



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:03 PM UTC

PDB ID : 1ZCC / pdb_00001zcc
Title : Crystal structure of glycerophosphodiester phosphodiesterase from *Agrobacterium tumefaciens* str.C58
Authors : Krishnamurthy, N.R.; Kumaran, D.; Swaminathan, S.; Burley, S.K.; New York
SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2005-04-11
Resolution : 2.50 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:

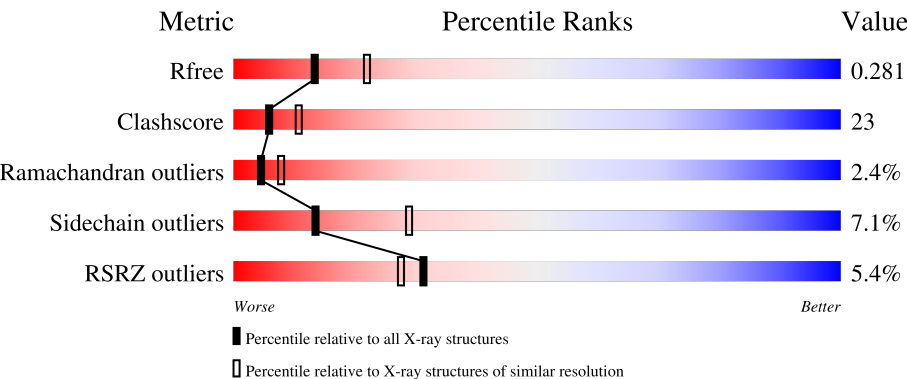
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	248	
1	B	248	
1	C	248	
1	D	248	
1	E	248	

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Mol	Chain	Length	Quality of chain
1	F	248	

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	SO4	F	4775	-	-	X	-

2 Entry composition [i](#)

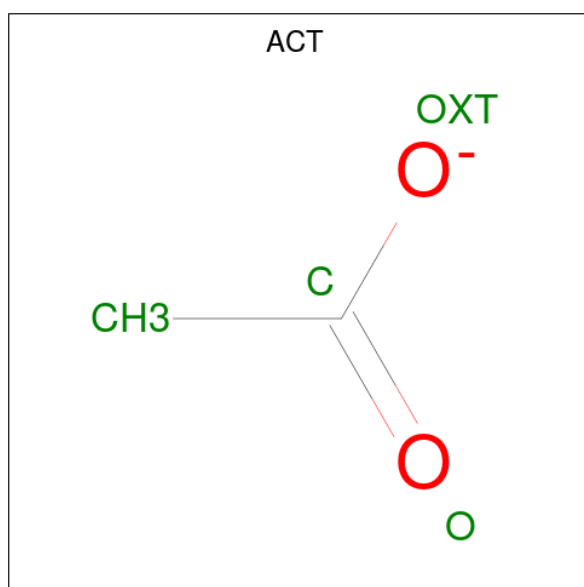
There are 4 unique types of molecules in this entry. The entry contains 10986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycerophosphodiester phosphodiesterase.

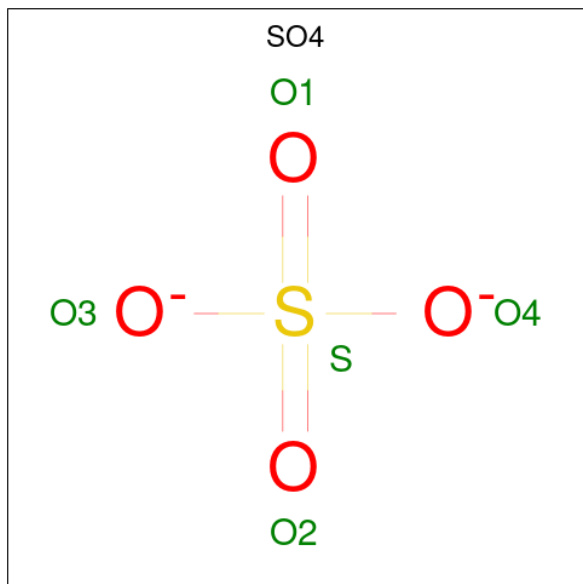
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1855	1167	326	352	10			
1	B	228	Total	C	N	O	S	0	0	0
			1705	1077	296	324	8			
1	C	233	Total	C	N	O	S	0	0	0
			1786	1124	311	342	9			
1	D	231	Total	C	N	O	S	0	0	0
			1736	1094	304	330	8			
1	E	233	Total	C	N	O	S	0	0	0
			1780	1119	312	341	8			
1	F	235	Total	C	N	O	S	0	0	0
			1794	1130	314	341	9			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

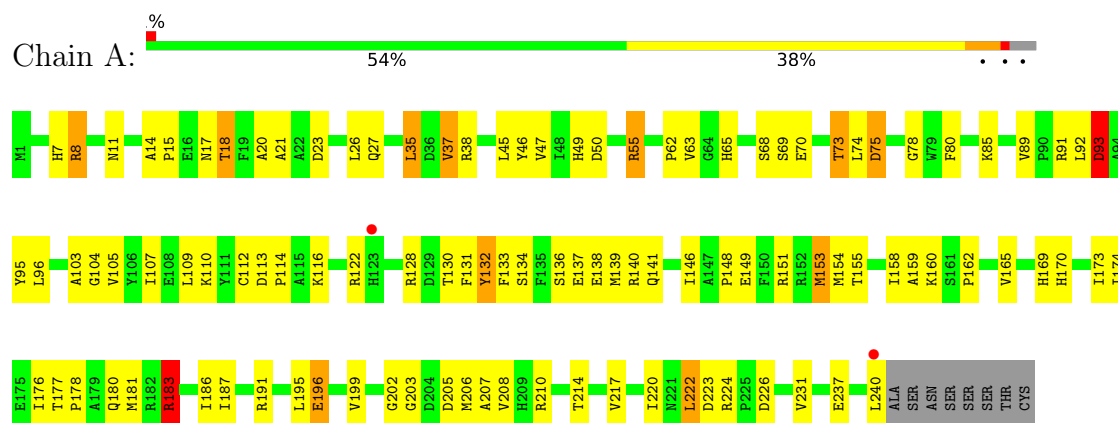
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total 68	O 68	0	0
4	B	34	Total 34	O 34	0	0
4	C	46	Total 46	O 46	0	0
4	D	55	Total 55	O 55	0	0
4	E	36	Total 36	O 36	0	0
4	F	37	Total 37	O 37	0	0

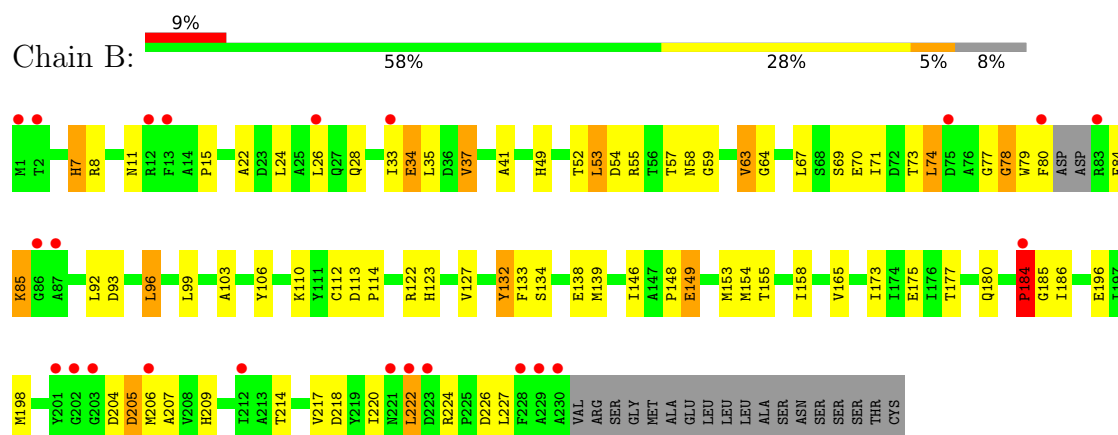
3 Residue-property plots [i](#)

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.

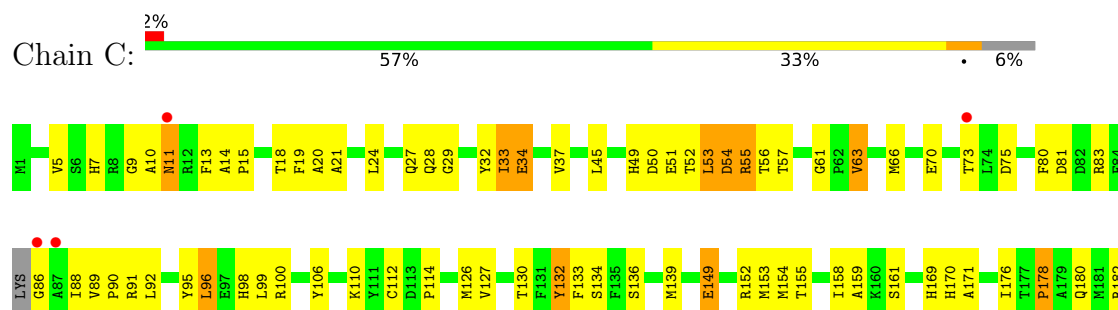
- Molecule 1: glycerophosphodiester phosphodiesterase



- Molecule 1: glycerophosphodiester phosphodiesterase

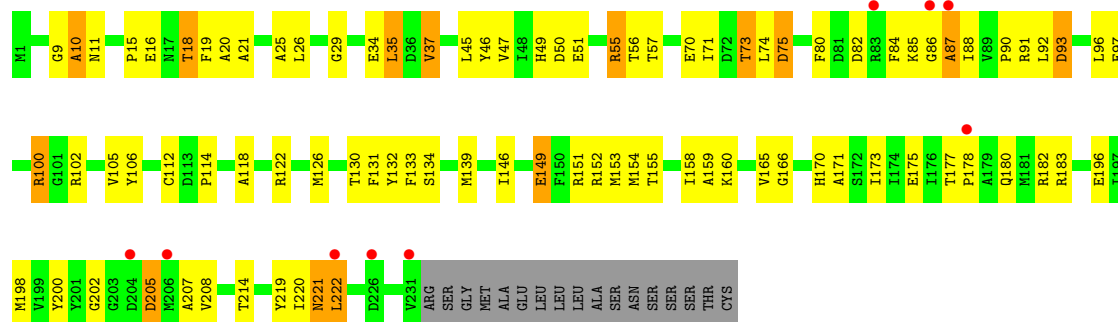


- Molecule 1: glycerophosphodiester phosphodiesterase

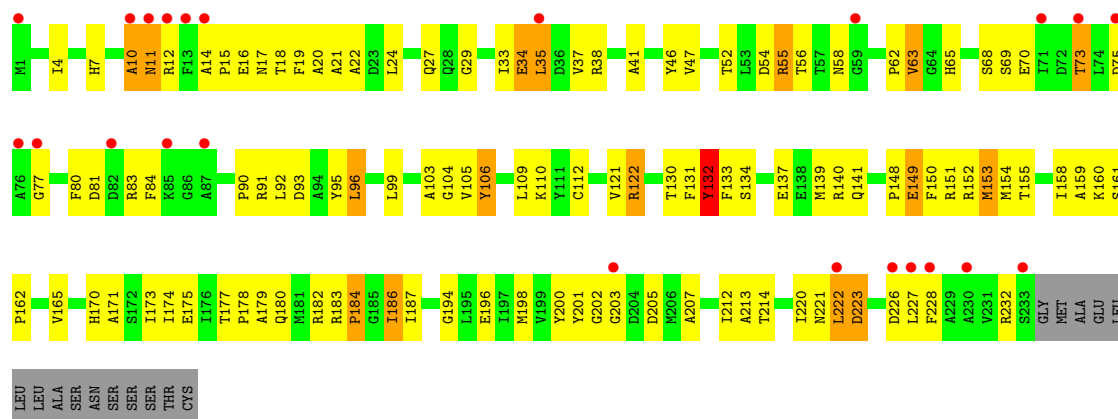




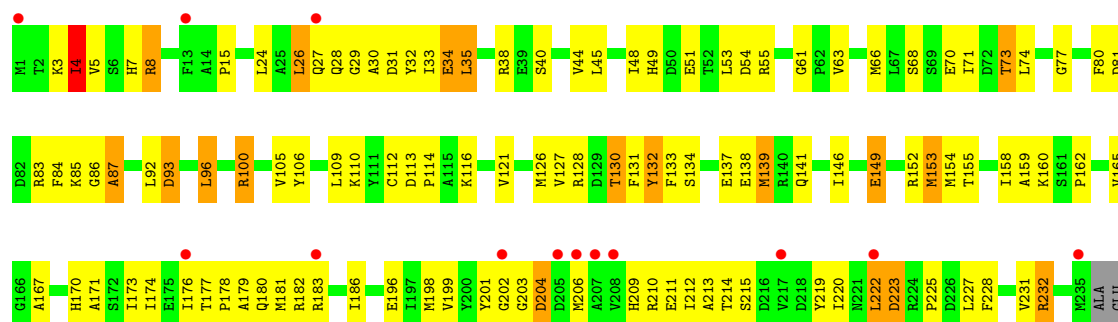
- Molecule 1: glycerophosphodiester phosphodiesterase



- Molecule 1: glycerophosphodiester phosphodiesterase



- Molecule 1: glycerophosphodiester phosphodiesterase



LEU
LEU
LEU
ALA
SER
ASN
SER
SER
SER
THR
CYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.56Å 140.22Å 88.60Å 90.00° 90.53° 90.00°	Depositor
Resolution (Å)	45.17 – 2.50 45.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (45.17-2.50) 94.2 (45.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.281 0.244 , 0.281	Depositor DCC
R_{free} test set	1264 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10986	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/1891	1.06	12/2560 (0.5%)
1	B	0.45	0/1738	1.01	7/2360 (0.3%)
1	C	0.48	0/1821	1.02	12/2467 (0.5%)
1	D	0.47	0/1770	1.01	6/2404 (0.2%)
1	E	0.45	0/1816	1.02	9/2464 (0.4%)
1	F	0.47	0/1830	1.04	11/2482 (0.4%)
All	All	0.47	0/10866	1.03	57/14737 (0.4%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	GLU	N-CA-C	-9.58	97.61	110.55
1	D	55	ARG	N-CA-C	8.10	119.80	110.97
1	E	11	ASN	N-CA-C	7.97	120.98	111.33
1	D	222	LEU	N-CA-C	7.97	122.45	109.85
1	D	196	GLU	N-CA-C	-7.86	97.82	110.32
1	F	55	ARG	N-CA-C	7.29	119.23	111.28
1	F	128	ARG	N-CA-C	7.28	119.84	111.11
1	A	55	ARG	N-CA-C	7.15	118.86	111.14
1	E	196	GLU	N-CA-C	-7.12	99.00	110.32
1	A	222	LEU	N-CA-C	6.93	119.02	109.18
1	A	203	GLY	N-CA-C	-6.92	103.10	112.57
1	B	37	VAL	N-CA-C	6.81	117.71	108.17
1	A	196	GLU	N-CA-C	-6.73	99.61	110.32
1	B	132	TYR	N-CA-C	6.72	120.09	109.81
1	B	196	GLU	N-CA-C	-6.72	99.64	110.32
1	D	37	VAL	N-CA-C	6.67	117.72	108.12
1	C	55	ARG	N-CA-C	6.48	119.18	111.33
1	A	49	HIS	N-CA-C	6.31	119.38	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	132	TYR	N-CA-C	6.22	119.68	109.85
1	F	196	GLU	N-CA-C	-6.20	100.19	110.17
1	C	132	TYR	N-CA-C	6.18	119.62	109.85
1	C	110	LYS	N-CA-C	-6.12	104.55	112.68
1	A	89	VAL	N-CA-C	-6.08	102.02	107.56
1	F	51	GLU	N-CA-C	-5.98	105.48	112.89
1	E	222	LEU	N-CA-C	5.94	119.25	110.46
1	C	49	HIS	N-CA-C	5.89	117.57	111.03
1	F	222	LEU	N-CA-C	5.89	119.13	110.59
1	E	104	GLY	N-CA-C	-5.88	104.14	112.37
1	B	224	ARG	CA-C-N	5.87	125.34	119.24
1	B	224	ARG	C-N-CA	5.87	125.34	119.24
1	B	127	VAL	N-CA-C	5.85	116.03	110.42
1	E	103	ALA	N-CA-C	5.81	117.36	108.42
1	F	223	ASP	N-CA-C	-5.78	106.01	114.39
1	A	104	GLY	N-CA-C	-5.75	103.87	113.02
1	C	222	LEU	N-CA-C	5.75	118.14	109.41
1	E	90	PRO	N-CA-C	5.69	119.39	110.80
1	B	209	HIS	N-CA-C	-5.65	105.22	111.71
1	A	183	ARG	CA-C-N	5.61	126.85	119.84
1	A	183	ARG	C-N-CA	5.61	126.85	119.84
1	E	223	ASP	N-CA-C	-5.61	106.33	114.12
1	C	61	GLY	CA-C-N	5.57	125.89	119.93
1	C	61	GLY	C-N-CA	5.57	125.89	119.93
1	A	11	ASN	N-CA-C	5.52	119.12	112.38
1	E	132	TYR	N-CA-C	5.51	117.79	109.41
1	C	37	VAL	N-CA-C	5.35	116.68	108.71
1	D	56	THR	N-CA-C	5.33	118.80	112.72
1	A	37	VAL	N-CA-C	5.30	116.11	108.48
1	F	61	GLY	CA-C-N	5.27	125.03	119.76
1	F	61	GLY	C-N-CA	5.27	125.03	119.76
1	C	89	VAL	N-CA-C	-5.24	97.56	108.88
1	A	132	TYR	N-CA-C	5.22	118.09	109.85
1	F	4	ILE	N-CA-C	5.18	115.77	108.36
1	F	167	ALA	N-CA-C	5.17	116.91	111.28
1	E	151	ARG	N-CA-C	-5.16	102.05	110.20
1	D	29	GLY	N-CA-C	5.10	122.94	115.08
1	C	56	THR	N-CA-C	5.05	118.98	112.41
1	C	91	ARG	N-CA-C	-5.03	101.52	109.96

There are no chirality outliers.

There are no planarity outliers.

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	1855	0	1816	80	0
1	B	1705	0	1636	73	0
1	C	1786	0	1725	63	0
1	D	1736	0	1667	75	0
1	E	1780	0	1709	108	0
1	F	1794	0	1735	101	0
2	A	4	0	3	0	0
2	B	4	0	3	1	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	2	0
4	A	68	0	0	3	0
4	B	34	0	0	1	0
4	C	46	0	0	0	0
4	D	55	0	0	3	0
4	E	36	0	0	2	0
4	F	37	0	0	0	0
All	All	10986	0	10306	484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (484) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MET:HE3	1:D:155:THR:H	1.11	1.05
1:C:154:MET:HE2	1:C:158:ILE:HB	1.37	1.02
1:C:154:MET:HE3	1:C:155:THR:H	1.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MET:HE2	1:D:158:ILE:HB	1.43	1.01
1:A:176:ILE:HG23	1:A:180:GLN:HB2	1.41	1.01
1:A:18:THR:HG22	1:A:21:ALA:H	1.23	1.01
1:E:154:MET:HE2	1:E:158:ILE:HB	1.45	0.99
1:B:57:THR:HG21	1:B:74:LEU:HD13	1.46	0.97
1:A:154:MET:HE2	1:A:158:ILE:HB	1.46	0.96
1:E:154:MET:HE3	1:E:155:THR:H	1.29	0.95
1:F:154:MET:HE3	1:F:155:THR:H	1.26	0.95
1:F:154:MET:HE2	1:F:158:ILE:HB	1.49	0.94
1:B:154:MET:HE3	1:B:155:THR:H	1.33	0.93
1:C:18:THR:HG22	1:C:20:ALA:H	1.32	0.92
1:F:176:ILE:HG23	1:F:180:GLN:HB2	1.53	0.91
1:F:139:MET:HE3	1:F:139:MET:HA	1.56	0.87
1:A:154:MET:HE3	1:A:155:THR:H	1.39	0.86
1:E:4:ILE:HG23	1:E:222:LEU:HD12	1.58	0.85
1:B:154:MET:HE2	1:B:158:ILE:HB	1.57	0.85
1:C:70:GLU:O	1:C:73:THR:HG22	1.78	0.83
1:A:35:LEU:HD21	1:A:107:ILE:HG12	1.60	0.83
1:A:18:THR:HG23	1:A:20:ALA:H	1.43	0.82
1:A:70:GLU:O	1:A:73:THR:HB	1.78	0.82
1:E:154:MET:HE1	1:E:158:ILE:HD12	1.61	0.81
1:A:112:CYS:O	1:A:139:MET:HE1	1.81	0.80
1:A:176:ILE:CG2	1:A:180:GLN:HB2	2.14	0.78
1:C:81:ASP:OD2	1:C:83:ARG:HB3	1.84	0.77
1:D:154:MET:HE3	1:D:155:THR:N	1.94	0.77
1:B:149:GLU:HG3	1:F:170:HIS:HA	1.67	0.77
1:E:37:VAL:HG12	1:E:109:LEU:HA	1.67	0.77
1:D:70:GLU:O	1:D:73:THR:HB	1.85	0.76
1:E:137:GLU:O	1:E:141:GLN:HG3	1.85	0.76
1:C:45:LEU:HD13	1:C:92:LEU:HD23	1.67	0.76
1:E:148:PRO:HD2	1:E:149:GLU:OE2	1.85	0.76
1:B:57:THR:HG22	1:B:59:GLY:H	1.51	0.75
1:F:212:ILE:HG21	1:F:220:ILE:HD12	1.66	0.75
1:F:154:MET:HE1	1:F:158:ILE:HD12	1.69	0.74
1:B:33:ILE:HD12	1:B:99:LEU:HD21	1.67	0.74
1:E:92:LEU:HG	1:E:96:LEU:HD22	1.69	0.73
1:D:93:ASP:HB2	4:D:4775:HOH:O	1.89	0.73
1:B:205:ASP:OD1	1:B:207:ALA:HB3	1.89	0.73
1:D:47:VAL:HB	1:D:90:PRO:HG2	1.70	0.73
1:F:178:PRO:HA	1:F:181:MET:HE2	1.69	0.72
1:D:154:MET:HE1	1:D:158:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:THR:OG1	1:F:180:GLN:HG3	1.90	0.71
1:F:5:VAL:HG21	1:F:198:MET:CE	2.20	0.71
1:A:137:GLU:O	1:A:141:GLN:HG3	1.90	0.71
1:D:220:ILE:HD11	1:D:222:LEU:HD21	1.71	0.71
1:F:154:MET:HE3	1:F:155:THR:N	2.03	0.70
1:B:7:HIS:CE1	1:B:8:ARG:HD3	2.26	0.70
1:B:15:PRO:HG3	1:B:80:PHE:HB3	1.73	0.70
1:D:105:VAL:HB	1:D:130:THR:HG22	1.73	0.70
1:C:34:GLU:HG3	1:C:106:TYR:CD2	2.27	0.70
1:E:105:VAL:HB	1:E:130:THR:HG22	1.74	0.70
1:B:149:GLU:CG	1:F:170:HIS:HA	2.22	0.69
1:B:92:LEU:HG	1:B:96:LEU:HD22	1.75	0.69
1:E:154:MET:HE3	1:E:155:THR:N	2.07	0.69
1:F:211:GLU:O	1:F:214:THR:HB	1.93	0.68
1:F:232:ARG:HB3	1:F:232:ARG:HH11	1.57	0.68
1:B:53:LEU:CD1	1:B:63:VAL:HG12	2.24	0.68
1:F:232:ARG:HH11	1:F:232:ARG:CB	2.06	0.68
1:D:154:MET:HE2	1:D:158:ILE:CB	2.23	0.67
1:A:15:PRO:HG3	1:A:80:PHE:HB3	1.77	0.67
1:A:112:CYS:O	1:A:114:PRO:HD3	1.94	0.67
1:E:15:PRO:HG3	1:E:80:PHE:HB3	1.78	0.66
1:F:154:MET:CE	1:F:158:ILE:HD12	2.25	0.66
1:E:7:HIS:HB3	1:E:222:LEU:O	1.96	0.66
1:D:50:ASP:OD1	1:D:55:ARG:HD3	1.95	0.66
1:F:26:LEU:HD13	1:F:33:ILE:HD11	1.77	0.66
1:B:78:GLY:HA2	1:B:85:LYS:HD2	1.78	0.65
1:D:18:THR:HG22	1:D:20:ALA:H	1.60	0.65
1:F:15:PRO:HG3	1:F:80:PHE:HB3	1.77	0.65
1:F:7:HIS:CE1	3:F:4775:SO4:O2	2.49	0.65
1:B:15:PRO:HG3	1:B:80:PHE:CB	2.27	0.65
1:B:53:LEU:HD13	1:B:63:VAL:HG12	1.79	0.65
1:B:57:THR:HG22	1:B:59:GLY:N	2.11	0.65
1:A:202:GLY:HA2	1:A:223:ASP:H	1.61	0.65
1:B:7:HIS:O	1:B:8:ARG:HG2	1.96	0.64
1:F:4:ILE:HG13	1:F:222:LEU:HD12	1.78	0.64
1:F:44:VAL:HG21	1:F:68:SER:HB3	1.78	0.64
1:F:92:LEU:HG	1:F:96:LEU:HD22	1.80	0.64
1:B:177:THR:OG1	1:B:180:GLN:HG3	1.98	0.64
1:E:35:LEU:CD1	1:E:105:VAL:HG13	2.27	0.64
1:F:139:MET:HA	1:F:139:MET:CE	2.27	0.64
1:E:4:ILE:HG13	1:E:232:ARG:NH1	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:MET:CE	1:D:155:THR:H	2.00	0.64
1:D:51:GLU:OE2	1:E:160:LYS:HE2	1.98	0.64
1:E:220:ILE:HG23	1:E:222:LEU:HG	1.80	0.63
1:F:220:ILE:CD1	1:F:222:LEU:HD21	2.28	0.63
1:C:230:ALA:O	1:C:233:SER:HB2	1.99	0.63
1:F:70:GLU:O	1:F:73:THR:HB	1.98	0.63
1:B:154:MET:HE3	1:B:155:THR:N	2.08	0.63
1:F:206:MET:HE1	1:F:227:LEU:HD22	1.81	0.63
1:C:112:CYS:O	1:C:139:MET:HE1	1.97	0.63
1:E:134:SER:O	1:E:140:ARG:HD3	1.99	0.63
1:F:35:LEU:HD11	1:F:105:VAL:HG13	1.81	0.63
1:A:7:HIS:C	1:A:8:ARG:HG2	2.24	0.63
1:A:154:MET:HE2	1:A:158:ILE:CB	2.25	0.63
1:C:170:HIS:HA	1:D:149:GLU:CG	2.29	0.63
1:D:19:PHE:CE1	1:D:90:PRO:HB3	2.34	0.63
1:F:121:VAL:HG21	1:F:132:TYR:OH	1.99	0.63
1:A:18:THR:HG23	1:A:20:ALA:N	2.12	0.63
1:E:213:ALA:HB2	1:E:228:PHE:CE1	2.33	0.63
1:E:35:LEU:HD11	1:E:105:VAL:HG13	1.81	0.62
1:D:18:THR:HG22	1:D:20:ALA:N	2.14	0.62
1:A:15:PRO:HG3	1:A:80:PHE:CB	2.29	0.62
1:F:77:GLY:HA3	1:F:87:ALA:HB3	1.81	0.62
1:A:35:LEU:O	1:A:35:LEU:HD23	2.00	0.62
1:A:173:ILE:HG12	1:A:196:GLU:HB2	1.80	0.62
1:B:92:LEU:O	1:B:96:LEU:HB2	1.99	0.62
1:E:11:ASN:ND2	1:E:223:ASP:OD1	2.33	0.62
1:E:15:PRO:HG3	1:E:80:PHE:CB	2.30	0.62
1:E:37:VAL:CG1	1:E:109:LEU:HA	2.30	0.62
1:B:33:ILE:HD12	1:B:99:LEU:CD2	2.30	0.61
1:E:56:THR:HG22	1:E:56:THR:O	1.99	0.61
1:E:4:ILE:HD11	1:E:228:PHE:HD2	1.66	0.61
1:E:152:ARG:HD3	1:E:170:HIS:O	2.00	0.61
1:E:34:GLU:HA	1:E:106:TYR:HB3	1.82	0.61
1:C:7:HIS:HB2	1:C:221:ASN:ND2	2.15	0.61
1:C:95:TYR:O	1:C:99:LEU:HG	2.00	0.61
1:F:202:GLY:HA2	1:F:223:ASP:HB2	1.82	0.61
1:B:112:CYS:O	1:B:139:MET:HE1	2.00	0.61
1:C:18:THR:HG22	1:C:20:ALA:N	2.12	0.61
1:B:154:MET:CE	1:B:155:THR:H	2.11	0.60
1:C:154:MET:HE3	1:C:155:THR:N	2.06	0.60
1:B:175:GLU:OE2	2:B:802:ACT:H2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:GLN:O	1:E:186:ILE:HD12	2.02	0.60
1:F:202:GLY:CA	1:F:223:ASP:HB2	2.32	0.60
1:E:154:MET:CE	1:E:158:ILE:HD12	2.31	0.60
1:B:78:GLY:O	1:B:80:PHE:N	2.35	0.60
1:C:170:HIS:HA	1:D:149:GLU:HG3	1.83	0.60
1:F:4:ILE:HG22	1:F:31:ASP:OD2	2.02	0.60
1:C:127:VAL:O	1:C:130:THR:HG22	2.01	0.60
1:C:210:ARG:HA	1:C:231:VAL:HG11	1.83	0.59
1:D:165:VAL:HG12	1:D:171:ALA:HB3	1.85	0.59
1:F:35:LEU:HD12	1:F:35:LEU:N	2.18	0.59
1:E:214:THR:O	1:E:214:THR:HG22	2.01	0.59
1:B:26:LEU:HD11	1:B:103:ALA:HB2	1.84	0.59
1:E:112:CYS:O	1:E:139:MET:HE1	2.03	0.59
1:F:210:ARG:HA	1:F:231:VAL:HG11	1.85	0.59
1:F:5:VAL:HG21	1:F:198:MET:HE2	1.83	0.58
1:C:14:ALA:HB3	1:C:21:ALA:HA	1.83	0.58
1:E:37:VAL:O	1:E:110:LYS:HB2	2.04	0.58
1:D:112:CYS:H	1:D:139:MET:CE	2.17	0.58
1:C:154:MET:HE1	1:C:158:ILE:HD12	1.84	0.58
1:C:133:PHE:CG	1:C:153:MET:HE3	2.39	0.58
1:D:205:ASP:OD1	1:D:207:ALA:HB3	2.03	0.58
1:F:53:LEU:HD13	1:F:74:LEU:HD11	1.86	0.58
1:D:175:GLU:OE1	1:D:198:MET:HE3	2.04	0.57
1:D:9:GLY:O	1:D:11:ASN:N	2.38	0.57
1:E:77:GLY:HA3	1:E:84:PHE:O	2.03	0.57
1:F:131:PHE:HZ	1:F:198:MET:HE1	1.70	0.57
1:C:100:ARG:HA	1:C:126:MET:HE3	1.87	0.57
1:D:132:TYR:CD1	1:D:132:TYR:N	2.73	0.57
1:E:133:PHE:HB2	1:E:153:MET:HG3	1.86	0.57
1:F:127:VAL:O	1:F:130:THR:HG22	2.04	0.57
1:A:176:ILE:HG22	1:A:177:THR:O	2.05	0.56
1:E:200:TYR:CD1	1:E:221:ASN:HB3	2.41	0.56
1:E:81:ASP:OD2	1:E:83:ARG:HG3	2.05	0.56
1:B:57:THR:HG22	1:B:58:ASN:N	2.19	0.56
1:F:35:LEU:HD11	1:F:105:VAL:CG1	2.35	0.56
1:F:114:PRO:HB2	1:F:146:ILE:HD12	1.88	0.56
1:D:198:MET:HA	1:D:219:TYR:O	2.06	0.56
1:D:220:ILE:CD1	1:D:222:LEU:HD21	2.34	0.55
1:F:165:VAL:HG21	1:F:174:ILE:HD12	1.88	0.55
1:A:205:ASP:OD1	1:A:207:ALA:HB3	2.07	0.55
1:D:154:MET:HB3	1:D:165:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:THR:OG1	1:D:180:GLN:HG3	2.06	0.55
1:A:153:MET:SD	1:A:153:MET:C	2.90	0.55
1:B:24:LEU:O	1:B:28:GLN:HG3	2.06	0.55
1:D:153:MET:SD	1:D:153:MET:C	2.89	0.55
1:A:35:LEU:HD12	1:A:95:TYR:CD2	2.42	0.55
1:E:7:HIS:HB2	1:E:221:ASN:ND2	2.22	0.55
1:C:154:MET:HE2	1:C:158:ILE:CB	2.25	0.55
1:E:154:MET:HB3	1:E:165:VAL:HG13	1.88	0.54
1:B:226:ASP:OD1	1:B:227:LEU:N	2.39	0.54
1:F:5:VAL:HG21	1:F:198:MET:HE1	1.89	0.54
1:A:35:LEU:CD2	1:A:107:ILE:HA	2.36	0.54
1:C:75:ASP:CG	1:C:86:GLY:HA2	2.31	0.54
1:D:91:ARG:O	1:D:92:LEU:C	2.51	0.54
1:A:18:THR:CG2	1:A:21:ALA:H	2.07	0.54
1:B:133:PHE:CG	1:B:153:MET:HE3	2.43	0.54
1:F:7:HIS:HE1	3:F:4775:SO4:O2	1.91	0.54
1:B:148:PRO:HD2	1:B:149:GLU:OE2	2.07	0.54
1:D:105:VAL:O	1:D:130:THR:HA	2.08	0.54
1:E:187:ILE:HG13	4:E:4782:HOH:O	2.08	0.54
1:F:114:PRO:HG3	1:F:139:MET:HE2	1.89	0.54
1:A:220:ILE:HD13	1:A:222:LEU:HD23	1.89	0.54
1:E:152:ARG:O	1:E:171:ALA:HB1	2.07	0.54
1:B:22:ALA:O	1:B:26:LEU:HB2	2.07	0.54
1:B:70:GLU:O	1:B:73:THR:HB	2.08	0.53
1:D:133:PHE:CG	1:D:153:MET:HE3	2.42	0.53
1:A:23:ASP:O	1:A:27:GLN:HG3	2.08	0.53
1:A:128:ARG:NE	1:A:128:ARG:HA	2.23	0.53
1:A:26:LEU:HD11	1:A:103:ALA:HB2	1.90	0.53
1:F:38:ARG:HB3	1:F:63:VAL:HG21	1.90	0.53
1:B:154:MET:HB3	1:B:165:VAL:HG13	1.91	0.53
1:C:133:PHE:CG	1:C:134:SER:N	2.76	0.53
1:C:149:GLU:CG	1:D:170:HIS:HA	2.39	0.53
1:E:220:ILE:HD13	1:E:222:LEU:HD21	1.91	0.53
1:E:175:GLU:OE1	1:E:198:MET:HE3	2.08	0.53
1:B:57:THR:HG23	1:B:74:LEU:HB3	1.90	0.53
1:E:18:THR:HG22	1:E:20:ALA:H	1.74	0.53
1:E:178:PRO:O	1:E:182:ARG:HG3	2.08	0.53
1:F:8:ARG:NH1	1:F:49:HIS:CD2	2.76	0.53
1:A:223:ASP:O	1:A:224:ARG:HG2	2.09	0.52
1:F:232:ARG:HB3	1:F:232:ARG:NH1	2.23	0.52
1:D:205:ASP:CG	1:D:208:VAL:HG23	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:TYR:N	1:B:132:TYR:CD1	2.77	0.52
1:F:201:TYR:CZ	1:F:203:GLY:HA3	2.45	0.52
1:A:205:ASP:HB3	1:A:208:VAL:HG23	1.92	0.52
1:D:165:VAL:CG1	1:D:171:ALA:HB3	2.39	0.52
1:F:198:MET:HA	1:F:219:TYR:O	2.09	0.52
1:D:198:MET:HB2	1:D:219:TYR:HB2	1.92	0.52
1:F:220:ILE:HG12	1:F:222:LEU:HG	1.91	0.52
1:A:50:ASP:CG	1:A:55:ARG:NH1	2.68	0.52
1:A:132:TYR:N	1:A:132:TYR:CD1	2.77	0.52
1:C:132:TYR:CD1	1:C:132:TYR:N	2.77	0.52
1:A:140:ARG:HD2	4:A:4804:HOH:O	2.10	0.52
1:B:204:ASP:O	1:B:206:MET:N	2.42	0.52
1:B:217:VAL:HG12	1:B:218:ASP:N	2.24	0.52
1:C:33:ILE:HD12	1:C:34:GLU:N	2.25	0.52
1:F:100:ARG:HA	1:F:126:MET:HE3	1.92	0.52
1:A:114:PRO:HB2	1:A:146:ILE:HD12	1.92	0.51
1:D:220:ILE:HG12	1:D:222:LEU:HG	1.91	0.51
1:B:149:GLU:CD	1:B:149:GLU:H	2.17	0.51
1:E:4:ILE:HG23	1:E:222:LEU:CD1	2.33	0.51
1:C:133:PHE:CD1	1:C:153:MET:HE3	2.46	0.51
1:E:35:LEU:N	1:E:35:LEU:HD12	2.26	0.51
1:F:133:PHE:CG	1:F:134:SER:N	2.78	0.51
1:C:88:ILE:O	1:C:90:PRO:HD3	2.09	0.51
1:A:133:PHE:CD1	1:A:153:MET:HE3	2.45	0.50
1:C:75:ASP:OD1	1:C:86:GLY:HA2	2.11	0.50
1:B:133:PHE:CG	1:B:134:SER:N	2.79	0.50
1:E:153:MET:HA	1:E:173:ILE:O	2.12	0.50
1:A:131:PHE:HA	1:A:151:ARG:O	2.11	0.50
1:F:7:HIS:CD2	1:F:8:ARG:HG2	2.46	0.50
1:F:71:ILE:C	1:F:73:THR:H	2.20	0.50
1:A:35:LEU:HD23	1:A:107:ILE:HA	1.93	0.50
1:A:170:HIS:HA	1:E:149:GLU:HG3	1.92	0.50
1:C:206:MET:HE3	1:C:231:VAL:HG23	1.94	0.50
1:C:7:HIS:HB2	1:C:221:ASN:HD21	1.74	0.50
1:E:22:ALA:HB1	1:E:33:ILE:HD13	1.94	0.50
1:A:7:HIS:O	1:A:8:ARG:HG2	2.11	0.50
1:E:165:VAL:HG21	1:E:174:ILE:HD12	1.94	0.50
1:E:212:ILE:HG21	1:E:220:ILE:HD12	1.93	0.50
1:D:96:LEU:HD22	1:D:126:MET:HE1	1.92	0.50
1:D:131:PHE:HA	1:D:151:ARG:O	2.11	0.50
1:B:73:THR:O	1:B:74:LEU:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:HIS:C	1:F:8:ARG:HG2	2.36	0.49
1:C:53:LEU:HB3	1:C:57:THR:OG1	2.11	0.49
1:F:44:VAL:HG21	1:F:68:SER:CB	2.43	0.49
1:C:15:PRO:HG3	1:C:80:PHE:CB	2.43	0.49
1:A:15:PRO:O	1:A:18:THR:HB	2.11	0.49
1:B:123:HIS:C	1:B:123:HIS:CD2	2.91	0.49
1:B:153:MET:HA	1:B:173:ILE:O	2.12	0.49
1:D:97:GLU:O	1:D:100:ARG:HB3	2.12	0.49
1:A:18:THR:CG2	1:A:20:ALA:HB3	2.43	0.49
1:B:175:GLU:OE1	1:B:198:MET:HE3	2.13	0.49
1:F:66:MET:HE2	1:F:70:GLU:OE2	2.13	0.49
1:F:149:GLU:CD	1:F:149:GLU:H	2.20	0.49
1:A:154:MET:HE1	1:A:158:ILE:HD12	1.95	0.49
1:F:220:ILE:HD13	1:F:222:LEU:HD21	1.93	0.49
1:A:37:VAL:CG1	1:A:109:LEU:HA	2.42	0.49
1:A:187:ILE:O	1:A:191:ARG:HG2	2.12	0.49
4:A:4784:HOH:O	1:E:148:PRO:HB2	2.13	0.49
1:D:15:PRO:O	1:D:21:ALA:HB2	2.12	0.49
1:E:159:ALA:C	1:E:161:SER:H	2.21	0.49
1:B:7:HIS:HE1	1:B:8:ARG:NH1	2.11	0.49
1:E:18:THR:HG22	1:E:19:PHE:N	2.28	0.49
1:E:27:GLN:C	1:E:29:GLY:H	2.19	0.49
1:F:4:ILE:HD11	1:F:225:PRO:HA	1.95	0.49
1:F:176:ILE:HG22	1:F:177:THR:O	2.12	0.49
1:F:130:THR:HG23	1:F:132:TYR:CE1	2.48	0.48
1:A:133:PHE:CG	1:A:134:SER:N	2.81	0.48
1:D:46:TYR:CE2	1:D:91:ARG:HG2	2.49	0.48
1:D:10:ALA:H	1:D:25:ALA:HB2	1.78	0.48
1:D:214:THR:HA	4:D:4815:HOH:O	2.13	0.48
1:E:152:ARG:HG2	1:E:171:ALA:HA	1.96	0.48
1:C:51:GLU:O	1:C:63:VAL:HG13	2.13	0.48
1:E:46:TYR:OH	1:E:68:SER:HB2	2.12	0.48
1:A:133:PHE:CG	1:A:153:MET:HE3	2.48	0.48
1:B:57:THR:CG2	1:B:58:ASN:N	2.76	0.48
1:C:136:SER:OG	1:C:139:MET:HG2	2.14	0.48
1:E:10:ALA:HB3	1:E:24:LEU:HD23	1.96	0.48
1:D:75:ASP:OD2	1:D:85:LYS:O	2.32	0.48
1:D:178:PRO:O	1:D:182:ARG:HG3	2.14	0.48
1:B:35:LEU:C	1:B:35:LEU:HD12	2.39	0.48
1:E:41:ALA:HA	1:F:162:PRO:HD2	1.96	0.48
1:F:81:ASP:OD2	1:F:83:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PRO:O	1:B:186:ILE:N	2.47	0.48
1:F:213:ALA:HB2	1:F:228:PHE:CE1	2.49	0.48
1:B:67:LEU:O	1:B:71:ILE:HG13	2.14	0.47
1:E:202:GLY:CA	1:E:223:ASP:HB2	2.44	0.47
1:F:38:ARG:HG3	1:F:48:ILE:HG23	1.95	0.47
1:A:170:HIS:HA	1:E:149:GLU:CG	2.44	0.47
1:B:78:GLY:C	1:B:80:PHE:H	2.22	0.47
1:C:15:PRO:O	1:C:21:ALA:HB2	2.14	0.47
1:C:176:ILE:HB	1:C:180:GLN:HB2	1.96	0.47
1:A:153:MET:SD	1:A:154:MET:N	2.86	0.47
1:C:149:GLU:HG3	1:D:170:HIS:HA	1.95	0.47
1:E:12:ARG:HD3	1:E:12:ARG:N	2.30	0.47
1:F:34:GLU:HG3	1:F:106:TYR:CD2	2.50	0.47
1:B:33:ILE:CD1	1:B:99:LEU:HD21	2.39	0.47
1:B:154:MET:HE3	1:B:154:MET:HA	1.96	0.47
1:E:202:GLY:HA2	1:E:223:ASP:HB2	1.96	0.47
1:A:35:LEU:HD12	1:A:95:TYR:HD2	1.80	0.47
1:B:220:ILE:CB	1:B:222:LEU:HD21	2.44	0.47
1:D:71:ILE:C	1:D:73:THR:H	2.21	0.47
1:D:134:SER:HA	4:D:4783:HOH:O	2.14	0.47
1:E:132:TYR:CD1	1:E:132:TYR:N	2.82	0.47
1:E:46:TYR:CE2	1:E:91:ARG:HG2	2.49	0.47
1:D:34:GLU:C	1:D:35:LEU:HD12	2.40	0.47
1:E:121:VAL:HG21	1:E:132:TYR:OH	2.15	0.47
1:D:88:ILE:O	1:D:90:PRO:HD3	2.15	0.47
1:E:226:ASP:CG	1:E:227:LEU:N	2.73	0.47
1:A:210:ARG:HA	1:A:231:VAL:HG11	1.97	0.46
1:F:7:HIS:NE2	1:F:8:ARG:HD3	2.30	0.46
1:A:62:PRO:HG2	1:A:65:HIS:HB2	1.97	0.46
1:A:105:VAL:O	1:A:130:THR:HA	2.15	0.46
1:B:217:VAL:CG1	1:B:218:ASP:N	2.78	0.46
1:E:162:PRO:HA	1:E:165:VAL:HG23	1.97	0.46
1:F:53:LEU:HD23	1:F:63:VAL:HG12	1.97	0.46
1:F:152:ARG:HG2	1:F:171:ALA:HA	1.97	0.46
1:E:15:PRO:HD3	1:E:84:PHE:CD1	2.50	0.46
1:E:201:TYR:CZ	1:E:203:GLY:HA3	2.51	0.46
1:A:154:MET:CE	1:A:158:ILE:HD12	2.46	0.46
1:C:205:ASP:HB3	1:C:208:VAL:HG23	1.97	0.46
1:C:213:ALA:HB2	1:C:228:PHE:CE1	2.50	0.46
1:E:11:ASN:HD22	1:E:223:ASP:HA	1.79	0.46
1:E:68:SER:O	1:E:69:SER:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HA	1:A:240:LEU:HD12	1.97	0.46
1:B:112:CYS:O	1:B:114:PRO:HD3	2.15	0.46
1:E:106:TYR:CD1	1:E:106:TYR:C	2.93	0.46
1:A:91:ARG:O	1:A:92:LEU:C	2.55	0.46
1:E:200:TYR:HD1	1:E:221:ASN:HB3	1.81	0.46
1:F:26:LEU:CD1	1:F:33:ILE:HD11	2.44	0.46
1:D:114:PRO:HB2	1:D:146:ILE:HD12	1.97	0.46
1:C:159:ALA:C	1:C:161:SER:H	2.24	0.46
1:D:57:THR:HA	1:D:75:ASP:O	2.16	0.46
1:D:202:GLY:H	1:D:222:LEU:HD23	1.81	0.46
1:A:237:GLU:O	1:A:240:LEU:HB2	2.15	0.46
1:E:65:HIS:HB3	1:F:186:ILE:HD11	1.97	0.46
1:A:91:ARG:C	1:A:93:ASP:N	2.69	0.46
1:A:109:LEU:HD13	1:A:139:MET:HE3	1.98	0.46
1:C:170:HIS:HA	1:D:149:GLU:HG2	1.98	0.46
1:D:153:MET:CB	1:D:173:ILE:HB	2.46	0.45
1:E:95:TYR:O	1:E:99:LEU:HG	2.16	0.45
1:E:96:LEU:HD11	1:E:105:VAL:HG11	1.97	0.45
1:F:154:MET:HE2	1:F:158:ILE:CB	2.32	0.45
1:B:8:ARG:NH1	1:B:49:HIS:CD2	2.84	0.45
1:C:24:LEU:O	1:C:28:GLN:HG3	2.15	0.45
1:E:179:ALA:HA	1:E:182:ARG:NH1	2.32	0.45
1:E:16:GLU:OE2	1:E:55:ARG:NH2	2.50	0.45
1:E:52:THR:HA	1:E:62:PRO:HA	1.98	0.45
1:C:18:THR:HG22	1:C:19:PHE:N	2.31	0.45
1:D:16:GLU:OE1	1:D:55:ARG:NH2	2.50	0.45
1:E:149:GLU:CD	1:E:149:GLU:H	2.25	0.45
1:F:4:ILE:CG1	1:F:222:LEU:HD12	2.44	0.45
1:C:152:ARG:HG2	1:C:171:ALA:HA	1.99	0.45
1:D:86:GLY:O	1:D:87:ALA:C	2.59	0.45
1:D:154:MET:CE	1:D:158:ILE:HD12	2.44	0.45
1:E:109:LEU:HD13	1:E:139:MET:HE3	1.98	0.45
1:F:114:PRO:CG	1:F:139:MET:HE2	2.46	0.45
1:B:7:HIS:C	1:B:8:ARG:HG2	2.42	0.45
1:F:5:VAL:HG22	1:F:32:TYR:HB2	1.98	0.45
1:C:34:GLU:HA	1:C:106:TYR:O	2.17	0.45
1:C:112:CYS:O	1:C:114:PRO:HD3	2.16	0.45
1:F:159:ALA:O	1:F:160:LYS:HB2	2.17	0.45
1:C:92:LEU:O	1:C:96:LEU:HB2	2.17	0.45
1:E:154:MET:HE2	1:E:158:ILE:CB	2.30	0.44
1:E:202:GLY:HA2	1:E:223:ASP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:LEU:HD13	1:F:92:LEU:HD23	2.00	0.44
1:E:35:LEU:HD13	1:E:105:VAL:HG13	2.00	0.44
1:F:4:ILE:HG23	1:F:31:ASP:H	1.82	0.44
1:B:78:GLY:C	1:B:80:PHE:N	2.76	0.44
1:B:154:MET:HE1	1:B:158:ILE:HD12	2.00	0.44
1:E:174:ILE:HG23	1:E:174:ILE:O	2.16	0.44
1:F:180:GLN:O	1:F:186:ILE:HG13	2.17	0.44
1:A:159:ALA:O	1:A:160:LYS:HB2	2.18	0.44
1:C:9:GLY:O	1:C:11:ASN:N	2.42	0.44
1:C:176:ILE:O	1:C:199:VAL:HA	2.18	0.44
1:E:62:PRO:HG2	1:E:65:HIS:CG	2.53	0.44
1:A:165:VAL:O	1:A:169:HIS:HB2	2.18	0.44
1:A:183:ARG:HB2	1:A:186:ILE:HD12	1.99	0.44
1:B:57:THR:CG2	1:B:74:LEU:HB3	2.48	0.44
1:B:149:GLU:HG3	1:F:170:HIS:CA	2.43	0.43
1:C:206:MET:CE	1:C:231:VAL:HG23	2.48	0.43
1:B:133:PHE:CD1	1:B:153:MET:HE3	2.52	0.43
1:D:82:ASP:C	1:D:84:PHE:H	2.26	0.43
1:D:159:ALA:O	1:D:160:LYS:HB2	2.19	0.43
1:E:14:ALA:HB3	1:E:21:ALA:HA	2.00	0.43
1:F:109:LEU:HD22	1:F:112:CYS:SG	2.58	0.43
1:F:179:ALA:HA	1:F:182:ARG:NH1	2.34	0.43
1:B:77:GLY:O	1:B:78:GLY:C	2.61	0.43
1:C:19:PHE:HD2	1:C:98:HIS:CD2	2.36	0.43
1:A:113:ASP:OD2	1:A:116:LYS:HG3	2.19	0.43
1:F:113:ASP:OD2	1:F:116:LYS:HG3	2.19	0.43
1:C:5:VAL:HG22	1:C:32:TYR:HB2	2.00	0.43
1:D:49:HIS:HD2	1:D:50:ASP:OD2	2.01	0.43
1:E:17:ASN:HB3	1:E:47:VAL:HG12	2.01	0.43
1:A:136:SER:HB3	1:A:139:MET:HG2	2.01	0.43
1:A:162:PRO:HD2	1:B:41:ALA:HA	2.01	0.43
1:F:4:ILE:HG23	1:F:30:ALA:HA	2.00	0.43
1:D:19:PHE:HE1	1:D:90:PRO:HB3	1.78	0.43
1:D:75:ASP:OD1	1:D:75:ASP:C	2.62	0.43
1:E:38:ARG:HD3	1:E:63:VAL:HG11	2.01	0.43
1:C:210:ARG:HA	1:C:231:VAL:CG1	2.48	0.42
1:D:200:TYR:HA	1:D:221:ASN:HB3	2.00	0.42
1:E:175:GLU:HB2	1:E:198:MET:HE2	2.01	0.42
1:F:209:HIS:HE1	1:F:222:LEU:HD22	1.84	0.42
1:A:14:ALA:HB3	1:A:21:ALA:HA	2.00	0.42
1:B:34:GLU:HG3	1:B:106:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LEU:HD13	1:D:92:LEU:HD23	2.00	0.42
1:E:170:HIS:HD2	4:E:4791:HOH:O	2.01	0.42
1:E:177:THR:OG1	1:E:180:GLN:HG3	2.19	0.42
1:F:84:PHE:O	1:F:85:LYS:C	2.62	0.42
1:A:174:ILE:HB	1:A:195:LEU:HD13	2.00	0.42
1:C:27:GLN:C	1:C:29:GLY:H	2.27	0.42
1:D:118:ALA:O	1:D:122:ARG:HG3	2.19	0.42
1:F:3:LYS:O	1:F:219:TYR:HA	2.18	0.42
1:F:110:LYS:HA	1:F:110:LYS:HD3	1.76	0.42
1:A:178:PRO:O	1:A:181:MET:HB3	2.20	0.42
1:E:213:ALA:HB2	1:E:228:PHE:CZ	2.54	0.42
1:F:77:GLY:CA	1:F:87:ALA:HB3	2.48	0.42
1:A:46:TYR:CE2	1:A:91:ARG:HG2	2.54	0.42
1:A:75:ASP:OD1	1:A:85:LYS:O	2.36	0.42
1:B:114:PRO:HB2	1:B:146:ILE:HD12	2.02	0.42
1:E:205:ASP:OD1	1:E:207:ALA:HB3	2.19	0.42
1:F:71:ILE:C	1:F:73:THR:N	2.78	0.42
1:C:50:ASP:OD2	1:C:55:ARG:NH1	2.53	0.42
1:A:220:ILE:HG23	1:A:220:ILE:O	2.20	0.42
1:E:131:PHE:C	1:E:132:TYR:CD1	2.97	0.42
1:A:17:ASN:HB3	1:A:47:VAL:HG12	2.01	0.42
1:A:128:ARG:HG2	1:E:194:GLY:HA3	2.01	0.42
1:E:112:CYS:H	1:E:139:MET:CE	2.33	0.42
1:E:133:PHE:CG	1:E:134:SER:N	2.88	0.42
1:A:38:ARG:CZ	1:A:110:LYS:HB3	2.50	0.42
1:D:91:ARG:C	1:D:93:ASP:N	2.77	0.42
1:A:47:VAL:HG12	1:A:47:VAL:O	2.19	0.42
1:D:166:GLY:O	1:D:170:HIS:HA	2.20	0.42
1:B:113:ASP:OD1	1:B:113:ASP:C	2.62	0.41
1:D:16:GLU:CD	1:D:55:ARG:HH22	2.28	0.41
1:B:11:ASN:HB2	4:B:4775:HOH:O	2.19	0.41
1:C:52:THR:HB	1:C:54:ASP:OD2	2.20	0.41
1:B:73:THR:O	1:B:74:LEU:C	2.63	0.41
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.83	0.41
1:E:150:PHE:N	1:E:150:PHE:CD1	2.88	0.41
1:B:41:ALA:HB2	1:B:64:GLY:O	2.21	0.41
1:F:137:GLU:HB3	1:F:141:GLN:HE21	1.84	0.41
1:C:178:PRO:O	1:C:182:ARG:HG3	2.20	0.41
1:D:34:GLU:CG	1:D:106:TYR:CD2	3.04	0.41
1:D:152:ARG:HG2	1:D:171:ALA:HA	2.02	0.41
1:A:199:VAL:HG23	1:A:217:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:GLU:HG3	1:E:106:TYR:CD2	2.56	0.41
1:E:70:GLU:O	1:E:73:THR:HG22	2.21	0.41
1:E:202:GLY:HA2	1:E:223:ASP:H	1.85	0.41
1:E:55:ARG:O	1:E:55:ARG:HG2	2.21	0.41
1:F:40:SER:HB3	1:F:71:ILE:HD12	2.03	0.41
1:C:149:GLU:HG2	1:D:170:HIS:HA	2.02	0.41
1:D:26:LEU:HD21	1:D:102:ARG:HB3	2.03	0.41
1:E:58:ASN:CG	1:E:75:ASP:HB3	2.45	0.41
1:E:92:LEU:CG	1:E:96:LEU:HD22	2.47	0.41
1:F:132:TYR:CD1	1:F:132:TYR:N	2.89	0.41
1:E:149:GLU:O	1:E:150:PHE:C	2.64	0.41
1:A:46:TYR:OH	1:A:68:SER:HB2	2.21	0.40
1:A:224:ARG:NH2	1:A:226:ASP:OD2	2.46	0.40
1:A:148:PRO:HD2	1:A:149:GLU:OE2	2.21	0.40
4:A:4783:HOH:O	1:E:122:ARG:HG2	2.21	0.40
1:B:63:VAL:CG2	1:B:64:GLY:N	2.84	0.40
1:C:66:MET:SD	1:C:70:GLU:HG2	2.61	0.40
1:D:71:ILE:C	1:D:73:THR:N	2.79	0.40
1:F:96:LEU:HD12	1:F:96:LEU:HA	1.91	0.40
1:C:154:MET:HG2	1:C:169:HIS:CG	2.57	0.40
1:F:153:MET:CB	1:F:173:ILE:HB	2.52	0.40
1:A:50:ASP:CG	1:A:55:ARG:HH11	2.28	0.40
1:B:205:ASP:C	1:B:207:ALA:H	2.30	0.40
1:C:13:PHE:HB2	1:C:24:LEU:HD21	2.04	0.40
1:E:91:ARG:C	1:E:93:ASP:N	2.80	0.40
1:F:24:LEU:O	1:F:28:GLN:HG3	2.21	0.40
1:F:27:GLN:C	1:F:29:GLY:H	2.28	0.40
1:F:86:GLY:O	1:F:87:ALA:C	2.64	0.40
1:F:176:ILE:O	1:F:199:VAL:HA	2.21	0.40
1:F:204:ASP:OD1	1:F:204:ASP:N	2.54	0.40

There are no symmetry-related clashes.

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	238/248 (96%)	220 (92%)	15 (6%)	3 (1%)	9	18
1	B	224/248 (90%)	198 (88%)	15 (7%)	11 (5%)	1	2
1	C	229/248 (92%)	211 (92%)	15 (7%)	3 (1%)	9	18
1	D	229/248 (92%)	202 (88%)	20 (9%)	7 (3%)	3	5
1	E	231/248 (93%)	200 (87%)	26 (11%)	5 (2%)	5	9
1	F	233/248 (94%)	210 (90%)	19 (8%)	4 (2%)	7	13
All	All	1384/1488 (93%)	1241 (90%)	110 (8%)	33 (2%)	4	8

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	ASP
1	B	74	LEU
1	B	79	TRP
1	B	184	PRO
1	D	10	ALA
1	F	87	ALA
1	A	93	ASP
1	B	55	ARG
1	B	185	GLY
1	B	205	ASP
1	D	87	ALA
1	D	205	ASP
1	E	54	ASP
1	E	55	ARG
1	E	184	PRO
1	F	93	ASP
1	A	74	LEU
1	B	93	ASP
1	D	100	ARG
1	F	215	SER
1	B	7	HIS
1	B	85	LYS
1	C	10	ALA
1	C	11	ASN
1	C	54	ASP
1	D	74	LEU
1	E	10	ALA

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Mol	Chain	Res	Type
1	F	54	ASP
1	B	78	GLY
1	D	80	PHE
1	D	93	ASP
1	A	78	GLY
1	E	186	ILE

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	191/201 (95%)	175 (92%)	16 (8%)	10	22
1	B	169/201 (84%)	155 (92%)	14 (8%)	10	22
1	C	182/201 (90%)	173 (95%)	9 (5%)	22	45
1	D	173/201 (86%)	165 (95%)	8 (5%)	24	48
1	E	180/201 (90%)	168 (93%)	12 (7%)	15	31
1	F	182/201 (90%)	165 (91%)	17 (9%)	8	18
All	All	1077/1206 (89%)	1001 (93%)	76 (7%)	13	29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	18	THR
1	A	35	LEU
1	A	45	LEU
1	A	63	VAL
1	A	69	SER
1	A	73	THR
1	A	75	ASP
1	A	93	ASP
1	A	96	LEU
1	A	122	ARG
1	A	138	GLU

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Mol	Chain	Res	Type
1	A	153	MET
1	A	183	ARG
1	A	206	MET
1	A	214	THR
1	B	34	GLU
1	B	37	VAL
1	B	52	THR
1	B	53	LEU
1	B	63	VAL
1	B	69	SER
1	B	84	PHE
1	B	96	LEU
1	B	122	ARG
1	B	138	GLU
1	B	149	GLU
1	B	184	PRO
1	B	214	THR
1	B	222	LEU
1	C	33	ILE
1	C	34	GLU
1	C	53	LEU
1	C	63	VAL
1	C	96	LEU
1	C	149	GLU
1	C	178	PRO
1	C	183	ARG
1	C	184	PRO
1	D	18	THR
1	D	35	LEU
1	D	37	VAL
1	D	73	THR
1	D	75	ASP
1	D	149	GLU
1	D	183	ARG
1	D	221	ASN
1	E	34	GLU
1	E	35	LEU
1	E	63	VAL
1	E	73	THR
1	E	96	LEU
1	E	106	TYR
1	E	122	ARG

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Mol	Chain	Res	Type
1	E	132	TYR
1	E	149	GLU
1	E	153	MET
1	E	183	ARG
1	E	184	PRO
1	F	4	ILE
1	F	8	ARG
1	F	26	LEU
1	F	34	GLU
1	F	35	LEU
1	F	73	THR
1	F	93	ASP
1	F	96	LEU
1	F	100	ARG
1	F	130	THR
1	F	138	GLU
1	F	139	MET
1	F	149	GLU
1	F	153	MET
1	F	183	ARG
1	F	204	ASP
1	F	232	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	17	ASN
1	A	144	GLN
1	A	170	HIS
1	A	221	ASN
1	B	17	ASN
1	B	28	GLN
1	B	123	HIS
1	B	221	ASN
1	C	17	ASN
1	C	98	HIS
1	C	221	ASN
1	D	17	ASN
1	D	49	HIS
1	D	65	HIS
1	D	144	GLN

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Mol	Chain	Res	Type
1	D	221	ASN
1	E	11	ASN
1	E	17	ASN
1	E	65	HIS
1	E	123	HIS
1	E	170	HIS
1	E	209	HIS
1	E	221	ASN
1	F	7	HIS
1	F	17	ASN
1	F	123	HIS
1	F	141	GLN
1	F	221	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	F	806	-	3,3,3	2.12	1 (33%)	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	C	803	-	3,3,3	2.11	1 (33%)	3,3,3	0.87	0
3	SO4	F	4775	-	4,4,4	1.39	0	6,6,6	1.26	1 (16%)
3	SO4	C	4772	-	4,4,4	1.45	2 (50%)	6,6,6	1.31	1 (16%)
3	SO4	E	4774	-	4,4,4	1.52	2 (50%)	6,6,6	1.29	1 (16%)
3	SO4	D	4773	-	4,4,4	1.47	1 (25%)	6,6,6	1.36	1 (16%)
3	SO4	B	4771	-	4,4,4	1.33	0	6,6,6	1.31	1 (16%)
2	ACT	B	802	-	3,3,3	2.16	2 (66%)	3,3,3	0.74	0
2	ACT	D	804	-	3,3,3	2.07	2 (66%)	3,3,3	0.86	0
3	SO4	A	4770	-	4,4,4	1.35	0	6,6,6	1.38	1 (16%)
2	ACT	E	805	-	3,3,3	2.11	1 (33%)	3,3,3	0.88	0
2	ACT	A	801	-	3,3,3	1.99	1 (33%)	3,3,3	0.86	0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	805	ACT	O-C	3.06	1.35	1.22
2	B	802	ACT	O-C	3.05	1.35	1.22
2	F	806	ACT	O-C	3.03	1.35	1.22
2	C	803	ACT	O-C	3.01	1.35	1.22
2	D	804	ACT	O-C	2.88	1.34	1.22
2	A	801	ACT	O-C	2.77	1.34	1.22
3	D	4773	SO4	O2-S	2.29	1.58	1.44
3	E	4774	SO4	O2-S	2.26	1.58	1.44
2	B	802	ACT	OXT-C	-2.14	1.21	1.30
3	C	4772	SO4	O1-S	2.09	1.57	1.44
3	E	4774	SO4	O1-S	2.02	1.56	1.44
2	D	804	ACT	OXT-C	-2.01	1.21	1.30
3	C	4772	SO4	O2-S	2.00	1.56	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4770	SO4	O4-S-O3	3.03	125.25	108.54
3	D	4773	SO4	O4-S-O3	2.95	124.79	108.54
3	B	4771	SO4	O4-S-O3	2.86	124.31	108.54
3	C	4772	SO4	O4-S-O3	2.86	124.29	108.54
3	E	4774	SO4	O4-S-O3	2.84	124.21	108.54
3	F	4775	SO4	O4-S-O3	2.79	123.94	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4775	SO4	2	0
2	B	802	ACT	1	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	240/248 (96%)	0.05	2 (0%) 82 80	17, 32, 50, 73	0
1	B	228/248 (91%)	0.83	23 (10%) 12 10	20, 47, 65, 73	0
1	C	233/248 (93%)	0.25	5 (2%) 63 59	17, 36, 55, 66	0
1	D	231/248 (93%)	0.47	9 (3%) 43 38	22, 40, 56, 66	0
1	E	233/248 (93%)	0.73	23 (9%) 13 11	19, 44, 63, 72	0
1	F	235/248 (94%)	0.52	13 (5%) 30 27	20, 39, 61, 70	0
All	All	1400/1488 (94%)	0.47	75 (5%) 31 27	17, 39, 61, 73	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	ALA	4.4
1	F	235	MET	4.3
1	B	223	ASP	4.1
1	C	234	GLY	4.0
1	D	231	VAL	3.9
1	B	1	MET	3.8
1	E	203	GLY	3.6
1	C	86	GLY	3.6
1	E	1	MET	3.5
1	C	87	ALA	3.5
1	B	201	TYR	3.3
1	B	206	MET	3.2
1	E	82	ASP	3.1
1	F	202	GLY	3.1
1	C	73	THR	3.0
1	B	228	PHE	3.0
1	E	13	PHE	3.0
1	B	83	ARG	2.9
1	D	222	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	59	GLY	2.9
1	F	176	ILE	2.9
1	D	86	GLY	2.9
1	E	85	LYS	2.9
1	B	222	LEU	2.8
1	E	87	ALA	2.8
1	B	80	PHE	2.8
1	A	240	LEU	2.7
1	B	184	PRO	2.7
1	E	11	ASN	2.7
1	B	33	ILE	2.7
1	B	203	GLY	2.6
1	B	2	THR	2.6
1	D	206	MET	2.6
1	F	183	ARG	2.5
1	F	205	ASP	2.5
1	E	12	ARG	2.5
1	B	87	ALA	2.5
1	D	226	ASP	2.5
1	E	233	SER	2.5
1	E	76	ALA	2.4
1	B	86	GLY	2.4
1	B	202	GLY	2.4
1	F	1	MET	2.4
1	E	230	ALA	2.4
1	E	228	PHE	2.3
1	C	11	ASN	2.3
1	E	14	ALA	2.3
1	E	222	LEU	2.3
1	F	222	LEU	2.3
1	F	208	VAL	2.3
1	F	207	ALA	2.3
1	D	178	PRO	2.2
1	B	12	ARG	2.2
1	F	27	GLN	2.2
1	E	35	LEU	2.2
1	D	204	ASP	2.2
1	B	212	ILE	2.2
1	E	71	ILE	2.2
1	E	75	ASP	2.1
1	E	73	THR	2.1
1	D	83	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	75	ASP	2.1
1	A	123	HIS	2.1
1	F	206	MET	2.1
1	F	13	PHE	2.1
1	B	221	ASN	2.1
1	E	226	ASP	2.1
1	B	13	PHE	2.0
1	B	229	ALA	2.0
1	D	87	ALA	2.0
1	E	10	ALA	2.0
1	B	26	LEU	2.0
1	E	77	GLY	2.0
1	F	217	VAL	2.0
1	E	227	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	F	4775	5/5	0.62	0.36	40,41,46,53	0
3	SO4	A	4770	5/5	0.67	0.36	37,38,44,48	0
3	SO4	B	4771	5/5	0.74	0.30	38,39,41,45	0
2	ACT	C	803	4/4	0.75	0.20	45,45,47,48	0
2	ACT	A	801	4/4	0.76	0.19	41,42,42,44	0
3	SO4	E	4774	5/5	0.77	0.30	42,43,44,54	0
3	SO4	C	4772	5/5	0.77	0.29	41,42,44,54	0
2	ACT	E	805	4/4	0.79	0.15	37,38,39,40	0
2	ACT	B	802	4/4	0.81	0.17	46,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	F	806	4/4	0.82	0.17	48,48,49,49	0
3	SO4	D	4773	5/5	0.85	0.31	37,41,43,52	0
2	ACT	D	804	4/4	0.86	0.13	46,46,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.