2:B:66:THR:HG21	2:B:113:ILE:HD11	1.94	0.48
2:B:222:ASP:OD2	2:B:224:LYS:HG2	2.14	0.47
1:C:9:ARG:HA	1:C:9:ARG:NE	2.29	0.47
2:F:123:ASN:C	2:F:125:ASN:H	2.17	0.47
2:D:13:LYS:HD2	2:D:181:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:ASN:O	2:D:171:LEU:C	2.50	0.47
1:E:19:VAL:HG23	1:E:82:ALA:HB2	1.95	0.47
2:B:53:ILE:HB	2:B:64:VAL:HG21	1.97	0.47
2:F:123:ASN:N	2:F:123:ASN:ND2	2.61	0.47
1:A:25:GLN:OE1	1:A:29:HIS:N	2.44	0.47
1:E:31:ASN:HA	1:E:49:SER:O	2.15	0.47
2:F:77:TYR:CE2	2:F:115:LYS:HE2	2.45	0.47
2:F:89:TYR:CD1	2:F:212:LEU:HD12	2.47	0.47
2:F:158:ASP:OD2	2:F:162:ARG:NH1	2.47	0.47
1:G:14:VAL:O	1:G:15:THR:C	2.51	0.47
1:G:25:GLN:O	1:G:25:GLN:HG3	2.15	0.47
2:H:184:ILE:HD12	2:H:186:PHE:CE1	2.49	0.47
2:B:229:GLU:HB3	2:B:231:HIS:HE2	1.80	0.47
2:F:42:ASP:CG	2:F:43:LYS:H	2.16	0.47
1:G:23:CYS:HB2	1:G:34:TRP:CZ2	2.50	0.47
1:A:41:HIS:O	1:A:43:LEU:N	2.47	0.47
2:D:82:VAL:HG21	2:D:113:ILE:HG23	1.96	0.47
1:E:11:LYS:HD3	1:E:19:VAL:CG1	2.45	0.47
2:H:187:ILE:HA	2:H:193:THR:HG22	1.97	0.47
2:B:27:LEU:HA	2:B:31:HIS:CD2	2.50	0.46
2:D:6:PRO:HD3	2:D:195:TRP:CE2	2.50	0.46
2:D:131:VAL:HG22	2:D:228:ILE:HG13	1.97	0.46
1:E:16:GLY:N	1:E:82:ALA:O	2.45	0.46
2:F:48:ASP:CB	2:F:67:GLU:HA	2.45	0.46
2:F:158:ASP:O	2:F:162:ARG:HG2	2.15	0.46
2:H:127:GLN:NE2	2:H:224:LYS:HB3	2.31	0.46
2:B:139:ASN:C	2:B:139:ASN:ND2	2.63	0.46
1:G:87:THR:HG23	1:G:115:SER:HA	1.96	0.46
2:D:155:GLN:O	2:D:159:ILE:HG13	2.16	0.46
1:G:36:ARG:HE	1:G:36:ARG:HB2	1.61	0.46
1:E:27:ASN:HB3	1:E:29:HIS:NE2	2.30	0.46
2:B:152:VAL:HG11	2:B:157:LEU:HD21	1.97	0.46
2:D:6:PRO:HB3	2:D:195:TRP:CZ2	2.51	0.46
1:E:11:LYS:HD3	1:E:19:VAL:HG11	1.98	0.46
2:H:21:MET:O	2:H:21:MET:HG3	2.16	0.46
1:A:15:THR:O	1:A:15:THR:CG2	2.64	0.46
2:D:37:LYS:HG3	2:D:81:VAL:HG11	1.98	0.46
2:B:37:LYS:HG3	2:B:81:VAL:CG1	2.46	0.46
2:B:56:LYS:NZ	2:B:56:LYS:CB	2.79	0.46
1:C:38:ASP:CG	1:C:44:ARG:HH11	2.20	0.46
2:H:123:ASN:HB2	2:H:125:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:227:LYS:NZ	2:H:227:LYS:HA	2.31	0.46
1:A:38:ASP:OD1	1:A:38:ASP:N	2.50	0.45
1:C:39:THR:CG2	1:C:39:THR:CA	2.85	0.45
2:D:219:LYS:HD3	2:D:220:THR:H	1.81	0.45
2:H:43:LYS:HA	2:H:50:ILE:HD12	1.98	0.45
2:H:65:LYS:HE2	2:H:95:PHE:HB3	1.97	0.45
1:A:98:THR:HG23	1:G:100:LEU:O	2.16	0.45
2:B:89:TYR:CZ	2:B:108:CYS:HB2	2.51	0.45
2:D:227:LYS:HA	2:D:227:LYS:HZ2	1.81	0.45
2:F:49:LEU:HD12	2:F:68:LEU:HD21	1.97	0.45
2:B:133:VAL:HB	2:B:141:ILE:HG23	1.97	0.45
1:C:43:LEU:HD12	1:C:43:LEU:HA	1.73	0.45
1:E:2:ALA:O	1:G:2:ALA:HB3	2.16	0.45
1:A:25:GLN:NE2	1:A:32:MET:SD	2.89	0.45
1:A:36:ARG:HH21	1:A:36:ARG:HD3	1.52	0.45
1:A:79:GLU:H	1:A:79:GLU:HG3	1.45	0.45
1:E:35:TYR:HA	1:E:44:ARG:O	2.17	0.45
1:A:24:GLN:NE2	1:A:24:GLN:N	2.64	0.45
2:D:214:MET:C	2:D:216:ASN:H	2.20	0.45
2:F:136:ASN:HD21	2:F:234:THR:H	1.64	0.45
2:F:199:MET:HE3	2:F:199:MET:HA	1.99	0.45
1:C:31:ASN:HA	1:C:49:SER:O	2.17	0.45
2:B:170:ASN:N	2:B:170:ASN:HD22	2.15	0.45
1:C:57:LYS:HZ3	2:D:175:ASN:HD21	1.65	0.45
2:D:166:ILE:HG21	2:D:166:ILE:HD13	1.64	0.45
2:F:172:TYR:HE2	2:F:199:MET:CE	2.29	0.45
2:D:43:LYS:HG3	2:D:48:ASP:O	2.17	0.45
2:F:61:TYR:CD2	2:F:107:THR:CG2	3.00	0.45
1:C:23:CYS:HB2	1:C:34:TRP:CZ2	2.52	0.45
2:F:224:LYS:HE3	2:F:224:LYS:HB2	1.67	0.45
2:H:24:MET:HG2	2:H:172:TYR:CE2	2.52	0.45
2:H:33:VAL:O	2:H:85:TYR:HA	2.17	0.45
1:G:88:SER:OG	1:G:89:VAL:N	2.50	0.45
2:B:136:ASN:ND2	2:B:233:THR:HA	2.32	0.44
2:B:140:THR:O	2:B:141:ILE:HB	2.18	0.44
1:C:66:LYS:NZ	1:C:66:LYS:HB2	2.32	0.44
1:C:83:THR:C	1:C:116:VAL:HG11	2.38	0.44
2:D:20:THR:HG22	2:D:22:GLY:H	1.82	0.44
2:F:123:ASN:O	2:F:125:ASN:N	2.51	0.44
1:E:46:ILE:HG21	1:E:65:TYR:CD2	2.52	0.44
1:C:6:GLN:O	1:C:9:ARG:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:ASN:HD22	2:F:88:ASN:N	1.96	0.44
2:B:58:LEU:HD12	2:B:60:ASN:HD21	1.83	0.44
2:B:75:LYS:CE	2:B:78:LYS:HD2	2.47	0.44
1:C:113:ARG:HG3	1:C:113:ARG:HH11	1.83	0.44
1:E:12:VAL:HA	1:E:115:SER:O	2.17	0.44
2:B:37:LYS:NZ	2:B:37:LYS:CB	2.79	0.44
2:H:112:GLY:HA2	2:H:153:THR:HG21	1.98	0.44
2:D:119:ASN:ND2	2:D:151:SER:H	2.05	0.44
1:E:69:ARG:HD2	1:E:74:GLN:O	2.17	0.44
1:G:27:ASN:O	1:G:29:HIS:N	2.50	0.44
2:B:190:ASN:OD1	2:B:192:ASN:N	2.40	0.43
2:H:123:ASN:CB	2:H:125:ASN:OD1	2.66	0.43
2:F:33:VAL:O	2:F:85:TYR:HA	2.18	0.43
2:H:87:SER:OG	2:H:159:ILE:HD13	2.18	0.43
1:C:25:GLN:HG2	1:C:73:GLU:HA	2.00	0.43
2:F:134:TYR:CE2	2:F:139:ASN:HB2	2.53	0.43
2:H:170:ASN:O	2:H:178:PRO:HD3	2.18	0.43
2:B:65:LYS:HE2	2:B:108:CYS:SG	2.59	0.43
2:B:168:LYS:HB2	2:B:168:LYS:HE2	1.84	0.43
2:D:7:MET:O	2:D:9:ASP:N	2.51	0.43
2:D:28:TYR:CD2	2:D:162:ARG:HG3	2.54	0.43
1:E:100:LEU:HD13	1:E:108:PHE:CZ	2.53	0.43
2:B:73:LEU:O	2:B:76:LYS:HB3	2.19	0.43
1:C:4:VAL:CG2	1:C:94:SER:HB3	2.49	0.43
2:F:199:MET:HA	2:F:199:MET:CE	2.49	0.43
2:H:49:LEU:HD21	2:H:78:LYS:HA	2.00	0.43
2:H:70:ASN:OD1	2:H:73:LEU:HD23	2.18	0.43
1:A:31:ASN:HA	1:A:49:SER:O	2.18	0.43
2:B:110:TYR:CD1	2:B:110:TYR:N	2.86	0.43
2:D:169:LYS:O	2:D:170:ASN:HB2	2.19	0.43
1:E:26:THR:HG21	1:G:2:ALA:CB	2.47	0.43
2:H:11:LEU:CD1	2:H:183:TYR:HD2	2.17	0.43
2:H:200:PRO:HB3	2:H:206:PHE:CE1	2.53	0.43
2:D:119:ASN:HD22	2:D:119:ASN:HA	1.63	0.43
2:F:25:LYS:HB2	2:F:172:TYR:HB2	2.01	0.43
1:C:24:GLN:HA	1:C:73:GLU:O	2.19	0.43
2:F:187:ILE:HG12	2:F:193:THR:HG22	2.00	0.43
2:D:185:LYS:HE2	2:D:187:ILE:CD1	2.48	0.43
2:F:61:TYR:CG	2:F:107:THR:HG22	2.54	0.43
2:F:99:ASP:N	2:F:102:THR:HG22	2.33	0.43
2:F:158:ASP:CG	2:F:162:ARG:NH1	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:TYR:CE2	2:H:162:ARG:HD2	2.53	0.43
2:H:35:ALA:CB	2:H:53:ILE:CD1	2.96	0.43
2:H:201:ALA:HB1	2:H:202:PRO:HD3	2.01	0.43
2:D:136:ASN:HD22	2:D:233:THR:HG22	1.84	0.42
1:E:65:TYR:HB3	1:E:77:LEU:HD11	2.00	0.42
2:H:95:PHE:O	2:H:106:LYS:NZ	2.41	0.42
2:H:197:ASP:OD1	2:H:198:MET:N	2.52	0.42
1:A:54:SER:HB2	2:B:91:VAL:HG21	2.02	0.42
2:D:131:VAL:HA	2:D:228:ILE:HB	2.01	0.42
2:H:216:ASN:HD22	2:H:216:ASN:HA	1.38	0.42
2:B:119:ASN:O	2:B:149:LYS:HA	2.18	0.42
2:D:127:GLN:OE1	2:D:224:LYS:HA	2.19	0.42
1:G:46:ILE:HG21	1:G:65:TYR:CD2	2.54	0.42
2:H:75:LYS:HD3	2:H:75:LYS:HA	1.58	0.42
2:H:136:ASN:OD1	2:H:233:THR:HA	2.19	0.42
1:C:52:ALA:CB	1:C:52:ALA:C	2.78	0.42
2:D:183:TYR:CE2	2:D:231:HIS:HB2	2.54	0.42
1:E:74:GLN:HE21	1:E:75:PHE:C	2.23	0.42
2:F:126:LEU:HD12	2:F:146:GLN:NE2	2.34	0.42
2:F:132:ARG:HA	2:F:142:SER:OG	2.19	0.42
2:H:109:MET:C	2:H:110:TYR:CD1	2.93	0.42
1:E:52:ALA:HA	1:E:69:ARG:HG3	2.01	0.42
1:G:93:ALA:CB	1:G:101:TYR:O	2.67	0.42
1:A:14:VAL:O	1:A:17:GLU:HB2	2.19	0.42
2:F:6:PRO:HB3	2:F:195:TRP:CH2	2.55	0.42
1:C:86:GLN:O	1:C:90:TYR:OH	2.25	0.42
1:G:93:ALA:HB1	1:G:101:TYR:O	2.19	0.42
2:H:81:VAL:O	2:H:116:HIS:HB3	2.19	0.42
1:C:66:LYS:HG3	1:C:66:LYS:HZ2	1.57	0.42
2:F:155:GLN:HG3	2:F:215:TYR:CE1	2.55	0.42
2:H:6:PRO:HB3	2:H:10:ASP:HB2	2.01	0.42
2:B:5:ASP:HA	2:B:6:PRO:HD3	1.89	0.42
2:B:211:TYR:O	2:B:214:MET:HG2	2.20	0.42
2:F:158:ASP:OD1	2:F:162:ARG:NH1	2.45	0.42
2:H:195:TRP:O	2:H:196:TYR:HD2	2.03	0.42
2:H:201:ALA:HB1	2:H:202:PRO:CD	2.50	0.42
2:B:56:LYS:HZ2	2:B:56:LYS:HA	1.85	0.42
1:C:18:LYS:HA	1:C:79:LEU:O	2.20	0.42
1:E:23:CYS:HB3	1:E:75:PHE:O	2.19	0.42
2:F:162:ARG:HD2	2:F:198:MET:HE2	2.02	0.42
2:H:157:LEU:HD13	2:H:228:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:MET:O	2:B:8:PRO:C	2.59	0.41
2:B:229:GLU:HB3	2:B:231:HIS:NE2	2.34	0.41
2:D:27:LEU:HA	2:D:31:HIS:HD2	1.85	0.41
2:D:113:ILE:HG21	2:D:113:ILE:HD13	1.52	0.41
2:D:227:LYS:NZ	2:D:228:ILE:H	2.18	0.41
1:E:46:ILE:HG21	1:E:46:ILE:HD13	1.77	0.41
1:E:78:ILE:HD12	1:E:78:ILE:N	2.35	0.41
2:F:119:ASN:HD21	2:F:149:LYS:HB3	1.85	0.41
2:H:55:ASP:HB3	2:H:58:LEU:O	2.20	0.41
1:A:33:TYR:O	1:A:91:CYS:HA	2.20	0.41
1:A:37:GLN:HE21	1:A:37:GLN:HB2	1.63	0.41
2:F:43:LYS:HE2	2:F:48:ASP:O	2.20	0.41
1:G:82:ALA:HB1	1:G:116:VAL:HG11	2.02	0.41
2:D:219:LYS:HD3	2:D:220:THR:O	2.20	0.41
1:E:45:LEU:O	1:E:59:ASP:N	2.50	0.41
1:C:57:LYS:HZ2	2:D:175:ASN:HD21	1.66	0.41
2:F:230:VAL:O	2:F:230:VAL:HG12	2.19	0.41
1:G:6:GLN:OE1	1:G:91:PHE:HA	2.21	0.41
1:G:55:THR:CG2	2:H:20:THR:HG21	2.40	0.41
2:B:114:THR:HG22	2:B:153:THR:HG23	2.02	0.41
2:F:2:SER:N	2:F:192:ASN:OD1	2.54	0.41
2:H:128:ASN:HB3	2:H:144:GLU:OE1	2.20	0.41
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.86	0.41
1:C:60:ILE:O	1:C:60:ILE:HG13	2.21	0.41
2:D:153:THR:HA	2:D:220:THR:HA	2.03	0.41
2:F:37:LYS:HB2	2:F:116:HIS:CE1	2.56	0.41
2:F:129:VAL:O	2:F:144:GLU:HA	2.20	0.41
1:G:9:ARG:HG3	1:G:9:ARG:HH11	1.86	0.41
1:A:67:SER:C	1:A:69:PRO:HD3	2.40	0.41
2:B:29:ASP:O	2:B:30:ASP:C	2.59	0.41
2:B:68:LEU:N	2:B:68:LEU:HD22	2.36	0.41
2:B:103:TRP:O	2:B:104:HIS:C	2.59	0.41
2:D:13:LYS:N	2:D:13:LYS:HD3	2.36	0.41
1:G:10:ASN:O	1:G:11:LYS:HB2	2.20	0.41
1:G:24:GLN:HE22	1:G:74:GLN:CD	2.22	0.41
2:H:71:GLU:O	2:H:71:GLU:HG2	2.21	0.41
1:C:88:SER:HB3	1:C:89:VAL:H	1.68	0.41
1:E:12:VAL:HG12	1:E:117:LEU:HD12	2.02	0.41
1:E:84:PRO:HA	1:E:116:VAL:HB	2.02	0.41
2:H:184:ILE:CD1	2:H:228:ILE:HG23	2.50	0.41
2:H:200:PRO:HB3	2:H:206:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:LYS:HB2	2:D:116:HIS:CE1	2.56	0.41
1:E:69:ARG:HD2	1:E:69:ARG:HA	1.88	0.41
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.71	0.41
2:F:48:ASP:HB2	2:F:67:GLU:HA	2.02	0.41
1:G:26:THR:HG22	1:G:27:ASN:H	1.86	0.41
1:G:69:ARG:CG	1:G:69:ARG:NH2	2.63	0.41
1:A:25:GLN:HG2	1:A:72:GLU:HA	2.03	0.40
1:E:77:LEU:C	1:E:78:ILE:HD12	2.40	0.40
2:F:29:ASP:O	2:F:30:ASP:C	2.57	0.40
2:F:41:VAL:O	2:F:42:ASP:HB2	2.20	0.40
2:F:43:LYS:HD3	2:F:45:LEU:O	2.21	0.40
2:D:158:ASP:O	2:D:161:ALA:HB3	2.21	0.40
2:D:222:ASP:OD1	2:D:225:SER:HB3	2.21	0.40
1:E:87:THR:CG2	1:E:114:LEU:O	2.68	0.40
2:F:36:THR:HG23	2:F:83:ASP:OD2	2.21	0.40
1:G:100:LEU:HA	1:G:100:LEU:HD23	1.87	0.40
2:B:49:LEU:HD23	2:B:49:LEU:HA	1.86	0.40
2:B:160:LYS:HD3	3:B:252:HOH:O	2.22	0.40
1:G:27:ASN:C	1:G:27:ASN:HD22	2.25	0.40
2:D:37:LYS:HB3	2:D:37:LYS:NZ	2.35	0.40
2:F:177:SER:C	2:F:179:TYR:H	2.25	0.40
1:C:36:ARG:CD	1:C:60:ILE:CD1	3.00	0.40
2:D:48:ASP:HB2	2:D:66:THR:O	2.21	0.40
1:E:17:GLU:HG2	1:E:18:LYS:N	2.36	0.40

All (1) 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)
2:D:56:LYS:NZ	2:F:123:ASN:OD1[1_554]	2.08	0.12

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	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	6	6
1	C	107/109 (98%)	97 (91%)	6 (6%)	4 (4%)	2	1
1	E	107/109 (98%)	90 (84%)	14 (13%)	3 (3%)	4	3
1	G	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2	1
2	B	228/239 (95%)	183 (80%)	34 (15%)	11 (5%)	2	1
2	D	229/239 (96%)	195 (85%)	30 (13%)	4 (2%)	7	7
2	F	230/239 (96%)	183 (80%)	35 (15%)	12 (5%)	1	1
2	H	226/239 (95%)	197 (87%)	22 (10%)	7 (3%)	3	2
All	All	1341/1392 (96%)	1136 (85%)	157 (12%)	48 (4%)	3	1

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	57	LYS
2	B	104	HIS
2	B	125	ASN
2	F	57	LYS
2	F	236	ASN
1	G	28	ASN
1	G	74	GLN
2	H	122	ASP
2	H	235	LYS
2	B	122	ASP
2	B	137	LYS
2	B	224	LYS
1	C	3	ALA
1	C	39	THR
2	D	102	THR
2	D	124	GLY
2	F	19	GLY
2	F	98	LYS
2	F	122	ASP
2	F	136	ASN
2	F	217	ASP
2	H	217	ASP
2	B	96	SER
1	C	27	ASN
2	F	9	ASP

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Mol	Chain	Res	Type
2	F	42	ASP
2	F	47	HIS
1	G	27	ASN
2	H	216	ASN
1	E	62	ASP
1	G	39	THR
2	H	116	HIS
2	H	137	LYS
2	B	56	LYS
2	B	95	PHE
2	D	57	LYS
2	H	8	PRO
2	B	124	GLY
1	E	42	GLY
1	E	97	GLY
2	F	73	LEU
2	F	123	ASN
1	G	97	GLY
1	C	97	GLY
1	A	42	GLY
2	B	8	PRO
2	D	191	GLY
1	A	97	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	88/88 (100%)	76 (86%)	12 (14%)	3 3
1	C	88/88 (100%)	78 (89%)	10 (11%)	4 5
1	E	88/88 (100%)	78 (89%)	10 (11%)	4 5
1	G	88/88 (100%)	77 (88%)	11 (12%)	3 4
2	B	214/220 (97%)	193 (90%)	21 (10%)	6 8
2	D	215/220 (98%)	195 (91%)	20 (9%)	7 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	216/220 (98%)	192 (89%)	24 (11%)	5 6
2	H	211/220 (96%)	196 (93%)	15 (7%)	12 17
All	All	1208/1232 (98%)	1085 (90%)	123 (10%)	6 7

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	27	ASN
1	A	33	TYR
1	A	37	GLN
1	A	55	THR
1	A	56	GLU
1	A	62	ASP
1	A	68	ARG
1	A	71	GLN
1	A	75	SER
1	A	83	PRO
1	A	84	SER
2	B	3	GLN
2	B	40	SER
2	B	43	LYS
2	B	56	LYS
2	B	57	LYS
2	B	68	LEU
2	B	72	ASP
2	B	73	LEU
2	B	75	LYS
2	B	76	LYS
2	B	103	TRP
2	B	114	THR
2	B	117	GLU
2	B	125	ASN
2	B	138	ARG
2	B	139	ASN
2	B	170	ASN
2	B	176	SER
2	B	216	ASN
2	B	233	THR
2	B	236	ASN
1	C	7	SER

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Mol	Chain	Res	Type
1	C	9	ARG
1	C	10	ASN
1	C	39	THR
1	C	43	LEU
1	C	56	GLU
1	C	66	LYS
1	C	72	GLN
1	C	73	GLU
1	C	94	SER
2	D	2	SER
2	D	3	GLN
2	D	13	LYS
2	D	24	MET
2	D	45	LEU
2	D	68	LEU
2	D	69	LEU
2	D	72	ASP
2	D	73	LEU
2	D	102	THR
2	D	104	HIS
2	D	115	LYS
2	D	138	ARG
2	D	139	ASN
2	D	144	GLU
2	D	162	ARG
2	D	216	ASN
2	D	219	LYS
2	D	227	LYS
2	D	234	THR
1	E	18	LYS
1	E	22	SER
1	E	37	GLN
1	E	41	HIS
1	E	44	ARG
1	E	46	ILE
1	E	72	GLN
1	E	80	GLU
1	E	99	THR
1	E	113	ARG
2	F	2	SER
2	F	69	LEU
2	F	73	LEU

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Mol	Chain	Res	Type
2	F	88	ASN
2	F	98	LYS
2	F	103	TRP
2	F	104	HIS
2	F	115	LYS
2	F	122	ASP
2	F	123	ASN
2	F	141	ILE
2	F	151	SER
2	F	153	THR
2	F	162	ARG
2	F	167	ASN
2	F	168	LYS
2	F	202	PRO
2	F	209	SER
2	F	216	ASN
2	F	218	ASN
2	F	220	THR
2	F	224	LYS
2	F	229	GLU
2	F	235	LYS
1	G	6	GLN
1	G	10	ASN
1	G	26	THR
1	G	27	ASN
1	G	43	LEU
1	G	69	ARG
1	G	72	GLN
1	G	73	GLU
1	G	80	GLU
1	G	84	PRO
1	G	113	ARG
2	H	3	GLN
2	H	41	VAL
2	H	56	LYS
2	H	58	LEU
2	H	65	LYS
2	H	68	LEU
2	H	73	LEU
2	H	88	ASN
2	H	97	SER
2	H	110	TYR

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Mol	Chain	Res	Type
2	H	153	THR
2	H	184	ILE
2	H	194	PHE
2	H	205	LYS
2	H	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	30	ASN
1	A	37	GLN
1	A	71	GLN
1	A	73	GLN
2	B	47	HIS
2	B	88	ASN
2	B	92	ASN
2	B	136	ASN
2	B	139	ASN
2	B	163	ASN
2	B	170	ASN
2	B	216	ASN
1	C	24	GLN
1	C	27	ASN
1	C	30	ASN
1	C	72	GLN
2	D	47	HIS
2	D	88	ASN
2	D	92	ASN
2	D	119	ASN
2	D	125	ASN
2	D	128	ASN
2	D	136	ASN
2	D	155	GLN
2	D	167	ASN
2	D	175	ASN
2	D	216	ASN
1	E	24	GLN
1	E	30	ASN
1	E	72	GLN
1	E	74	GLN
2	F	3	GLN

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Mol	Chain	Res	Type
2	F	88	ASN
2	F	92	ASN
2	F	123	ASN
2	F	128	ASN
2	F	136	ASN
2	F	163	ASN
2	F	167	ASN
2	F	170	ASN
2	F	216	ASN
1	G	27	ASN
1	G	28	ASN
1	G	30	ASN
1	G	72	GLN
2	H	3	GLN
2	H	88	ASN
2	H	92	ASN
2	H	163	ASN
2	H	167	ASN
2	H	175	ASN
2	H	216	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	109/109 (100%)	-0.40	1 (0%) 81 81	24, 39, 60, 68	0
1	C	109/109 (100%)	-0.54	0 100 100	21, 34, 55, 64	0
1	E	109/109 (100%)	-0.39	0 100 100	25, 39, 60, 71	0
1	G	109/109 (100%)	-0.26	2 (1%) 67 68	26, 46, 67, 76	0
2	B	232/239 (97%)	-0.38	1 (0%) 89 89	23, 44, 75, 88	0
2	D	233/239 (97%)	-0.50	1 (0%) 89 89	18, 38, 62, 84	0
2	F	234/239 (97%)	-0.21	1 (0%) 89 89	26, 46, 76, 105	0
2	H	230/239 (96%)	-0.34	1 (0%) 89 89	25, 43, 72, 90	0
All	All	1365/1392 (98%)	-0.37	7 (0%) 87 88	18, 42, 69, 105	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	3.7
2	B	103	TRP	2.9
2	D	97	SER	2.7
2	F	104	HIS	2.6
1	G	41	HIS	2.3
2	H	96	SER	2.1
1	G	3	ALA	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.