



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:14 AM EDT

PDB ID : 3VS8 / pdb_00003vs8
Title : Crystal structure of type III PKS ArsC
Authors : Satou, R.; Miyanaga, A.; Ozawa, H.; Funa, N.; Miyazono, K.; Tanokura, M.;
Ohnishi, Y.; Horinouchi, S.
Deposited on : 2012-04-23
Resolution : 1.76 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 Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

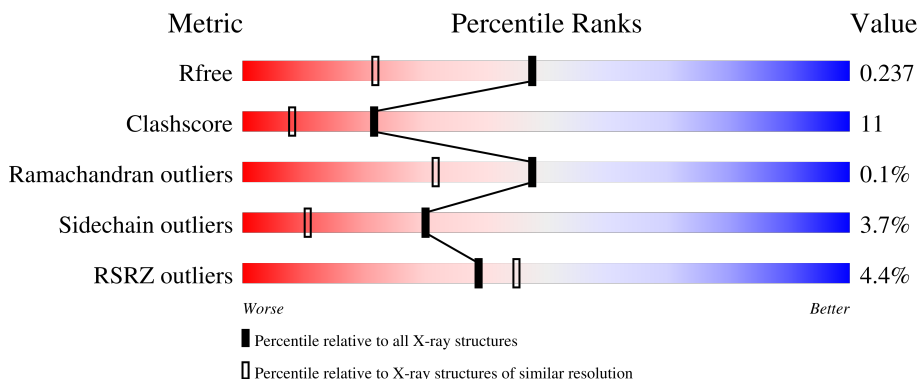
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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.



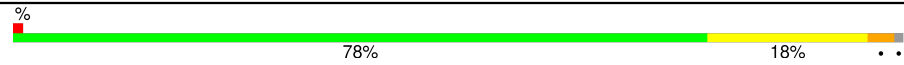

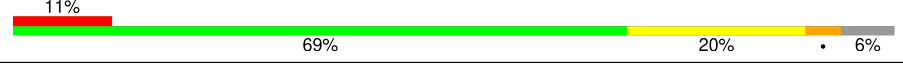
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	410	 80% 17% •
1	B	410	 71% 24% ••
1	C	410	 78% 17% ••
1	D	410	 78% 17% ••
1	E	410	 80% 17% ••

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Mol	Chain	Length	Quality of chain
1	F	410	 <p>% 78% 18% • •</p>
1	G	410	 <p>4% 76% 18% • •</p>
1	H	410	 <p>11% 69% 20% • 6%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 27375 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	Total 3123	C 1984	N 542	O 582	S 15	0	0	0
1	B	399	Total 3084	C 1961	N 537	O 571	S 15	0	0	0
1	C	402	Total 3108	C 1973	N 540	O 580	S 15	0	0	0
1	D	401	Total 3100	C 1969	N 539	O 577	S 15	0	0	0
1	E	401	Total 3107	C 1976	N 539	O 577	S 15	0	0	0
1	F	404	Total 3123	C 1984	N 542	O 582	S 15	0	0	0
1	G	398	Total 3078	C 1958	N 536	O 569	S 15	0	0	0
1	H	384	Total 2968	C 1891	N 518	O 544	S 15	0	0	0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Na 1	0	0
2	B	1	Total 1	Na 1	0	0
2	C	1	Total 1	Na 1	0	0
2	D	1	Total 1	Na 1	0	0
2	E	1	Total 1	Na 1	0	0
2	F	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Na 1	0	0
2	H	1	Total 1	Na 1	0	0

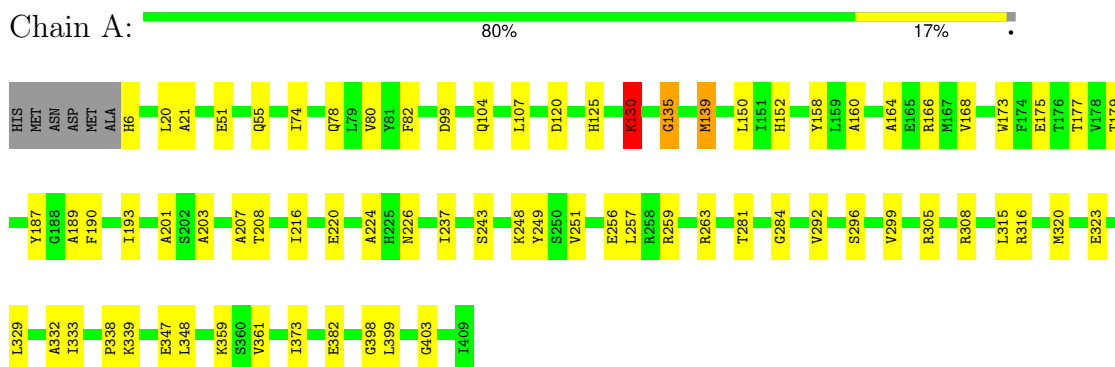
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total 437	O 437	0	0
3	B	258	Total 258	O 258	0	0
3	C	361	Total 361	O 361	0	0
3	D	356	Total 356	O 356	0	0
3	E	417	Total 417	O 417	0	0
3	F	330	Total 330	O 330	0	0
3	G	283	Total 283	O 283	0	0
3	H	234	Total 234	O 234	0	0

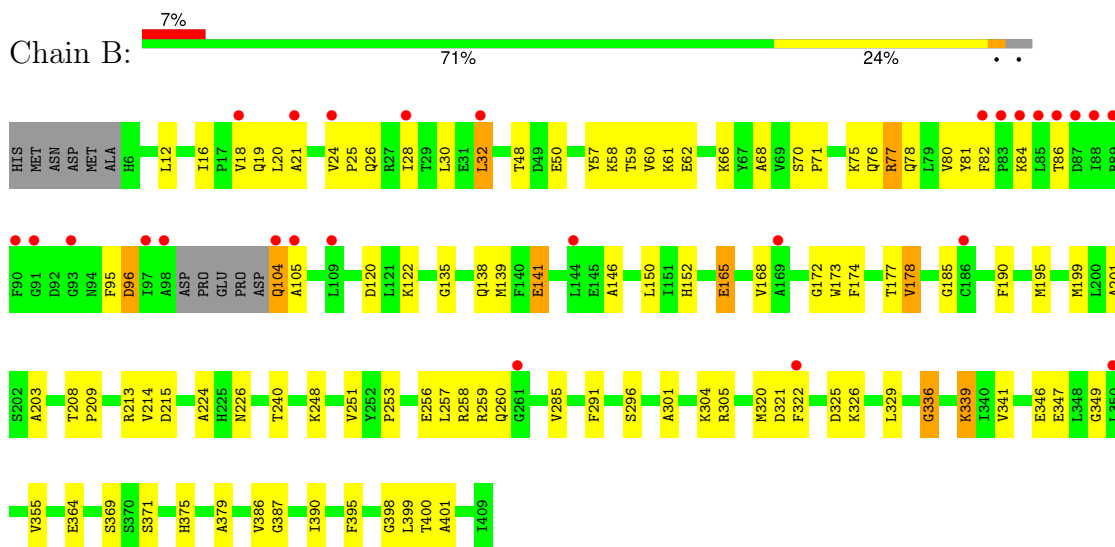
3 Residue-property plots

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.

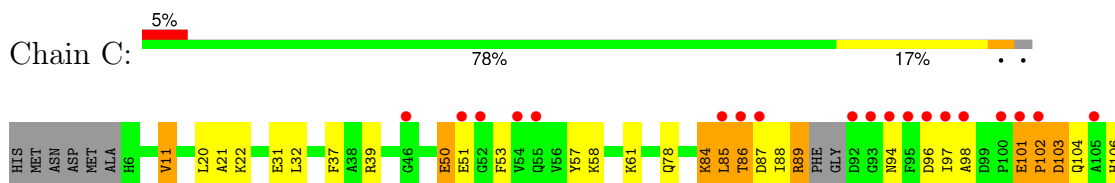
- Molecule 1: Type III polyketide synthase

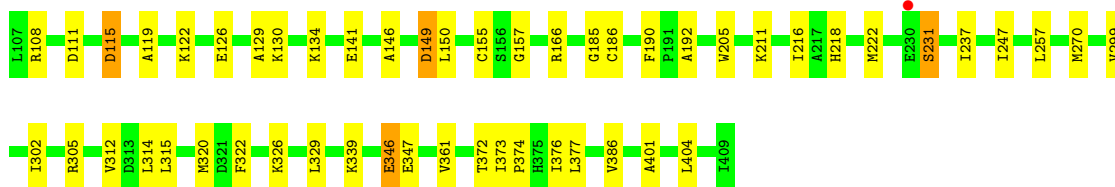


- Molecule 1: Type III polyketide synthase

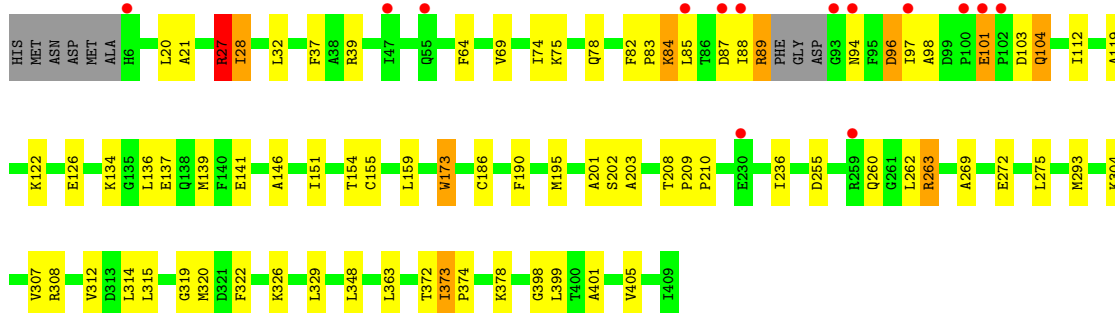
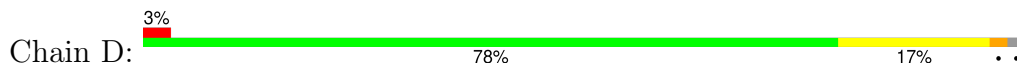


- Molecule 1: Type III polyketide synthase

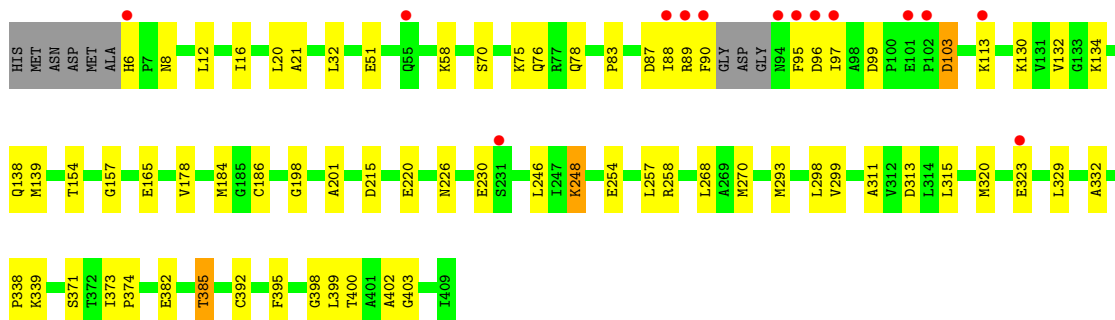
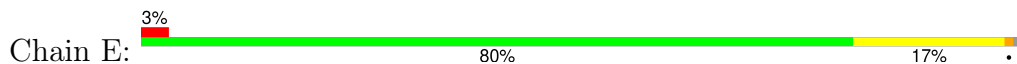




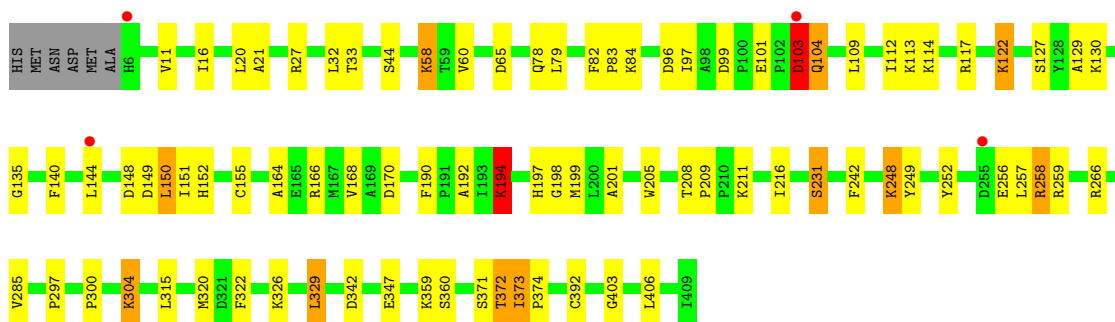
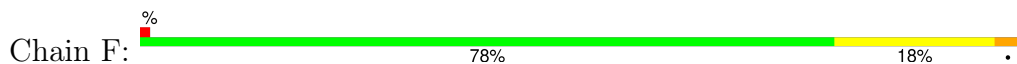
- Molecule 1: Type III polyketide synthase



- Molecule 1: Type III polyketide synthase



- Molecule 1: Type III polyketide synthase



- Molecule 1: Type III polyketide synthase

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.32Å 143.39Å 129.62Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	37.57 – 1.76 37.57 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.57-1.76) 97.3 (37.57-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.183 , 0.230 0.194 , 0.237	Depositor DCC
R_{free} test set	16976 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27375	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.42 % 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 2.2090e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	1.66	35/3194 (1.1%)	1.35	10/4331 (0.2%)
1	B	1.44	19/3152 (0.6%)	1.34	22/4270 (0.5%)
1	C	1.54	26/3177 (0.8%)	1.30	14/4307 (0.3%)
1	D	1.48	19/3169 (0.6%)	1.29	17/4296 (0.4%)
1	E	1.55	18/3177 (0.6%)	1.33	11/4307 (0.3%)
1	F	1.49	23/3194 (0.7%)	1.35	17/4331 (0.4%)
1	G	1.31	7/3148 (0.2%)	1.25	10/4267 (0.2%)
1	H	1.32	12/3034 (0.4%)	1.32	15/4110 (0.4%)
All	All	1.48	159/25245 (0.6%)	1.32	116/34219 (0.3%)

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	F	0	1
1	G	0	2
All	All	0	3

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	299	VAL	CA-CB	-16.56	1.45	1.54
1	A	373	ILE	CA-CB	14.55	1.62	1.54
1	B	195	MET	C-O	10.43	1.36	1.24
1	E	186	CYS	CA-CB	10.26	1.70	1.53
1	C	222	MET	SD-CE	-10.01	1.54	1.79
1	E	373	ILE	CA-C	9.14	1.60	1.52
1	G	373	ILE	CA-CB	8.91	1.59	1.53
1	A	332	ALA	CA-CB	8.73	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	386	VAL	CA-CB	8.53	1.63	1.54
1	C	149	ASP	N-CA	8.27	1.56	1.45
1	F	168	VAL	C-O	8.07	1.33	1.24
1	C	190	PHE	N-CA	8.06	1.53	1.46
1	B	209	PRO	CA-C	8.04	1.59	1.52
1	D	209	PRO	CA-C	7.79	1.59	1.52
1	E	299	VAL	CA-CB	7.69	1.59	1.53
1	F	27	ARG	N-CA	7.45	1.55	1.46
1	A	190	PHE	N-CA	7.44	1.53	1.46
1	D	312	VAL	CA-CB	7.38	1.63	1.54
1	A	189	ALA	CA-CB	7.20	1.65	1.53
1	B	301	ALA	CA-CB	7.19	1.64	1.53
1	C	401	ALA	CA-CB	7.10	1.64	1.53
1	F	60	VAL	CA-CB	-7.04	1.46	1.54
1	A	299	VAL	CA-CB	6.90	1.57	1.54
1	F	164	ALA	C-O	6.87	1.32	1.24
1	A	333	ILE	CA-CB	-6.80	1.46	1.54
1	F	198	GLY	C-O	6.71	1.31	1.23
1	H	195	MET	N-CA	-6.70	1.38	1.46
1	F	242	PHE	N-CA	6.65	1.53	1.45
1	H	16	ILE	CA-C	6.63	1.59	1.52
1	D	203	ALA	N-CA	6.63	1.54	1.46
1	A	243	SER	N-CA	-6.60	1.37	1.45
1	C	129	ALA	N-CA	6.59	1.54	1.46
1	D	173	TRP	C-O	6.50	1.32	1.23
1	A	166	ARG	N-CA	6.50	1.54	1.46
1	H	299	VAL	CA-CB	6.41	1.57	1.54
1	G	284	GLY	N-CA	6.34	1.52	1.45
1	H	208	THR	N-CA	6.29	1.50	1.46
1	A	373	ILE	CA-C	6.27	1.58	1.52
1	D	28	ILE	CA-CB	6.26	1.62	1.54
1	B	201	ALA	CA-CB	6.24	1.63	1.53
1	F	122	LYS	N-CA	6.20	1.53	1.46
1	F	192	ALA	C-O	6.20	1.31	1.24
1	B	60	VAL	C-O	6.18	1.31	1.24
1	B	190	PHE	C-O	6.17	1.30	1.24
1	F	197	HIS	C-O	6.17	1.31	1.24
1	D	137	GLU	N-CA	6.14	1.53	1.46
1	E	201	ALA	CA-CB	6.12	1.63	1.53
1	A	284	GLY	N-CA	6.09	1.54	1.45
1	A	338	PRO	C-O	-6.07	1.16	1.24
1	H	168	VAL	CA-CB	-6.02	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	379	ALA	CA-CB	6.02	1.62	1.53
1	E	198	GLY	CA-C	5.99	1.59	1.52
1	G	391	ALA	CA-CB	5.94	1.61	1.53
1	B	213	ARG	N-CA	5.93	1.52	1.46
1	C	299	VAL	CA-C	5.93	1.58	1.52
1	E	338	PRO	C-O	-5.87	1.16	1.24
1	G	209	PRO	CA-C	5.85	1.57	1.52
1	C	119	ALA	CA-CB	5.85	1.63	1.53
1	F	209	PRO	C-O	5.83	1.31	1.24
1	C	186	CYS	CA-CB	5.82	1.62	1.53
1	F	166	ARG	N-CA	5.81	1.53	1.46
1	F	170	ASP	N-CA	5.76	1.53	1.46
1	E	332	ALA	N-CA	5.73	1.53	1.46
1	D	374	PRO	N-CA	5.73	1.55	1.47
1	C	386	VAL	CA-CB	5.71	1.60	1.54
1	A	177	THR	CA-CB	5.71	1.62	1.53
1	C	166	ARG	N-CA	5.70	1.53	1.46
1	A	99	ASP	CA-C	-5.69	1.47	1.53
1	C	186	CYS	N-CA	5.68	1.53	1.46
1	F	194	LYS	N-CA	5.68	1.53	1.46
1	D	190	PHE	CA-C	5.66	1.59	1.52
1	A	333	ILE	C-O	-5.65	1.18	1.24
1	A	320	MET	SD-CE	-5.64	1.65	1.79
1	B	208	THR	CA-CB	-5.62	1.47	1.54
1	A	164	ALA	CA-CB	5.60	1.62	1.53
1	B	185	GLY	C-O	5.59	1.31	1.23
1	F	190	PHE	CA-C	5.59	1.58	1.52
1	F	190	PHE	C-O	5.58	1.30	1.24
1	H	278	SER	C-O	-5.57	1.17	1.24
1	D	272	GLU	N-CA	5.57	1.52	1.46
1	B	178	VAL	CA-CB	5.56	1.60	1.54
1	A	359	LYS	N-CA	5.55	1.53	1.46
1	F	155	CYS	CA-CB	5.55	1.60	1.53
1	F	129	ALA	N-CA	5.55	1.53	1.46
1	C	247	ILE	CA-CB	5.55	1.61	1.55
1	E	12	LEU	N-CA	5.53	1.53	1.46
1	E	16	ILE	N-CA	5.52	1.53	1.46
1	B	401	ALA	N-CA	5.51	1.52	1.46
1	F	79	LEU	CG-CD1	5.50	1.70	1.52
1	D	201	ALA	CA-CB	5.50	1.62	1.53
1	G	357	ILE	C-O	5.49	1.30	1.24
1	A	135	GLY	N-CA	5.49	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	MET	N-CA	5.48	1.52	1.46
1	C	237	ILE	CA-CB	5.45	1.60	1.54
1	D	154	THR	CA-CB	5.44	1.62	1.53
1	B	203	ALA	N-CA	5.44	1.52	1.46
1	D	151	ILE	N-CA	5.41	1.52	1.46
1	A	237	ILE	CA-CB	5.40	1.60	1.54
1	F	360	SER	CA-C	5.40	1.59	1.52
1	H	214	VAL	N-CA	5.40	1.52	1.46
1	A	203	ALA	CA-CB	5.39	1.61	1.53
1	A	139	MET	N-CA	5.39	1.52	1.46
1	B	355	VAL	CA-CB	5.37	1.60	1.54
1	A	152	HIS	CA-C	5.36	1.59	1.52
1	C	155	CYS	CA-CB	5.34	1.61	1.53
1	C	247	ILE	C-O	-5.31	1.17	1.23
1	A	347	GLU	N-CA	5.31	1.52	1.46
1	C	377	LEU	C-O	5.29	1.30	1.24
1	A	361	VAL	N-CA	5.29	1.52	1.46
1	E	313	ASP	CA-C	5.28	1.59	1.52
1	C	146	ALA	N-CA	5.28	1.52	1.45
1	F	208	THR	C-O	5.27	1.28	1.24
1	F	140	PHE	N-CA	5.27	1.52	1.46
1	C	185	GLY	C-O	5.25	1.31	1.24
1	B	386	VAL	N-CA	-5.24	1.40	1.46
1	A	249	TYR	C-O	5.22	1.30	1.23
1	D	203	ALA	C-O	5.22	1.30	1.24
1	E	270	MET	C-O	5.22	1.30	1.23
1	G	372	THR	CA-CB	5.22	1.61	1.53
1	A	187	TYR	CA-CB	5.22	1.61	1.53
1	A	216	ILE	C-O	5.21	1.29	1.24
1	F	127	SER	CA-C	5.20	1.59	1.52
1	C	270	MET	CG-SD	5.20	1.93	1.80
1	D	269	ALA	CA-CB	5.20	1.62	1.53
1	D	401	ALA	CA-CB	5.19	1.61	1.53
1	H	151	ILE	CA-CB	5.18	1.60	1.54
1	H	190	PHE	C-N	5.18	1.40	1.34
1	A	179	THR	C-O	5.18	1.30	1.23
1	E	339	LYS	N-CA	5.17	1.52	1.46
1	F	199	MET	N-CA	5.17	1.52	1.46
1	D	210	PRO	CA-CB	5.16	1.60	1.53
1	E	70	SER	N-CA	5.14	1.52	1.45
1	H	201	ALA	CA-CB	5.14	1.61	1.53
1	A	80	VAL	N-CA	5.13	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	312	VAL	CA-CB	5.12	1.60	1.54
1	H	209	PRO	CA-C	5.11	1.56	1.52
1	E	132	VAL	CA-C	5.10	1.59	1.52
1	H	312	VAL	CA-CB	5.09	1.59	1.54
1	B	199	MET	C-O	5.08	1.30	1.24
1	E	154	THR	CA-CB	5.08	1.62	1.53
1	A	208	THR	N-CA	5.07	1.50	1.45
1	A	292	VAL	CA-CB	-5.07	1.47	1.54
1	C	216	ILE	CA-CB	5.07	1.61	1.54
1	A	220	GLU	CB-CG	5.06	1.67	1.52
1	A	160	ALA	C-O	-5.06	1.19	1.24
1	D	119	ALA	CA-CB	5.05	1.61	1.53
1	C	157	GLY	N-CA	5.05	1.52	1.45
1	D	209	PRO	C-O	5.05	1.30	1.24
1	A	403	GLY	N-CA	5.04	1.50	1.45
1	G	237	ILE	CA-C	5.04	1.58	1.52
1	C	166	ARG	CD-NE	5.04	1.53	1.46
1	E	402	ALA	CA-CB	5.04	1.66	1.54
1	A	80	VAL	C-O	5.04	1.30	1.24
1	E	215	ASP	CA-CB	5.04	1.61	1.53
1	E	157	GLY	N-CA	5.03	1.52	1.45
1	D	195	MET	C-O	-5.02	1.18	1.24
1	C	218	HIS	N-CA	5.01	1.52	1.46
1	C	11	VAL	CA-CB	5.01	1.61	1.54
1	B	253	PRO	N-CA	-5.00	1.41	1.47

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	276	PRO	CA-C-N	-17.58	99.47	123.03
1	H	276	PRO	C-N-CA	-17.58	99.47	123.03
1	F	103	ASP	N-CA-C	10.19	126.01	113.17
1	E	186	CYS	CA-CB-SG	-9.58	92.37	114.40
1	E	298	LEU	CA-C-N	-9.56	114.22	120.24
1	E	298	LEU	C-N-CA	-9.56	114.22	120.24
1	D	27	ARG	CB-CG-CD	9.27	132.63	111.30
1	H	309	ALA	N-CA-C	-9.16	101.37	111.36
1	C	186	CYS	CA-CB-SG	-7.88	96.27	114.40
1	D	27	ARG	NE-CZ-NH2	-7.57	112.38	119.20
1	A	207	ALA	N-CA-C	-7.51	104.09	113.18
1	F	372	THR	N-CA-C	7.46	120.06	111.11
1	C	37	PHE	N-CA-C	-7.43	103.26	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LYS	N-CA-C	7.43	119.38	111.28
1	D	202	SER	N-CA-C	-7.18	103.49	111.82
1	A	251	VAL	N-CA-C	-7.04	97.99	108.12
1	A	82	PHE	CA-C-N	-6.94	113.16	120.03
1	A	82	PHE	C-N-CA	-6.94	113.16	120.03
1	B	104	GLN	CA-C-N	-6.71	114.64	126.32
1	B	104	GLN	C-N-CA	-6.71	114.64	126.32
1	B	141	GLU	CB-CA-C	-6.71	99.61	110.74
1	F	164	ALA	N-CA-C	-6.68	104.08	111.36
1	C	115	ASP	CA-C-N	6.67	126.80	119.87
1	C	115	ASP	C-N-CA	6.67	126.80	119.87
1	B	28	ILE	N-CA-C	6.54	117.29	110.62
1	F	99	ASP	CA-C-N	-6.49	113.27	120.14
1	F	99	ASP	C-N-CA	-6.49	113.27	120.14
1	E	186	CYS	N-CA-C	-6.47	104.31	111.82
1	E	99	ASP	CA-C-N	-6.44	114.00	120.31
1	E	99	ASP	C-N-CA	-6.44	114.00	120.31
1	E	6	HIS	CA-C-N	-6.44	114.03	120.21
1	E	6	HIS	C-N-CA	-6.44	114.03	120.21
1	G	103	ASP	N-CA-C	-6.34	105.60	113.15
1	B	77	ARG	CD-NE-CZ	6.26	133.16	124.40
1	F	252	TYR	CA-C-N	-6.22	113.35	119.76
1	F	252	TYR	C-N-CA	-6.22	113.35	119.76
1	B	336	GLY	N-CA-C	-6.21	107.84	114.67
1	D	139	MET	CA-CB-CG	-6.19	101.71	114.10
1	B	96	ASP	N-CA-C	-6.18	100.08	109.85
1	G	146	ALA	CA-C-N	-6.18	114.41	120.52
1	G	146	ALA	C-N-CA	-6.18	114.41	120.52
1	H	323	GLU	N-CA-C	6.04	118.64	111.33
1	G	101	GLU	C-N-CD	-6.00	107.41	120.60
1	H	276	PRO	N-CA-C	5.93	121.66	113.65
1	C	150	LEU	N-CA-C	-5.92	98.20	108.69
1	H	103	ASP	N-CA-C	-5.90	106.43	113.21
1	F	152	HIS	N-CA-C	-5.86	98.85	108.41
1	B	82	PHE	CA-C-N	-5.85	113.94	119.85
1	B	82	PHE	C-N-CA	-5.85	113.94	119.85
1	B	77	ARG	CG-CD-NE	-5.84	99.14	112.00
1	D	307	VAL	N-CA-C	5.84	116.58	110.62
1	H	200	LEU	N-CA-C	-5.82	105.02	111.36
1	G	400	THR	OG1-CB-CG2	5.81	120.92	109.30
1	G	99	ASP	CA-C-N	-5.81	114.77	120.98
1	G	99	ASP	C-N-CA	-5.81	114.77	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	ALA	N-CA-C	-5.79	105.05	111.36
1	B	59	THR	N-CA-C	-5.78	105.06	111.36
1	B	77	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	F	103	ASP	O-C-N	-5.70	115.21	122.34
1	B	387	GLY	N-CA-C	-5.69	107.52	114.92
1	H	259	ARG	N-CA-C	-5.67	104.47	111.33
1	D	319	GLY	N-CA-C	-5.65	106.38	115.08
1	H	47	ILE	CB-CA-C	-5.62	102.08	111.29
1	D	373	ILE	CA-C-N	-5.60	113.12	119.28
1	D	373	ILE	C-N-CA	-5.60	113.12	119.28
1	A	74	ILE	CB-CA-C	-5.57	102.55	110.12
1	C	314	LEU	N-CA-C	-5.56	105.12	111.07
1	F	65	ASP	N-CA-C	-5.55	105.38	111.82
1	B	152	HIS	CA-C-O	-5.54	114.34	120.38
1	C	302	ILE	N-CA-C	-5.53	104.97	111.00
1	E	130	LYS	N-CA-C	5.52	116.98	111.07
1	H	186	CYS	CA-CB-SG	-5.52	101.70	114.40
1	F	33	THR	CA-C-N	-5.52	113.26	120.44
1	F	33	THR	C-N-CA	-5.52	113.26	120.44
1	B	48	THR	N-CA-C	-5.50	106.57	113.72
1	H	276	PRO	O-C-N	-5.49	115.14	122.22
1	C	150	LEU	CA-C-N	-5.49	116.39	123.19
1	C	150	LEU	C-N-CA	-5.49	116.39	123.19
1	A	6	HIS	CA-C-N	-5.48	114.94	120.31
1	A	6	HIS	C-N-CA	-5.48	114.94	120.31
1	H	260	GLN	N-CA-C	5.46	119.57	113.02
1	C	372	THR	N-CA-C	5.45	116.91	111.07
1	G	101	GLU	CA-C-N	5.45	140.08	127.00
1	G	101	GLU	C-N-CA	5.45	140.08	127.00
1	F	117	ARG	N-CA-C	-5.42	106.17	112.89
1	A	193	ILE	N-CA-C	-5.41	104.33	111.09
1	B	369	SER	CB-CA-C	-5.41	108.77	116.34
1	C	305	ARG	N-CA-C	5.40	117.92	111.71
1	D	155	CYS	N-CA-C	-5.35	105.02	112.30
1	F	103	ASP	CA-C-N	5.35	131.33	121.70
1	F	103	ASP	C-N-CA	5.35	131.33	121.70
1	B	208	THR	CA-C-N	-5.35	114.87	120.38
1	B	208	THR	C-N-CA	-5.35	114.87	120.38
1	B	253	PRO	N-CA-C	-5.34	102.89	111.38
1	D	208	THR	N-CA-C	-5.33	100.23	108.55
1	A	224	ALA	N-CA-C	-5.32	106.05	112.54
1	H	187	TYR	N-CA-C	-5.30	106.68	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	164	ALA	CA-C-O	5.24	125.97	120.42
1	C	361	VAL	N-CA-C	-5.19	105.48	110.72
1	B	80	VAL	CB-CA-C	-5.18	104.12	112.16
1	H	172	GLY	N-CA-C	-5.18	107.10	115.08
1	G	165	GLU	N-CA-C	-5.14	105.75	111.36
1	E	184	MET	CB-CA-C	5.11	119.29	111.02
1	B	165	GLU	N-CA-C	-5.10	105.80	111.36
1	D	372	THR	N-CA-C	5.10	116.52	111.07
1	H	390	ILE	CB-CG1-CD1	-5.10	103.10	113.80
1	F	82	PHE	N-CA-C	-5.05	103.35	110.31
1	D	112	ILE	N-CA-C	-5.04	107.79	112.43
1	D	186	CYS	CA-CB-SG	-5.04	102.80	114.40
1	D	27	ARG	NE-CZ-NH1	5.03	126.53	121.50
1	B	214	VAL	N-CA-C	-5.02	101.08	108.11
1	E	385	THR	CB-CA-C	-5.02	100.31	109.54
1	C	376	ILE	CA-CB-CG1	-5.01	101.88	110.40
1	D	136	LEU	N-CA-C	-5.01	105.90	111.36
1	D	275	LEU	CA-C-N	-5.00	115.08	120.03
1	D	275	LEU	C-N-CA	-5.00	115.08	120.03

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	103	ASP	Peptide
1	G	100	PRO	Peptide
1	G	92	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3123	0	3112	30	0
1	B	3084	0	3083	88	0
1	C	3108	0	3099	72	0
1	D	3100	0	3095	57	0
1	E	3107	0	3101	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3123	0	3112	66	0
1	G	3078	0	3074	80	0
1	H	2968	0	2986	104	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	437	0	0	8	1
3	B	258	0	0	13	0
3	C	361	0	0	8	1
3	D	356	0	0	14	2
3	E	417	0	0	10	0
3	F	330	0	0	13	0
3	G	283	0	0	11	0
3	H	234	0	0	7	0
All	All	27375	0	24662	531	2

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 11.

All (531) 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:C:89:ARG:CB	1:C:96:ASP:HB3	1.55	1.35
1:C:89:ARG:HB2	1:C:96:ASP:CB	1.62	1.29
1:D:122:LYS:HD3	3:D:872:HOH:O	1.32	1.26
1:C:39:ARG:NH2	1:C:94:ASN:ND2	1.86	1.22
1:H:104:GLN:HE21	1:H:104:GLN:CA	1.51	1.22
1:F:103:ASP:N	1:F:104:GLN:HB2	1.56	1.20
1:F:103:ASP:OD2	1:F:104:GLN:HG2	1.41	1.18
1:C:39:ARG:HH21	1:C:94:ASN:ND2	1.37	1.18
1:H:104:GLN:HA	1:H:104:GLN:NE2	1.46	1.14
1:F:101:GLU:O	1:F:104:GLN:HB3	1.48	1.13
1:B:304:LYS:HE2	1:B:346:GLU:OE1	1.47	1.12
1:G:111:ASP:OD2	1:G:114:LYS:HD3	1.52	1.09
1:C:84:LYS:HB2	1:C:86:THR:O	1.53	1.08
1:F:258:ARG:HG2	1:F:258:ARG:HH11	1.16	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:324:ARG:HG2	1:H:324:ARG:HH11	1.18	1.07
1:B:18:VAL:HG21	1:B:139:MET:HG3	1.37	1.06
1:C:39:ARG:NH2	1:C:94:ASN:HD21	1.49	1.06
1:B:66:LYS:HD2	1:B:66:LYS:O	1.54	1.05
1:B:104:GLN:O	1:B:105:ALA:HB3	1.56	1.05
1:F:101:GLU:O	1:F:104:GLN:CB	2.07	1.03
1:D:122:LYS:HE3	3:D:910:HOH:O	1.59	1.03
1:B:339:LYS:HE2	3:B:753:HOH:O	1.57	1.02
1:H:320:MET:HE1	1:H:389:ARG:HD3	1.41	1.02
1:F:320:MET:HE1	1:F:329:LEU:HD11	1.40	1.01
1:B:18:VAL:HG21	1:B:139:MET:CG	1.91	1.00
1:B:26:GLN:OE1	1:B:77:ARG:HD2	1.61	0.99
1:G:134:LYS:HE3	1:G:138:GLN:HE22	1.25	0.98
1:C:346:GLU:C	1:C:346:GLU:OE1	2.07	0.97
1:E:382:GLU:OE2	3:E:993:HOH:O	1.82	0.97
1:F:20:LEU:H	1:F:78:GLN:NE2	1.62	0.97
1:H:305:ARG:HD3	3:H:834:HOH:O	1.65	0.95
1:D:39:ARG:NH2	1:D:94:ASN:OD1	1.99	0.95
1:C:84:LYS:HZ3	1:C:108:ARG:HH21	1.14	0.94
1:B:20:LEU:H	1:B:78:GLN:HE22	1.12	0.93
1:C:320:MET:HE1	1:C:329:LEU:HD21	1.51	0.92
1:B:320:MET:HE1	1:B:329:LEU:HD11	1.52	0.92
1:D:37:PHE:CE2	1:D:236:ILE:HD13	2.05	0.91
1:A:382:GLU:OE2	3:A:824:HOH:O	1.87	0.91
1:G:111:ASP:OD2	1:G:114:LYS:CD	2.19	0.89
1:E:89:ARG:O	1:E:96:ASP:N	2.04	0.89
1:D:104:GLN:OE1	1:D:104:GLN:HA	1.71	0.89
1:F:20:LEU:H	1:F:78:GLN:HE22	1.18	0.89
1:C:86:THR:HB	1:C:87:ASP:OD1	1.73	0.89
1:F:103:ASP:H	1:F:104:GLN:HB2	1.36	0.89
1:F:103:ASP:OD2	1:F:104:GLN:CG	2.22	0.87
1:D:263:ARG:HG2	1:D:263:ARG:HH11	1.39	0.87
1:D:320:MET:HE1	1:D:329:LEU:HD21	1.57	0.87
1:C:84:LYS:NZ	1:C:108:ARG:HH21	1.73	0.86
1:B:104:GLN:O	1:B:105:ALA:CB	2.25	0.85
1:G:20:LEU:H	1:G:78:GLN:HE22	1.25	0.85
1:A:20:LEU:H	1:A:78:GLN:HE22	1.21	0.84
1:B:20:LEU:H	1:B:78:GLN:NE2	1.75	0.84
1:C:20:LEU:H	1:C:78:GLN:HE22	1.24	0.84
1:G:134:LYS:HE3	1:G:138:GLN:NE2	1.92	0.84
1:H:324:ARG:HG2	1:H:324:ARG:NH1	1.81	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:320:MET:HE2	1:H:389:ARG:NH1	1.92	0.83
1:H:104:GLN:HE21	1:H:104:GLN:HA	0.70	0.83
1:H:35:TYR:CZ	1:H:39:ARG:HD2	2.13	0.82
1:B:21:ALA:H	1:B:78:GLN:HE21	1.25	0.82
1:D:20:LEU:H	1:D:78:GLN:NE2	1.77	0.82
1:H:320:MET:CE	1:H:389:ARG:HH11	1.92	0.81
1:H:324:ARG:HH11	1:H:324:ARG:CG	1.92	0.81
1:D:20:LEU:H	1:D:78:GLN:HE22	1.26	0.81
1:C:57:TYR:CZ	1:C:61:LYS:HE3	2.15	0.81
1:H:39:ARG:NH1	1:H:53:PHE:HE1	1.79	0.80
1:C:20:LEU:H	1:C:78:GLN:NE2	1.79	0.80
1:F:258:ARG:HG2	1:F:258:ARG:NH1	1.93	0.79
1:G:111:ASP:OD2	1:G:114:LYS:CE	2.30	0.79
1:H:20:LEU:H	1:H:78:GLN:HE22	1.29	0.79
1:A:305:ARG:HD2	3:A:758:HOH:O	1.80	0.79
1:H:141:GLU:OE1	3:H:829:HOH:O	2.01	0.79
1:H:320:MET:HE2	1:H:389:ARG:HH11	1.48	0.78
1:C:51:GLU:H	1:C:51:GLU:CD	1.91	0.78
1:A:139:MET:HE3	1:A:248:LYS:HB3	1.64	0.78
1:G:139:MET:HE3	1:G:248:LYS:HB3	1.66	0.78
1:H:351:ALA:H	1:H:354:GLN:HE21	1.29	0.78
1:G:293:MET:HE3	3:G:669:HOH:O	1.83	0.77
1:G:111:ASP:OD2	1:G:114:LYS:HE2	1.84	0.77
1:C:126:GLU:OE2	3:C:903:HOH:O	2.03	0.77
1:E:20:LEU:H	1:E:78:GLN:HE22	1.31	0.77
1:A:305:ARG:CD	3:A:758:HOH:O	2.33	0.76
1:H:300:PRO:O	1:H:304:LYS:HG3	1.85	0.76
1:G:20:LEU:H	1:G:78:GLN:NE2	1.82	0.76
1:B:18:VAL:CG2	1:B:139:MET:CG	2.64	0.76
1:C:103:ASP:C	1:C:103:ASP:OD1	2.28	0.76
1:A:20:LEU:H	1:A:78:GLN:NE2	1.83	0.75
1:B:321:ASP:O	1:B:325:ASP:HB2	1.86	0.75
1:E:139:MET:HG3	1:E:248:LYS:HG2	1.68	0.75
1:H:21:ALA:H	1:H:78:GLN:HE21	1.34	0.75
1:A:21:ALA:H	1:A:78:GLN:HE21	1.34	0.74
1:D:37:PHE:HE2	1:D:236:ILE:HD13	1.50	0.74
1:G:21:ALA:H	1:G:78:GLN:HE21	1.36	0.74
1:B:84:LYS:HE3	3:B:781:HOH:O	1.87	0.74
1:D:37:PHE:CE2	1:D:236:ILE:CD1	2.71	0.74
1:D:304:LYS:HE3	3:D:777:HOH:O	1.88	0.74
1:A:175:GLU:O	3:A:873:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:TYR:CE1	1:H:61:LYS:HD2	2.23	0.73
1:D:126:GLU:OE2	3:D:910:HOH:O	2.06	0.73
1:E:21:ALA:H	1:E:78:GLN:HE21	1.36	0.73
1:C:57:TYR:CE1	1:C:61:LYS:HE3	2.22	0.73
1:E:75:LYS:HE2	3:E:695:HOH:O	1.88	0.73
1:F:103:ASP:CA	1:F:104:GLN:HB2	2.18	0.73
1:H:33:THR:HG21	3:H:804:HOH:O	1.90	0.72
1:D:89:ARG:NH2	1:D:98:ALA:HB2	2.04	0.72
1:B:304:LYS:HZ3	1:B:347:GLU:HB2	1.54	0.72
1:D:89:ARG:HG2	1:D:96:ASP:O	1.89	0.72
1:E:139:MET:CG	1:E:248:LYS:HG2	2.20	0.72
1:B:122:LYS:HZ1	1:H:285:VAL:HG21	1.55	0.72
1:H:230:GLU:OE1	1:H:232:ARG:NH2	2.23	0.72
1:B:139:MET:HE3	1:B:248:LYS:HB2	1.70	0.71
1:C:87:ASP:HB2	1:C:98:ALA:HB3	1.72	0.71
1:F:194:LYS:NZ	1:G:179:THR:OG1	2.23	0.71
1:F:101:GLU:O	1:F:104:GLN:HB2	1.90	0.71
1:G:97:ILE:HD12	1:G:97:ILE:N	2.05	0.71
1:A:323:GLU:OE2	3:A:1030:HOH:O	2.07	0.71
1:E:75:LYS:CE	3:E:695:HOH:O	2.39	0.70
1:C:21:ALA:H	1:C:78:GLN:HE21	1.36	0.70
1:E:89:ARG:HB3	1:E:90:PHE:CD2	2.26	0.70
1:B:18:VAL:CG2	1:B:139:MET:HG2	2.22	0.70
1:H:37:PHE:CE2	1:H:236:ILE:HD13	2.26	0.70
1:F:21:ALA:H	1:F:78:GLN:HE21	1.38	0.70
1:C:86:THR:CB	1:C:87:ASP:OD1	2.40	0.70
1:F:113:LYS:NZ	3:F:895:HOH:O	2.22	0.70
1:D:89:ARG:CZ	1:D:98:ALA:HB2	2.22	0.69
1:E:89:ARG:HB2	1:E:96:ASP:HB3	1.74	0.69
1:G:66:LYS:HE3	1:G:67:TYR:OH	1.92	0.69
1:D:21:ALA:H	1:D:78:GLN:HE21	1.40	0.69
1:D:64:PHE:CE1	1:D:236:ILE:HD12	2.28	0.69
1:D:126:GLU:OE1	3:D:890:HOH:O	2.11	0.69
1:A:125:HIS:HE1	1:A:158:TYR:H	1.41	0.68
1:B:326:LYS:NZ	1:B:349:GLY:O	2.27	0.68
1:B:18:VAL:CG2	1:B:139:MET:HG3	2.20	0.68
1:C:101:GLU:O	1:C:103:ASP:N	2.26	0.68
1:E:320:MET:HE1	1:E:329:LEU:HD21	1.76	0.68
1:G:315:LEU:HG	1:G:320:MET:HE3	1.76	0.68
1:F:150:LEU:C	1:F:150:LEU:HD23	2.19	0.67
1:F:258:ARG:HH11	1:F:258:ARG:CG	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ASP:OD2	3:A:929:HOH:O	2.12	0.66
1:C:86:THR:CA	1:C:87:ASP:OD1	2.43	0.66
1:H:320:MET:CE	1:H:389:ARG:NH1	2.56	0.66
1:C:106:HIS:NE2	1:C:130:LYS:HE2	2.10	0.66
1:G:388:THR:OG1	3:G:844:HOH:O	2.14	0.66
1:C:89:ARG:HB2	1:C:96:ASP:HB3	0.72	0.65
1:F:101:GLU:HB2	1:F:104:GLN:HG3	1.77	0.65
1:C:31:GLU:OE2	3:C:769:HOH:O	2.14	0.65
1:C:86:THR:HA	1:C:87:ASP:OD1	1.96	0.65
1:B:304:LYS:CE	1:B:346:GLU:OE1	2.37	0.65
1:G:111:ASP:CG	1:G:114:LYS:HD3	2.21	0.65
1:H:102:PRO:C	1:H:104:GLN:H	2.05	0.65
1:C:39:ARG:HH21	1:C:94:ASN:HD22	1.42	0.65
1:G:293:MET:CE	3:G:669:HOH:O	2.41	0.65
1:D:101:GLU:HG3	1:D:104:GLN:HB2	1.79	0.65
1:H:27:ARG:HG3	1:H:28:ILE:N	2.11	0.65
1:C:89:ARG:CZ	1:C:98:ALA:HB2	2.27	0.64
1:H:64:PHE:CE1	1:H:236:ILE:HD12	2.33	0.64
1:C:84:LYS:HZ3	1:C:108:ARG:NH2	1.90	0.64
1:H:324:ARG:HG3	1:H:325:ASP:OD1	1.97	0.64
1:F:231:SER:HB2	3:F:679:HOH:O	1.95	0.64
1:F:256:GLU:CD	1:F:259:ARG:HH21	2.06	0.64
1:H:39:ARG:HD3	1:H:112:ILE:HD12	1.80	0.63
1:G:321:ASP:HB3	1:G:324:ARG:HD3	1.81	0.63
1:H:320:MET:HB2	1:H:325:ASP:OD2	1.98	0.63
1:C:103:ASP:OD1	1:C:104:GLN:HG3	1.98	0.63
1:H:102:PRO:CD	1:H:104:GLN:HB2	2.27	0.63
1:H:308:ARG:NH2	1:H:323:GLU:OE2	2.31	0.63
1:D:104:GLN:OE1	1:D:104:GLN:CA	2.45	0.62
1:F:103:ASP:CG	1:F:104:GLN:HG2	2.22	0.62
1:A:308:ARG:NH2	1:A:323:GLU:OE2	2.31	0.62
1:E:89:ARG:N	1:E:89:ARG:HD3	2.13	0.62
1:H:39:ARG:NH1	1:H:53:PHE:CE1	2.66	0.62
1:E:134:LYS:HE3	1:E:138:GLN:NE2	2.14	0.62
1:F:150:LEU:HD23	1:F:151:ILE:N	2.14	0.62
1:C:103:ASP:OD1	1:C:103:ASP:O	2.18	0.61
1:A:125:HIS:CE1	1:A:158:TYR:H	2.18	0.61
1:B:20:LEU:N	1:B:78:GLN:NE2	2.48	0.61
1:H:112:ILE:HG13	1:H:112:ILE:O	2.00	0.61
1:C:101:GLU:C	1:C:103:ASP:N	2.57	0.61
1:B:76:GLN:HG3	3:B:757:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TYR:CZ	1:C:61:LYS:CE	2.83	0.61
1:H:102:PRO:HG2	1:H:103:ASP:OD2	2.01	0.61
1:E:20:LEU:H	1:E:78:GLN:NE2	1.99	0.60
1:H:37:PHE:CE2	1:H:236:ILE:CD1	2.83	0.60
1:D:32:LEU:HD21	1:D:83:PRO:HG2	1.83	0.60
1:G:101:GLU:HG2	1:G:104:GLN:HG3	1.83	0.60
1:G:97:ILE:N	1:G:97:ILE:CD1	2.63	0.60
1:G:353:ASP:OD1	1:G:354:GLN:N	2.34	0.60
1:C:32:LEU:HD11	1:C:88:ILE:HG12	1.84	0.60
1:H:53:PHE:C	1:H:53:PHE:CD2	2.80	0.60
1:D:84:LYS:HB2	1:D:87:ASP:HB2	1.84	0.60
1:E:89:ARG:HB3	1:E:90:PHE:CE2	2.36	0.60
1:H:263:ARG:HH11	1:H:263:ARG:HG2	1.67	0.60
1:G:55:GLN:HE21	1:G:55:GLN:HA	1.66	0.60
1:B:371:SER:O	1:B:375:HIS:HD2	1.84	0.59
1:F:258:ARG:NH1	1:F:258:ARG:CG	2.57	0.59
1:C:101:GLU:O	1:C:102:PRO:C	2.46	0.59
1:G:371:SER:C	1:G:374:PRO:HD2	2.28	0.59
1:F:11:VAL:HG11	1:F:257:LEU:HD22	1.85	0.59
1:H:258:ARG:O	1:H:259:ARG:C	2.46	0.59
1:H:20:LEU:H	1:H:78:GLN:NE2	2.00	0.58
1:C:39:ARG:HD3	1:C:53:PHE:CE1	2.38	0.58
1:F:101:GLU:CB	1:F:104:GLN:HG3	2.33	0.58
1:F:285:VAL:HG13	3:F:734:HOH:O	2.03	0.58
1:H:102:PRO:CG	1:H:103:ASP:H	2.15	0.58
1:H:139:MET:HE3	1:H:248:LYS:HB3	1.86	0.58
1:E:323:GLU:CD	1:E:323:GLU:H	2.11	0.58
1:H:29:THR:O	1:H:33:THR:CG2	2.51	0.58
1:G:102:PRO:HD2	1:G:103:ASP:H	1.68	0.58
1:G:134:LYS:CE	1:G:138:GLN:NE2	2.64	0.58
1:H:102:PRO:HD2	1:H:104:GLN:HG2	1.86	0.58
1:B:305:ARG:NH2	1:F:103:ASP:O	2.37	0.58
1:D:101:GLU:HB2	1:D:103:ASP:OD1	2.04	0.58
1:B:75:LYS:HE3	3:B:741:HOH:O	2.01	0.58
1:B:75:LYS:HE3	1:B:76:GLN:HE22	1.69	0.58
1:E:20:LEU:HD11	1:E:246:LEU:HD22	1.84	0.58
1:E:293:MET:HE1	3:E:985:HOH:O	2.04	0.57
1:F:326:LYS:HA	1:F:329:LEU:HD22	1.86	0.57
1:B:66:LYS:HD2	1:B:66:LYS:C	2.23	0.57
1:H:29:THR:O	1:H:33:THR:HG23	2.04	0.57
1:E:134:LYS:HE3	1:E:138:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PHE:HD2	3:B:653:HOH:O	1.88	0.56
1:D:32:LEU:CD2	1:D:83:PRO:HG2	2.35	0.56
1:G:134:LYS:HD3	1:G:138:GLN:NE2	2.20	0.56
1:C:315:LEU:HD12	1:C:322:PHE:HA	1.86	0.56
1:C:89:ARG:CB	1:C:96:ASP:CB	2.47	0.56
1:H:75:LYS:NZ	3:H:796:HOH:O	2.37	0.56
1:A:315:LEU:HD21	1:A:329:LEU:HD11	1.88	0.56
1:D:263:ARG:NH2	1:F:44:SER:O	2.38	0.56
1:E:103:ASP:OD2	1:E:103:ASP:N	2.39	0.56
1:C:346:GLU:OE1	1:C:346:GLU:O	2.23	0.56
1:E:88:ILE:C	1:E:89:ARG:HD3	2.31	0.56
1:H:226:ASN:ND2	3:H:707:HOH:O	2.39	0.56
1:B:285:VAL:HG13	3:B:695:HOH:O	2.05	0.55
1:H:60:VAL:HA	1:H:63:LYS:HE2	1.88	0.55
1:A:315:LEU:HD21	1:A:329:LEU:CD1	2.36	0.55
1:C:141:GLU:HG3	3:C:603:HOH:O	2.07	0.55
1:G:141:GLU:OE1	3:G:803:HOH:O	2.18	0.55
1:G:100:PRO:HA	1:G:101:GLU:OE1	2.07	0.55
1:H:58:LYS:O	1:H:62:GLU:HG3	2.06	0.55
1:G:102:PRO:C	1:G:104:GLN:H	2.13	0.55
1:A:139:MET:CE	1:A:248:LYS:HB3	2.35	0.55
1:E:113:LYS:HD3	3:E:770:HOH:O	2.07	0.55
1:G:89:ARG:HG3	1:G:96:ASP:HB3	1.89	0.54
1:A:305:ARG:HD3	3:A:758:HOH:O	2.05	0.54
1:B:150:LEU:HD12	1:B:215:ASP:O	2.07	0.54
1:B:122:LYS:HZ1	1:H:285:VAL:CG2	2.20	0.54
1:D:87:ASP:OD1	1:D:98:ALA:HB3	2.08	0.54
3:F:921:HOH:O	1:G:175:GLU:HG2	2.06	0.54
1:F:256:GLU:OE2	1:F:259:ARG:NH2	2.38	0.53
1:H:315:LEU:HD22	1:H:322:PHE:HA	1.90	0.53
1:C:106:HIS:CD2	1:C:130:LYS:HE2	2.43	0.53
1:D:263:ARG:HH11	1:D:263:ARG:CG	2.17	0.53
1:C:89:ARG:CA	1:C:96:ASP:HB3	2.34	0.53
1:A:51:GLU:OE2	1:A:55:GLN:HG2	2.08	0.53
1:H:85:LEU:N	1:H:85:LEU:HD23	2.23	0.53
1:H:150:LEU:C	1:H:150:LEU:HD23	2.34	0.53
1:B:18:VAL:HG23	1:B:139:MET:HG2	1.89	0.53
1:F:16:ILE:HD12	1:F:248:LYS:HE3	1.90	0.53
1:G:285:VAL:HG22	3:G:789:HOH:O	2.09	0.53
1:H:315:LEU:CD2	1:H:322:PHE:HA	2.38	0.53
1:B:21:ALA:H	1:B:78:GLN:NE2	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:LYS:HE3	1:H:62:GLU:OE2	2.08	0.52
1:B:122:LYS:NZ	3:B:775:HOH:O	2.38	0.52
1:B:258:ARG:HH11	1:B:258:ARG:HG2	1.74	0.52
1:B:84:LYS:HD3	3:B:807:HOH:O	2.10	0.52
1:G:66:LYS:HE3	1:G:67:TYR:CZ	2.44	0.52
1:C:89:ARG:HB2	1:C:96:ASP:CG	2.32	0.52
1:C:101:GLU:C	1:C:103:ASP:H	2.16	0.52
1:G:110:PHE:HB3	1:G:226:ASN:OD1	2.10	0.52
1:G:150:LEU:C	1:G:150:LEU:HD23	2.35	0.52
1:G:22:LYS:HE3	3:G:771:HOH:O	2.10	0.52
1:D:27:ARG:HG2	3:D:641:HOH:O	2.09	0.51
1:G:226:ASN:ND2	1:G:228:ILE:HG23	2.25	0.51
1:H:102:PRO:HG2	1:H:103:ASP:H	1.74	0.51
1:H:35:TYR:OH	1:H:39:ARG:HD2	2.10	0.51
1:H:232:ARG:HH11	1:H:234:ASP:HB3	1.74	0.51
1:C:89:ARG:N	1:C:96:ASP:O	2.39	0.51
1:H:102:PRO:HD2	1:H:103:ASP:OD2	2.11	0.51
1:F:342:ASP:OD1	1:F:359:LYS:HE2	2.11	0.51
1:G:12:LEU:HD23	1:G:251:VAL:HG22	1.93	0.51
1:C:39:ARG:HH22	1:C:94:ASN:HD21	1.48	0.51
1:B:364:GLU:OE1	3:B:662:HOH:O	2.20	0.50
1:F:194:LYS:CE	3:F:666:HOH:O	2.59	0.50
1:B:341:VAL:HG23	3:B:828:HOH:O	2.11	0.50
1:F:315:LEU:HD12	1:F:322:PHE:HD1	1.77	0.50
1:G:102:PRO:CD	1:G:103:ASP:H	2.23	0.50
1:H:35:TYR:CE2	1:H:39:ARG:HD2	2.47	0.50
1:H:53:PHE:C	1:H:53:PHE:HD2	2.18	0.50
1:C:106:HIS:CE1	1:C:130:LYS:CE	2.95	0.50
1:E:89:ARG:N	1:E:89:ARG:CD	2.73	0.50
1:C:86:THR:O	1:C:86:THR:OG1	2.29	0.50
1:B:81:TYR:CE1	1:B:224:ALA:HB2	2.47	0.50
1:B:138:GLN:O	1:B:141:GLU:HG3	2.12	0.50
1:H:27:ARG:HG3	1:H:28:ILE:H	1.74	0.50
1:D:89:ARG:HD3	1:D:89:ARG:N	2.27	0.50
1:F:148:ASP:HB3	1:F:211:LYS:NZ	2.26	0.50
1:D:27:ARG:HG3	1:D:28:ILE:N	2.26	0.49
1:F:148:ASP:HB3	1:F:211:LYS:HZ3	1.77	0.49
1:G:134:LYS:CE	1:G:138:GLN:HE22	2.11	0.49
1:F:20:LEU:N	1:F:78:GLN:NE2	2.45	0.49
1:H:263:ARG:HD2	1:H:409:ILE:O	2.13	0.49
1:D:255:ASP:OD1	3:D:785:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282:MET:HE3	1:G:399:LEU:HD11	1.95	0.49
1:E:89:ARG:O	1:E:95:PHE:HA	2.13	0.49
1:F:113:LYS:CD	3:F:895:HOH:O	2.60	0.49
1:G:101:GLU:HG2	1:G:101:GLU:O	2.13	0.49
1:B:165:GLU:HG3	1:B:178:VAL:HG11	1.94	0.49
1:D:20:LEU:N	1:D:78:GLN:NE2	2.54	0.49
1:B:24:VAL:HG12	1:B:25:PRO:O	2.12	0.49
1:H:313:ASP:OD1	1:H:316:ARG:NH2	2.46	0.49
1:F:373:ILE:N	1:F:374:PRO:CD	2.76	0.48
1:F:149:ASP:OD2	1:F:211:LYS:NZ	2.45	0.48
1:H:75:LYS:CE	3:H:796:HOH:O	2.60	0.48
1:G:101:GLU:CG	1:G:104:GLN:HG3	2.43	0.48
1:C:51:GLU:CD	1:C:51:GLU:N	2.63	0.48
1:D:82:PHE:CG	1:D:83:PRO:HD2	2.48	0.48
1:C:89:ARG:N	1:C:89:ARG:HD3	2.28	0.48
1:D:134:LYS:HD3	3:D:870:HOH:O	2.14	0.48
1:B:21:ALA:N	1:B:78:GLN:HE21	2.01	0.48
1:G:101:GLU:OE1	1:G:101:GLU:N	2.47	0.48
1:G:103:ASP:OD1	1:G:103:ASP:N	2.46	0.48
1:B:122:LYS:NZ	1:H:285:VAL:CG2	2.77	0.48
1:F:144:LEU:HD23	1:F:144:LEU:HA	1.68	0.48
1:G:134:LYS:CD	1:G:138:GLN:NE2	2.77	0.48
1:A:130:LYS:NZ	1:A:130:LYS:HB3	2.28	0.48
1:B:75:LYS:HE2	1:B:364:GLU:OE1	2.14	0.48
1:C:106:HIS:CE1	1:C:130:LYS:HE2	2.48	0.48
1:B:68:ALA:HB1	1:B:240:THR:HG21	1.96	0.48
1:F:130:LYS:HB3	1:F:130:LYS:HE3	1.63	0.48
1:G:315:LEU:CD2	1:G:322:PHE:HA	2.43	0.47
1:B:122:LYS:NZ	1:H:285:VAL:HG21	2.26	0.47
1:H:103:ASP:O	1:H:104:GLN:NE2	2.47	0.47
1:G:139:MET:HE1	1:G:217:ALA:HB1	1.96	0.47
1:D:314:LEU:HG	1:D:405:VAL:CG2	2.44	0.47
1:E:20:LEU:CD1	1:E:246:LEU:HD22	2.44	0.47
1:F:150:LEU:C	1:F:150:LEU:CD2	2.87	0.47
1:B:32:LEU:CD2	1:B:95:PHE:CD2	2.97	0.47
1:C:32:LEU:HD11	1:C:88:ILE:CD1	2.44	0.47
1:F:201:ALA:HA	1:G:205:TRP:CZ2	2.50	0.47
1:F:304:LYS:HZ2	1:F:347:GLU:HB2	1.78	0.47
1:F:103:ASP:CA	1:F:104:GLN:CB	2.92	0.47
1:H:398:GLY:N	1:H:399:LEU:HA	2.28	0.47
1:A:150:LEU:C	1:A:150:LEU:HD23	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:PHE:HA	1:B:400:THR:O	2.15	0.47
1:C:20:LEU:N	1:C:78:GLN:NE2	2.56	0.47
1:B:32:LEU:HA	1:B:32:LEU:HD22	1.56	0.46
1:C:346:GLU:OE1	1:C:347:GLU:N	2.47	0.46
1:E:20:LEU:HD11	1:E:246:LEU:CD2	2.45	0.46
1:F:216:ILE:HD12	1:F:249:TYR:CE1	2.50	0.46
1:E:293:MET:HE2	3:E:723:HOH:O	2.13	0.46
1:H:39:ARG:HH11	1:H:53:PHE:HE1	1.56	0.46
1:B:322:PHE:O	1:B:326:LYS:HB3	2.15	0.46
1:F:266:ARG:O	1:F:406:LEU:HA	2.15	0.46
1:E:83:PRO:HG3	1:E:97:ILE:HD13	1.97	0.46
1:E:89:ARG:CB	1:E:96:ASP:HB3	2.44	0.46
1:C:111:ASP:HB3	1:C:115:ASP:O	2.16	0.46
1:H:168:VAL:HG13	1:H:173:TRP:HB2	1.96	0.46
1:A:339:LYS:HA	1:A:339:LYS:HD3	1.58	0.46
1:B:305:ARG:HD3	3:F:620:HOH:O	2.15	0.46
1:F:194:LYS:HE2	3:F:666:HOH:O	2.15	0.46
1:G:299:VAL:HB	1:G:300:PRO:HD3	1.98	0.46
1:A:398:GLY:HA3	1:A:399:LEU:C	2.40	0.46
1:C:89:ARG:NH2	1:C:98:ALA:HB2	2.31	0.46
1:F:194:LYS:HE3	3:F:666:HOH:O	2.16	0.46
1:B:304:LYS:NZ	1:B:347:GLU:OE1	2.49	0.46
1:E:8:ASN:ND2	3:E:970:HOH:O	2.43	0.46
1:D:37:PHE:CD2	1:D:236:ILE:CD1	2.99	0.46
1:B:174:PHE:CE1	1:H:276:PRO:HA	2.51	0.45
1:D:263:ARG:CG	1:D:263:ARG:NH1	2.77	0.45
1:H:21:ALA:H	1:H:78:GLN:NE2	2.09	0.45
1:H:280:ASP:HB3	3:H:751:HOH:O	2.15	0.45
1:A:201:ALA:HA	1:C:205:TRP:CZ2	2.51	0.45
1:B:20:LEU:N	1:B:78:GLN:HE22	1.95	0.45
1:B:177:THR:HG23	1:H:272:GLU:HB3	1.98	0.45
1:C:101:GLU:HG3	1:C:103:ASP:CG	2.41	0.45
1:H:20:LEU:N	1:H:78:GLN:HE22	2.06	0.45
1:H:320:MET:HE1	1:H:389:ARG:HH11	1.79	0.45
1:C:11:VAL:HG11	1:C:257:LEU:HD22	1.97	0.45
1:E:51:GLU:O	1:E:51:GLU:HG3	2.16	0.45
1:F:20:LEU:HD21	1:F:135:GLY:HA2	1.98	0.45
1:H:312:VAL:HA	1:H:322:PHE:HB2	1.98	0.45
1:B:146:ALA:HB2	1:B:173:TRP:CD1	2.51	0.45
1:B:256:GLU:OE2	1:B:259:ARG:NH1	2.50	0.45
1:B:259:ARG:NH1	1:B:260:GLN:HE21	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:MET:CE	1:B:329:LEU:HD11	2.36	0.45
1:C:87:ASP:HB3	1:C:89:ARG:NH1	2.31	0.45
1:G:100:PRO:CA	1:G:101:GLU:OE1	2.65	0.45
1:B:248:LYS:NZ	3:B:621:HOH:O	2.27	0.45
1:E:139:MET:HG2	1:E:248:LYS:HG2	1.98	0.45
1:A:135:GLY:O	1:A:139:MET:HG3	2.16	0.45
1:G:285:VAL:CG2	3:G:789:HOH:O	2.64	0.45
1:H:304:LYS:HE3	1:H:304:LYS:HB3	1.71	0.45
1:H:232:ARG:O	1:H:233:VAL:C	2.59	0.45
1:B:32:LEU:HD21	1:B:95:PHE:CG	2.51	0.45
1:B:285:VAL:HG13	1:B:285:VAL:O	2.17	0.45
1:F:392:CYS:O	1:F:403:GLY:HA2	2.17	0.45
1:A:20:LEU:HD23	1:A:20:LEU:HA	1.82	0.44
1:B:16:ILE:HD12	1:B:248:LYS:HE3	1.99	0.44
1:D:101:GLU:H	1:D:101:GLU:HG2	1.34	0.44
1:B:12:LEU:HD23	1:B:251:VAL:HG22	2.00	0.44
1:D:315:LEU:HD12	1:D:322:PHE:HA	1.99	0.44
1:E:230:GLU:OE2	3:E:951:HOH:O	2.20	0.44
1:D:304:LYS:CE	3:D:777:HOH:O	2.57	0.44
1:E:87:ASP:OD2	3:E:978:HOH:O	2.21	0.44
1:F:285:VAL:HG11	3:F:794:HOH:O	2.16	0.44
1:H:102:PRO:CD	1:H:103:ASP:N	2.80	0.44
1:C:85:LEU:HD12	1:C:88:ILE:HD12	2.00	0.44
1:G:89:ARG:HE	1:G:89:ARG:HB2	1.64	0.44
1:H:102:PRO:CG	1:H:103:ASP:N	2.80	0.44
1:D:146:ALA:HB2	1:D:173:TRP:CD1	2.52	0.44
1:E:89:ARG:HG2	1:E:96:ASP:HB3	2.00	0.44
1:G:226:ASN:HD21	1:G:228:ILE:HG23	1.82	0.44
1:B:18:VAL:HG21	1:B:139:MET:HG2	1.78	0.44
1:C:134:LYS:CE	3:C:690:HOH:O	2.65	0.44
1:F:83:PRO:HG3	1:F:97:ILE:HD12	2.00	0.44
1:G:32:LEU:HD11	1:G:97:ILE:HD11	2.00	0.44
1:B:76:GLN:NE2	3:B:741:HOH:O	2.50	0.44
1:D:398:GLY:N	1:D:399:LEU:HA	2.33	0.44
1:H:29:THR:O	1:H:33:THR:HG22	2.18	0.43
1:B:75:LYS:HB3	1:B:76:GLN:NE2	2.33	0.43
1:C:32:LEU:HD11	1:C:88:ILE:CG1	2.47	0.43
1:C:339:LYS:HE3	3:C:801:HOH:O	2.17	0.43
1:D:141:GLU:HG3	3:D:642:HOH:O	2.18	0.43
1:E:254:GLU:O	1:E:258:ARG:HG2	2.18	0.43
1:G:20:LEU:N	1:G:78:GLN:NE2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLN:OE1	1:B:77:ARG:CD	2.49	0.43
1:C:50:GLU:N	1:C:50:GLU:CD	2.76	0.43
1:F:58:LYS:HB2	1:F:58:LYS:HE2	1.68	0.43
1:F:122:LYS:HE2	3:G:765:HOH:O	2.18	0.43
1:A:168:VAL:HG13	1:A:173:TRP:HB2	2.00	0.43
3:A:938:HOH:O	1:C:122:LYS:HD3	2.18	0.43
1:B:291:PHE:N	1:B:291:PHE:CD1	2.86	0.43
1:D:326:LYS:HD2	3:D:737:HOH:O	2.18	0.43
1:G:134:LYS:HD3	1:G:138:GLN:HE21	1.84	0.43
1:G:134:LYS:HE2	3:G:818:HOH:O	2.18	0.43
1:B:58:LYS:O	1:B:62:GLU:HG3	2.19	0.43
1:B:75:LYS:CB	1:B:76:GLN:NE2	2.82	0.43
1:B:120:ASP:C	1:B:120:ASP:OD1	2.62	0.43
1:D:260:GLN:O	1:D:262:LEU:HD13	2.19	0.43
1:F:32:LEU:HD21	1:F:97:ILE:HD11	2.00	0.43
1:G:101:GLU:CD	1:G:104:GLN:HG3	2.43	0.43
1:H:102:PRO:C	1:H:104:GLN:N	2.72	0.43
1:H:303:ILE:O	1:H:304:LYS:C	2.59	0.43
1:A:104:GLN:HE21	1:A:107:LEU:HD11	1.84	0.43
1:B:172:GLY:HA2	1:B:174:PHE:CE2	2.54	0.43
1:D:314:LEU:HG	1:D:405:VAL:HG23	2.00	0.43
1:F:300:PRO:HD2	3:F:809:HOH:O	2.17	0.43
1:G:96:ASP:C	1:G:97:ILE:HD12	2.43	0.43
1:G:398:GLY:N	1:G:399:LEU:HA	2.33	0.43
1:H:395:PHE:HA	1:H:400:THR:O	2.18	0.43
1:H:226:ASN:ND2	1:H:226:ASN:C	2.75	0.43
1:C:106:HIS:HE1	3:C:690:HOH:O	2.00	0.43
1:G:256:GLU:OE2	1:G:259:ARG:NH2	2.52	0.43
1:G:316:ARG:HG3	3:G:881:HOH:O	2.19	0.43
1:B:66:LYS:C	1:B:66:LYS:CD	2.90	0.43
1:H:103:ASP:OD2	1:H:103:ASP:N	2.50	0.43
1:C:87:ASP:HB2	1:C:98:ALA:CB	2.45	0.42
1:D:89:ARG:N	1:D:89:ARG:CD	2.82	0.42
1:H:139:MET:HE1	1:H:217:ALA:HB1	2.01	0.42
1:G:256:GLU:O	1:G:260:GLN:CG	2.67	0.42
1:D:263:ARG:HG2	1:D:263:ARG:NH1	2.15	0.42
1:F:205:TRP:HE1	1:G:204:GLN:HE21	1.67	0.42
1:G:321:ASP:OD2	1:G:324:ARG:CD	2.67	0.42
1:C:134:LYS:HE3	3:C:690:HOH:O	2.17	0.42
1:D:308:ARG:HA	1:D:348:LEU:HD21	2.01	0.42
1:G:339:LYS:HB2	1:G:339:LYS:HE2	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LYS:HE3	1:D:363:LEU:HD21	2.01	0.42
1:D:85:LEU:HA	1:D:88:ILE:HD12	2.02	0.42
1:E:165:GLU:HG3	1:E:178:VAL:HG11	2.01	0.42
1:G:308:ARG:O	1:G:312:VAL:HG23	2.19	0.42
1:F:297:PRO:HD2	3:F:804:HOH:O	2.19	0.42
1:H:59:THR:O	1:H:63:LYS:HG3	2.20	0.42
1:H:263:ARG:HA	1:H:263:ARG:HD3	1.74	0.42
1:D:32:LEU:HD21	1:D:83:PRO:CG	2.49	0.42
1:H:183:ASN:CG	1:H:183:ASN:O	2.63	0.42
1:H:308:ARG:O	1:H:312:VAL:HG23	2.19	0.42
1:B:66:LYS:O	1:B:66:LYS:CD	2.45	0.42
1:C:149:ASP:OD2	1:C:211:LYS:NZ	2.51	0.42
1:H:232:ARG:NH1	1:H:234:ASP:HB3	2.35	0.42
1:B:20:LEU:HD21	1:B:135:GLY:HA2	2.01	0.42
1:G:102:PRO:CD	1:G:103:ASP:N	2.81	0.42
1:G:256:GLU:O	1:G:260:GLN:HG3	2.20	0.42
1:G:304:LYS:NZ	1:G:347:GLU:HB2	2.35	0.42
1:A:104:GLN:NE2	1:A:107:LEU:HD11	2.35	0.41
1:C:231:SER:HB2	3:C:898:HOH:O	2.19	0.41
1:D:122:LYS:HD2	3:D:718:HOH:O	2.20	0.41
1:E:311:ALA:O	1:E:315:LEU:HD13	2.20	0.41
1:B:398:GLY:N	1:B:399:LEU:HA	2.36	0.41
1:E:398:GLY:HA3	1:E:399:LEU:C	2.44	0.41
1:F:371:SER:C	1:F:374:PRO:HD2	2.46	0.41
1:B:57:TYR:CZ	1:B:61:LYS:HE3	2.55	0.41
1:G:97:ILE:HD13	1:G:112:ILE:HD11	2.01	0.41
1:G:329:LEU:HD22	1:G:389:ARG:HB2	2.02	0.41
1:A:256:GLU:OE1	1:A:259:ARG:NH2	2.45	0.41
1:G:91:GLY:O	1:G:92:ASP:C	2.63	0.41
1:H:102:PRO:N	1:H:104:GLN:HB2	2.35	0.41
1:E:315:LEU:HD21	1:E:329:LEU:CD1	2.51	0.41
1:E:392:CYS:O	1:E:403:GLY:HA2	2.20	0.41
1:H:256:GLU:O	1:H:260:GLN:HG3	2.20	0.41
1:H:263:ARG:HG2	1:H:263:ARG:NH1	2.34	0.41
1:A:281:THR:HB	1:A:296:SER:HB3	2.03	0.41
1:B:336:GLY:HA3	3:B:795:HOH:O	2.20	0.41
1:B:104:GLN:HB3	1:B:105:ALA:H	1.64	0.41
1:E:395:PHE:HA	1:E:400:THR:O	2.20	0.41
1:G:208:THR:HB	1:G:209:PRO:HD2	2.03	0.41
1:H:18:VAL:O	1:H:18:VAL:HG13	2.20	0.41
1:E:75:LYS:NZ	3:E:695:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:353:ASP:OD1	1:G:353:ASP:C	2.63	0.41
1:H:22:LYS:HA	1:H:23:PRO:HD3	1.97	0.41
1:F:101:GLU:HB3	3:F:894:HOH:O	2.20	0.41
1:F:109:LEU:HD23	1:F:109:LEU:HA	1.89	0.41
1:G:168:VAL:HG13	1:G:173:TRP:HB2	2.02	0.41
1:H:339:LYS:HA	1:H:339:LYS:HD2	1.96	0.41
1:B:168:VAL:HG13	1:B:173:TRP:HB2	2.03	0.40
1:G:18:VAL:HG22	3:G:849:HOH:O	2.21	0.40
1:D:293:MET:HE2	3:D:685:HOH:O	2.20	0.40
1:D:378:LYS:NZ	3:D:846:HOH:O	2.49	0.40
1:F:112:ILE:HG13	1:F:113:LYS:HD2	2.03	0.40
1:F:149:ASP:OD2	1:F:211:LYS:CE	2.69	0.40
1:H:102:PRO:HD2	1:H:104:GLN:HB2	2.01	0.40
1:B:75:LYS:CB	1:B:76:GLN:HE22	2.34	0.40
1:B:398:GLY:HA3	1:B:399:LEU:C	2.46	0.40
1:D:69:VAL:HG11	1:D:74:ILE:HD12	2.04	0.40
1:G:392:CYS:O	1:G:403:GLY:HA2	2.21	0.40
1:H:121:LEU:HD12	1:H:121:LEU:HA	1.91	0.40
1:B:325:ASP:O	1:B:329:LEU:HD13	2.20	0.40
1:E:371:SER:C	1:E:374:PRO:HD2	2.46	0.40
1:H:298:LEU:O	1:H:299:VAL:C	2.64	0.40
1:B:70:SER:HA	1:B:71:PRO:HD3	1.89	0.40
1:E:89:ARG:HB2	1:E:96:ASP:CB	2.46	0.40
1:E:220:GLU:HA	1:E:220:GLU:OE1	2.22	0.40
1:H:390:ILE:HG21	1:H:390:ILE:HD13	1.93	0.40

All (2) 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)
3:C:864:HOH:O	3:D:864:HOH:O[1_655]	2.04	0.16
3:A:998:HOH:O	3:D:946:HOH:O[2_646]	2.16	0.04

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	402/410 (98%)	391 (97%)	11 (3%)	0	100	100
1	B	395/410 (96%)	381 (96%)	14 (4%)	0	100	100
1	C	398/410 (97%)	386 (97%)	11 (3%)	1 (0%)	36	21
1	D	397/410 (97%)	385 (97%)	12 (3%)	0	100	100
1	E	397/410 (97%)	386 (97%)	11 (3%)	0	100	100
1	F	402/410 (98%)	389 (97%)	12 (3%)	1 (0%)	43	27
1	G	394/410 (96%)	376 (95%)	16 (4%)	2 (0%)	24	11
1	H	378/410 (92%)	360 (95%)	18 (5%)	0	100	100
All	All	3163/3280 (96%)	3054 (97%)	105 (3%)	4 (0%)	48	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	104	GLN
1	G	92	ASP
1	C	102	PRO
1	G	102	PRO

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	333/338 (98%)	327 (98%)	6 (2%)	51	33
1	B	328/338 (97%)	317 (97%)	11 (3%)	32	13
1	C	332/338 (98%)	316 (95%)	16 (5%)	23	6
1	D	331/338 (98%)	321 (97%)	10 (3%)	36	16
1	E	332/338 (98%)	323 (97%)	9 (3%)	39	19
1	F	333/338 (98%)	319 (96%)	14 (4%)	26	8
1	G	328/338 (97%)	316 (96%)	12 (4%)	30	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	317/338 (94%)	298 (94%)	19 (6%)	17 3
All	All	2634/2704 (97%)	2537 (96%)	97 (4%)	30 11

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LYS
1	A	226	ASN
1	A	257	LEU
1	A	263	ARG
1	A	316	ARG
1	A	348	LEU
1	B	19	GLN
1	B	30	LEU
1	B	32	LEU
1	B	50	GLU
1	B	86	THR
1	B	96	ASP
1	B	226	ASN
1	B	257	LEU
1	B	296	SER
1	B	339	LYS
1	B	390	ILE
1	C	22	LYS
1	C	50	GLU
1	C	58	LYS
1	C	84	LYS
1	C	85	LEU
1	C	86	THR
1	C	89	ARG
1	C	97	ILE
1	C	101	GLU
1	C	103	ASP
1	C	231	SER
1	C	326	LYS
1	C	346	GLU
1	C	373	ILE
1	C	374	PRO
1	C	404	LEU
1	D	27	ARG
1	D	84	LYS
1	D	89	ARG

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Mol	Chain	Res	Type
1	D	96	ASP
1	D	97	ILE
1	D	101	GLU
1	D	104	GLN
1	D	159	LEU
1	D	263	ARG
1	D	373	ILE
1	E	32	LEU
1	E	58	LYS
1	E	76	GLN
1	E	103	ASP
1	E	226	ASN
1	E	248	LYS
1	E	257	LEU
1	E	268	LEU
1	E	385	THR
1	F	58	LYS
1	F	84	LYS
1	F	96	ASP
1	F	103	ASP
1	F	114	LYS
1	F	150	LEU
1	F	194	LYS
1	F	231	SER
1	F	248	LYS
1	F	258	ARG
1	F	304	LYS
1	F	329	LEU
1	F	372	THR
1	F	373	ILE
1	G	55	GLN
1	G	84	LYS
1	G	97	ILE
1	G	114	LYS
1	G	134	LYS
1	G	226	ASN
1	G	255	ASP
1	G	298	LEU
1	G	339	LYS
1	G	346	GLU
1	G	397	PRO
1	G	399	LEU

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Mol	Chain	Res	Type
1	H	33	THR
1	H	53	PHE
1	H	56	VAL
1	H	66	LYS
1	H	103	ASP
1	H	104	GLN
1	H	134	LYS
1	H	226	ASN
1	H	231	SER
1	H	248	LYS
1	H	257	LEU
1	H	285	VAL
1	H	300	PRO
1	H	305	ARG
1	H	324	ARG
1	H	339	LYS
1	H	346	GLU
1	H	348	LEU
1	H	374	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	78	GLN
1	A	94	ASN
1	A	104	GLN
1	A	125	HIS
1	A	290	GLN
1	B	19	GLN
1	B	41	HIS
1	B	76	GLN
1	B	78	GLN
1	B	106	HIS
1	B	260	GLN
1	B	375	HIS
1	C	78	GLN
1	C	94	ASN
1	C	106	HIS
1	C	290	GLN
1	D	41	HIS
1	D	45	ASN

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Mol	Chain	Res	Type
1	D	78	GLN
1	D	290	GLN
1	E	8	ASN
1	E	41	HIS
1	E	55	GLN
1	E	76	GLN
1	E	78	GLN
1	E	138	GLN
1	E	226	ASN
1	E	343	HIS
1	F	78	GLN
1	F	343	HIS
1	G	55	GLN
1	G	78	GLN
1	G	104	GLN
1	G	138	GLN
1	G	204	GLN
1	G	343	HIS
1	H	41	HIS
1	H	78	GLN
1	H	104	GLN
1	H	226	ASN
1	H	260	GLN
1	H	354	GLN

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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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	404/410 (98%)	-0.19	0 100 100	13, 21, 37, 48	0
1	B	399/410 (97%)	0.66	27 (6%) 23 27	21, 32, 52, 67	0
1	C	402/410 (98%)	0.05	20 (4%) 34 39	14, 23, 51, 79	0
1	D	401/410 (97%)	0.05	14 (3%) 47 53	14, 24, 53, 68	0
1	E	401/410 (97%)	-0.03	14 (3%) 47 53	13, 22, 46, 63	0
1	F	404/410 (98%)	0.24	4 (0%) 79 84	18, 28, 45, 58	0
1	G	398/410 (97%)	0.46	17 (4%) 40 46	19, 31, 54, 68	0
1	H	384/410 (93%)	0.85	46 (11%) 9 10	19, 33, 63, 85	0
All	All	3193/3280 (97%)	0.26	142 (4%) 39 45	13, 27, 52, 85	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	54	VAL	5.7
1	G	52	GLY	5.6
1	H	53	PHE	5.2
1	E	90	PHE	5.1
1	H	312	VAL	4.9
1	B	98	ALA	4.6
1	C	86	THR	4.4
1	D	93	GLY	4.3
1	B	104	GLN	4.2
1	H	102	PRO	4.2
1	H	114	LYS	4.2
1	H	322	PHE	3.9
1	F	144	LEU	3.9
1	H	43	LEU	3.9
1	H	85	LEU	3.8
1	G	7	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	48	THR	3.8
1	B	88	ILE	3.7
1	E	95	PHE	3.7
1	H	229	ALA	3.7
1	B	24	VAL	3.6
1	G	102	PRO	3.5
1	D	94	ASN	3.5
1	C	102	PRO	3.5
1	G	6	HIS	3.5
1	C	98	ALA	3.5
1	H	47	ILE	3.5
1	C	87	ASP	3.4
1	C	100	PRO	3.4
1	H	324	ARG	3.4
1	C	46	GLY	3.3
1	C	94	ASN	3.3
1	H	42	CYS	3.3
1	H	316	ARG	3.3
1	H	6	HIS	3.3
1	F	6	HIS	3.2
1	B	90	PHE	3.2
1	G	100	PRO	3.1
1	D	230	GLU	3.1
1	C	54	VAL	3.0
1	H	56	VAL	3.0
1	C	105	ALA	3.0
1	B	97	ILE	3.0
1	G	93	GLY	3.0
1	B	87	ASP	3.0
1	C	97	ILE	2.9
1	B	91	GLY	2.9
1	D	97	ILE	2.9
1	C	95	PHE	2.8
1	H	40	ALA	2.8
1	H	309	ALA	2.8
1	H	46	GLY	2.8
1	D	87	ASP	2.8
1	H	301	ALA	2.8
1	B	144	LEU	2.8
1	H	277	ASP	2.8
1	H	306	HIS	2.8
1	H	228	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	101	GLU	2.7
1	B	350	LEU	2.7
1	E	94	ASN	2.7
1	D	85	LEU	2.7
1	B	28	ILE	2.7
1	D	47	ILE	2.7
1	G	92	ASP	2.7
1	H	308	ARG	2.6
1	D	101	GLU	2.6
1	C	52	GLY	2.6
1	B	105	ALA	2.6
1	G	328	ALA	2.6
1	D	102	PRO	2.6
1	C	93	GLY	2.6
1	D	259	ARG	2.6
1	H	111	ASP	2.6
1	H	234	ASP	2.6
1	H	328	ALA	2.6
1	B	85	LEU	2.5
1	B	32	LEU	2.5
1	H	38	ALA	2.5
1	C	230	GLU	2.5
1	H	66	LYS	2.4
1	E	88	ILE	2.4
1	B	83	PRO	2.4
1	C	85	LEU	2.4
1	D	100	PRO	2.4
1	H	59	THR	2.4
1	H	255	ASP	2.4
1	H	321	ASP	2.4
1	B	84	LYS	2.4
1	E	97	ILE	2.4
1	C	96	ASP	2.3
1	H	110	PHE	2.3
1	H	398	GLY	2.3
1	G	114	LYS	2.3
1	G	409	ILE	2.3
1	H	238	SER	2.3
1	E	102	PRO	2.3
1	C	51	GLU	2.2
1	E	101	GLU	2.2
1	G	318	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	ARG	2.2
1	G	144	LEU	2.2
1	F	103	ASP	2.2
1	B	18	VAL	2.2
1	G	54	VAL	2.2
1	B	86	THR	2.2
1	E	89	ARG	2.2
1	B	186	CYS	2.2
1	E	96	ASP	2.2
1	B	261	GLY	2.2
1	H	112	ILE	2.2
1	H	297	PRO	2.2
1	B	169	ALA	2.2
1	C	92	ASP	2.2
1	H	105	ALA	2.2
1	H	57	TYR	2.2
1	H	71	PRO	2.2
1	E	231	SER	2.2
1	H	285	VAL	2.1
1	D	6	HIS	2.1
1	H	399	LEU	2.1
1	E	113	LYS	2.1
1	B	93	GLY	2.1
1	B	109	LEU	2.1
1	H	32	LEU	2.1
1	B	322	PHE	2.1
1	D	88	ILE	2.1
1	B	21	ALA	2.1
1	E	55	GLN	2.1
1	G	55	GLN	2.1
1	H	350	LEU	2.1
1	G	23	PRO	2.1
1	E	323	GLU	2.0
1	C	55	GLN	2.0
1	D	55	GLN	2.0
1	B	82	PHE	2.0
1	G	380	TYR	2.0
1	H	35	TYR	2.0
1	F	255	ASP	2.0
1	H	279	ALA	2.0
1	G	386	VAL	2.0
1	E	6	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	B	501	1/1	0.97	0.04	25,25,25,25	0
2	NA	G	501	1/1	0.97	0.05	25,25,25,25	0
2	NA	H	501	1/1	0.97	0.04	28,28,28,28	0
2	NA	A	501	1/1	0.98	0.03	20,20,20,20	0
2	NA	F	501	1/1	0.98	0.05	27,27,27,27	0
2	NA	E	501	1/1	0.99	0.04	19,19,19,19	0
2	NA	C	501	1/1	0.99	0.03	19,19,19,19	0
2	NA	D	501	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.