Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 01:23 PM JST

PDB ID	:	4XLZ
Title	:	N,N'-diacetylchitobiose deacetylase (SeMet derivative) from Pyrococcus furiosus in the presence of cadmium
Authors	:	Nakamura, T.; Niiyama, M.; Hashimoto, W.; Ida, K.; Uegaki, K.
Deposited on	:	2015-01-14
Resolution	:	1.51 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 (i) 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 (i)) were used in the production of this report:

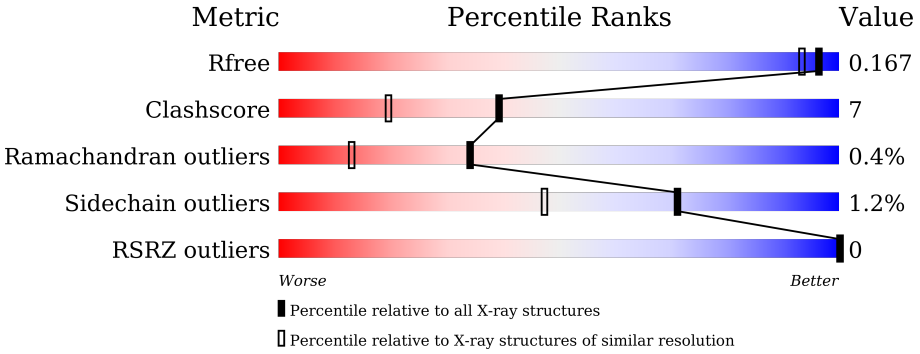
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	267	77% 21% •
1	B	267	75% 23% •
1	C	267	73% 23% •
1	D	267	79% 18% •
1	E	267	72% 25% •
1	F	267	80% 18% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEZ	A	306	-	-	X	-
3	HEZ	D	307	-	-	X	-
3	HEZ	D	311	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15060 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.

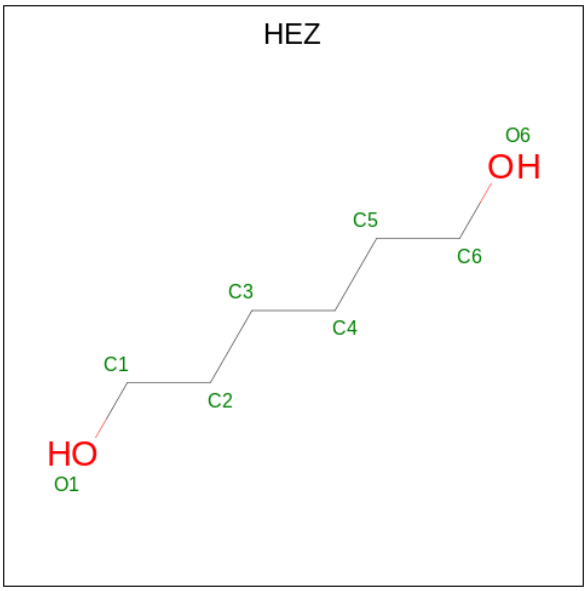
- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	267	2197	1421	362	404	3	7	0	1	0
1	B	267	2197	1421	362	404	3	7	0	1	0
1	C	267	2197	1421	362	404	3	7	0	1	0
1	D	267	2197	1421	362	404	3	7	0	1	0
1	E	267	2197	1421	362	404	3	7	0	1	0
1	F	267	2197	1421	362	404	3	7	0	1	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	A	4	4	4	0	0
2	B	3	3	3	0	0
2	C	2	2	2	0	0
2	D	4	4	4	0	0
2	E	3	3	3	0	0
2	F	2	2	2	0	0

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	B	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	C	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	D	1	8	6	2		0	0
3	E	1	8	6	2		0	0
3	E	1	8	6	2		0	0
3	E	1	8	6	2		0	0
3	E	1	8	6	2		0	0
3	E	1	8	6	2		0	0

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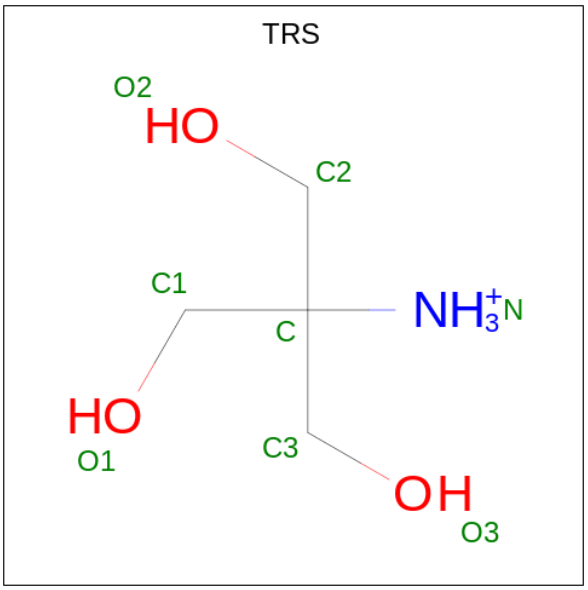
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	E	1	8	6	2		0	0
			Total	C	O			
3	E	1	8	6	2		0	0
			Total	C	O			
3	E	1	8	6	2		0	0
			Total	C	O			
3	E	1	8	6	2		0	0
			Total	C	O			
3	F	1	8	6	2		0	0
			Total	C	O			
3	F	1	8	6	2		0	0
			Total	C	O			
3	F	1	8	6	2		0	0
			Total	C	O			
3	F	1	8	6	2		0	0
			Total	C	O			
3	F	1	8	6	2		0	0
			Total	C	O			
3	F	1	8	6	2		0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0
4	B	1	8	4	1	3	0	0
4	C	1	8	4	1	3	0	0
4	D	1	8	4	1	3	0	0
4	D	1	8	4	1	3	0	0
4	E	1	8	4	1	3	0	0
4	F	1	8	4	1	3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	5	5	5	0	0
5	B	4	4	4	0	0
5	C	3	3	3	0	0
5	D	5	5	5	0	0
5	E	4	4	4	0	0
5	F	3	3	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	238	238	238	0	0
6	B	219	219	219	0	0
6	C	243	243	243	0	0
6	D	236	236	236	0	0

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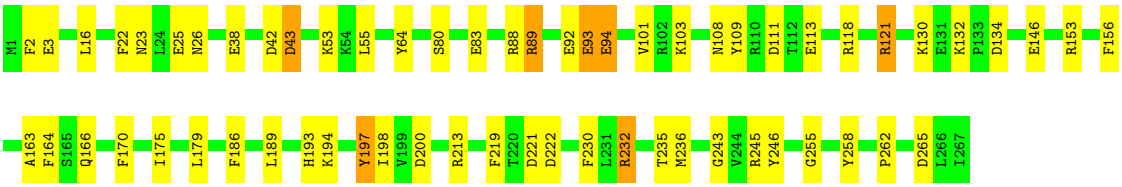
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	E	235	235	235	0	0
			Total	O		
6	F	241	241	241	0	0

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.

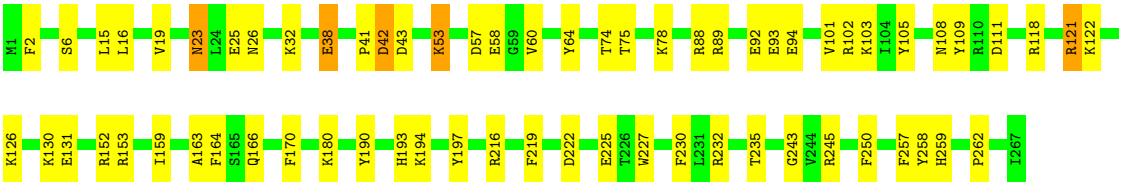
• Molecule 1: Uncharacterized protein

Chain A:



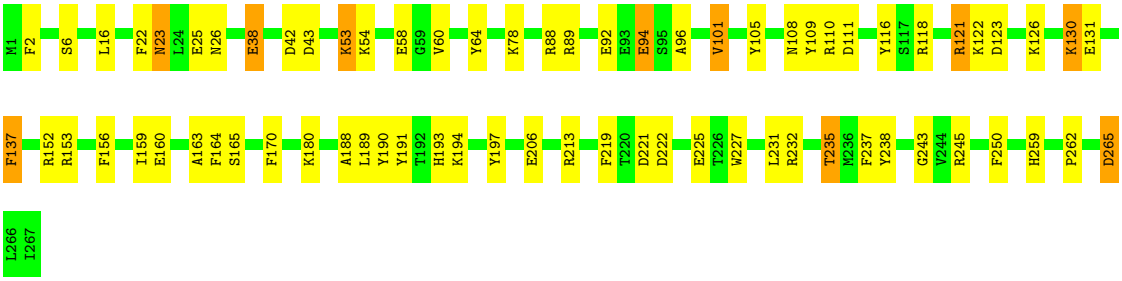
• Molecule 1: Uncharacterized protein

Chain B:



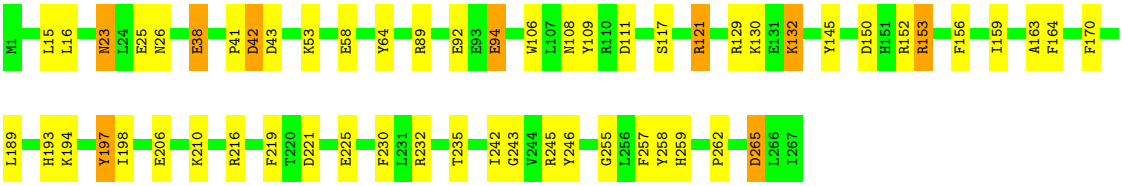
• Molecule 1: Uncharacterized protein

Chain C:



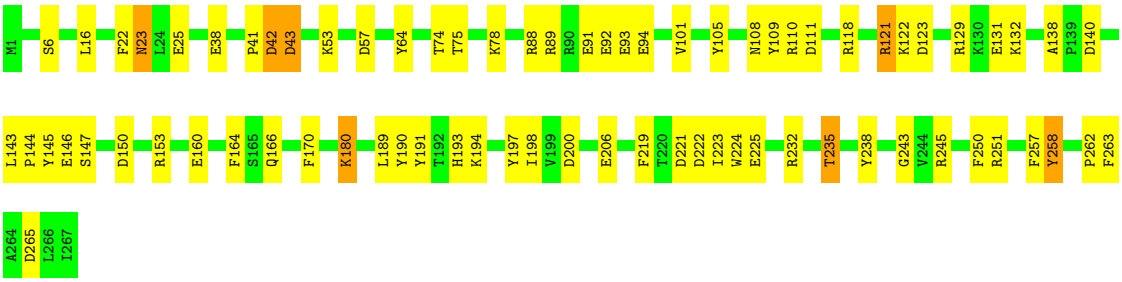
• Molecule 1: Uncharacterized protein

Chain D:



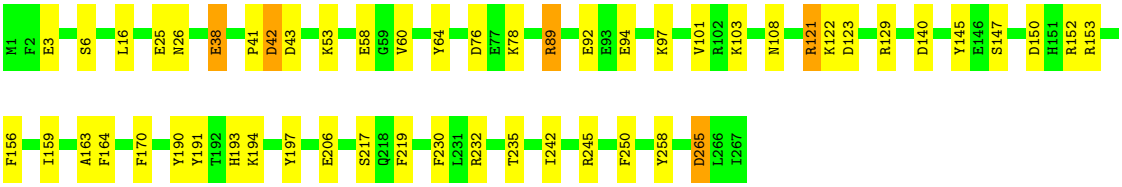
- Molecule 1: Uncharacterized protein

Chain E:



- Molecule 1: Uncharacterized protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.89Å 93.88Å 93.88Å 74.69° 74.68° 74.68°	Depositor
Resolution (Å)	31.16 – 1.51 31.16 – 1.51	Depositor EDS
% Data completeness (in resolution range)	95.7 (31.16-1.51) 95.5 (31.16-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.152 , 0.167 0.152 , 0.167	Depositor DCC
R_{free} test set	21852 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.457 for k,l,h 0.457 for l,h,k 0.458 for -h,-l,-k 0.457 for -k,-h,-l 0.459 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	15060	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEZ, TRS, CD, CL

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	1.68	25/2253 (1.1%)	1.61	37/3038 (1.2%)
1	B	1.66	28/2253 (1.2%)	1.63	38/3038 (1.3%)
1	C	1.72	25/2253 (1.1%)	1.64	40/3038 (1.3%)
1	D	1.68	19/2253 (0.8%)	1.63	35/3038 (1.2%)
1	E	1.69	26/2253 (1.2%)	1.68	41/3038 (1.3%)
1	F	1.65	19/2253 (0.8%)	1.54	30/3038 (1.0%)
All	All	1.68	142/13518 (1.1%)	1.62	221/18228 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	7

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	94	GLU	CD-OE2	15.69	1.43	1.25
1	C	94	GLU	CG-CD	13.87	1.72	1.51
1	D	132	LYS	CG-CD	-11.52	1.13	1.52
1	E	166	GLN	CB-CG	-8.00	1.30	1.52
1	C	219	PHE	CE1-CZ	7.76	1.52	1.37
1	F	217	SER	C-O	-7.73	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLN	CB-CG	-7.67	1.31	1.52
1	F	190	TYR	CG-CD1	7.50	1.48	1.39
1	F	53	LYS	CD-CE	7.38	1.69	1.51
1	E	6	SER	CB-OG	-7.31	1.32	1.42
1	C	64	TYR	CD1-CE1	7.16	1.50	1.39
1	B	6	SER	CB-OG	-7.14	1.32	1.42
1	F	153	ARG	CZ-NH2	7.04	1.42	1.33
1	D	108	ASN	CG-ND2	-7.02	1.15	1.32
1	B	108	ASN	CG-ND2	-6.94	1.15	1.32
1	E	219	PHE	CE1-CZ	6.92	1.50	1.37
1	C	108	ASN	CG-ND2	-6.89	1.15	1.32
1	D	206	GLU	CG-CD	6.84	1.62	1.51
1	D	219	PHE	CE1-CZ	6.82	1.50	1.37
1	A	108	ASN	CG-ND2	-6.80	1.15	1.32
1	A	93	GLU	CB-CG	6.80	1.65	1.52
1	F	147	SER	CB-OG	6.73	1.51	1.42
1	C	160	GLU	CG-CD	6.71	1.62	1.51
1	D	64	TYR	CD1-CE1	6.71	1.49	1.39
1	C	197	TYR	CD2-CE2	6.62	1.49	1.39
1	A	113	GLU	CD-OE2	6.57	1.32	1.25
1	D	225	GLU	CG-CD	6.55	1.61	1.51
1	B	216	ARG	CG-CD	6.47	1.68	1.51
1	F	64	TYR	CD1-CE1	6.46	1.49	1.39
1	F	206	GLU	CD-OE2	6.44	1.32	1.25
1	A	94	GLU	CG-CD	6.35	1.61	1.51
1	C	122	LYS	CE-NZ	6.30	1.64	1.49
1	C	2	PHE	CE2-CZ	6.29	1.49	1.37
1	E	243	GLY	N-CA	6.22	1.55	1.46
1	D	92	GLU	CD-OE2	6.17	1.32	1.25
1	D	132	LYS	CB-CG	-6.17	1.35	1.52
1	C	243	GLY	N-CA	6.15	1.55	1.46
1	B	170	PHE	CD2-CE2	6.15	1.51	1.39
1	C	131	GLU	CD-OE1	-6.12	1.19	1.25
1	F	108	ASN	CG-ND2	-6.11	1.17	1.32
1	C	130	LYS	CD-CE	6.05	1.66	1.51
1	E	122	LYS	CE-NZ	6.05	1.64	1.49
1	A	3	GLU	CG-CD	-6.04	1.42	1.51
1	B	219	PHE	CE1-CZ	6.02	1.48	1.37
1	E	140	ASP	CG-OD2	-6.02	1.11	1.25
1	A	219	PHE	N-CA	6.00	1.58	1.46
1	A	243	GLY	N-CA	5.93	1.54	1.46
1	A	153	ARG	CZ-NH2	5.91	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	ARG	CZ-NH2	5.91	1.40	1.33
1	B	216	ARG	CZ-NH2	5.91	1.40	1.33
1	E	92	GLU	CD-OE2	5.91	1.32	1.25
1	A	101	VAL	CB-CG1	5.91	1.65	1.52
1	E	225	GLU	CD-OE1	5.91	1.32	1.25
1	B	93	GLU	CB-CG	5.89	1.63	1.52
1	C	190	TYR	CG-CD1	5.89	1.46	1.39
1	C	250	PHE	CE1-CZ	5.89	1.48	1.37
1	A	213	ARG	CZ-NH1	5.88	1.40	1.33
1	E	91	GLU	CD-OE1	5.86	1.32	1.25
1	C	101	VAL	CB-CG1	5.85	1.65	1.52
1	A	53	LYS	CD-CE	5.82	1.65	1.51
1	F	219	PHE	CE1-CZ	5.81	1.48	1.37
1	B	225	GLU	CG-CD	5.79	1.60	1.51
1	C	6	SER	CA-CB	5.78	1.61	1.52
1	A	53	LYS	CB-CG	5.77	1.68	1.52
1	E	146	GLU	CG-CD	5.77	1.60	1.51
1	B	243	GLY	N-CA	5.76	1.54	1.46
1	F	122	LYS	CE-NZ	5.74	1.63	1.49
1	B	250	PHE	CE1-CZ	5.74	1.48	1.37
1	D	38	GLU	CD-OE1	-5.72	1.19	1.25
1	C	109	TYR	CD2-CE2	5.69	1.47	1.39
1	B	216	ARG	NE-CZ	5.69	1.40	1.33
1	D	170	PHE	CD2-CE2	5.68	1.50	1.39
1	C	94	GLU	CB-CG	5.67	1.62	1.52
1	A	130	LYS	CD-CE	5.65	1.65	1.51
1	B	216	ARG	CD-NE	5.63	1.56	1.46
1	B	19	VAL	CB-CG2	5.62	1.64	1.52
1	D	219	PHE	N-CA	5.61	1.57	1.46
1	E	206	GLU	CG-CD	5.59	1.60	1.51
1	F	103	LYS	CE-NZ	5.58	1.63	1.49
1	B	258	TYR	CG-CD2	5.58	1.46	1.39
1	A	132	LYS	CE-NZ	5.57	1.62	1.49
1	F	101	VAL	CB-CG1	5.57	1.64	1.52
1	D	106	TRP	CD1-NE1	5.52	1.47	1.38
1	B	126	LYS	CE-NZ	5.52	1.62	1.49
1	F	6	SER	CA-CB	5.49	1.61	1.52
1	A	64	TYR	CD1-CE1	5.47	1.47	1.39
1	E	197	TYR	CD2-CE2	5.47	1.47	1.39
1	F	38	GLU	CD-OE1	-5.47	1.19	1.25
1	F	3	GLU	CG-CD	-5.43	1.43	1.51
1	C	225	GLU	CG-CD	5.42	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	GLU	CD-OE2	5.42	1.31	1.25
1	E	110	ARG	CZ-NH2	5.42	1.40	1.33
1	F	250	PHE	CE1-CZ	5.41	1.47	1.37
1	C	38	GLU	CD-OE1	-5.41	1.19	1.25
1	E	64	TYR	CD2-CE2	5.40	1.47	1.39
1	C	105	TYR	CG-CD1	5.40	1.46	1.39
1	D	206	GLU	CD-OE2	5.40	1.31	1.25
1	E	160	GLU	CG-CD	5.40	1.60	1.51
1	C	191	TYR	CD2-CE2	5.39	1.47	1.39
1	B	166	GLN	CG-CD	5.38	1.63	1.51
1	B	53	LYS	CB-CG	5.37	1.67	1.52
1	E	143	LEU	N-CA	5.35	1.57	1.46
1	D	117	SER	C-O	-5.34	1.13	1.23
1	C	206	GLU	CG-CD	5.34	1.59	1.51
1	B	190	TYR	C-O	-5.33	1.13	1.23
1	E	108	ASN	CG-ND2	-5.32	1.19	1.32
1	F	206	GLU	CG-CD	5.30	1.59	1.51
1	C	53	LYS	CB-CG	5.30	1.66	1.52
1	B	122	LYS	CE-NZ	5.27	1.62	1.49
1	A	2	PHE	CE1-CZ	5.25	1.47	1.37
1	F	53	LYS	CB-CG	5.25	1.66	1.52
1	B	130	LYS	CD-CE	5.23	1.64	1.51
1	D	243	GLY	N-CA	5.23	1.53	1.46
1	B	227	TRP	CG-CD1	5.22	1.44	1.36
1	A	255	GLY	N-CA	5.22	1.53	1.46
1	A	230	PHE	CD1-CE1	5.21	1.49	1.39
1	E	147	SER	CB-OG	5.20	1.49	1.42
1	C	213	ARG	CG-CD	5.19	1.65	1.51
1	A	219	PHE	CE1-CZ	5.16	1.47	1.37
1	B	60	VAL	N-CA	5.16	1.56	1.46
1	A	94	GLU	CB-CG	5.15	1.61	1.52
1	A	186	PHE	CG-CD2	5.15	1.46	1.38
1	A	134	ASP	CA-CB	5.14	1.65	1.53
1	D	130	LYS	CD-CE	5.13	1.64	1.51
1	E	224	TRP	CG-CD1	5.13	1.44	1.36
1	F	258	TYR	CG-CD2	5.11	1.45	1.39
1	E	180	LYS	CD-CE	5.09	1.64	1.51
1	E	88	ARG	NE-CZ	5.09	1.39	1.33
1	A	83	GLU	CD-OE2	5.09	1.31	1.25
1	E	219	PHE	N-CA	5.08	1.56	1.46
1	D	94	GLU	CG-CD	5.08	1.59	1.51
1	D	258	TYR	C-O	-5.05	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	153	ARG	CZ-NH2	5.05	1.39	1.33
1	E	93	GLU	CB-CG	5.05	1.61	1.52
1	A	103	LYS	CE-NZ	5.04	1.61	1.49
1	B	103	LYS	CE-NZ	5.04	1.61	1.49
1	E	101	VAL	CB-CG2	-5.04	1.42	1.52
1	A	170	PHE	CD2-CE2	5.04	1.49	1.39
1	B	101	VAL	CB-CG1	5.03	1.63	1.52
1	B	170	PHE	CD1-CE1	5.03	1.49	1.39
1	D	255	GLY	N-CA	5.03	1.53	1.46
1	E	190	TYR	CG-CD1	5.03	1.45	1.39

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	140	ASP	CB-CG-OD1	-15.82	104.06	118.30
1	B	216	ARG	NE-CZ-NH2	14.64	127.62	120.30
1	D	153	ARG	NE-CZ-NH2	-14.15	113.22	120.30
1	E	129	ARG	NE-CZ-NH1	-11.97	114.31	120.30
1	E	232	ARG	NE-CZ-NH2	-11.89	114.36	120.30
1	B	153	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	F	164	PHE	CB-CG-CD2	-11.69	112.62	120.80
1	E	121	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	64	TYR	CB-CG-CD2	-11.52	114.09	121.00
1	F	170	PHE	CB-CG-CD1	-11.46	112.78	120.80
1	B	232	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	D	64	TYR	CB-CG-CD2	-10.53	114.68	121.00
1	C	153	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	B	153	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	B	164	PHE	CB-CG-CD2	-10.00	113.80	120.80
1	C	64	TYR	CB-CG-CD2	-9.98	115.02	121.00
1	C	152	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	E	153	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	A	88	ARG	NE-CZ-NH1	-9.78	115.41	120.30
1	E	140	ASP	CB-CG-OD2	9.76	127.08	118.30
1	F	121	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	B	245	ARG	NE-CZ-NH2	9.28	124.94	120.30
1	A	170	PHE	CB-CG-CD1	-9.20	114.36	120.80
1	E	64	TYR	CB-CG-CD2	-9.18	115.50	121.00
1	E	121	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	D	153	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	A	121	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	121	ARG	NE-CZ-NH1	8.91	124.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	A	111	ASP	CB-CG-OD1	8.84	126.25	118.30
1	C	245	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	D	121	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	D	245	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	A	245	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	B	16	LEU	CB-CG-CD1	-8.20	97.05	111.00
1	B	2	PHE	CB-CG-CD1	8.19	126.53	120.80
1	F	153	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	16	LEU	CB-CG-CD1	-8.09	97.24	111.00
1	B	118	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	F	16	LEU	CB-CG-CD1	-7.92	97.54	111.00
1	B	152	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	232	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	F	64	TYR	CB-CG-CD2	-7.83	116.31	121.00
1	D	111	ASP	CB-CG-OD1	7.75	125.28	118.30
1	A	164	PHE	CB-CG-CD2	-7.74	115.38	120.80
1	C	232	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	221	ASP	CB-CG-OD2	7.72	125.25	118.30
1	D	64	TYR	CD1-CE1-CZ	-7.65	112.91	119.80
1	F	53	LYS	CD-CE-NZ	-7.60	94.23	111.70
1	C	238	TYR	CB-CG-CD2	-7.56	116.46	121.00
1	A	265	ASP	CB-CG-OD1	7.55	125.10	118.30
1	C	170	PHE	CB-CG-CD1	-7.49	115.56	120.80
1	C	92	GLU	OE1-CD-OE2	-7.47	114.33	123.30
1	B	111	ASP	CB-CG-OD1	7.46	125.01	118.30
1	B	216	ARG	NE-CZ-NH1	-7.36	116.62	120.30
1	F	92	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	E	170	PHE	CB-CG-CD1	-7.36	115.65	120.80
1	F	245	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	E	153	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	E	43	ASP	CB-CG-OD2	7.23	124.81	118.30
1	B	216	ARG	CD-NE-CZ	7.17	133.64	123.60
1	F	235	THR	CA-CB-CG2	-7.13	102.42	112.40
1	B	235	THR	CA-CB-CG2	-7.12	102.43	112.40
1	C	111	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	C	111	ASP	CB-CG-OD1	7.10	124.69	118.30
1	E	88	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	E	16	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	D	232	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	D	129	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	C	16	LEU	CB-CG-CD1	-6.97	99.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2	PHE	CB-CG-CD2	-6.95	115.93	120.80
1	D	265	ASP	CB-CG-OD1	6.94	124.54	118.30
1	A	153	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	C	110	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	B	121	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	B	64	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C	237	PHE	CB-CG-CD1	-6.89	115.98	120.80
1	D	16	LEU	CB-CG-CD1	-6.86	99.33	111.00
1	B	121	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	152	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	53	LYS	CD-CE-NZ	-6.76	96.16	111.70
1	C	130	LYS	CD-CE-NZ	-6.67	96.35	111.70
1	E	64	TYR	CD1-CE1-CZ	-6.67	113.80	119.80
1	B	131	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	F	123	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	57	ASP	CB-CG-OD1	6.64	124.27	118.30
1	E	265	ASP	CB-CG-OD1	6.62	124.26	118.30
1	E	145	TYR	CB-CG-CD1	-6.61	117.04	121.00
1	C	235	THR	CA-CB-CG2	-6.51	103.28	112.40
1	C	121	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	197	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	C	265	ASP	CB-CG-OD1	6.46	124.12	118.30
1	D	117	SER	CA-C-N	-6.45	103.01	117.20
1	B	227	TRP	CA-CB-CG	-6.42	101.51	113.70
1	F	265	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	64	TYR	CD1-CE1-CZ	-6.35	114.08	119.80
1	C	118	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	D	132	LYS	CA-CB-CG	-6.32	99.50	113.40
1	C	126	LYS	CD-CE-NZ	-6.29	97.25	111.70
1	C	94	GLU	CG-CD-OE2	6.28	130.86	118.30
1	E	118	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	E	92	GLU	OE1-CD-OE2	-6.25	115.81	123.30
1	D	89	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	102	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	D	164	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	A	153	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	F	232	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	111	ASP	CB-CG-OD2	-6.08	112.82	118.30
1	A	118	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	B	109	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	C	64	TYR	CD1-CE1-CZ	-6.02	114.38	119.80
1	A	175	ILE	CG1-CB-CG2	-6.02	98.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	88	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	C	156	PHE	CB-CG-CD2	-5.96	116.63	120.80
1	B	92	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	D	235	THR	CA-CB-CG2	-5.90	104.14	112.40
1	D	92	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	E	109	TYR	CZ-CE2-CD2	-5.89	114.50	119.80
1	A	64	TYR	CD1-CE1-CZ	-5.88	114.51	119.80
1	F	140	ASP	CB-CG-OD2	5.86	123.57	118.30
1	F	230	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	E	105	TYR	CB-CG-CD2	-5.82	117.50	121.00
1	F	191	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	15	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	F	164	PHE	CB-CG-CD1	5.72	124.80	120.80
1	E	250	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	E	111	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	137	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	F	129	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	C	165	SER	O-C-N	5.66	131.75	122.70
1	E	57	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	246	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	A	179	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	A	189	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	C	60	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	B	105	TYR	CD1-CE1-CZ	-5.57	114.79	119.80
1	E	111	ASP	N-CA-CB	-5.57	100.58	110.60
1	E	257	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	258	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	F	89	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	230	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	C	227	TRP	CA-CB-CG	-5.53	103.19	113.70
1	B	126	LYS	CD-CE-NZ	-5.52	99.00	111.70
1	E	238	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
1	E	263	PHE	CB-CG-CD2	5.50	124.65	120.80
1	C	123	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	E	22	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	A	235	THR	CA-CB-CG2	-5.49	104.71	112.40
1	E	200	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	164	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	E	235	THR	CA-CB-CG2	-5.47	104.75	112.40
1	E	123	ASP	CB-CG-OD1	5.46	123.22	118.30
1	E	258	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	B	102	ARG	NE-CZ-NH2	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	TYR	CZ-CE2-CD2	-5.44	114.91	119.80
1	A	156	PHE	CB-CG-CD2	-5.44	117.00	120.80
1	D	109	TYR	CZ-CE2-CD2	-5.42	114.92	119.80
1	A	55	LEU	CB-CG-CD2	5.42	120.21	111.00
1	C	164	PHE	CB-CG-CD2	-5.42	117.01	120.80
1	B	258	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	D	15	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	F	60	VAL	CG1-CB-CG2	-5.38	102.30	110.90
1	B	257	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	A	146	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	A	265	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	E	131	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	F	156	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	D	132	LYS	CG-CD-CE	-5.34	95.88	111.90
1	B	170	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	C	111	ASP	N-CA-CB	-5.32	101.02	110.60
1	F	152	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	200	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	257	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	43	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	88	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	C	109	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	C	152	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	22	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	A	22	PHE	CZ-CE2-CD2	-5.28	113.76	120.10
1	C	153	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	164	PHE	CB-CG-CD1	5.28	124.50	120.80
1	D	246	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	C	116	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	F	150	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	150	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	190	TYR	CG-CD1-CE1	-5.25	117.10	121.30
1	D	156	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	C	122	LYS	CD-CE-NZ	-5.23	99.66	111.70
1	A	111	ASP	N-CA-CB	-5.23	101.19	110.60
1	F	265	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	219	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	E	251	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	C	190	TYR	CG-CD1-CE1	-5.20	117.14	121.30
1	A	164	PHE	CB-CG-CD1	5.19	124.43	120.80
1	F	197	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	D	197	TYR	CG-CD1-CE1	-5.17	117.16	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	245	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	E	245	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	23	ASN	N-CA-CB	5.17	119.90	110.60
1	F	153	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	109	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	D	189	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	E	132	LYS	CD-CE-NZ	-5.14	99.88	111.70
1	D	210	LYS	CD-CE-NZ	-5.12	99.93	111.70
1	A	64	TYR	CB-CG-CD1	5.10	124.06	121.00
1	A	92	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	D	150	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	64	TYR	CE1-CZ-CE2	5.08	127.93	119.80
1	B	131	GLU	O-C-N	-5.07	114.58	122.70
1	E	219	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	D	145	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	B	111	ASP	N-CA-CB	-5.05	101.50	110.60
1	C	189	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	F	197	TYR	CG-CD1-CE1	-5.05	117.26	121.30
1	C	238	TYR	CD1-CG-CD2	5.05	123.45	117.90
1	F	170	PHE	CB-CG-CD2	5.05	124.33	120.80
1	D	230	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	E	64	TYR	CE1-CZ-CE2	5.02	127.83	119.80
1	B	64	TYR	CZ-CE2-CD2	-5.01	115.30	119.80
1	F	145	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	A	64	TYR	CE1-CZ-CE2	5.00	127.81	119.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	B	121	ARG	Sidechain
1	C	121	ARG	Sidechain
1	D	121	ARG	Sidechain
1	E	121	ARG	Sidechain
1	E	191	TYR	Sidechain
1	F	121	ARG	Sidechain

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	2197	0	2168	29	0
1	B	2197	0	2168	31	0
1	C	2197	0	2168	34	0
1	D	2197	0	2168	38	0
1	E	2197	0	2168	32	0
1	F	2197	0	2168	19	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
3	A	64	0	112	13	0
3	B	56	0	98	10	0
3	C	48	0	84	5	0
3	D	72	0	126	24	0
3	E	72	0	126	10	0
3	F	48	0	84	5	0
4	A	16	0	22	4	0
4	B	8	0	10	3	0
4	C	8	0	10	4	0
4	D	16	0	22	3	0
4	E	8	0	10	4	0
4	F	8	0	10	3	0
5	A	5	0	0	0	0
5	B	4	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	0	0
5	E	4	0	0	0	0
5	F	3	0	0	0	0
6	A	238	0	0	11	3
6	B	219	0	0	14	3
6	C	243	0	0	21	3
6	D	236	0	0	12	3
6	E	235	0	0	17	3
6	F	241	0	0	10	3
All	All	15060	0	13722	202	9

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 7.

All (202) 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:A:166:GLN:NE2	3:A:306:HEZ:H62	1.23	1.42
3:D:311:HEZ:H11	3:D:311:HEZ:C5	1.41	1.38
1:A:89:ARG:HD3	6:A:554:HOH:O	1.23	1.33
1:C:54:LYS:HE2	6:C:531:HOH:O	1.17	1.30
1:A:166:GLN:NE2	3:A:306:HEZ:C6	1.92	1.29
3:D:311:HEZ:H52	3:D:311:HEZ:C1	1.64	1.26
1:C:89:ARG:HD3	6:C:534:HOH:O	1.05	1.18
1:A:166:GLN:HE21	3:A:306:HEZ:C6	1.58	1.10
1:F:89:ARG:HD3	6:F:543:HOH:O	1.53	1.08
4:A:313:TRS:C3	6:A:637:HOH:O	2.02	1.07
4:D:314:TRS:C3	6:D:633:HOH:O	2.03	1.06
4:E:313:TRS:H21	6:E:634:HOH:O	1.56	1.06
4:E:313:TRS:C2	6:E:634:HOH:O	2.03	1.03
4:D:314:TRS:H31	6:D:633:HOH:O	1.55	1.02
1:D:153:ARG:HH12	3:D:311:HEZ:H62	1.21	1.02
3:D:311:HEZ:C5	3:D:311:HEZ:C1	2.29	1.02
4:C:309:TRS:C1	6:C:640:HOH:O	2.08	1.00
1:D:153:ARG:NH1	3:D:311:HEZ:H62	1.76	0.99
1:B:89:ARG:HD3	6:B:566:HOH:O	1.64	0.98
3:D:311:HEZ:H11	3:D:311:HEZ:H51	1.43	0.96
4:A:313:TRS:H31	6:A:637:HOH:O	1.63	0.94
1:E:23:ASN:HD21	1:E:25:GLU:HB2	1.30	0.94
4:A:313:TRS:O3	6:A:637:HOH:O	1.84	0.92
1:A:166:GLN:HE22	3:A:306:HEZ:C6	1.75	0.91
1:B:180:LYS:HE3	6:B:509:HOH:O	1.71	0.91
6:E:504:HOH:O	1:F:193[A]:HIS:CE1	2.23	0.90
1:D:216:ARG:HD3	6:D:591:HOH:O	1.72	0.89
1:D:23:ASN:HD21	1:D:25:GLU:HG2	1.37	0.89
1:E:222:ASP:HB2	6:E:406:HOH:O	1.72	0.89
4:F:309:TRS:C1	6:F:637:HOH:O	2.19	0.89
1:E:89:ARG:HD3	6:E:553:HOH:O	1.74	0.88
4:C:309:TRS:H11	6:C:640:HOH:O	1.70	0.88
3:D:311:HEZ:H11	3:D:311:HEZ:H52	0.88	0.87
1:D:193[A]:HIS:CE1	6:F:533:HOH:O	2.25	0.87
1:C:222:ASP:HB2	6:C:403:HOH:O	1.76	0.86
4:B:311:TRS:C3	6:B:619:HOH:O	2.23	0.85
1:B:222:ASP:HB2	6:B:402:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:309:TRS:O1	6:C:640:HOH:O	1.92	0.81
1:A:166:GLN:HE21	3:A:306:HEZ:H62	0.72	0.81
1:D:23:ASN:ND2	1:D:25:GLU:HG2	1.95	0.81
6:A:520:HOH:O	1:B:193[A]:HIS:CE1	2.32	0.80
4:F:309:TRS:H11	6:F:637:HOH:O	1.82	0.80
1:A:193[B]:HIS:CD2	6:A:525:HOH:O	2.35	0.80
1:B:75:THR:H	3:B:308:HEZ:H11	1.46	0.79
1:F:76:ASP:OD2	1:F:78:LYS:HG2	1.82	0.79
4:B:311:TRS:H31	6:B:619:HOH:O	1.80	0.78
3:A:308:HEZ:H61	6:C:591:HOH:O	1.84	0.77
1:D:153:ARG:HH12	3:D:311:HEZ:C6	1.97	0.77
1:A:166:GLN:NE2	3:A:306:HEZ:O6	2.17	0.77
1:D:23:ASN:HD21	1:D:25:GLU:CG	1.98	0.77
1:E:23:ASN:HD21	1:E:25:GLU:CB	1.98	0.77
1:B:53:LYS:HE2	6:B:524:HOH:O	1.83	0.76
1:C:159:ILE:CG2	3:C:306:HEZ:H51	2.15	0.76
1:E:23:ASN:ND2	1:E:25:GLU:HB2	2.01	0.75
1:C:23:ASN:HD22	1:C:25:GLU:H	1.34	0.75
1:D:58:GLU:HG3	3:D:313:HEZ:H22	1.72	0.72
1:C:222:ASP:CB	6:C:403:HOH:O	2.37	0.71
6:D:512:HOH:O	1:E:193[A]:HIS:HE1	1.69	0.70
3:E:309:HEZ:C6	6:E:562:HOH:O	2.42	0.68
1:A:193[A]:HIS:HE1	6:C:524:HOH:O	1.66	0.68
1:B:53:LYS:CE	6:B:524:HOH:O	2.37	0.68
1:E:223:ILE:CD1	3:E:307:HEZ:H31	2.24	0.66
1:A:80:SER:HB3	3:A:308:HEZ:H31	1.77	0.66
1:E:193[B]:HIS:CD2	6:E:523:HOH:O	2.47	0.65
1:D:265:ASP:OD2	6:D:512:HOH:O	2.14	0.65
1:C:159:ILE:HG23	3:C:306:HEZ:H51	1.78	0.64
1:E:193[B]:HIS:CE1	1:E:194:LYS:HE2	2.33	0.64
1:B:75:THR:H	3:B:308:HEZ:C1	2.11	0.64
1:F:265:ASP:OD2	6:F:533:HOH:O	2.15	0.64
1:B:222:ASP:CB	6:B:402:HOH:O	2.44	0.62
1:F:58:GLU:HG3	3:F:307:HEZ:H51	1.81	0.62
1:F:94:GLU:HG3	6:F:618:HOH:O	1.99	0.62
1:A:23:ASN:HD21	1:A:25:GLU:HB2	1.65	0.62
1:C:159:ILE:HG22	3:C:306:HEZ:H51	1.83	0.61
1:A:163:ALA:HB2	3:A:309:HEZ:H31	1.82	0.60
1:E:74:THR:HA	3:E:307:HEZ:H11	1.84	0.60
3:E:309:HEZ:H61	6:E:562:HOH:O	2.00	0.60
1:F:193[B]:HIS:CD2	6:F:518:HOH:O	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ASP:OD1	6:C:401:HOH:O	2.17	0.59
1:D:159:ILE:CG2	3:D:308:HEZ:H22	2.31	0.59
1:B:23:ASN:HD22	1:B:25:GLU:H	1.50	0.59
6:E:504:HOH:O	1:F:193[A]:HIS:HE1	1.72	0.58
1:E:222:ASP:CB	6:E:406:HOH:O	2.40	0.58
1:F:38:GLU:HB2	1:F:43:ASP:HB2	1.86	0.58
4:F:309:TRS:O1	6:F:637:HOH:O	2.02	0.58
1:D:193[A]:HIS:HE1	6:F:533:HOH:O	1.75	0.58
1:F:159:ILE:CG2	3:F:305:HEZ:H51	2.33	0.58
1:F:159:ILE:HG22	3:F:305:HEZ:H51	1.86	0.57
1:D:53:LYS:CE	6:D:511:HOH:O	2.51	0.57
1:E:258:TYR:HB2	3:E:308:HEZ:H51	1.85	0.57
4:A:313:TRS:O3	1:C:259:HIS:NE2	2.36	0.57
1:B:38:GLU:HB2	1:B:43:ASP:HB2	1.87	0.57
4:B:311:TRS:O3	6:B:619:HOH:O	2.05	0.56
1:D:23:ASN:HD21	1:D:25:GLU:CB	2.18	0.56
1:D:38:GLU:HB2	1:D:43:ASP:HB2	1.87	0.56
1:B:193[B]:HIS:HD2	6:B:417:HOH:O	1.89	0.55
1:E:75:THR:H	3:E:307:HEZ:C1	2.19	0.55
1:C:265:ASP:OD2	6:C:524:HOH:O	2.18	0.55
1:A:193[A]:HIS:HD2	1:C:262:PRO:O	1.88	0.55
4:E:313:TRS:O2	6:E:634:HOH:O	1.95	0.55
1:A:38:GLU:HB2	1:A:43:ASP:HB2	1.88	0.55
1:B:193[B]:HIS:CD2	6:B:497:HOH:O	2.59	0.54
1:E:193[B]:HIS:HD2	6:E:419:HOH:O	1.90	0.54
1:B:58:GLU:HG3	3:B:310:HEZ:H41	1.87	0.54
3:D:310:HEZ:H52	1:E:144:PRO:HB3	1.89	0.54
1:D:242:ILE:CG2	3:D:307:HEZ:H32	2.38	0.54
1:B:193[B]:HIS:CE1	1:B:194:LYS:HE2	2.43	0.54
1:A:23:ASN:HD21	1:A:25:GLU:CB	2.22	0.53
1:D:197:TYR:HA	3:D:307:HEZ:H22	1.90	0.53
1:E:38:GLU:HB2	1:E:43:ASP:HB2	1.89	0.53
1:A:80:SER:HA	3:A:308:HEZ:H51	1.91	0.53
1:C:193[B]:HIS:CD2	1:C:194:LYS:HG2	2.44	0.52
1:A:193[B]:HIS:CD2	1:A:194:LYS:HG2	2.45	0.52
1:D:153:ARG:CZ	3:D:311:HEZ:H62	2.38	0.52
3:B:308:HEZ:H22	6:B:577:HOH:O	2.09	0.51
1:A:221:ASP:OD1	6:A:401:HOH:O	2.19	0.51
1:D:198:ILE:O	3:D:307:HEZ:H12	2.10	0.51
1:C:38:GLU:HB2	1:C:43:ASP:HB2	1.92	0.51
1:F:242:ILE:CG2	3:F:308:HEZ:H51	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193[A]:HIS:CD2	1:C:262:PRO:O	2.63	0.51
1:B:75:THR:N	3:B:308:HEZ:H11	2.23	0.51
6:A:520:HOH:O	1:B:193[A]:HIS:HE1	1.83	0.50
1:B:94:GLU:HG2	6:B:584:HOH:O	2.11	0.50
1:C:180:LYS:HD3	6:C:599:HOH:O	2.12	0.50
1:C:58:GLU:HG3	3:C:307:HEZ:H22	1.94	0.50
1:A:193[B]:HIS:CE1	1:A:194:LYS:HE2	2.46	0.50
1:B:159:ILE:CG2	3:B:307:HEZ:H32	2.42	0.49
1:E:223:ILE:HD11	3:E:307:HEZ:H31	1.94	0.49
1:F:193[B]:HIS:CE1	1:F:194:LYS:HE2	2.46	0.49
1:C:193[B]:HIS:CE1	1:C:194:LYS:HE2	2.47	0.49
1:E:221:ASP:OD1	6:E:401:HOH:O	2.19	0.49
1:D:262:PRO:O	1:E:193[A]:HIS:HD2	1.96	0.48
1:B:163:ALA:HB2	3:B:307:HEZ:H31	1.94	0.48
1:A:94:GLU:HG3	6:A:527:HOH:O	2.12	0.48
1:D:198:ILE:H	3:D:307:HEZ:C2	2.26	0.48
1:C:193[B]:HIS:CD2	6:C:495:HOH:O	2.66	0.48
1:D:159:ILE:HG23	3:D:308:HEZ:H22	1.94	0.48
1:B:159:ILE:HG22	3:B:307:HEZ:H32	1.96	0.48
1:B:259:HIS:NE2	4:C:309:TRS:O1	2.44	0.48
1:D:41:PRO:O	1:D:42:ASP:CG	2.52	0.47
1:E:53:LYS:CE	6:E:564:HOH:O	2.62	0.47
1:E:193[B]:HIS:CD2	1:E:194:LYS:HG2	2.50	0.47
1:E:53:LYS:NZ	6:E:564:HOH:O	2.36	0.47
1:D:193[B]:HIS:CD2	6:D:532:HOH:O	2.67	0.47
1:D:53:LYS:NZ	6:D:511:HOH:O	2.46	0.47
3:E:308:HEZ:H42	3:E:308:HEZ:H11	1.39	0.47
1:F:193[B]:HIS:CD2	1:F:194:LYS:HG2	2.50	0.47
1:D:23:ASN:HD21	1:D:25:GLU:HB2	1.80	0.46
1:D:262:PRO:O	1:E:193[A]:HIS:CD2	2.69	0.46
1:F:193[B]:HIS:HD2	6:F:421:HOH:O	1.97	0.46
1:C:23:ASN:ND2	6:C:593:HOH:O	2.47	0.46
1:D:159:ILE:HG22	3:D:308:HEZ:H22	1.97	0.46
1:E:235:THR:HG22	6:E:530:HOH:O	2.16	0.46
4:D:314:TRS:O3	6:D:633:HOH:O	2.00	0.46
1:D:259:HIS:NE2	4:E:313:TRS:O2	2.45	0.45
1:D:53:LYS:HE2	6:D:511:HOH:O	2.14	0.45
1:D:198:ILE:O	3:D:307:HEZ:C1	2.64	0.45
1:E:144:PRO:HD3	1:E:193[B]:HIS:CD2	2.51	0.45
1:F:163:ALA:HB2	3:F:305:HEZ:H52	1.99	0.44
1:D:193[B]:HIS:CD2	1:D:194:LYS:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:GLU:HG2	6:E:538:HOH:O	2.17	0.44
1:C:53:LYS:CE	6:C:579:HOH:O	2.66	0.44
1:C:53:LYS:NZ	6:C:579:HOH:O	2.31	0.44
1:D:153:ARG:HH12	3:D:311:HEZ:C5	2.30	0.44
1:C:54:LYS:NZ	6:C:493:HOH:O	2.50	0.44
1:B:262:PRO:O	1:C:193[A]:HIS:CD2	2.72	0.43
1:D:163:ALA:HB2	3:D:308:HEZ:H21	2.01	0.43
1:A:193[B]:HIS:HD2	6:A:418:HOH:O	2.00	0.43
1:A:93:GLU:HG2	3:A:307:HEZ:H42	2.00	0.43
1:C:163:ALA:HB2	3:C:306:HEZ:H52	2.01	0.43
1:E:198:ILE:HG12	3:E:311:HEZ:H32	2.00	0.43
1:E:258:TYR:CB	3:E:308:HEZ:H51	2.49	0.43
1:C:96:ALA:HB1	1:C:101:VAL:HB	2.00	0.42
1:D:198:ILE:HG12	3:D:307:HEZ:H31	2.01	0.42
1:E:41:PRO:O	1:E:42:ASP:CG	2.58	0.42
1:C:130:LYS:HE3	6:C:573:HOH:O	2.18	0.42
1:B:262:PRO:O	1:C:193[A]:HIS:HD2	2.03	0.42
1:D:193[B]:HIS:HD2	6:D:418:HOH:O	2.02	0.42
1:D:242:ILE:HG21	3:D:307:HEZ:H32	2.02	0.42
1:A:197:TYR:HA	3:A:312:HEZ:H11	2.02	0.42
1:B:163:ALA:HB2	3:B:307:HEZ:C3	2.50	0.42
1:D:94:GLU:HG2	6:D:583:HOH:O	2.19	0.42
1:B:41:PRO:O	1:B:42:ASP:CG	2.58	0.41
1:B:193[B]:HIS:CD2	1:B:194:LYS:HG2	2.54	0.41
1:C:235:THR:HG22	6:C:618:HOH:O	2.20	0.41
1:A:193[B]:HIS:HD2	6:A:525:HOH:O	1.90	0.41
1:A:232:ARG:O	1:A:236:MSE:HG3	2.20	0.41
1:B:23:ASN:ND2	6:B:558:HOH:O	2.54	0.41
1:C:94:GLU:HB2	6:C:634:HOH:O	2.20	0.41
1:C:137:PHE:CD2	1:C:188:ALA:HB3	2.56	0.41
1:A:262:PRO:O	1:B:193[A]:HIS:HD2	2.04	0.41
1:C:231:LEU:O	1:C:235:THR:HG23	2.20	0.41
1:A:262:PRO:O	1:B:193[A]:HIS:CD2	2.73	0.41
1:E:138:ALA:O	1:E:189:LEU:HA	2.20	0.41
1:E:262:PRO:O	1:F:193[A]:HIS:HD2	2.03	0.40
1:E:262:PRO:O	1:F:193[A]:HIS:CD2	2.74	0.40
1:B:74:THR:HA	3:B:308:HEZ:H11	2.03	0.40
1:C:137:PHE:HA	1:C:188:ALA:O	2.21	0.40
3:D:311:HEZ:C1	3:D:311:HEZ:H51	2.26	0.40
1:A:198:ILE:HG12	3:A:312:HEZ:H12	2.02	0.40
1:F:41:PRO:O	1:F:42:ASP:CG	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193[B]:HIS:HD2	6:C:418:HOH:O	2.04	0.40

All (9) 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)
6:B:407:HOH:O	6:E:401:HOH:O[1_655]	2.08	0.12
6:A:401:HOH:O	6:F:405:HOH:O[1_556]	2.11	0.09
6:B:401:HOH:O	6:E:405:HOH:O[1_565]	2.12	0.08
6:C:401:HOH:O	6:D:406:HOH:O[1_655]	2.13	0.07
6:C:406:HOH:O	6:D:401:HOH:O[1_556]	2.15	0.05
6:B:415:HOH:O	6:E:416:HOH:O[1_565]	2.17	0.03
6:A:401:HOH:O	6:F:402:HOH:O[1_556]	2.18	0.02
6:C:401:HOH:O	6:D:403:HOH:O[1_655]	2.18	0.02
6:A:416:HOH:O	6:F:412:HOH:O[1_565]	2.19	0.01

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	266/267 (100%)	260 (98%)	5 (2%)	1 (0%)	34	13
1	B	266/267 (100%)	261 (98%)	4 (2%)	1 (0%)	34	13
1	C	266/267 (100%)	260 (98%)	5 (2%)	1 (0%)	34	13
1	D	266/267 (100%)	262 (98%)	3 (1%)	1 (0%)	34	13
1	E	266/267 (100%)	261 (98%)	4 (2%)	1 (0%)	34	13
1	F	266/267 (100%)	259 (97%)	6 (2%)	1 (0%)	34	13
All	All	1596/1602 (100%)	1563 (98%)	27 (2%)	6 (0%)	34	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	B	42	ASP
1	C	42	ASP
1	D	42	ASP
1	E	42	ASP
1	F	42	ASP

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	240/232 (103%)	238 (99%)	2 (1%)	81	65
1	B	240/232 (103%)	237 (99%)	3 (1%)	69	43
1	C	240/232 (103%)	237 (99%)	3 (1%)	69	43
1	D	240/232 (103%)	237 (99%)	3 (1%)	69	43
1	E	240/232 (103%)	237 (99%)	3 (1%)	69	43
1	F	240/232 (103%)	237 (99%)	3 (1%)	69	43
All	All	1440/1392 (103%)	1423 (99%)	17 (1%)	71	47

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	222	ASP
1	B	26	ASN
1	B	32	LYS
1	B	78	LYS
1	C	23	ASN
1	C	26	ASN
1	C	78	LYS
1	D	23	ASN
1	D	26	ASN
1	D	132	LYS
1	E	23	ASN
1	E	78	LYS

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Mol	Chain	Res	Type
1	E	180	LYS
1	F	25	GLU
1	F	26	ASN
1	F	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	166	GLN
1	B	23	ASN
1	B	166	GLN
1	C	23	ASN
1	D	23	ASN
1	D	26	ASN
1	E	23	ASN
1	E	166	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 95 ligands modelled in this entry, 42 are monoatomic - leaving 53 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEZ	D	310	-	7,7,7	0.58	0	6,6,6	1.03	1 (16%)
4	TRS	D	314	2	7,7,7	1.21	0	9,9,9	1.76	3 (33%)
3	HEZ	C	306	-	7,7,7	1.02	0	6,6,6	2.02	4 (66%)
3	HEZ	B	304	-	7,7,7	0.83	0	6,6,6	0.99	0
3	HEZ	A	311	-	7,7,7	0.15	0	6,6,6	1.73	1 (16%)
3	HEZ	E	304	-	7,7,7	0.78	0	6,6,6	0.98	0
3	HEZ	C	304	-	7,7,7	1.01	0	6,6,6	1.10	1 (16%)
3	HEZ	E	309	-	7,7,7	0.61	0	6,6,6	0.44	0
3	HEZ	A	310	-	7,7,7	0.38	0	6,6,6	0.81	0
3	HEZ	E	311	-	7,7,7	0.71	0	6,6,6	1.33	1 (16%)
3	HEZ	B	309	-	7,7,7	0.39	0	6,6,6	1.24	0
3	HEZ	F	305	-	7,7,7	1.08	0	6,6,6	1.78	2 (33%)
4	TRS	B	311	2	7,7,7	1.12	1 (14%)	9,9,9	1.23	1 (11%)
3	HEZ	D	305	-	7,7,7	0.99	0	6,6,6	0.86	0
3	HEZ	D	313	-	7,7,7	0.21	0	6,6,6	1.37	1 (16%)
3	HEZ	C	307	-	7,7,7	0.18	0	6,6,6	1.59	1 (16%)
3	HEZ	E	308	-	7,7,7	1.03	0	6,6,6	1.90	2 (33%)
3	HEZ	F	306	-	7,7,7	0.50	0	6,6,6	1.20	0
3	HEZ	F	308	-	7,7,7	0.38	0	6,6,6	1.78	2 (33%)
3	HEZ	D	306	-	7,7,7	1.04	0	6,6,6	0.81	0
3	HEZ	B	310	-	7,7,7	0.25	0	6,6,6	1.25	0
3	HEZ	D	309	-	7,7,7	0.56	0	6,6,6	1.01	0
3	HEZ	F	304	-	7,7,7	0.98	0	6,6,6	0.87	0
3	HEZ	D	312	-	7,7,7	0.37	0	6,6,6	1.43	1 (16%)
3	HEZ	A	312	-	7,7,7	0.58	0	6,6,6	1.18	0
4	TRS	D	315	-	7,7,7	2.19	4 (57%)	9,9,9	0.49	0
4	TRS	A	314	-	7,7,7	2.10	3 (42%)	9,9,9	1.08	0
4	TRS	E	313	2	7,7,7	1.34	2 (28%)	9,9,9	1.34	1 (11%)
4	TRS	C	309	2	7,7,7	1.35	1 (14%)	9,9,9	2.00	3 (33%)
3	HEZ	F	307	-	7,7,7	0.27	0	6,6,6	1.09	1 (16%)
3	HEZ	D	311	-	7,7,7	0.92	0	6,6,6	0.83	0
3	HEZ	D	307	-	7,7,7	1.01	0	6,6,6	2.07	2 (33%)
3	HEZ	C	308	-	7,7,7	0.68	0	6,6,6	1.24	1 (16%)
3	HEZ	E	306	-	7,7,7	1.22	0	6,6,6	0.90	0
3	HEZ	E	310	-	7,7,7	0.42	0	6,6,6	1.41	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEZ	D	308	-	7,7,7	0.88	0	6,6,6	1.78	2 (33%)
3	HEZ	A	308	-	7,7,7	1.20	1 (14%)	6,6,6	0.74	0
3	HEZ	E	307	-	7,7,7	0.45	0	6,6,6	0.47	0
4	TRS	F	309	2	7,7,7	1.46	2 (28%)	9,9,9	1.71	3 (33%)
4	TRS	A	313	2	7,7,7	1.31	2 (28%)	9,9,9	1.62	3 (33%)
3	HEZ	B	307	-	7,7,7	1.11	0	6,6,6	2.11	3 (50%)
3	HEZ	C	303	-	7,7,7	0.89	0	6,6,6	0.80	0
3	HEZ	E	305	-	7,7,7	0.55	0	6,6,6	1.02	0
3	HEZ	A	306	-	7,7,7	1.04	0	6,6,6	1.19	0
3	HEZ	A	307	-	7,7,7	0.61	0	6,6,6	1.48	1 (16%)
3	HEZ	A	305	-	7,7,7	0.79	0	6,6,6	0.68	0
3	HEZ	B	305	-	7,7,7	0.78	0	6,6,6	1.18	1 (16%)
3	HEZ	E	312	-	7,7,7	0.23	0	6,6,6	1.88	2 (33%)
3	HEZ	F	303	-	7,7,7	1.00	0	6,6,6	0.94	0
3	HEZ	C	305	-	7,7,7	0.45	0	6,6,6	1.19	0
3	HEZ	A	309	-	7,7,7	0.65	0	6,6,6	1.61	2 (33%)
3	HEZ	B	306	-	7,7,7	0.50	0	6,6,6	1.14	0
3	HEZ	B	308	-	7,7,7	0.66	0	6,6,6	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEZ	D	310	-	-	1/5/5/5	-
4	TRS	D	314	2	-	3/9/9/9	-
3	HEZ	C	306	-	-	2/5/5/5	-
3	HEZ	B	304	-	-	0/5/5/5	-
3	HEZ	A	311	-	-	2/5/5/5	-
3	HEZ	E	304	-	-	0/5/5/5	-
3	HEZ	C	304	-	-	0/5/5/5	-
3	HEZ	E	309	-	-	5/5/5/5	-
3	HEZ	A	310	-	-	1/5/5/5	-
3	HEZ	E	311	-	-	2/5/5/5	-
3	HEZ	B	309	-	-	2/5/5/5	-
3	HEZ	F	305	-	-	2/5/5/5	-
4	TRS	B	311	2	-	3/9/9/9	-
3	HEZ	D	305	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEZ	D	313	-	-	2/5/5/5	-
3	HEZ	C	307	-	-	2/5/5/5	-
3	HEZ	E	308	-	-	4/5/5/5	-
3	HEZ	F	306	-	-	2/5/5/5	-
3	HEZ	F	308	-	-	4/5/5/5	-
3	HEZ	D	306	-	-	0/5/5/5	-
3	HEZ	B	310	-	-	3/5/5/5	-
3	HEZ	D	309	-	-	1/5/5/5	-
3	HEZ	F	304	-	-	0/5/5/5	-
3	HEZ	D	312	-	-	1/5/5/5	-
3	HEZ	A	312	-	-	2/5/5/5	-
4	TRS	D	315	-	-	0/9/9/9	-
4	TRS	A	314	-	-	0/9/9/9	-
4	TRS	E	313	2	-	3/9/9/9	-
4	TRS	C	309	2	-	3/9/9/9	-
3	HEZ	F	307	-	-	3/5/5/5	-
3	HEZ	D	311	-	-	4/5/5/5	-
3	HEZ	D	307	-	-	4/5/5/5	-
3	HEZ	C	308	-	-	2/5/5/5	-
3	HEZ	E	306	-	-	0/5/5/5	-
3	HEZ	E	310	-	-	3/5/5/5	-
3	HEZ	D	308	-	-	2/5/5/5	-
3	HEZ	A	308	-	-	3/5/5/5	-
3	HEZ	E	307	-	-	3/5/5/5	-
4	TRS	F	309	2	-	3/9/9/9	-
4	TRS	A	313	2	-	3/9/9/9	-
3	HEZ	B	307	-	-	3/5/5/5	-
3	HEZ	C	303	-	-	0/5/5/5	-
3	HEZ	E	305	-	-	1/5/5/5	-
3	HEZ	A	306	-	-	0/5/5/5	-
3	HEZ	A	307	-	-	4/5/5/5	-
3	HEZ	A	305	-	-	0/5/5/5	-
3	HEZ	B	305	-	-	2/5/5/5	-
3	HEZ	E	312	-	-	3/5/5/5	-
3	HEZ	F	303	-	-	0/5/5/5	-
3	HEZ	C	305	-	-	2/5/5/5	-
3	HEZ	A	309	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEZ	B	306	-	-	3/5/5/5	-
3	HEZ	B	308	-	-	1/5/5/5	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	315	TRS	O2-C2	3.07	1.52	1.42
4	D	315	TRS	O1-C1	3.01	1.52	1.42
4	C	309	TRS	O2-C2	2.97	1.52	1.42
4	A	314	TRS	O3-C3	2.81	1.51	1.42
4	A	314	TRS	O2-C2	2.72	1.51	1.42
4	A	314	TRS	O1-C1	2.66	1.51	1.42
4	D	315	TRS	O3-C3	2.65	1.51	1.42
4	E	313	TRS	O3-C3	2.64	1.51	1.42
4	F	309	TRS	C3-C	2.64	1.61	1.53
4	B	311	TRS	O1-C1	2.63	1.51	1.42
4	F	309	TRS	O2-C2	2.48	1.50	1.42
4	A	313	TRS	O1-C1	2.44	1.50	1.42
4	A	313	TRS	C-N	2.29	1.57	1.49
3	A	308	HEZ	O6-C6	2.26	1.53	1.42
4	D	315	TRS	C3-C	2.07	1.59	1.53
4	E	313	TRS	C1-C	2.07	1.59	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	307	HEZ	C4-C3-C2	3.98	134.63	114.42
3	B	307	HEZ	C4-C3-C2	3.89	134.19	114.42
3	E	308	HEZ	C3-C2-C1	-3.45	91.43	114.02
4	C	309	TRS	C3-C-C2	-3.28	100.64	110.81
3	F	308	HEZ	C5-C4-C3	-3.17	98.33	114.42
3	D	308	HEZ	O1-C1-C2	-3.13	91.06	111.66
4	C	309	TRS	C2-C-C1	3.13	120.51	110.81
3	A	311	HEZ	C4-C3-C2	-3.07	98.84	114.42
3	E	312	HEZ	C5-C4-C3	-3.02	99.09	114.42
3	E	312	HEZ	O1-C1-C2	-3.00	91.92	111.66
3	C	307	HEZ	C4-C3-C2	-2.99	99.22	114.42
3	E	308	HEZ	C4-C5-C6	2.99	133.61	114.02
3	A	309	HEZ	C3-C2-C1	-2.85	95.33	114.02
3	D	312	HEZ	C4-C3-C2	-2.81	100.16	114.42
4	F	309	TRS	C2-C-N	2.79	116.30	107.98
3	C	306	HEZ	O6-C6-C5	-2.75	93.56	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	314	TRS	C3-C-C1	2.70	119.17	110.81
3	A	307	HEZ	C5-C4-C3	-2.67	100.85	114.42
4	D	314	TRS	C3-C-N	-2.60	100.20	107.98
3	C	306	HEZ	C3-C2-C1	-2.58	97.13	114.02
3	F	305	HEZ	O6-C6-C5	-2.56	94.83	111.66
3	B	305	HEZ	C4-C5-C6	-2.53	97.44	114.02
4	A	313	TRS	O1-C1-C	-2.52	103.01	111.00
3	D	313	HEZ	C4-C3-C2	-2.49	101.77	114.42
3	F	305	HEZ	C4-C5-C6	2.49	130.32	114.02
4	E	313	TRS	C3-C-C2	2.46	118.44	110.81
4	C	309	TRS	O2-C2-C	-2.42	103.32	111.00
4	F	309	TRS	C3-C-C1	-2.42	103.31	110.81
4	F	309	TRS	O2-C2-C	-2.39	103.41	111.00
3	B	307	HEZ	C3-C2-C1	-2.37	98.49	114.02
3	C	308	HEZ	O1-C1-C2	2.36	127.19	111.66
3	A	309	HEZ	C4-C5-C6	-2.36	98.58	114.02
3	C	304	HEZ	C4-C3-C2	-2.33	102.60	114.42
3	B	307	HEZ	C5-C4-C3	-2.32	102.63	114.42
3	C	306	HEZ	C4-C5-C6	-2.31	98.90	114.02
4	A	313	TRS	C2-C-C1	-2.31	103.66	110.81
3	D	308	HEZ	C4-C5-C6	-2.28	99.06	114.02
4	A	313	TRS	C3-C-C1	2.18	117.56	110.81
3	F	307	HEZ	C5-C4-C3	-2.16	103.47	114.42
3	E	311	HEZ	C5-C4-C3	-2.14	103.56	114.42
3	F	308	HEZ	C4-C3-C2	2.13	125.26	114.42
3	D	310	HEZ	C5-C4-C3	-2.10	103.76	114.42
3	E	310	HEZ	C5-C4-C3	-2.09	103.84	114.42
4	B	311	TRS	C3-C-C1	2.08	117.27	110.81
4	D	314	TRS	O1-C1-C	-2.08	104.42	111.00
3	D	307	HEZ	C4-C5-C6	2.05	127.45	114.02
3	C	306	HEZ	C4-C3-C2	2.04	124.77	114.42

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	313	TRS	C1-C-C3-O3
4	A	313	TRS	C2-C-C3-O3
4	A	313	TRS	N-C-C3-O3
4	B	311	TRS	C1-C-C3-O3
4	B	311	TRS	C2-C-C3-O3
4	B	311	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	309	TRS	C2-C-C1-O1
4	C	309	TRS	C3-C-C1-O1
4	C	309	TRS	N-C-C1-O1
4	D	314	TRS	C1-C-C3-O3
4	D	314	TRS	C2-C-C3-O3
4	D	314	TRS	N-C-C3-O3
4	E	313	TRS	C1-C-C2-O2
4	E	313	TRS	C3-C-C2-O2
4	E	313	TRS	N-C-C2-O2
4	F	309	TRS	C2-C-C1-O1
4	F	309	TRS	C3-C-C1-O1
4	F	309	TRS	N-C-C1-O1
3	B	307	HEZ	C1-C2-C3-C4
3	D	311	HEZ	C2-C3-C4-C5
3	C	306	HEZ	C2-C3-C4-C5
3	E	307	HEZ	C1-C2-C3-C4
3	D	311	HEZ	C1-C2-C3-C4
3	A	312	HEZ	C1-C2-C3-C4
3	D	308	HEZ	C2-C3-C4-C5
3	C	306	HEZ	C4-C5-C6-O6
3	F	307	HEZ	C1-C2-C3-C4
3	B	310	HEZ	O1-C1-C2-C3
3	E	309	HEZ	C2-C3-C4-C5
3	E	312	HEZ	C1-C2-C3-C4
3	F	308	HEZ	C3-C4-C5-C6
3	B	310	HEZ	C2-C3-C4-C5
3	F	305	HEZ	C4-C5-C6-O6
3	A	307	HEZ	C1-C2-C3-C4
3	A	311	HEZ	C1-C2-C3-C4
3	E	310	HEZ	C1-C2-C3-C4
3	D	307	HEZ	C2-C3-C4-C5
3	B	305	HEZ	C3-C4-C5-C6
3	E	309	HEZ	C3-C4-C5-C6
3	E	312	HEZ	C3-C4-C5-C6
3	C	307	HEZ	C1-C2-C3-C4
3	A	307	HEZ	C3-C4-C5-C6
3	B	308	HEZ	C2-C3-C4-C5
3	D	308	HEZ	O1-C1-C2-C3
3	F	308	HEZ	C1-C2-C3-C4
3	E	308	HEZ	C3-C4-C5-C6
3	A	308	HEZ	C2-C3-C4-C5
3	E	312	HEZ	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	307	HEZ	C1-C2-C3-C4
3	D	310	HEZ	C1-C2-C3-C4
3	E	311	HEZ	C3-C4-C5-C6
3	A	308	HEZ	C4-C5-C6-O6
3	D	311	HEZ	C4-C5-C6-O6
3	F	306	HEZ	O1-C1-C2-C3
3	F	307	HEZ	C3-C4-C5-C6
3	F	308	HEZ	C2-C3-C4-C5
3	E	308	HEZ	C1-C2-C3-C4
3	C	305	HEZ	O1-C1-C2-C3
3	E	305	HEZ	C4-C5-C6-O6
3	E	308	HEZ	O1-C1-C2-C3
3	A	312	HEZ	C4-C5-C6-O6
3	C	308	HEZ	C4-C5-C6-O6
3	D	307	HEZ	O1-C1-C2-C3
3	D	309	HEZ	O1-C1-C2-C3
3	D	311	HEZ	O1-C1-C2-C3
3	D	313	HEZ	C4-C5-C6-O6
3	E	309	HEZ	C4-C5-C6-O6
3	F	307	HEZ	O1-C1-C2-C3
3	A	311	HEZ	C4-C5-C6-O6
3	B	306	HEZ	C4-C5-C6-O6
3	C	307	HEZ	C4-C5-C6-O6
3	D	307	HEZ	C4-C5-C6-O6
3	D	312	HEZ	C4-C5-C6-O6
3	F	308	HEZ	O1-C1-C2-C3
3	A	307	HEZ	C4-C5-C6-O6
3	F	305	HEZ	C1-C2-C3-C4
3	B	310	HEZ	C3-C4-C5-C6
3	E	310	HEZ	O1-C1-C2-C3
3	D	313	HEZ	C1-C2-C3-C4
3	A	308	HEZ	O1-C1-C2-C3
3	E	309	HEZ	C1-C2-C3-C4
3	B	306	HEZ	C2-C3-C4-C5
3	A	307	HEZ	C2-C3-C4-C5
3	E	307	HEZ	C2-C3-C4-C5
3	C	305	HEZ	C2-C3-C4-C5
3	F	306	HEZ	C2-C3-C4-C5
3	B	305	HEZ	C4-C5-C6-O6
3	B	309	HEZ	C3-C4-C5-C6
3	E	308	HEZ	C4-C5-C6-O6
3	E	311	HEZ	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	306	HEZ	O1-C1-C2-C3
3	A	310	HEZ	C3-C4-C5-C6
3	C	308	HEZ	C3-C4-C5-C6
3	E	309	HEZ	O1-C1-C2-C3
3	B	307	HEZ	O1-C1-C2-C3
3	E	310	HEZ	C4-C5-C6-O6
3	B	307	HEZ	C2-C3-C4-C5
3	B	309	HEZ	O1-C1-C2-C3
3	E	307	HEZ	C4-C5-C6-O6

There are no ring outliers.

28 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	310	HEZ	1	0
4	D	314	TRS	3	0
3	C	306	HEZ	4	0
3	E	309	HEZ	2	0
3	E	311	HEZ	1	0
3	F	305	HEZ	3	0
4	B	311	TRS	3	0
3	D	313	HEZ	1	0
3	C	307	HEZ	1	0
3	E	308	HEZ	3	0
3	F	308	HEZ	1	0
3	B	310	HEZ	1	0
3	A	312	HEZ	2	0
4	E	313	TRS	4	0
4	C	309	TRS	4	0
3	F	307	HEZ	1	0
3	D	311	HEZ	11	0
3	D	307	HEZ	7	0
3	D	308	HEZ	4	0
3	A	308	HEZ	3	0
3	E	307	HEZ	4	0
4	F	309	TRS	3	0
4	A	313	TRS	4	0
3	B	307	HEZ	4	0
3	A	306	HEZ	6	0
3	A	307	HEZ	1	0
3	A	309	HEZ	1	0
3	B	308	HEZ	5	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	260/267 (97%)	-0.81	0	100	100	12, 18, 35, 55	0
1	B	260/267 (97%)	-0.80	0	100	100	12, 18, 34, 52	0
1	C	260/267 (97%)	-0.84	0	100	100	12, 18, 34, 54	0
1	D	260/267 (97%)	-0.80	0	100	100	12, 18, 35, 55	0
1	E	260/267 (97%)	-0.85	0	100	100	12, 18, 35, 54	0
1	F	260/267 (97%)	-0.78	0	100	100	12, 18, 35, 53	0
All	All	1560/1602 (97%)	-0.81	0	100	100	12, 18, 35, 55	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEZ	E	308	8/8	0.78	0.13	28,35,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEZ	E	305	8/8	0.80	0.19	29,33,41,41	0
3	HEZ	B	307	8/8	0.82	0.13	30,35,40,46	0
3	HEZ	F	306	8/8	0.82	0.20	28,32,36,40	0
3	HEZ	A	309	8/8	0.85	0.13	32,35,38,38	0
3	HEZ	A	307	8/8	0.85	0.15	29,33,41,41	0
3	HEZ	D	308	8/8	0.85	0.12	28,36,40,43	0
3	HEZ	A	308	8/8	0.86	0.11	38,43,49,49	0
3	HEZ	D	309	8/8	0.86	0.16	29,32,34,38	0
3	HEZ	B	310	8/8	0.86	0.13	38,48,59,64	0
3	HEZ	C	305	8/8	0.86	0.17	28,33,35,39	0
3	HEZ	C	306	8/8	0.86	0.12	30,34,39,40	0
4	TRS	D	315	8/8	0.86	0.13	23,25,26,26	0
3	HEZ	A	311	8/8	0.87	0.12	39,45,55,55	0
3	HEZ	F	307	8/8	0.87	0.12	40,47,54,58	0
3	HEZ	C	308	8/8	0.87	0.12	25,41,45,51	0
3	HEZ	B	308	8/8	0.88	0.12	34,37,45,48	0
4	TRS	A	314	8/8	0.88	0.11	23,25,27,28	0
3	HEZ	C	307	8/8	0.88	0.12	40,46,54,60	0
3	HEZ	D	313	8/8	0.89	0.15	38,48,56,56	0
3	HEZ	A	305	8/8	0.90	0.09	22,26,31,34	0
3	HEZ	B	306	8/8	0.90	0.16	27,33,35,40	0
3	HEZ	E	312	8/8	0.91	0.10	35,43,52,55	0
3	HEZ	F	305	8/8	0.91	0.12	27,32,41,42	0
3	HEZ	D	311	8/8	0.91	0.11	21,34,38,42	0
3	HEZ	E	306	8/8	0.91	0.10	21,29,31,31	0
3	HEZ	E	307	8/8	0.91	0.12	38,41,49,49	0
3	HEZ	D	306	8/8	0.91	0.11	20,28,32,34	0
3	HEZ	D	305	8/8	0.92	0.08	21,26,30,32	0
3	HEZ	D	307	8/8	0.92	0.12	18,38,41,43	0
3	HEZ	B	305	8/8	0.93	0.11	20,31,33,47	0
3	HEZ	F	308	8/8	0.93	0.13	24,41,45,51	0
4	TRS	A	313	8/8	0.93	0.09	18,19,22,29	0
3	HEZ	B	304	8/8	0.93	0.11	23,25,31,32	0
3	HEZ	E	311	8/8	0.93	0.09	25,41,48,53	0
4	TRS	F	309	8/8	0.93	0.10	17,19,24,32	0
3	HEZ	D	310	8/8	0.94	0.09	25,35,49,50	0
3	HEZ	A	306	8/8	0.94	0.10	19,28,31,34	0
3	HEZ	A	312	8/8	0.94	0.10	25,42,45,53	0
3	HEZ	C	303	8/8	0.94	0.10	24,26,30,32	0
3	HEZ	F	303	8/8	0.94	0.07	23,27,31,31	0
4	TRS	B	311	8/8	0.94	0.10	15,19,22,32	0
3	HEZ	F	304	8/8	0.94	0.09	21,29,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRS	E	313	8/8	0.94	0.09	16,20,22,28	0
3	HEZ	A	310	8/8	0.94	0.12	29,45,55,60	0
4	TRS	D	314	8/8	0.95	0.09	16,19,21,30	0
3	HEZ	C	304	8/8	0.95	0.09	21,28,30,33	0
3	HEZ	B	309	8/8	0.95	0.09	29,41,49,54	0
4	TRS	C	309	8/8	0.95	0.11	16,21,23,29	0
3	HEZ	E	304	8/8	0.96	0.09	22,26,31,31	0
3	HEZ	E	309	8/8	0.96	0.07	22,41,58,59	0
3	HEZ	D	312	8/8	0.97	0.10	28,42,50,51	0
3	HEZ	E	310	8/8	0.97	0.10	27,40,52,52	0
2	CD	D	303	1/1	0.99	0.05	19,19,19,19	1
5	CL	A	317	1/1	0.99	0.08	20,20,20,20	0
5	CL	B	314	1/1	0.99	0.06	21,21,21,21	0
5	CL	D	316	1/1	0.99	0.04	21,21,21,21	0
5	CL	E	316	1/1	0.99	0.05	22,22,22,22	0
5	CL	F	311	1/1	0.99	0.05	21,21,21,21	0
5	CL	F	312	1/1	0.99	0.03	17,17,17,17	0
2	CD	D	301	1/1	1.00	0.06	14,14,14,14	0
2	CD	D	302	1/1	1.00	0.06	19,19,19,19	0
2	CD	A	301	1/1	1.00	0.07	14,14,14,14	0
2	CD	D	304	1/1	1.00	0.04	19,19,19,19	1
2	CD	E	301	1/1	1.00	0.07	14,14,14,14	0
2	CD	E	302	1/1	1.00	0.06	19,19,19,19	0
2	CD	E	303	1/1	1.00	0.04	19,19,19,19	1
2	CD	F	301	1/1	1.00	0.06	14,14,14,14	0
2	CD	F	302	1/1	1.00	0.06	19,19,19,19	0
2	CD	A	302	1/1	1.00	0.06	19,19,19,19	0
2	CD	A	303	1/1	1.00	0.03	19,19,19,19	1
5	CL	A	315	1/1	1.00	0.06	22,22,22,22	0
5	CL	A	316	1/1	1.00	0.05	22,22,22,22	0
2	CD	A	304	1/1	1.00	0.04	19,19,19,19	1
5	CL	A	318	1/1	1.00	0.03	21,21,21,21	0
5	CL	A	319	1/1	1.00	0.03	17,17,17,17	0
5	CL	B	312	1/1	1.00	0.07	19,19,19,19	0
5	CL	B	313	1/1	1.00	0.03	21,21,21,21	0
2	CD	B	301	1/1	1.00	0.07	14,14,14,14	0
5	CL	B	315	1/1	1.00	0.03	17,17,17,17	0
5	CL	C	310	1/1	1.00	0.04	19,19,19,19	0
5	CL	C	311	1/1	1.00	0.04	21,21,21,21	0
5	CL	C	312	1/1	1.00	0.02	17,17,17,17	0
2	CD	B	302	1/1	1.00	0.07	19,19,19,19	0
5	CL	D	317	1/1	1.00	0.07	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	D	318	1/1	1.00	0.05	21,21,21,21	0
5	CL	D	319	1/1	1.00	0.03	22,22,22,22	0
5	CL	D	320	1/1	1.00	0.03	17,17,17,17	0
5	CL	E	314	1/1	1.00	0.08	19,19,19,19	0
5	CL	E	315	1/1	1.00	0.05	21,21,21,21	0
2	CD	B	303	1/1	1.00	0.04	19,19,19,19	1
5	CL	E	317	1/1	1.00	0.03	17,17,17,17	0
5	CL	F	310	1/1	1.00	0.04	20,20,20,20	0
2	CD	C	301	1/1	1.00	0.07	14,14,14,14	0
2	CD	C	302	1/1	1.00	0.06	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.