



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:40 PM UTC

PDB ID : 4XLZ / pdb_00004xlz
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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

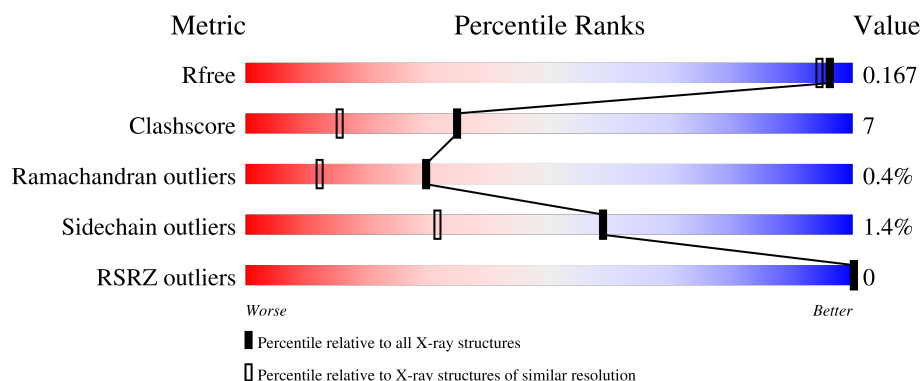
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

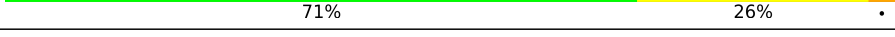
The reported resolution of this entry is 1.51 Å.

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}	180053	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (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 $\leq 5\%$. 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	267	
1	B	267	
1	C	267	
1	D	267	
1	E	267	

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Mol	Chain	Length	Quality of chain
1	F	267	 79% 20%

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

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.

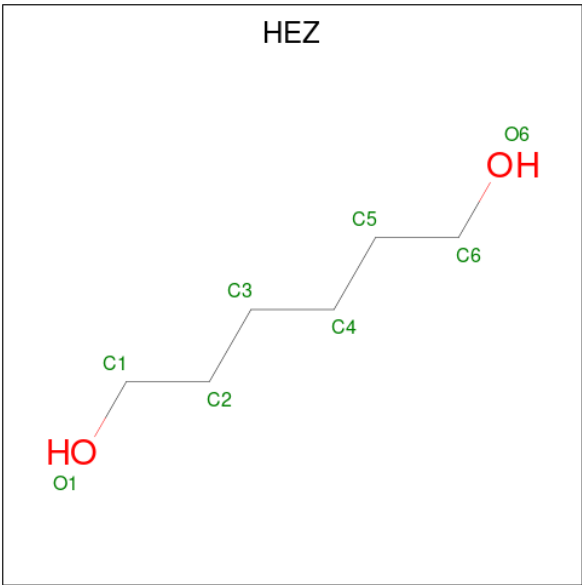
- Molecule 1 is a protein called Uncharacterized protein.

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

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 3 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: C₆H₁₄O₂).



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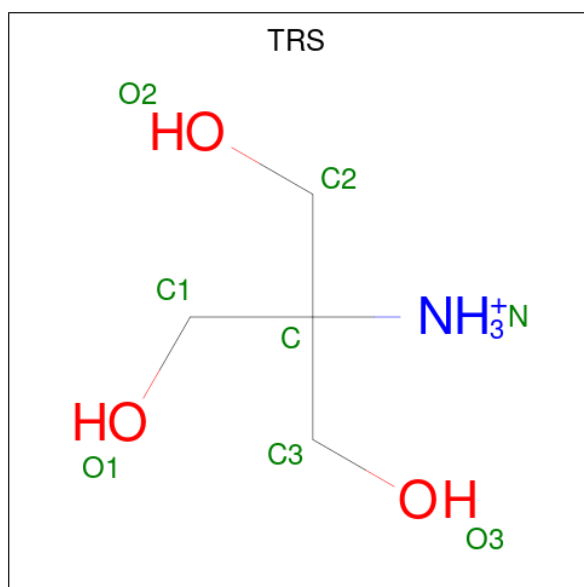
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total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

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

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

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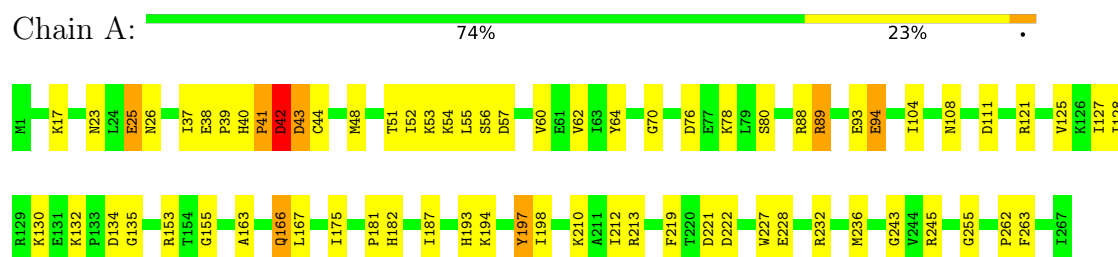
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	235	Total 235	O 235	0	0
6	F	241	Total 241	O 241	0	0

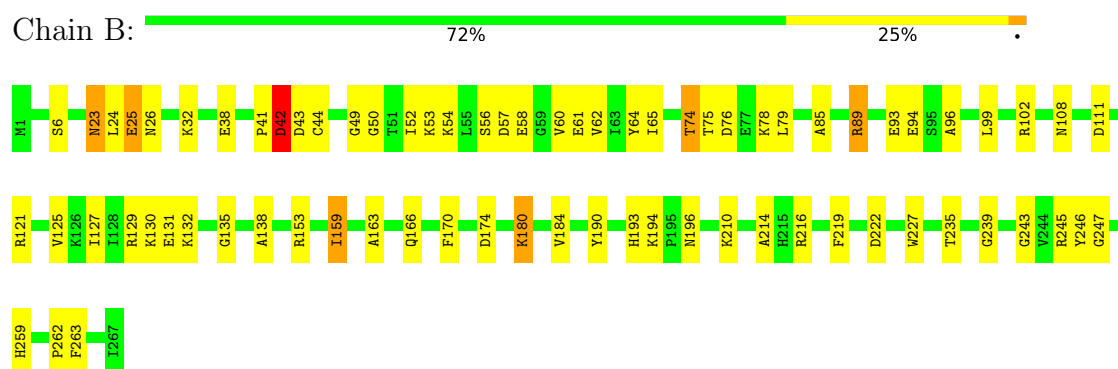
3 Residue-property plots

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.

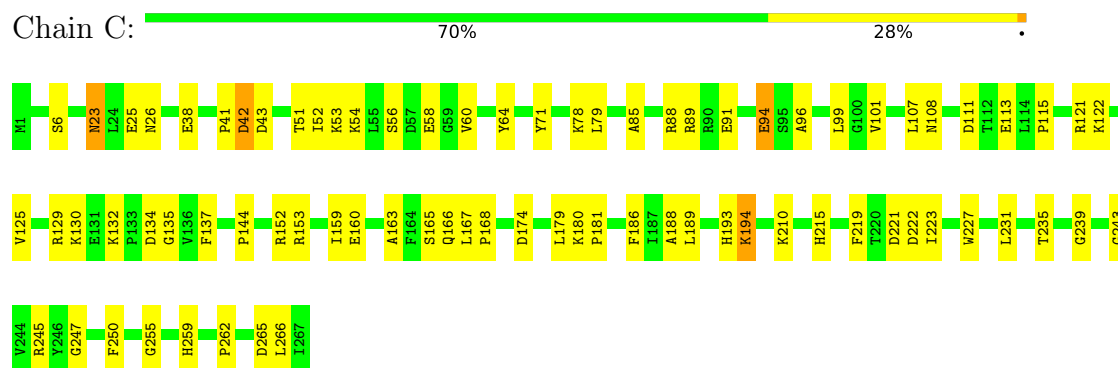
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



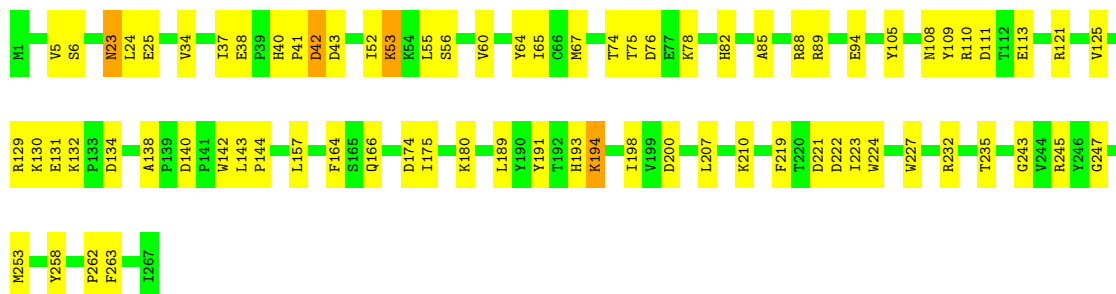
- Molecule 1: Uncharacterized protein

Chain D:  71% 26% .



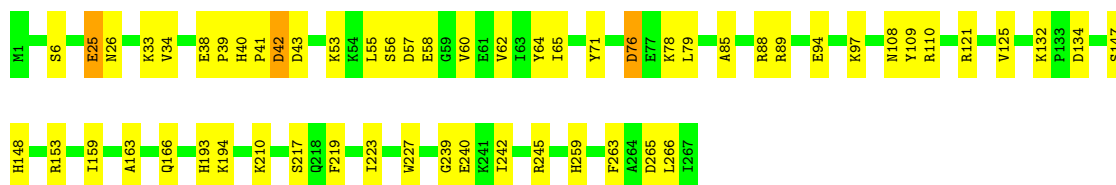
• Molecule 1: Uncharacterized protein

Chain E:  72% 27% .



• Molecule 1: Uncharacterized protein

Chain F:  79% 20% .



4 Data and refinement statistics

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) 95.6 (31.16-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.80%)	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)	0.36 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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

5.1 Standard geometry

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

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	2.01	40/2253 (1.8%)	1.75	25/3038 (0.8%)
1	B	1.95	46/2253 (2.0%)	1.73	26/3038 (0.9%)
1	C	1.98	40/2253 (1.8%)	1.76	21/3038 (0.7%)
1	D	2.04	50/2253 (2.2%)	1.77	27/3038 (0.9%)
1	E	1.98	31/2253 (1.4%)	1.78	25/3038 (0.8%)
1	F	1.96	34/2253 (1.5%)	1.69	18/3038 (0.6%)
All	All	1.99	241/13518 (1.8%)	1.75	142/18228 (0.8%)

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 (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	132	LYS	CG-CD	-13.06	1.13	1.52
1	F	217	SER	C-O	-12.01	1.08	1.24
1	C	94	GLU	CD-OE2	9.24	1.43	1.25
1	A	132	LYS	C-O	8.98	1.28	1.23
1	D	117	SER	C-O	-8.85	1.13	1.23
1	B	60	VAL	N-CA	8.85	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	PRO	CA-C	8.62	1.61	1.52
1	D	108	ASN	CG-ND2	-8.55	1.15	1.33
1	B	108	ASN	CG-ND2	-8.45	1.15	1.33
1	C	108	ASN	CG-ND2	-8.40	1.15	1.33
1	F	132	LYS	CA-CB	8.36	1.60	1.52
1	A	108	ASN	CG-ND2	-8.29	1.15	1.33
1	C	94	GLU	CG-CD	8.28	1.72	1.52
1	D	60	VAL	N-CA	8.19	1.56	1.46
1	D	183	SER	C-O	-8.13	1.14	1.24
1	E	132	LYS	C-O	8.11	1.27	1.23
1	B	190	TYR	C-O	-8.06	1.13	1.23
1	A	219	PHE	N-CA	8.01	1.58	1.46
1	E	143	LEU	N-CA	7.98	1.57	1.46
1	D	5	VAL	CA-CB	7.93	1.63	1.54
1	F	148	HIS	CA-C	7.78	1.61	1.52
1	E	194	LYS	CA-CB	7.74	1.61	1.53
1	C	60	VAL	N-CA	7.63	1.55	1.46
1	F	132	LYS	C-O	7.57	1.27	1.23
1	B	44	CYS	N-CA	7.54	1.55	1.46
1	E	243	GLY	N-CA	7.54	1.55	1.45
1	D	219	PHE	N-CA	7.48	1.57	1.46
1	F	108	ASN	CG-ND2	-7.47	1.17	1.33
1	E	130	LYS	N-CA	7.42	1.55	1.46
1	C	132	LYS	C-O	7.42	1.27	1.23
1	E	140	ASP	CG-OD2	-7.29	1.11	1.25
1	A	134	ASP	CA-CB	7.29	1.65	1.53
1	E	166	GLN	CB-CG	-7.17	1.30	1.52
1	C	243	GLY	N-CA	7.11	1.55	1.45
1	C	179	LEU	C-O	7.10	1.32	1.23
1	D	261	THR	C-O	-7.08	1.18	1.25
1	D	258	TYR	C-O	-7.00	1.13	1.24
1	B	216	ARG	CD-NE	6.97	1.56	1.46
1	C	134	ASP	CA-CB	6.95	1.64	1.53
1	B	166	GLN	CB-CG	-6.87	1.31	1.52
1	A	243	GLY	N-CA	6.87	1.54	1.45
1	D	79	LEU	CA-CB	-6.86	1.43	1.53
1	F	34	VAL	N-CA	6.86	1.53	1.46
1	F	64	TYR	N-CA	6.81	1.53	1.45
1	C	166	GLN	N-CA	6.79	1.55	1.46
1	A	64	TYR	N-CA	6.78	1.53	1.45
1	E	219	PHE	N-CA	6.77	1.56	1.46
1	F	153	ARG	CZ-NH2	6.73	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	ARG	NE-CZ	6.72	1.40	1.33
1	C	215	HIS	CA-CB	6.71	1.61	1.52
1	E	253	MSE	CA-C	6.71	1.58	1.52
1	E	132	LYS	CA-CB	6.68	1.58	1.52
1	B	243	GLY	N-CA	6.68	1.54	1.45
1	D	166	GLN	N-CA	6.67	1.54	1.46
1	A	57	ASP	N-CA	6.67	1.54	1.46
1	E	108	ASN	CG-ND2	-6.52	1.19	1.33
1	D	57	ASP	N-CA	6.50	1.54	1.46
1	E	134	ASP	CA-CB	6.50	1.64	1.53
1	A	166	GLN	N-CA	6.50	1.54	1.46
1	A	135	GLY	N-CA	6.50	1.52	1.45
1	E	55	LEU	CA-CB	6.48	1.63	1.53
1	C	160	GLU	C-O	6.46	1.31	1.24
1	D	143	LEU	N-CA	6.43	1.54	1.46
1	E	53	LYS	N-CA	6.43	1.54	1.46
1	F	134	ASP	CA-CB	6.35	1.63	1.53
1	A	76	ASP	C-O	6.33	1.31	1.24
1	A	182	HIS	C-O	6.29	1.31	1.23
1	C	250	PHE	N-CA	6.28	1.53	1.45
1	D	48	MSE	C-O	-6.27	1.18	1.24
1	F	79	LEU	CA-CB	-6.25	1.45	1.53
1	B	49	GLY	CA-C	6.24	1.59	1.52
1	F	110	ARG	C-O	-6.19	1.16	1.23
1	C	153	ARG	N-CA	6.19	1.53	1.46
1	E	76	ASP	C-O	6.16	1.31	1.24
1	B	138	ALA	N-CA	6.13	1.51	1.46
1	D	243	GLY	N-CA	6.11	1.53	1.45
1	B	135	GLY	N-CA	6.10	1.51	1.45
1	C	132	LYS	CA-CB	6.09	1.58	1.52
1	B	132	LYS	CA-CB	6.08	1.58	1.52
1	A	255	GLY	N-CA	6.06	1.53	1.45
1	D	255	GLY	N-CA	6.04	1.53	1.45
1	C	219	PHE	N-CA	6.04	1.55	1.46
1	D	192	THR	C-O	6.03	1.31	1.24
1	E	88	ARG	NE-CZ	6.01	1.39	1.33
1	B	184	VAL	CA-CB	6.01	1.61	1.54
1	C	99	LEU	CA-CB	5.99	1.64	1.53
1	E	247	GLY	N-CA	5.98	1.51	1.45
1	B	159	ILE	C-O	5.96	1.30	1.24
1	A	60	VAL	N-CA	5.87	1.53	1.46
1	C	245	ARG	CA-C	5.87	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	239	GLY	CA-C	5.87	1.58	1.52
1	B	219	PHE	N-CA	5.87	1.55	1.46
1	D	76	ASP	C-O	5.85	1.31	1.24
1	B	131	GLU	C-O	5.84	1.31	1.24
1	B	246	TYR	N-CA	5.82	1.53	1.46
1	A	127	ILE	CA-C	-5.82	1.45	1.52
1	A	228	GLU	CA-CB	5.81	1.61	1.53
1	A	51	THR	N-CA	-5.79	1.39	1.46
1	D	134	ASP	CA-CB	5.79	1.62	1.53
1	F	245	ARG	CA-C	5.79	1.60	1.52
1	D	159	ILE	CA-CB	-5.78	1.47	1.54
1	F	53	LYS	CD-CE	5.75	1.69	1.52
1	C	247	GLY	CA-C	5.74	1.57	1.52
1	A	17	LYS	CA-C	-5.73	1.45	1.52
1	C	64	TYR	N-CA	5.71	1.52	1.45
1	D	183	SER	CA-C	5.71	1.60	1.52
1	D	189	LEU	N-CA	5.71	1.53	1.46
1	A	43	ASP	CA-CB	5.70	1.62	1.53
1	A	181	PRO	C-O	5.68	1.30	1.23
1	D	179	LEU	C-O	5.67	1.30	1.23
1	A	213	ARG	CZ-NH1	5.67	1.40	1.32
1	F	240	GLU	N-CA	5.66	1.53	1.46
1	A	37	ILE	C-O	5.63	1.30	1.24
1	A	187	ILE	N-CA	5.63	1.53	1.46
1	B	64	TYR	N-CA	5.62	1.52	1.45
1	F	223	ILE	CA-CB	5.62	1.62	1.54
1	B	235	THR	N-CA	5.61	1.53	1.46
1	F	263	PHE	CA-CB	5.61	1.60	1.53
1	A	153	ARG	CZ-NH2	5.61	1.40	1.33
1	B	62	VAL	C-N	5.61	1.41	1.33
1	B	85	ALA	CA-CB	5.61	1.62	1.53
1	B	102	ARG	CZ-NH2	5.61	1.40	1.33
1	C	129	ARG	C-O	5.61	1.31	1.24
1	E	67	MSE	CA-C	-5.60	1.45	1.52
1	B	216	ARG	CZ-NH2	5.60	1.40	1.33
1	D	45	ALA	N-CA	5.60	1.53	1.46
1	C	79	LEU	CA-CB	-5.59	1.45	1.53
1	F	219	PHE	N-CA	5.59	1.54	1.46
1	B	54	LYS	CA-C	-5.58	1.45	1.52
1	B	247	GLY	N-CA	5.58	1.51	1.45
1	C	115	PRO	CA-C	-5.58	1.45	1.52
1	A	39	PRO	C-N	5.57	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	136	VAL	CA-CB	5.55	1.61	1.54
1	B	96	ALA	CA-CB	5.55	1.61	1.53
1	E	131	GLU	C-O	5.54	1.31	1.24
1	E	157	LEU	N-CA	5.54	1.53	1.46
1	D	94	GLU	N-CA	5.54	1.53	1.46
1	C	181	PRO	C-O	5.53	1.30	1.23
1	B	74	THR	N-CA	5.52	1.52	1.45
1	D	132	LYS	CB-CG	-5.52	1.35	1.52
1	A	54	LYS	CA-C	-5.51	1.45	1.52
1	D	153	ARG	N-CA	5.51	1.53	1.46
1	D	258	TYR	N-CA	5.49	1.53	1.46
1	D	186	PHE	CA-CB	5.48	1.63	1.53
1	E	34	VAL	N-CA	5.47	1.52	1.46
1	D	55	LEU	CA-CB	5.47	1.61	1.53
1	B	129	ARG	C-O	5.47	1.30	1.24
1	D	93	GLU	N-CA	5.46	1.52	1.46
1	B	76	ASP	C-O	5.46	1.30	1.24
1	D	117	SER	C-N	5.45	1.41	1.33
1	F	109	TYR	N-CA	5.44	1.52	1.46
1	F	60	VAL	N-CA	5.44	1.52	1.46
1	D	167	LEU	CA-C	-5.43	1.46	1.52
1	D	184	VAL	CA-CB	5.43	1.60	1.54
1	F	71	TYR	CA-CB	5.43	1.62	1.53
1	F	166	GLN	CD-NE2	-5.43	1.21	1.33
1	C	223	ILE	CA-CB	5.42	1.61	1.54
1	C	51	THR	C-O	-5.42	1.17	1.24
1	A	167	LEU	CA-CB	5.41	1.62	1.53
1	D	2	PHE	CA-C	-5.39	1.46	1.53
1	A	130	LYS	N-CA	5.39	1.52	1.46
1	D	125	VAL	N-CA	5.39	1.53	1.46
1	F	110	ARG	CD-NE	5.36	1.53	1.46
1	C	6	SER	CA-CB	5.35	1.61	1.54
1	E	37	ILE	C-O	5.34	1.30	1.24
1	B	196	ASN	C-O	5.34	1.30	1.24
1	F	210	LYS	CA-C	5.33	1.59	1.52
1	C	107	LEU	CA-C	-5.33	1.45	1.52
1	B	79	LEU	CA-CB	-5.32	1.46	1.53
1	B	214	ALA	CA-C	5.32	1.60	1.52
1	D	248	GLU	N-CA	5.32	1.52	1.46
1	A	263	PHE	CA-CB	5.31	1.60	1.53
1	D	34	VAL	N-CA	5.30	1.52	1.46
1	A	55	LEU	CA-CB	5.29	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	74	THR	N-CA	5.29	1.52	1.45
1	A	104	ILE	N-CA	5.28	1.52	1.46
1	D	166	GLN	CD-NE2	-5.27	1.22	1.33
1	D	248	GLU	C-N	5.26	1.38	1.33
1	D	85	ALA	CA-CB	5.25	1.61	1.53
1	F	55	LEU	CA-CB	5.25	1.61	1.53
1	D	121	ARG	C-O	-5.25	1.18	1.24
1	B	93	GLU	N-CA	5.24	1.52	1.46
1	F	33	LYS	CA-C	5.24	1.58	1.52
1	E	105	TYR	N-CA	5.24	1.52	1.46
1	D	196	ASN	N-CA	5.23	1.52	1.46
1	F	166	GLN	N-CA	5.23	1.52	1.46
1	F	259	HIS	N-CA	5.23	1.52	1.46
1	A	53	LYS	CB-CG	5.23	1.68	1.52
1	D	54	LYS	CA-C	-5.22	1.46	1.52
1	D	208	LYS	N-CA	5.22	1.52	1.46
1	B	216	ARG	CG-CD	5.22	1.68	1.52
1	C	255	GLY	N-CA	5.22	1.52	1.45
1	B	159	ILE	C-N	-5.21	1.27	1.33
1	B	263	PHE	CA-CB	5.21	1.60	1.53
1	B	127	ILE	C-O	5.20	1.30	1.24
1	D	21	GLU	C-O	5.20	1.30	1.23
1	B	190	TYR	C-N	5.20	1.40	1.33
1	C	85	ALA	CA-CB	5.19	1.61	1.53
1	A	88	ARG	NE-CZ	5.17	1.38	1.33
1	F	57	ASP	N-CA	5.17	1.52	1.46
1	E	200	ASP	C-O	5.17	1.30	1.24
1	C	115	PRO	CA-CB	5.15	1.60	1.53
1	C	122	LYS	CE-NZ	5.15	1.64	1.49
1	C	144	PRO	C-O	5.15	1.29	1.23
1	F	266	LEU	N-CA	5.14	1.52	1.46
1	C	189	LEU	N-CA	5.13	1.52	1.46
1	B	170	PHE	N-CA	5.12	1.52	1.46
1	E	164	PHE	CA-C	-5.12	1.45	1.52
1	F	62	VAL	CA-CB	-5.11	1.48	1.54
1	E	110	ARG	CZ-NH2	5.11	1.40	1.33
1	E	263	PHE	CA-CB	5.11	1.60	1.53
1	A	245	ARG	CA-C	5.11	1.59	1.52
1	E	60	VAL	N-CA	5.11	1.52	1.46
1	C	186	PHE	CA-CB	5.10	1.62	1.53
1	D	2	PHE	CA-CB	5.10	1.61	1.53
1	E	64	TYR	N-CA	5.10	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	LYS	CA-CB	5.09	1.58	1.53
1	F	39	PRO	C-N	5.08	1.39	1.32
1	B	57	ASP	N-CA	5.08	1.52	1.46
1	C	168	PRO	CA-C	5.08	1.60	1.52
1	E	40	HIS	CA-CB	5.07	1.60	1.54
1	B	50	GLY	N-CA	5.07	1.52	1.45
1	E	140	ASP	CG-OD1	5.07	1.34	1.25
1	B	130	LYS	C-O	5.07	1.30	1.24
1	D	62	VAL	CA-C	-5.06	1.46	1.52
1	C	152	ARG	C-O	5.06	1.29	1.24
1	C	56	SER	CA-C	5.05	1.59	1.52
1	C	266	LEU	N-CA	5.05	1.52	1.46
1	A	197	TYR	C-O	5.04	1.29	1.23
1	B	239	GLY	C-O	5.04	1.30	1.23
1	A	94	GLU	N-CA	5.04	1.52	1.46
1	F	6	SER	CA-CB	5.04	1.61	1.54
1	B	210	LYS	CA-C	5.03	1.59	1.52
1	A	212	ILE	C-N	5.02	1.40	1.33
1	F	76	ASP	C-O	5.02	1.30	1.24
1	A	48	MSE	C-O	-5.02	1.19	1.24
1	A	53	LYS	N-CA	5.01	1.52	1.46
1	B	61	GLU	N-CA	-5.01	1.40	1.46
1	A	245	ARG	NE-CZ	5.01	1.38	1.33
1	C	255	GLY	C-O	5.00	1.29	1.23
1	B	99	LEU	CA-CB	5.00	1.62	1.53

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	NE-CZ-NH2	9.35	127.62	119.20
1	A	125	VAL	CA-C-O	-7.48	113.17	120.95
1	C	210	LYS	O-C-N	7.38	129.95	122.12
1	D	132	LYS	CA-CB-CG	-7.30	99.50	114.10
1	E	129	ARG	NE-CZ-NH1	-7.18	114.31	121.50
1	E	210	LYS	O-C-N	7.10	129.65	122.12
1	D	56	SER	O-C-N	7.03	129.57	122.12
1	C	165	SER	O-C-N	6.96	131.75	122.43
1	D	165	SER	CA-C-O	-6.94	110.84	119.38
1	C	165	SER	CA-C-O	-6.93	110.85	119.38
1	D	132	LYS	CG-CD-CE	-6.71	95.88	111.30
1	E	227	TRP	N-CA-C	6.70	119.59	111.82
1	A	227	TRP	N-CA-C	6.70	119.59	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	CYS	O-C-N	6.66	129.18	122.12
1	D	153	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	F	65	ILE	CA-C-O	-6.61	113.52	120.39
1	B	138	ALA	N-CA-CB	-6.61	104.48	111.29
1	B	216	ARG	CD-NE-CZ	6.60	133.64	124.40
1	E	125	VAL	CA-C-O	-6.58	113.37	120.47
1	B	44	CYS	O-C-N	6.55	129.62	122.15
1	C	125	VAL	CA-C-O	-6.51	113.44	120.47
1	A	175	ILE	N-CA-C	-6.41	104.25	110.72
1	C	6	SER	CA-CB-OG	-6.39	98.33	111.10
1	B	245	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	B	227	TRP	CA-CB-CG	-6.36	101.51	113.60
1	C	167	LEU	CA-C-O	6.35	125.43	119.59
1	E	56	SER	O-C-N	6.31	128.81	122.12
1	B	125	VAL	CA-C-O	-6.29	114.18	120.85
1	E	88	ARG	N-CA-C	6.29	120.21	112.54
1	C	245	ARG	O-C-N	6.24	128.77	122.03
1	E	140	ASP	CB-CG-OD1	-6.24	104.06	118.40
1	B	62	VAL	CA-C-O	6.21	127.07	120.48
1	F	166	GLN	CB-CG-CD	-6.17	102.12	112.60
1	D	166	GLN	CB-CG-CD	-6.15	102.14	112.60
1	D	135	GLY	O-C-N	6.15	128.78	123.37
1	F	88	ARG	N-CA-C	6.14	118.94	111.82
1	F	6	SER	CA-CB-OG	-6.14	98.83	111.10
1	D	210	LYS	O-C-N	6.11	128.37	122.07
1	A	88	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	A	127	ILE	O-C-N	-6.09	115.56	121.83
1	A	56	SER	O-C-N	6.05	128.53	122.12
1	D	113	GLU	CA-C-O	-6.03	113.42	120.53
1	D	50	GLY	CA-C-O	5.96	126.89	120.75
1	D	52	ILE	O-C-N	5.93	127.72	121.91
1	A	62	VAL	CA-C-O	5.93	127.05	120.59
1	E	207	LEU	N-CA-C	-5.91	104.76	111.14
1	D	245	ARG	NE-CZ-NH2	5.88	124.50	119.20
1	F	227	TRP	N-CA-C	5.87	118.63	111.82
1	C	167	LEU	O-C-N	-5.86	114.44	121.12
1	A	210	LYS	O-C-N	5.83	128.30	122.12
1	A	245	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	D	65	ILE	O-C-N	5.80	129.35	123.20
1	E	245	ARG	O-C-N	5.77	128.32	122.09
1	D	117	SER	CA-C-O	5.76	127.39	121.23
1	B	131	GLU	O-C-N	-5.75	114.58	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLY	CA-C-N	5.74	128.24	120.38
1	A	70	GLY	C-N-CA	5.74	128.24	120.38
1	E	24	LEU	N-CA-C	-5.73	105.60	112.59
1	B	52	ILE	O-C-N	5.73	127.43	121.87
1	D	117	SER	O-C-N	5.73	129.55	123.42
1	E	111	ASP	N-CA-CB	-5.73	100.58	109.69
1	A	40	HIS	O-C-N	5.72	126.01	121.55
1	A	245	ARG	O-C-N	5.72	127.97	122.03
1	B	56	SER	CA-CB-OG	-5.66	99.78	111.10
1	E	52	ILE	O-C-N	5.64	127.44	121.91
1	B	6	SER	CA-CB-OG	-5.61	99.88	111.10
1	F	62	VAL	CA-C-O	5.58	126.54	120.57
1	B	159	ILE	CA-C-O	-5.57	114.87	121.05
1	F	125	VAL	CA-C-O	-5.56	115.17	120.95
1	D	44	CYS	O-C-N	5.54	127.99	122.12
1	E	65	ILE	CA-C-O	-5.53	114.63	120.39
1	F	53	LYS	CD-CE-NZ	-5.52	94.23	111.90
1	C	56	SER	O-C-N	5.48	127.93	122.12
1	F	210	LYS	O-C-N	5.48	127.93	122.12
1	D	134	ASP	CA-C-N	-5.48	117.39	121.61
1	D	134	ASP	C-N-CA	-5.48	117.39	121.61
1	A	128	ILE	O-C-N	5.48	127.28	121.91
1	C	227	TRP	CA-CB-CG	-5.48	103.19	113.60
1	F	56	SER	CA-CB-OG	-5.46	100.17	111.10
1	C	111	ASP	N-CA-CB	-5.46	101.02	109.48
1	F	147	SER	CA-C-N	-5.46	113.32	121.83
1	F	147	SER	C-N-CA	-5.46	113.32	121.83
1	D	25	GLU	CA-C-N	-5.45	117.30	122.37
1	D	25	GLU	C-N-CA	-5.45	117.30	122.37
1	B	89	ARG	CA-CB-CG	-5.45	103.20	114.10
1	A	52	ILE	O-C-N	5.45	127.16	121.87
1	B	210	LYS	O-C-N	5.44	127.89	122.12
1	C	91	GLU	CA-C-O	5.43	126.31	120.55
1	C	94	GLU	CG-CD-OE2	5.42	130.86	118.40
1	C	71	TYR	N-CA-C	5.41	117.87	111.33
1	F	56	SER	O-C-N	5.41	127.85	122.12
1	D	89	ARG	CA-CB-CG	-5.40	103.31	114.10
1	B	25	GLU	CA-C-N	-5.38	117.54	122.28
1	B	25	GLU	C-N-CA	-5.38	117.54	122.28
1	E	232	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	D	62	VAL	CA-C-O	5.37	126.17	120.48
1	C	113	GLU	N-CA-C	-5.37	105.00	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ARG	N-CA-C	5.35	119.07	112.54
1	C	174	ASP	CA-C-O	-5.35	115.20	120.82
1	A	111	ASP	N-CA-CB	-5.35	101.19	109.48
1	C	227	TRP	N-CA-C	5.35	118.02	111.82
1	B	153	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	A	89	ARG	O-C-N	5.31	128.21	122.15
1	E	40	HIS	O-C-N	5.30	125.69	121.55
1	F	245	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	65	ILE	CA-C-O	-5.29	114.89	120.39
1	D	245	ARG	O-C-N	5.29	127.80	122.09
1	B	23	ASN	N-CA-CB	5.28	119.90	111.56
1	E	109	TYR	CA-C-O	-5.26	115.97	121.55
1	F	40	HIS	O-C-N	5.26	125.65	121.55
1	C	239	GLY	CA-C-O	-5.25	115.34	120.75
1	A	155	GLY	O-C-N	5.22	127.20	122.18
1	E	82	HIS	O-C-N	5.22	127.45	122.07
1	A	42	ASP	CA-C-N	-5.22	112.38	120.31
1	A	42	ASP	C-N-CA	-5.22	112.38	120.31
1	A	88	ARG	N-CA-C	5.22	117.87	111.82
1	F	25	GLU	CA-C-N	-5.21	117.70	122.28
1	F	25	GLU	C-N-CA	-5.21	117.70	122.28
1	D	24	LEU	N-CA-C	-5.19	105.66	112.41
1	D	174	ASP	N-CA-C	-5.17	105.64	111.28
1	B	111	ASP	N-CA-CB	-5.15	101.50	109.69
1	E	174	ASP	CA-C-O	-5.14	115.43	120.82
1	F	85	ALA	N-CA-C	5.13	117.61	111.71
1	E	5	VAL	CA-C-N	-5.12	114.19	122.23
1	E	5	VAL	C-N-CA	-5.12	114.19	122.23
1	C	135	GLY	O-C-N	5.11	127.91	123.36
1	E	85	ALA	O-C-N	5.10	127.52	122.12
1	E	175	ILE	N-CA-C	-5.09	105.43	110.62
1	B	50	GLY	CA-C-O	5.08	126.05	120.66
1	D	65	ILE	CA-C-O	-5.08	115.10	120.39
1	E	224	TRP	O-C-N	5.08	128.52	122.27
1	A	25	GLU	CA-C-N	-5.07	117.28	122.85
1	A	25	GLU	C-N-CA	-5.07	117.28	122.85
1	B	24	LEU	N-CA-C	-5.06	105.83	112.41
1	C	52	ILE	O-C-N	5.05	126.86	121.91
1	A	227	TRP	O-C-N	-5.05	116.06	122.27
1	B	174	ASP	CA-C-O	-5.05	115.52	120.82
1	B	42	ASP	N-CA-CB	5.04	119.01	110.49
1	E	6	SER	CA-CB-OG	-5.02	101.05	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	ARG	O-C-N	5.01	127.50	122.09
1	D	131	GLU	O-C-N	-5.01	115.78	122.49
1	E	113	GLU	CA-C-O	-5.01	113.97	119.78

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

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	30	0
1	B	2197	0	2168	31	0
1	C	2197	0	2168	35	0
1	D	2197	0	2168	38	0
1	E	2197	0	2168	33	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	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	205	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 (205) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:E:313:TRS:O2	6:E:634:HOH:O	1.95	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:309:TRS:O1	6:C:640:HOH:O	1.92	0.68
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:53:LYS:NZ	6:C:579:HOH:O	2.31	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:D:41:PRO:O	1:D:42:ASP:CG	2.52	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:53:LYS:NZ	6:E:564:HOH:O	2.36	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:53:LYS:NZ	6:D:511:HOH:O	2.46	0.47
1:E:53:LYS:CE	6:E:564:HOH:O	2.62	0.47
1:E:41:PRO:O	1:E:42:ASP:CG	2.58	0.47
1:E:193[B]:HIS:CD2	1:E:194:LYS:HG2	2.50	0.47
1:D:193[B]:HIS:CD2	6:D:532:HOH:O	2.67	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:B:41:PRO:O	1:B:42:ASP:CG	2.58	0.46
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:F:41:PRO:O	1:F:42:ASP:CG	2.60	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
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:D:153:ARG:HH12	3:D:311:HEZ:C5	2.30	0.44
1:C:41:PRO:O	1:C:42:ASP:CG	2.61	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:41:PRO:O	1:A:42:ASP:CG	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:ILE:HG12	3:D:307:HEZ:H31	2.01	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: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:E:142:TRP:CD1	3:E:309:HEZ:HO1	2.37	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: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

5.3.1 Protein backbone

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%)	30	12
1	B	266/267 (100%)	261 (98%)	4 (2%)	1 (0%)	30	12
1	C	266/267 (100%)	260 (98%)	5 (2%)	1 (0%)	30	12
1	D	266/267 (100%)	262 (98%)	3 (1%)	1 (0%)	30	12
1	E	266/267 (100%)	261 (98%)	4 (2%)	1 (0%)	30	12
1	F	266/267 (100%)	259 (97%)	6 (2%)	1 (0%)	30	12
All	All	1596/1602 (100%)	1563 (98%)	27 (2%)	6 (0%)	30	12

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

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%)	237 (99%)	3 (1%)	61	34
1	B	240/232 (103%)	236 (98%)	4 (2%)	53	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	240/232 (103%)	237 (99%)	3 (1%)	61	34
1	D	240/232 (103%)	236 (98%)	4 (2%)	53	24
1	E	240/232 (103%)	237 (99%)	3 (1%)	61	34
1	F	240/232 (103%)	237 (99%)	3 (1%)	61	34
All	All	1440/1392 (103%)	1420 (99%)	20 (1%)	59	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	78	LYS
1	A	222	ASP
1	B	26	ASN
1	B	32	LYS
1	B	78	LYS
1	B	180	LYS
1	C	23	ASN
1	C	26	ASN
1	C	78	LYS
1	D	23	ASN
1	D	26	ASN
1	D	97	LYS
1	D	132	LYS
1	E	23	ASN
1	E	78	LYS
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 (9) 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	C	23	ASN
1	C	26	ASN
1	D	23	ASN

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Mol	Chain	Res	Type
1	E	23	ASN
1	E	218	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	F	305	-	7,7,7	1.13	0	6,6,6	1.88	2 (33%)
3	HEZ	D	305	-	7,7,7	1.01	0	6,6,6	0.89	0
4	TRS	A	314	-	7,7,7	2.25	4 (57%)	9,9,9	1.20	0
3	HEZ	D	308	-	7,7,7	0.90	0	6,6,6	1.86	2 (33%)
3	HEZ	D	306	-	7,7,7	1.06	0	6,6,6	0.83	0
3	HEZ	A	307	-	7,7,7	0.65	0	6,6,6	1.52	1 (16%)
3	HEZ	D	309	-	7,7,7	0.56	0	6,6,6	1.06	0
3	HEZ	A	311	-	7,7,7	0.18	0	6,6,6	1.75	2 (33%)
3	HEZ	E	304	-	7,7,7	0.81	0	6,6,6	1.01	0
3	HEZ	E	310	-	7,7,7	0.42	0	6,6,6	1.43	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEZ	F	304	-	7,7,7	0.99	0	6,6,6	0.88	0
3	HEZ	C	305	-	7,7,7	0.46	0	6,6,6	1.20	0
3	HEZ	B	305	-	7,7,7	0.79	0	6,6,6	1.26	1 (16%)
3	HEZ	E	308	-	7,7,7	1.08	0	6,6,6	2.07	2 (33%)
3	HEZ	A	312	-	7,7,7	0.59	0	6,6,6	1.22	1 (16%)
3	HEZ	D	311	-	7,7,7	0.98	0	6,6,6	0.88	0
3	HEZ	B	308	-	7,7,7	0.67	0	6,6,6	0.86	0
4	TRS	B	311	2	7,7,7	1.20	1 (14%)	9,9,9	1.41	1 (11%)
3	HEZ	C	308	-	7,7,7	0.69	0	6,6,6	1.28	1 (16%)
3	HEZ	A	308	-	7,7,7	1.22	1 (14%)	6,6,6	0.78	0
3	HEZ	A	306	-	7,7,7	1.05	0	6,6,6	1.23	0
3	HEZ	A	310	-	7,7,7	0.38	0	6,6,6	0.82	0
3	HEZ	E	307	-	7,7,7	0.45	0	6,6,6	0.48	0
3	HEZ	D	310	-	7,7,7	0.59	0	6,6,6	1.05	1 (16%)
4	TRS	E	313	2	7,7,7	1.47	2 (28%)	9,9,9	1.56	2 (22%)
4	TRS	C	309	2	7,7,7	1.45	1 (14%)	9,9,9	2.30	5 (55%)
3	HEZ	E	305	-	7,7,7	0.56	0	6,6,6	1.03	0
3	HEZ	F	306	-	7,7,7	0.51	0	6,6,6	1.25	0
3	HEZ	C	303	-	7,7,7	0.92	0	6,6,6	0.83	0
3	HEZ	C	307	-	7,7,7	0.21	0	6,6,6	1.60	1 (16%)
3	HEZ	E	312	-	7,7,7	0.24	0	6,6,6	1.91	2 (33%)
3	HEZ	F	307	-	7,7,7	0.27	0	6,6,6	1.08	1 (16%)
3	HEZ	F	308	-	7,7,7	0.38	0	6,6,6	1.82	2 (33%)
4	TRS	D	314	2	7,7,7	1.36	0	9,9,9	2.03	3 (33%)
3	HEZ	E	306	-	7,7,7	1.24	0	6,6,6	0.92	0
3	HEZ	C	304	-	7,7,7	1.03	0	6,6,6	1.12	1 (16%)
4	TRS	D	315	-	7,7,7	2.34	4 (57%)	9,9,9	0.55	0
3	HEZ	E	309	-	7,7,7	0.62	0	6,6,6	0.48	0
3	HEZ	B	306	-	7,7,7	0.51	0	6,6,6	1.19	0
4	TRS	A	313	2	7,7,7	1.38	2 (28%)	9,9,9	1.86	4 (44%)
3	HEZ	B	309	-	7,7,7	0.39	0	6,6,6	1.25	0
3	HEZ	C	306	-	7,7,7	1.05	0	6,6,6	2.12	4 (66%)
3	HEZ	B	310	-	7,7,7	0.26	0	6,6,6	1.28	0
3	HEZ	D	312	-	7,7,7	0.36	0	6,6,6	1.44	1 (16%)
3	HEZ	E	311	-	7,7,7	0.72	0	6,6,6	1.37	1 (16%)
3	HEZ	B	304	-	7,7,7	0.85	0	6,6,6	1.04	0
3	HEZ	A	305	-	7,7,7	0.80	0	6,6,6	0.69	0
3	HEZ	D	307	-	7,7,7	1.07	0	6,6,6	2.16	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRS	F	309	2	7,7,7	1.62	2 (28%)	9,9,9	1.95	3 (33%)
3	HEZ	F	303	-	7,7,7	1.03	0	6,6,6	0.97	0
3	HEZ	A	309	-	7,7,7	0.67	0	6,6,6	1.73	2 (33%)
3	HEZ	D	313	-	7,7,7	0.21	0	6,6,6	1.38	1 (16%)
3	HEZ	B	307	-	7,7,7	1.19	0	6,6,6	2.16	3 (50%)

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	F	305	-	-	2/5/5/5	-
3	HEZ	D	305	-	-	0/5/5/5	-
4	TRS	A	314	-	-	0/9/9/9	-
3	HEZ	D	308	-	-	2/5/5/5	-
3	HEZ	D	306	-	-	0/5/5/5	-
3	HEZ	A	307	-	-	4/5/5/5	-
3	HEZ	D	309	-	-	1/5/5/5	-
3	HEZ	A	311	-	-	2/5/5/5	-
3	HEZ	E	304	-	-	0/5/5/5	-
3	HEZ	E	310	-	-	3/5/5/5	-
3	HEZ	F	304	-	-	0/5/5/5	-
3	HEZ	C	305	-	-	2/5/5/5	-
3	HEZ	B	305	-	-	2/5/5/5	-
3	HEZ	E	308	-	-	4/5/5/5	-
3	HEZ	A	312	-	-	2/5/5/5	-
3	HEZ	D	311	-	-	4/5/5/5	-
3	HEZ	B	308	-	-	1/5/5/5	-
4	TRS	B	311	2	-	3/9/9/9	-
3	HEZ	C	308	-	-	3/5/5/5	-
3	HEZ	A	308	-	-	3/5/5/5	-
3	HEZ	A	306	-	-	0/5/5/5	-
3	HEZ	A	310	-	-	1/5/5/5	-
3	HEZ	E	307	-	-	3/5/5/5	-
3	HEZ	D	310	-	-	1/5/5/5	-
4	TRS	E	313	2	-	3/9/9/9	-
4	TRS	C	309	2	-	3/9/9/9	-

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

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	315	TRS	O2-C2	3.19	1.52	1.42
4	F	309	TRS	C3-C	3.13	1.61	1.53
4	D	315	TRS	O1-C1	3.13	1.52	1.42
4	C	309	TRS	O2-C2	3.08	1.52	1.42
4	A	314	TRS	O3-C3	2.92	1.51	1.42
4	A	314	TRS	O2-C2	2.82	1.51	1.42
4	A	314	TRS	O1-C1	2.77	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	315	TRS	O3-C3	2.75	1.51	1.42
4	E	313	TRS	O3-C3	2.75	1.51	1.42
4	B	311	TRS	O1-C1	2.73	1.51	1.42
4	F	309	TRS	O2-C2	2.58	1.50	1.42
4	A	313	TRS	O1-C1	2.54	1.50	1.42
4	D	315	TRS	C3-C	2.46	1.59	1.53
4	E	313	TRS	C1-C	2.46	1.59	1.53
4	A	313	TRS	C-N	2.41	1.57	1.49
3	A	308	HEZ	O6-C6	2.29	1.53	1.42
4	A	314	TRS	C-N	2.10	1.56	1.49

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	307	HEZ	C4-C3-C2	4.01	134.63	114.37
3	B	307	HEZ	C4-C3-C2	3.92	134.19	114.37
4	C	309	TRS	C3-C-C2	-3.76	100.64	110.66
3	E	308	HEZ	C3-C2-C1	-3.75	91.43	113.83
4	C	309	TRS	C2-C-C1	3.70	120.51	110.66
3	E	308	HEZ	C4-C5-C6	3.31	133.61	113.83
3	D	308	HEZ	O1-C1-C2	-3.21	91.06	111.44
4	D	314	TRS	C3-C-C1	3.20	119.17	110.66
4	F	309	TRS	C2-C-N	3.19	116.30	108.17
3	F	308	HEZ	C5-C4-C3	-3.17	98.33	114.37
4	D	314	TRS	C3-C-N	-3.12	100.20	108.17
3	A	309	HEZ	C3-C2-C1	-3.10	95.33	113.83
3	E	312	HEZ	O1-C1-C2	-3.07	91.92	111.44
3	A	311	HEZ	C4-C3-C2	-3.07	98.84	114.37
3	E	312	HEZ	C5-C4-C3	-3.02	99.09	114.37
3	C	307	HEZ	C4-C3-C2	-3.00	99.22	114.37
4	E	313	TRS	C3-C-C2	2.92	118.44	110.66
4	A	313	TRS	O1-C1-C	-2.82	103.01	110.88
3	C	306	HEZ	O6-C6-C5	-2.81	93.56	111.44
3	D	312	HEZ	C4-C3-C2	-2.81	100.16	114.37
3	C	306	HEZ	C3-C2-C1	-2.80	97.13	113.83
3	F	305	HEZ	C4-C5-C6	2.76	130.32	113.83
4	F	309	TRS	C3-C-C1	-2.76	103.31	110.66
3	B	305	HEZ	C4-C5-C6	-2.75	97.44	113.83
4	C	309	TRS	O2-C2-C	-2.71	103.32	110.88
4	F	309	TRS	O2-C2-C	-2.68	103.41	110.88
3	A	307	HEZ	C5-C4-C3	-2.67	100.85	114.37
4	A	313	TRS	C2-C-C1	-2.63	103.66	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	305	HEZ	O6-C6-C5	-2.62	94.83	111.44
4	A	313	TRS	C3-C-C1	2.59	117.56	110.66
3	B	307	HEZ	C3-C2-C1	-2.57	98.49	113.83
3	A	309	HEZ	C4-C5-C6	-2.55	98.58	113.83
3	C	306	HEZ	C4-C5-C6	-2.50	98.90	113.83
3	D	313	HEZ	C4-C3-C2	-2.49	101.77	114.37
4	B	311	TRS	C3-C-C1	2.48	117.27	110.66
3	C	308	HEZ	O1-C1-C2	2.48	127.19	111.44
3	D	308	HEZ	C4-C5-C6	-2.47	99.06	113.83
4	A	313	TRS	C3-C-N	-2.34	102.21	108.17
3	C	304	HEZ	C4-C3-C2	-2.33	102.60	114.37
3	B	307	HEZ	C5-C4-C3	-2.32	102.63	114.37
4	D	314	TRS	O1-C1-C	-2.32	104.42	110.88
3	D	307	HEZ	C4-C5-C6	2.28	127.45	113.83
4	C	309	TRS	C1-C-N	-2.23	102.48	108.17
4	C	309	TRS	C2-C-N	2.22	113.83	108.17
3	F	307	HEZ	C5-C4-C3	-2.16	103.47	114.37
3	F	308	HEZ	C4-C3-C2	2.15	125.26	114.37
3	E	311	HEZ	C5-C4-C3	-2.14	103.56	114.37
4	E	313	TRS	C3-C-C1	-2.13	104.99	110.66
3	A	312	HEZ	O1-C1-C2	2.10	124.78	111.44
3	D	310	HEZ	C5-C4-C3	-2.10	103.76	114.37
3	E	310	HEZ	C5-C4-C3	-2.08	103.84	114.37
3	C	306	HEZ	C4-C3-C2	2.06	124.77	114.37
3	A	311	HEZ	O6-C6-C5	-2.02	98.60	111.44

There are no chirality outliers.

All (100) 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
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

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

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

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

There are no ring outliers.

28 monomers are involved in 89 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-1.25	0 100 100	10, 18, 35, 55	1 (0%)
1	B	260/267 (97%)	-1.24	0 100 100	10, 18, 34, 52	1 (0%)
1	C	260/267 (97%)	-1.24	0 100 100	10, 18, 34, 54	1 (0%)
1	D	260/267 (97%)	-1.24	0 100 100	11, 18, 35, 55	1 (0%)
1	E	260/267 (97%)	-1.24	0 100 100	10, 18, 35, 54	1 (0%)
1	F	260/267 (97%)	-1.26	0 100 100	11, 18, 35, 53	1 (0%)
All	All	1560/1602 (97%)	-1.24	0 100 100	10, 18, 35, 55	6 (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 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(Å ²)	Q<0.9
3	HEZ	F	306	8/8	0.96	0.08	28,32,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEZ	D	309	8/8	0.97	0.07	29,32,34,38	0
3	HEZ	E	305	8/8	0.97	0.08	29,33,41,41	0
3	HEZ	C	305	8/8	0.97	0.07	28,33,35,39	0
4	TRS	A	314	8/8	0.97	0.06	23,25,27,28	0
3	HEZ	C	303	8/8	0.98	0.05	24,26,30,32	0
3	HEZ	A	307	8/8	0.98	0.07	29,33,41,41	0
3	HEZ	A	309	8/8	0.98	0.06	32,35,38,38	0
3	HEZ	D	313	8/8	0.98	0.06	38,48,56,56	0
3	HEZ	B	304	8/8	0.98	0.04	23,25,31,32	0
3	HEZ	E	308	8/8	0.98	0.05	28,35,38,41	0
3	HEZ	F	305	8/8	0.98	0.06	27,32,41,42	0
3	HEZ	B	306	8/8	0.98	0.06	27,33,35,40	0
3	HEZ	F	307	8/8	0.98	0.06	40,47,54,58	0
3	HEZ	B	307	8/8	0.98	0.06	30,35,40,46	0
4	TRS	C	309	8/8	0.98	0.05	16,21,23,29	0
4	TRS	D	315	8/8	0.98	0.06	23,25,26,26	0
3	HEZ	A	311	8/8	0.99	0.05	39,45,55,55	0
3	HEZ	C	306	8/8	0.99	0.05	30,34,39,40	0
3	HEZ	C	307	8/8	0.99	0.05	40,46,54,60	0
3	HEZ	C	308	8/8	0.99	0.06	25,41,45,51	0
3	HEZ	D	305	8/8	0.99	0.04	21,26,30,32	0
3	HEZ	D	306	8/8	0.99	0.05	20,28,32,34	0
3	HEZ	D	307	8/8	0.99	0.06	18,38,41,43	0
3	HEZ	D	308	8/8	0.99	0.05	28,36,40,43	0
3	HEZ	A	312	8/8	0.99	0.05	25,42,45,53	0
3	HEZ	D	310	8/8	0.99	0.04	25,35,49,50	0
3	HEZ	D	311	8/8	0.99	0.06	21,34,38,42	0
3	HEZ	D	312	8/8	0.99	0.04	28,42,50,51	0
3	HEZ	A	305	8/8	0.99	0.04	22,26,31,34	0
3	HEZ	E	304	8/8	0.99	0.04	22,26,31,31	0
3	HEZ	B	305	8/8	0.99	0.04	20,31,33,47	0
3	HEZ	E	306	8/8	0.99	0.05	21,29,31,31	0
3	HEZ	E	307	8/8	0.99	0.06	38,41,49,49	0
3	HEZ	A	308	8/8	0.99	0.06	38,43,49,49	0
3	HEZ	E	309	8/8	0.99	0.05	22,41,58,59	0
3	HEZ	E	310	8/8	0.99	0.04	27,40,52,52	0
3	HEZ	E	311	8/8	0.99	0.06	25,41,48,53	0
3	HEZ	E	312	8/8	0.99	0.05	35,43,52,55	0
3	HEZ	F	303	8/8	0.99	0.04	23,27,31,31	0
3	HEZ	F	304	8/8	0.99	0.04	21,29,32,32	0
3	HEZ	A	306	8/8	0.99	0.04	19,28,31,34	0
3	HEZ	B	308	8/8	0.99	0.06	34,37,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEZ	B	309	8/8	0.99	0.04	29,41,49,54	0
3	HEZ	F	308	8/8	0.99	0.06	24,41,45,51	0
4	TRS	A	313	8/8	0.99	0.04	18,19,22,29	0
3	HEZ	B	310	8/8	0.99	0.06	38,48,59,64	0
4	TRS	B	311	8/8	0.99	0.04	15,19,22,32	0
3	HEZ	A	310	8/8	0.99	0.06	29,45,55,60	0
4	TRS	D	314	8/8	0.99	0.04	16,19,21,30	0
3	HEZ	C	304	8/8	0.99	0.04	21,28,30,33	0
4	TRS	E	313	8/8	0.99	0.04	16,20,22,28	0
4	TRS	F	309	8/8	0.99	0.04	17,19,24,32	0
2	CD	F	302	1/1	1.00	0.01	19,19,19,19	0
2	CD	A	301	1/1	1.00	0.01	14,14,14,14	0
2	CD	A	302	1/1	1.00	0.02	19,19,19,19	0
2	CD	A	303	1/1	1.00	0.02	19,19,19,19	1
2	CD	A	304	1/1	1.00	0.02	19,19,19,19	1
2	CD	B	301	1/1	1.00	0.01	14,14,14,14	0
2	CD	B	302	1/1	1.00	0.01	19,19,19,19	0
2	CD	B	303	1/1	1.00	0.02	19,19,19,19	1
2	CD	C	301	1/1	1.00	0.01	14,14,14,14	0
2	CD	C	302	1/1	1.00	0.02	20,20,20,20	0
2	CD	D	301	1/1	1.00	0.01	14,14,14,14	0
2	CD	D	302	1/1	1.00	0.02	19,19,19,19	0
2	CD	D	303	1/1	1.00	0.02	19,19,19,19	1
2	CD	D	304	1/1	1.00	0.02	19,19,19,19	1
2	CD	E	301	1/1	1.00	0.01	14,14,14,14	0
2	CD	E	302	1/1	1.00	0.02	19,19,19,19	0
2	CD	E	303	1/1	1.00	0.02	19,19,19,19	1
2	CD	F	301	1/1	1.00	0.01	14,14,14,14	0
5	CL	A	315	1/1	1.00	0.01	22,22,22,22	0
5	CL	A	316	1/1	1.00	0.04	22,22,22,22	0
5	CL	A	317	1/1	1.00	0.01	20,20,20,20	0
5	CL	A	318	1/1	1.00	0.03	21,21,21,21	0
5	CL	A	319	1/1	1.00	0.04	17,17,17,17	0
5	CL	B	312	1/1	1.00	0.01	19,19,19,19	0
5	CL	B	313	1/1	1.00	0.04	21,21,21,21	0
5	CL	B	314	1/1	1.00	0.03	21,21,21,21	0
5	CL	B	315	1/1	1.00	0.04	17,17,17,17	0
5	CL	C	310	1/1	1.00	0.02	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	0.04	17,17,17,17	0
5	CL	D	316	1/1	1.00	0.03	21,21,21,21	0
5	CL	D	317	1/1	1.00	0.01	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	318	1/1	1.00	0.03	21,21,21,21	0
5	CL	D	319	1/1	1.00	0.04	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	0.01	19,19,19,19	0
5	CL	E	315	1/1	1.00	0.02	21,21,21,21	0
5	CL	E	316	1/1	1.00	0.01	22,22,22,22	0
5	CL	E	317	1/1	1.00	0.04	17,17,17,17	0
5	CL	F	310	1/1	1.00	0.02	20,20,20,20	0
5	CL	F	311	1/1	1.00	0.02	21,21,21,21	0
5	CL	F	312	1/1	1.00	0.04	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.