



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 AM UTC

PDB ID : 4OGK / pdb_00004ogk
Title : X-ray structure of the uridine phosphorylase from Salmonella typhimurium in complex with thymidine at 2.40 Å resolution
Authors : Sotnichenko, S.E.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Mikhailov, A.M.
Deposited on : 2014-01-16
Resolution : 2.40 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

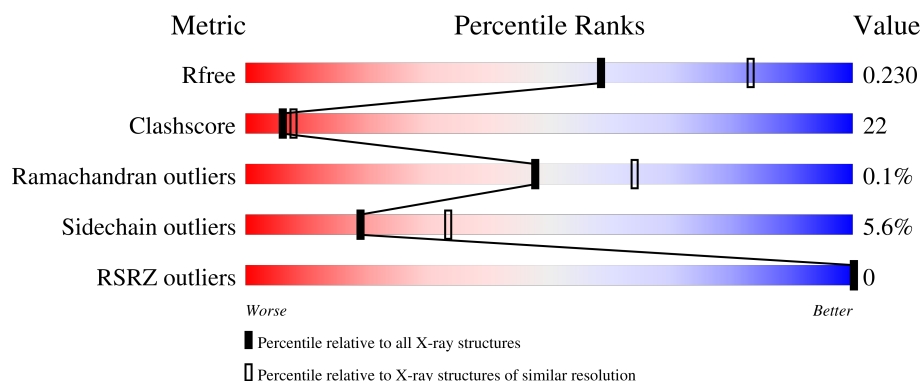
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

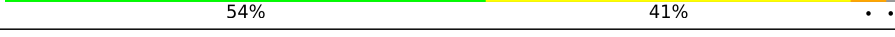
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	

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Mol	Chain	Length	Quality of chain
1	F	253	 A horizontal bar chart showing the quality of the chain. The bar is divided into three segments: a green segment representing 66%, a yellow segment representing 29%, and a small grey segment at the end. Below the bar, the percentages '66%' and '29%' are labeled. To the right of the bar, there are two small black dots.

2 Entry composition [i](#)

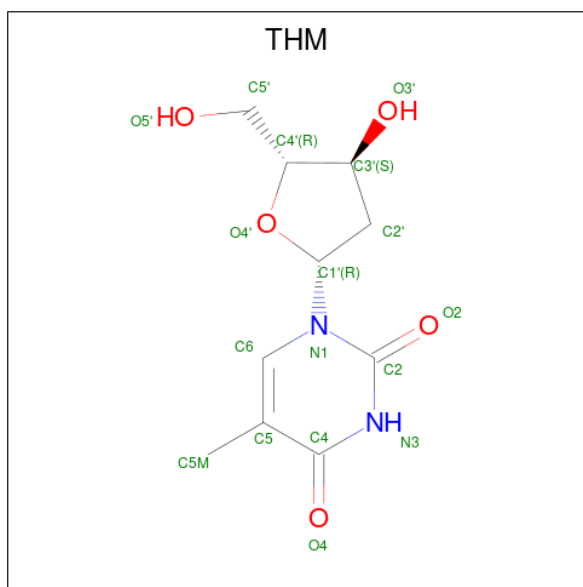
There are 8 unique types of molecules in this entry. The entry contains 11404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

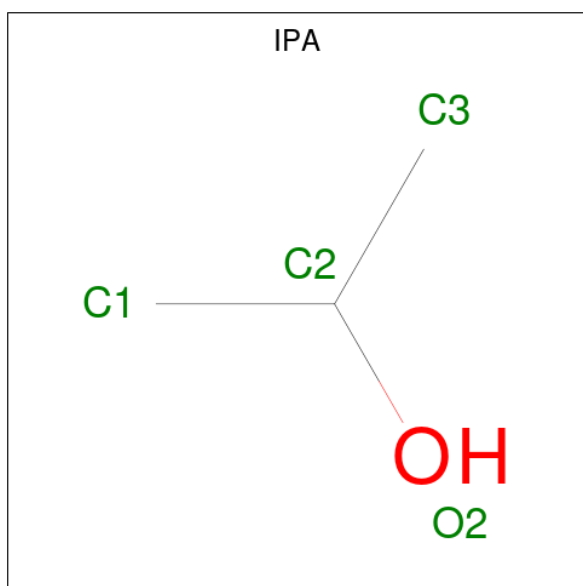
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	B	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	C	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	D	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	E	250	Total	C	N	O	S	0	0	0
			1877	1174	330	361	12			
1	F	245	Total	C	N	O	S	0	0	0
			1837	1151	323	351	12			

- Molecule 2 is THYMIDINE (CCD ID: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		
2	D	1	Total	C	N	O	0	0
			17	10	2	5		
2	E	1	Total	C	N	O	0	0
			17	10	2	5		
2	F	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



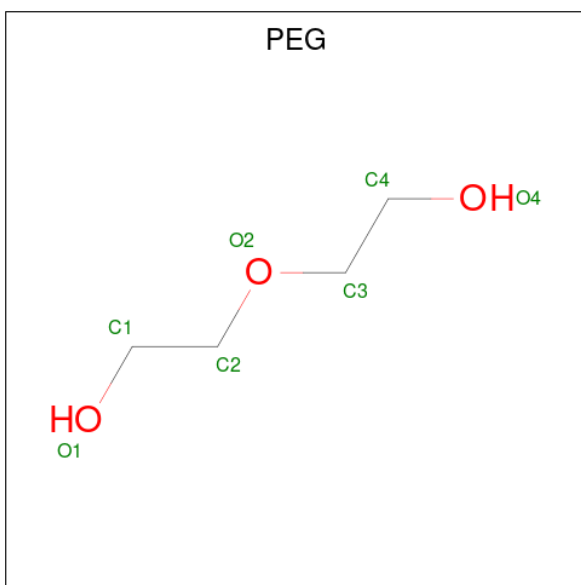
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



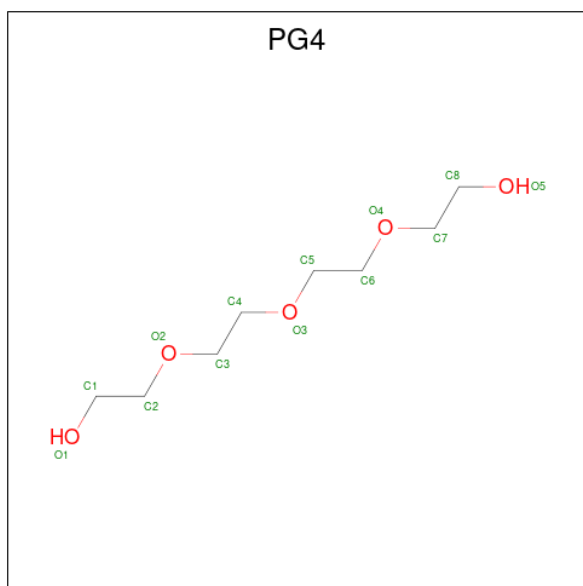
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	1	Total	K	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total	O	0	0
			10	10		
8	B	10	Total	O	0	0
			10	10		
8	C	11	Total	O	0	0
			11	11		
8	D	7	Total	O	0	0
			7	7		

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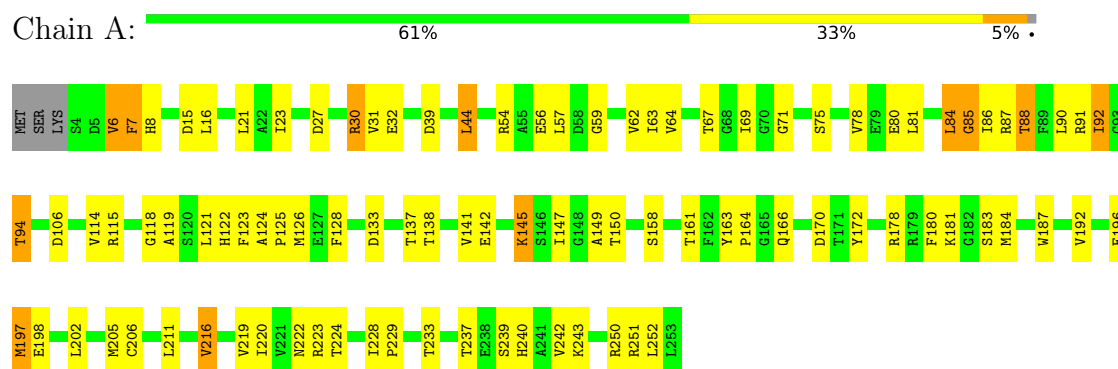
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	13	Total	O	0	0
			13	13		
8	F	5	Total	O	0	0
			5	5		

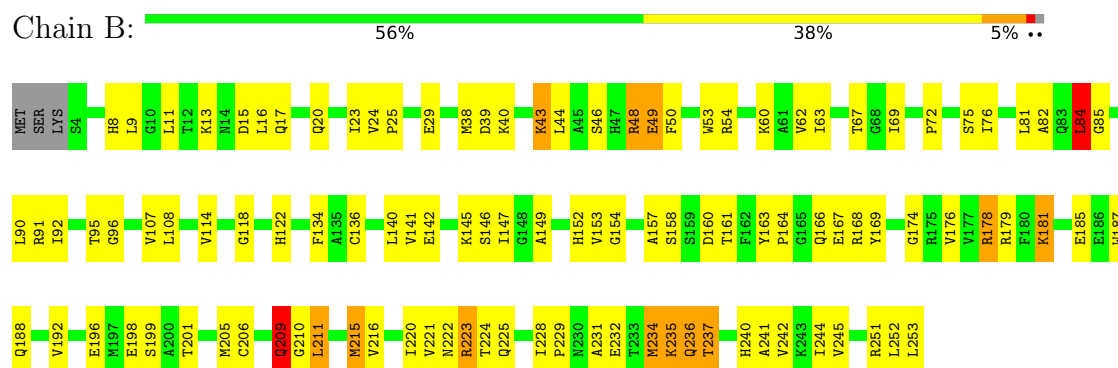
3 Residue-property plots

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.

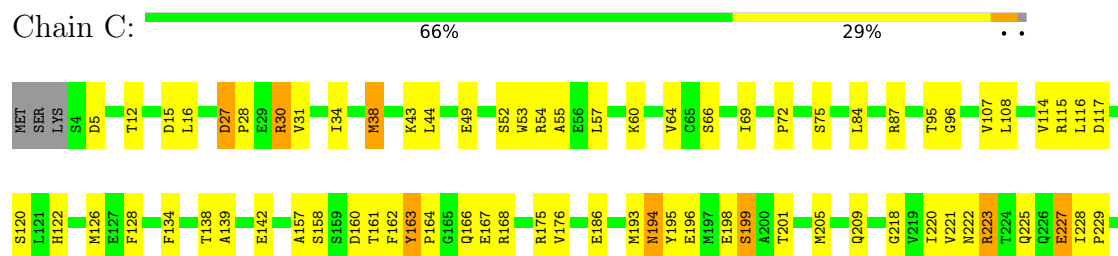
• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



• Molecule 1: Uridine phosphorylase



M234
K235
Q236
T237
E238
S239
V242
R250
R251
L252
L253

• Molecule 1: Uridine phosphorylase

Chain D:  54% 41%

MET SER LYS S4 D5 V6 F7 H8 L9 G10 L11 T12 K13 N14 D15 L16 Q17 A22 I23 V24 P25 R30 V31 E32 E33 I34 N38 D39 K40 P41 V42 K43 L44 R48 E49 F50 T51 S52 W53 R54 A55 E56 A61 V62 I63 V64 C65 S66 T67 G71 P72 S73 T74 S75

I76 A77 V78 L81 A82 Q83 R84 G85 I86 R87 T88 F89 L90 R91 I92 G93 T94 P100 H101 I102 L108 V109 T110 T111 V114 R115 L116 L121 A124 F128 P129 T137 T138 A139 L140 V141 K145 H152 V153 G154 S159 D160 Y163 G164 R168 Y169

D170 T171 Y172 S173 G174 R178 A179 F180 M184 Y185 E186 S189 A200 T201 T204 M205 S208 Q209 Q210 L211 V216 T220 R221 Q225 Q226 E227 P229 V236 A231 E232 T233 W234 K235 E238 S239 H240 A241 V242 V245 V246 E247 A248 L252 L253

• Molecule 1: Uridine phosphorylase

Chain E:  54% 39% 6%

MET SER LYS S4 H8 K13 L16 L21 A22 I23 V24 G26 D27 P28 V31 I34 A35 A36 L37 M38 D39 K40 P41 V42 K43 L44 R48 E49 F50 W53 R54 A55 E56 L57 A61 V62 I63 V64 S65 T67 G68 I69 W78 E79 E80 L81 A82 Q83

L84 G85 I86 R91 I92 T95 Q96 A97 Q99 L108 V114 R115 L121 H122 P125 M126 E127 F128 P129 V131 D133 A143 I147 G154 E155 T156 A157 S158 S159 D160 T161 F162 Y163 P164 G165 Q166 E167 R168 F180 S183 E186 W187 Q188 M190

G191 V192 M193 N194 Y195 E196 M197 E198 S199 L202 I98 L203 T204 M205 S208 Q209 V216 T220 V221 N222 Q225 T228 P229 T233 M234 K235 Q236 T237 E238 S239 H240 A241 V242 K243 I244 V245 V246 E247 R250 L251 L252 L253

• Molecule 1: Uridine phosphorylase

Chain F:  66% 29%

MET SER LYS S4 D5 V6 F7 H8 L9 T12 K13 N14 D15 L16 Q17 A22 I23 V24 D27 P28 E29 R30 A35 A36 L37 M38 D39 K40 P41 L44 R43 A55 K60 I63 V64 T69 V169 E80 N194 Y195 E196 M197 S199 A200 T216 N222 R223

L108 V109 V114 R115 L116 H122 P129 A130 F134 E142 K145 T150 T151 V153 A157 S158 D159 F161 Y163 P164 G165 Q166 E167 R168 Y172 R175 V176 V177 R178 W187 V192 N193 Y195 E196 M197 S199 A200 T216 N222 R223

T224 Q225 M234 LYS GLN THR SER A241 V242 K243 I244 V245 L253

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	89.97Å 89.97Å 256.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.99 – 2.40 9.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (9.99-2.40) 99.9 (9.99-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.220 , 0.236 (Not available) , 0.230	Depositor DCC
R_{free} test set	2283 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.459 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-h-k,-l	Depositor
Outliers	0 of 45659 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11404	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: PG4, PEG, EDO, IPA, THM, K

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	0.59	0/1907	0.93	5/2584 (0.2%)
1	B	0.85	0/1907	0.95	6/2584 (0.2%)
1	C	0.70	0/1907	0.95	7/2584 (0.3%)
1	D	0.68	0/1907	0.91	7/2584 (0.3%)
1	E	0.66	1/1907 (0.1%)	0.97	10/2584 (0.4%)
1	F	0.64	2/1866 (0.1%)	0.89	3/2528 (0.1%)
All	All	0.69	3/11401 (0.0%)	0.93	38/15448 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	8	HIS	CG-ND1	-5.37	1.32	1.38
1	E	69	ILE	C-O	-5.26	1.18	1.24
1	F	8	HIS	CD2-NE2	-5.19	1.32	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	N-CA-C	9.33	121.06	111.07
1	E	193	MET	N-CA-C	8.91	120.92	111.03
1	B	84	LEU	N-CA-C	8.75	120.81	111.28
1	E	84	LEU	N-CA-C	7.69	119.30	111.07
1	C	27	ASP	CA-C-N	7.53	126.80	118.97
1	C	27	ASP	C-N-CA	7.53	126.80	118.97
1	E	236	GLN	N-CA-C	-7.27	103.51	112.38
1	D	16	LEU	N-CA-C	7.11	118.82	111.14
1	E	24	VAL	N-CA-C	7.04	115.11	108.15
1	B	147	ILE	N-CA-C	6.98	117.77	110.72
1	E	199	SER	N-CA-C	6.97	118.67	111.14
1	D	208	SER	N-CA-C	6.79	118.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	GLY	N-CA-C	6.66	121.47	111.42
1	B	209	GLN	N-CA-C	6.61	118.14	111.07
1	A	7	PHE	N-CA-C	6.56	118.09	111.07
1	C	227	GLU	N-CA-C	6.36	118.74	110.53
1	C	223	ARG	N-CA-C	6.21	118.13	111.36
1	E	99	GLN	CA-C-N	6.05	125.77	119.05
1	E	99	GLN	C-N-CA	6.05	125.77	119.05
1	F	199	SER	N-CA-C	6.05	117.68	111.14
1	D	234	MET	N-CA-C	-6.02	105.70	113.16
1	B	224	THR	N-CA-C	5.91	117.40	111.07
1	B	48	ARG	CB-CA-C	-5.91	109.75	116.54
1	D	211	LEU	N-CA-C	5.78	118.62	109.50
1	E	251	ARG	N-CA-C	5.61	117.20	111.14
1	B	154	GLY	N-CA-C	5.59	118.40	110.74
1	A	7	PHE	CB-CA-C	-5.52	102.21	110.88
1	C	194	ASN	N-CA-C	5.44	116.25	108.74
1	D	204	THR	N-CA-C	5.37	116.81	111.07
1	C	116	LEU	N-CA-C	-5.28	107.01	112.93
1	D	84	LEU	O-C-N	-5.18	116.73	122.07
1	A	85	GLY	CA-C-N	5.18	128.52	120.34
1	A	85	GLY	C-N-CA	5.18	128.52	120.34
1	F	40	LYS	N-CA-C	5.15	121.19	109.81
1	D	220	ILE	CB-CA-C	-5.13	106.57	111.44
1	F	162	PHE	N-CA-C	5.13	116.95	111.36
1	C	199	SER	N-CA-C	5.05	116.59	111.14
1	E	48	ARG	CB-CA-C	-5.02	109.31	116.34

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	1877	0	1887	78	0
1	B	1877	0	1887	111	0
1	C	1877	0	1887	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1877	0	1887	104	0
1	E	1877	0	1887	110	0
1	F	1837	0	1847	64	0
2	A	17	0	14	4	0
2	B	17	0	14	1	0
2	D	17	0	14	0	0
2	E	17	0	14	1	0
2	F	17	0	14	0	0
3	A	4	0	8	0	0
4	A	4	0	6	0	0
4	C	4	0	6	0	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	D	7	0	10	0	0
6	E	13	0	18	2	0
7	F	1	0	0	0	0
8	A	10	0	0	0	0
8	B	10	0	0	0	0
8	C	11	0	0	0	0
8	D	7	0	0	0	0
8	E	13	0	0	0	0
8	F	5	0	0	0	0
All	All	11404	0	11412	510	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 22.

All (510) 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:B:140:LEU:HD22	1:B:216:VAL:CG2	1.63	1.28
1:E:108:LEU:HD13	1:E:194:ASN:ND2	1.60	1.16
1:F:196:GLU:HG3	1:F:197:MET:H	1.08	1.10
1:B:140:LEU:HD22	1:B:216:VAL:HG21	1.23	1.08
1:F:15:ASP:HB3	1:F:44:LEU:HD13	1.37	1.03
1:B:223:ARG:HG2	1:B:223:ARG:HH11	0.95	1.03
1:D:22:ALA:HB2	1:D:86:ILE:HG12	1.39	1.01
1:E:108:LEU:HD13	1:E:194:ASN:CG	1.85	1.01
1:E:199:SER:O	1:E:203:LEU:HG	1.63	0.98
1:F:196:GLU:HG3	1:F:197:MET:N	1.77	0.96
1:B:176:VAL:O	1:B:181:LYS:HE2	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ALA:CB	1:D:86:ILE:HG12	1.97	0.94
1:E:250:ARG:O	1:E:253:LEU:HD12	1.68	0.93
1:B:15:ASP:HB3	1:B:44:LEU:HD22	1.49	0.93
1:B:140:LEU:HD22	1:B:216:VAL:HG23	1.47	0.92
1:C:161:THR:OG1	1:C:164:PRO:HD2	1.68	0.92
1:A:250:ARG:O	1:A:251:ARG:HB2	1.71	0.90
1:B:223:ARG:HG2	1:B:223:ARG:NH1	1.75	0.89
1:E:156:THR:HG23	1:E:194:ASN:O	1.73	0.89
1:C:221:VAL:HB	1:C:229:PRO:HD3	1.54	0.89
1:D:16:LEU:CD1	1:D:84:LEU:HD13	2.04	0.88
1:B:206:CYS:O	1:B:210:GLY:HA2	1.74	0.88
1:B:223:ARG:HH11	1:B:223:ARG:CG	1.85	0.88
1:B:40:LYS:O	1:B:40:LYS:HG2	1.73	0.87
1:B:222:ASN:ND2	1:B:225:GLN:CB	2.37	0.87
1:D:81:LEU:O	1:D:85:GLY:HA2	1.75	0.87
1:D:16:LEU:HD13	1:D:84:LEU:HD13	1.58	0.86
1:D:22:ALA:HB2	1:D:86:ILE:CG1	2.06	0.85
1:F:92:ILE:HD11	1:F:241:ALA:HB1	1.60	0.83
1:A:197:MET:HG3	2:A:301:THM:H1'	1.61	0.82
1:E:143:ALA:HB1	1:E:247:GLU:HG3	1.61	0.82
1:E:8:HIS:HB3	1:E:50:PHE:CE1	2.16	0.81
1:B:222:ASN:ND2	1:B:225:GLN:HB3	1.97	0.80
1:B:60:LYS:HB2	1:B:253:LEU:HD13	1.64	0.79
1:F:95:THR:HG22	1:F:196:GLU:HB2	1.63	0.79
1:E:82:ALA:O	1:E:85:GLY:HA3	1.82	0.78
1:B:40:LYS:O	1:B:40:LYS:CG	2.30	0.78
1:A:57:LEU:HD11	1:A:250:ARG:HE	1.48	0.77
1:D:15:ASP:HB3	1:D:44:LEU:HD22	1.67	0.76
1:A:178:ARG:HA	1:A:181:LYS:HD3	1.68	0.76
1:B:222:ASN:ND2	1:B:225:GLN:HB2	1.99	0.76
1:E:86:ILE:N	1:E:86:ILE:HD13	2.00	0.76
1:B:81:LEU:HA	1:B:84:LEU:HD22	1.67	0.75
1:D:86:ILE:HG21	1:D:88:THR:O	1.86	0.75
1:D:22:ALA:HB2	1:D:86:ILE:CD1	2.17	0.75
1:E:252:LEU:O	1:E:253:LEU:OXT	2.05	0.74
1:D:86:ILE:CG2	1:D:88:THR:O	2.36	0.74
1:B:140:LEU:CD2	1:B:216:VAL:HG21	2.11	0.73
1:E:40:LYS:HD3	1:E:56:GLU:HB2	1.70	0.73
1:D:81:LEU:O	1:D:84:LEU:HB2	1.90	0.71
1:B:164:PRO:HB3	1:B:176:VAL:HG13	1.71	0.71
1:E:108:LEU:CD1	1:E:194:ASN:ND2	2.49	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASN:O	1:C:225:GLN:HB3	1.91	0.71
1:B:221:VAL:HA	1:B:229:PRO:HG3	1.71	0.71
1:E:238:GLU:O	1:E:242:VAL:N	2.22	0.70
1:B:16:LEU:HD21	1:B:84:LEU:HB3	1.73	0.70
1:E:108:LEU:CD1	1:E:194:ASN:CG	2.63	0.70
1:D:8:HIS:HB3	1:D:50:PHE:HE2	1.57	0.70
1:B:166:GLN:OE1	1:B:168:ARG:NH2	2.25	0.69
1:B:205:MET:O	1:B:209:GLN:HB2	1.93	0.69
1:E:22:ALA:HB2	1:E:86:ILE:HG13	1.75	0.69
1:B:13:LYS:HA	1:B:16:LEU:HD13	1.74	0.69
1:A:172:TYR:CE2	1:B:211:LEU:HD21	2.28	0.68
1:B:16:LEU:HA	1:B:63:ILE:HD11	1.75	0.68
1:B:222:ASN:HD22	1:B:225:GLN:HB3	1.58	0.68
1:F:81:LEU:O	1:F:84:LEU:HB2	1.94	0.68
1:A:39:ASP:HB2	1:A:56:GLU:HB2	1.75	0.68
1:E:92:ILE:HD11	1:E:241:ALA:HB1	1.76	0.68
1:F:163:TYR:HB2	1:F:164:PRO:HD3	1.77	0.67
1:C:196:GLU:CD	1:C:199:SER:H	2.01	0.67
1:F:22:ALA:HB2	1:F:86:ILE:HD13	1.77	0.67
1:A:92:ILE:HG23	1:A:92:ILE:O	1.92	0.67
1:E:166:GLN:NE2	2:E:301:THM:O2	2.28	0.67
1:E:108:LEU:HD13	1:E:194:ASN:HD21	1.60	0.66
1:A:122:HIS:CE1	1:B:160:ASP:HB2	2.31	0.66
1:C:87:ARG:NH1	1:D:172:TYR:OH	2.29	0.66
1:D:94:THR:HG22	1:D:220:ILE:HD11	1.76	0.66
1:A:166:GLN:NE2	2:A:301:THM:O2	2.28	0.66
1:D:25:PRO:HB3	1:D:92:ILE:HG23	1.78	0.65
1:D:171:THR:HG22	1:D:173:SER:H	1.62	0.65
1:A:172:TYR:CZ	1:B:211:LEU:HD21	2.31	0.65
1:D:94:THR:CG2	1:D:220:ILE:HD11	2.26	0.65
1:C:162:PHE:O	1:C:168:ARG:NH1	2.29	0.65
1:E:23:ILE:HB	1:E:64:VAL:HG22	1.78	0.65
1:A:196:GLU:CD	1:A:198:GLU:H	2.05	0.65
1:C:196:GLU:OE2	1:C:199:SER:N	2.30	0.65
1:B:206:CYS:O	1:B:210:GLY:CA	2.45	0.64
1:D:204:THR:O	1:D:208:SER:N	2.21	0.64
1:B:206:CYS:O	1:B:211:LEU:N	2.30	0.64
1:F:16:LEU:HA	1:F:63:ILE:HD11	1.79	0.64
1:C:5:ASP:HB2	1:C:12:THR:HA	1.80	0.64
1:C:38:MET:HB2	1:C:55:ALA:HB1	1.80	0.64
1:A:57:LEU:HD11	1:A:250:ARG:NE	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ARG:HA	1:E:253:LEU:HD11	1.80	0.63
1:E:252:LEU:O	1:E:253:LEU:C	2.38	0.63
1:C:49:GLU:HG2	1:D:49:GLU:HG3	1.80	0.63
1:B:141:VAL:HG12	1:B:145:LYS:HE2	1.79	0.63
1:E:42:VAL:HB	1:E:54:ARG:HB3	1.80	0.63
1:A:250:ARG:O	1:A:251:ARG:CB	2.45	0.63
1:D:16:LEU:CD1	1:D:84:LEU:CD1	2.75	0.63
1:E:234:MET:O	1:E:236:GLN:N	2.32	0.63
1:C:175:ARG:NH2	1:D:208:SER:OG	2.32	0.63
1:E:221:VAL:HG23	1:E:229:PRO:HD3	1.81	0.63
1:B:222:ASN:HD21	1:B:225:GLN:HB2	1.63	0.63
1:D:109:VAL:HB	1:D:153:VAL:HG22	1.81	0.63
1:A:86:ILE:HG22	1:A:88:THR:H	1.64	0.62
1:A:91:ARG:O	1:A:92:ILE:HG22	1.99	0.62
1:B:163:TYR:HA	1:B:168:ARG:HD2	1.81	0.62
1:D:11:LEU:HD11	1:D:44:LEU:HB3	1.81	0.62
1:D:205:MET:O	1:D:209:GLN:N	2.31	0.62
1:B:91:ARG:HG2	1:B:215:MET:CE	2.29	0.62
1:E:236:GLN:O	1:E:239:SER:N	2.33	0.62
1:D:82:ALA:O	1:D:85:GLY:HA3	2.00	0.61
1:C:166:GLN:OE1	1:C:168:ARG:NH1	2.30	0.61
1:E:16:LEU:HD11	1:E:84:LEU:HB3	1.82	0.61
1:B:242:VAL:HA	1:B:245:VAL:HG12	1.81	0.61
1:D:163:TYR:HA	1:D:168:ARG:HD2	1.81	0.61
1:E:234:MET:C	1:E:236:GLN:H	2.08	0.61
1:E:205:MET:O	1:E:209:GLN:NE2	2.27	0.61
1:C:205:MET:O	1:C:209:GLN:N	2.34	0.60
1:A:166:GLN:HB3	1:A:223:ARG:HH12	1.65	0.60
1:D:23:ILE:N	1:D:63:ILE:O	2.31	0.60
1:F:166:GLN:OE1	1:F:168:ARG:NH2	2.32	0.60
1:A:44:LEU:HD11	1:A:54:ARG:HB2	1.83	0.60
1:D:52:SER:HG	1:D:65:CYS:HG	1.49	0.60
1:A:166:GLN:HE22	2:A:301:THM:C2	2.13	0.60
1:B:181:LYS:O	1:D:178:ARG:NH2	2.34	0.60
1:E:196:GLU:CD	1:E:199:SER:H	2.10	0.60
1:A:114:VAL:HA	1:F:129:PRO:HD3	1.83	0.60
1:B:15:ASP:HB3	1:B:44:LEU:CD2	2.28	0.59
1:B:210:GLY:C	1:B:211:LEU:HG	2.27	0.59
1:C:115:ARG:NH1	1:C:128:PHE:O	2.36	0.59
1:D:196:GLU:CD	1:D:199:SER:H	2.10	0.59
1:D:205:MET:HA	1:D:208:SER:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH2	1:A:124:ALA:O	2.28	0.59
1:E:78:VAL:HG21	1:E:202:LEU:HD13	1.85	0.59
1:A:239:SER:HA	1:A:242:VAL:HB	1.83	0.59
1:D:16:LEU:HD11	1:D:84:LEU:CD1	2.33	0.59
1:C:167:GLU:O	1:C:223:ARG:NH1	2.36	0.59
1:D:90:LEU:HD21	1:D:140:LEU:HD21	1.83	0.59
1:D:13:LYS:O	1:D:16:LEU:HB2	2.03	0.59
1:E:81:LEU:O	1:E:85:GLY:HA2	2.03	0.59
1:F:92:ILE:HB	1:F:245:VAL:HG21	1.83	0.59
1:F:115:ARG:HD2	1:F:130:ALA:HB2	1.84	0.58
1:C:44:LEU:HB2	1:C:52:SER:O	2.04	0.58
1:C:122:HIS:HE1	1:D:160:ASP:H	1.52	0.58
1:E:143:ALA:CB	1:E:247:GLU:HG3	2.32	0.58
1:E:16:LEU:HD22	1:E:63:ILE:HG13	1.85	0.58
1:B:91:ARG:HG2	1:B:215:MET:HE1	1.85	0.58
1:E:154:GLY:N	1:E:193:MET:HE1	2.19	0.58
1:D:16:LEU:HD11	1:D:84:LEU:HD13	1.86	0.58
1:D:221:VAL:HG23	1:D:229:PRO:HD2	1.85	0.58
1:A:69:ILE:HD12	1:B:50:PHE:HZ	1.69	0.58
1:E:34:ILE:HG13	1:E:242:VAL:HG11	1.86	0.58
1:C:161:THR:OG1	1:C:164:PRO:CD	2.48	0.57
1:B:91:ARG:CG	1:B:215:MET:CE	2.83	0.57
1:C:114:VAL:HB	1:C:157:ALA:HA	1.86	0.57
1:C:43:LYS:HG2	1:C:53:TRP:CZ2	2.40	0.57
1:E:222:ASN:HD22	1:E:225:GLN:HB2	1.70	0.57
1:A:86:ILE:CG2	1:A:88:THR:H	2.18	0.57
1:B:198:GLU:O	1:B:201:THR:OG1	2.23	0.57
1:A:142:GLU:HG2	1:A:251:ARG:HH11	1.70	0.56
1:B:222:ASN:HD22	1:B:225:GLN:CB	2.12	0.56
1:B:237:THR:O	1:B:241:ALA:N	2.28	0.56
1:A:23:ILE:HG12	1:A:90:LEU:HD12	1.87	0.56
1:E:220:ILE:O	1:E:229:PRO:HG3	2.05	0.56
1:A:84:LEU:HB2	1:A:85:GLY:HA2	1.88	0.56
1:C:43:LYS:NZ	1:C:53:TRP:HE1	2.04	0.56
1:E:246:VAL:O	1:E:250:ARG:HG3	2.06	0.56
1:B:178:ARG:HA	1:B:181:LYS:HG2	1.88	0.56
1:D:141:VAL:O	1:D:145:LYS:HG2	2.06	0.56
1:C:16:LEU:HD21	1:C:84:LEU:HB3	1.88	0.56
1:B:91:ARG:CG	1:B:215:MET:HE1	2.36	0.55
1:F:115:ARG:HG2	1:F:200:ALA:HB1	1.88	0.55
1:B:84:LEU:N	1:B:85:GLY:HA2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ARG:NH1	1:E:125:PRO:O	2.39	0.55
1:D:139:ALA:HB3	1:D:252:LEU:HD11	1.88	0.55
1:B:23:ILE:HG22	1:B:25:PRO:HD3	1.89	0.55
1:B:43:LYS:HB2	1:B:53:TRP:CZ2	2.41	0.55
1:D:108:LEU:HD23	1:D:152:HIS:HB2	1.89	0.55
1:F:114:VAL:HB	1:F:157:ALA:HA	1.88	0.55
1:D:221:VAL:HG23	1:D:229:PRO:CD	2.36	0.55
1:C:234:MET:O	1:C:238:GLU:HG2	2.07	0.55
1:E:79:GLU:OE2	1:E:83:GLN:NE2	2.40	0.55
1:A:222:ASN:ND2	1:A:224:THR:OG1	2.40	0.55
1:D:90:LEU:HD22	1:D:245:VAL:HG23	1.89	0.55
1:D:16:LEU:O	1:D:54:ARG:HG3	2.07	0.54
1:E:114:VAL:HB	1:E:157:ALA:HA	1.88	0.54
1:A:121:LEU:HD21	1:A:126:MET:HE2	1.88	0.54
1:B:234:MET:O	1:B:236:GLN:N	2.41	0.54
1:D:56:GLU:HG2	1:D:61:ALA:HA	1.90	0.54
1:C:163:TYR:HB2	1:C:164:PRO:HD3	1.89	0.54
1:C:222:ASN:HB3	1:C:225:GLN:HB2	1.89	0.54
1:C:115:ARG:HH21	1:C:120:SER:HB2	1.72	0.54
1:B:206:CYS:HB3	1:B:211:LEU:O	2.07	0.54
1:A:6:VAL:HG11	1:A:80:GLU:HB3	1.90	0.54
1:C:196:GLU:CD	1:C:198:GLU:H	2.15	0.54
1:B:140:LEU:CD2	1:B:216:VAL:HG23	2.28	0.53
1:C:43:LYS:HZ2	1:C:53:TRP:HE1	1.55	0.53
1:C:122:HIS:CE1	1:D:160:ASP:H	2.26	0.53
1:B:67:THR:OG1	1:B:91:ARG:NH1	2.41	0.53
1:D:13:LYS:O	1:D:16:LEU:N	2.28	0.53
1:D:42:VAL:N	1:D:54:ARG:O	2.33	0.53
1:B:158:SER:OG	1:B:196:GLU:OE2	2.22	0.53
1:A:172:TYR:OH	1:B:211:LEU:HD21	2.08	0.53
1:C:108:LEU:HD13	1:C:193:MET:HB3	1.91	0.53
1:C:115:ARG:HH21	1:C:120:SER:CB	2.21	0.53
1:E:79:GLU:HG3	1:E:83:GLN:HE22	1.73	0.53
1:F:6:VAL:HG11	1:F:80:GLU:HG2	1.91	0.53
1:F:35:ALA:HB1	1:F:41:PRO:HG3	1.91	0.53
1:F:163:TYR:N	1:F:164:PRO:CD	2.72	0.53
1:A:69:ILE:N	1:B:49:GLU:OE2	2.42	0.53
1:B:136:CYS:HA	1:B:252:LEU:HD11	1.91	0.53
1:E:41:PRO:C	1:E:53:TRP:HE1	2.17	0.53
1:E:220:ILE:HG22	1:E:235:LYS:HD2	1.91	0.53
1:E:147:ILE:HD12	1:E:244:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:HG23	1:A:90:LEU:HB2	1.91	0.52
1:B:72:PRO:O	1:B:76:ILE:HG13	2.09	0.52
1:C:15:ASP:O	1:C:54:ARG:HD3	2.09	0.52
1:E:158:SER:O	1:E:158:SER:OG	2.24	0.52
1:B:17:GLN:O	1:B:17:GLN:HG2	2.07	0.52
1:B:81:LEU:O	1:B:84:LEU:HB2	2.09	0.52
1:D:16:LEU:HD13	1:D:84:LEU:CD1	2.33	0.52
1:B:16:LEU:HD11	1:B:84:LEU:HG	1.91	0.52
1:A:158:SER:HA	1:A:196:GLU:O	2.09	0.52
1:A:178:ARG:NH2	1:C:186:GLU:OE2	2.40	0.52
1:B:179:ARG:O	1:D:178:ARG:NH1	2.42	0.52
1:D:100:PRO:HA	1:D:222:ASN:HD21	1.75	0.52
1:B:196:GLU:OE2	1:B:199:SER:OG	2.24	0.52
1:E:190:MET:HB2	1:E:192:VAL:HG23	1.92	0.52
1:D:81:LEU:HB3	1:D:86:ILE:HD13	1.92	0.52
1:E:238:GLU:O	1:E:242:VAL:HG23	2.10	0.52
1:C:117:ASP:CG	1:C:120:SER:HG	2.17	0.51
1:E:91:ARG:NH2	1:E:198:GLU:OE1	2.43	0.51
1:B:43:LYS:HZ1	1:B:46:SER:HB2	1.75	0.51
1:C:158:SER:HA	1:C:196:GLU:O	2.09	0.51
1:D:115:ARG:NH2	1:D:121:LEU:HD23	2.26	0.51
1:C:134:PHE:O	1:C:138:THR:HG23	2.09	0.51
1:C:163:TYR:N	1:C:164:PRO:CD	2.73	0.51
1:A:56:GLU:HB3	1:A:59:GLY:HA2	1.92	0.51
1:B:134:PHE:CE1	1:C:138:THR:HG22	2.45	0.51
1:B:209:GLN:HG2	1:B:211:LEU:HD11	1.91	0.51
1:C:28:PRO:HD2	1:D:48:ARG:HG2	1.93	0.51
1:B:44:LEU:HD11	1:B:54:ARG:HB2	1.92	0.51
1:D:6:VAL:HG21	1:D:9:LEU:HB2	1.91	0.51
1:E:41:PRO:HB2	1:E:53:TRP:NE1	2.26	0.51
1:E:35:ALA:HA	1:E:38:MET:HE2	1.93	0.51
1:F:12:THR:HG23	1:F:14:ASN:H	1.75	0.51
1:B:185:GLU:HA	1:B:188:GLN:HB3	1.93	0.51
1:E:186:GLU:O	1:E:190:MET:HG2	2.11	0.51
1:A:7:PHE:HB3	1:A:8:HIS:ND1	2.26	0.51
1:A:142:GLU:HG2	1:A:251:ARG:NH1	2.24	0.50
1:C:117:ASP:OD1	1:C:120:SER:OG	2.29	0.50
1:A:161:THR:OG1	1:B:122:HIS:ND1	2.39	0.50
1:E:83:GLN:HG3	1:F:172:TYR:HB2	1.93	0.50
1:A:30:ARG:HH22	1:A:94:THR:CB	2.24	0.50
1:C:160:ASP:O	1:D:72:PRO:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TYR:H	1:C:164:PRO:HD3	1.75	0.50
1:C:139:ALA:HA	1:C:142:GLU:HB3	1.92	0.50
1:B:134:PHE:HE1	1:C:138:THR:HG22	1.77	0.50
1:C:238:GLU:O	1:C:242:VAL:HG23	2.10	0.50
1:E:34:ILE:HG13	1:E:242:VAL:CG1	2.41	0.50
1:A:133:ASP:O	1:A:137:THR:OG1	2.27	0.50
1:B:185:GLU:N	1:B:185:GLU:OE2	2.43	0.50
1:D:9:LEU:HD23	1:D:50:PHE:CG	2.47	0.50
1:B:142:GLU:HG3	1:B:251:ARG:NH1	2.27	0.50
1:D:220:ILE:O	1:D:229:PRO:HG3	2.12	0.49
1:E:163:TYR:OH	1:F:80:GLU:OE1	2.31	0.49
1:A:115:ARG:NH1	1:A:125:PRO:O	2.45	0.49
1:B:43:LYS:HA	1:B:53:TRP:CD2	2.47	0.49
1:D:226:GLN:NE2	1:D:227:GLU:OE2	2.40	0.49
1:A:118:GLY:HA3	1:B:118:GLY:HA3	1.93	0.49
1:A:149:ALA:HB2	1:A:240:HIS:CE1	2.47	0.49
1:C:117:ASP:OD1	1:C:120:SER:N	2.34	0.49
1:C:142:GLU:OE1	1:C:251:ARG:NH1	2.45	0.49
1:A:78:VAL:HG21	1:A:202:LEU:HD13	1.93	0.49
1:F:27:ASP:OD2	1:F:30:ARG:HG2	2.13	0.49
1:E:216:VAL:HG11	1:E:245:VAL:HB	1.95	0.49
1:A:8:HIS:HB2	1:A:80:GLU:OE1	2.13	0.49
1:C:95:THR:OG1	1:C:195:TYR:O	2.20	0.49
1:E:97:ALA:HA	1:E:194:ASN:HA	1.94	0.49
1:F:80:GLU:O	1:F:84:LEU:HG	2.13	0.49
1:B:142:GLU:HA	1:B:145:LYS:HD2	1.94	0.49
1:D:222:ASN:HB3	1:D:225:GLN:HB3	1.95	0.49
1:E:41:PRO:HB2	1:E:53:TRP:HE1	1.78	0.49
1:E:42:VAL:HG21	1:E:54:ARG:HH21	1.78	0.49
1:E:154:GLY:CA	1:E:193:MET:CE	2.90	0.49
1:E:127:GLU:OE2	1:E:127:GLU:N	2.46	0.48
1:F:142:GLU:HA	1:F:145:LYS:HG2	1.96	0.48
1:D:30:ARG:O	1:D:34:ILE:HG12	2.13	0.48
1:D:74:THR:O	1:D:78:VAL:HG23	2.13	0.48
1:E:147:ILE:HD11	1:E:247:GLU:CD	2.37	0.48
1:B:92:ILE:HA	1:B:216:VAL:O	2.13	0.48
1:F:29:GLU:HB3	1:F:30:ARG:NH2	2.28	0.48
1:A:81:LEU:O	1:A:85:GLY:HA2	2.14	0.48
1:C:117:ASP:OD2	1:C:120:SER:OG	2.30	0.48
1:D:115:ARG:HH21	1:D:121:LEU:HD23	1.78	0.48
1:B:164:PRO:HB3	1:B:176:VAL:CG1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:SER:O	1:E:243:LYS:N	2.30	0.48
1:F:15:ASP:HB3	1:F:44:LEU:CD1	2.26	0.48
1:F:108:LEU:HD12	1:F:194:ASN:HB3	1.96	0.48
1:D:86:ILE:HG23	1:D:88:THR:H	1.78	0.48
1:E:21:LEU:HD11	1:E:252:LEU:HD12	1.95	0.48
1:F:163:TYR:H	1:F:164:PRO:HD3	1.79	0.48
1:B:209:GLN:N	1:B:210:GLY:HA2	2.29	0.48
1:E:95:THR:OG1	1:E:195:TYR:O	2.25	0.48
1:E:154:GLY:HA3	1:E:193:MET:CE	2.44	0.48
1:E:250:ARG:HA	1:E:253:LEU:CD1	2.43	0.48
1:E:143:ALA:HB1	1:E:247:GLU:CG	2.36	0.47
1:A:252:LEU:O	1:A:252:LEU:HD23	2.13	0.47
1:A:240:HIS:HA	1:A:243:LYS:HE3	1.95	0.47
1:C:60:LYS:HB2	1:C:253:LEU:HD11	1.95	0.47
1:F:194:ASN:OD1	1:F:194:ASN:N	2.47	0.47
1:D:201:THR:O	1:D:205:MET:HG2	2.14	0.47
1:B:15:ASP:O	1:B:54:ARG:HD3	2.13	0.47
1:C:72:PRO:O	1:C:75:SER:OG	2.31	0.47
1:C:167:GLU:HG3	1:C:176:VAL:HG11	1.97	0.47
1:E:196:GLU:OE1	1:E:199:SER:N	2.45	0.47
1:D:242:VAL:HA	1:D:245:VAL:HG12	1.97	0.47
1:F:92:ILE:HD13	1:F:216:VAL:HG13	1.96	0.47
1:A:163:TYR:N	1:A:164:PRO:CD	2.78	0.47
1:B:149:ALA:HB2	1:B:240:HIS:NE2	2.29	0.47
1:A:86:ILE:HG22	1:A:88:THR:N	2.29	0.47
1:D:238:GLU:O	1:D:242:VAL:HG23	2.15	0.47
1:E:98:ILE:O	1:E:188:GLN:NE2	2.40	0.47
1:E:115:ARG:NH2	1:E:121:LEU:HD23	2.31	0.46
1:A:187:TRP:HB3	1:A:192:VAL:HB	1.98	0.46
1:F:196:GLU:CG	1:F:197:MET:N	2.61	0.46
1:C:194:ASN:OD1	1:C:194:ASN:N	2.48	0.46
1:E:38:MET:HG3	1:E:57:LEU:HD22	1.97	0.46
1:E:208:SER:O	1:F:175:ARG:NH2	2.44	0.46
1:F:91:ARG:HH21	1:F:196:GLU:CD	2.24	0.46
1:C:239:SER:HA	1:C:242:VAL:HB	1.98	0.46
1:D:129:PRO:HD3	1:E:114:VAL:HA	1.97	0.46
1:F:187:TRP:CD1	1:F:195:TYR:HH	2.34	0.46
1:A:67:THR:OG1	1:A:91:ARG:NH1	2.45	0.46
1:F:9:LEU:HD11	1:F:81:LEU:HD12	1.96	0.46
1:B:72:PRO:O	1:B:75:SER:OG	2.30	0.46
1:B:114:VAL:HB	1:B:157:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ALA:HA	1:D:232:GLU:HA	1.57	0.46
1:E:161:THR:OG1	1:F:122:HIS:ND1	2.46	0.46
1:B:91:ARG:CG	1:B:215:MET:HE2	2.45	0.46
1:E:48:ARG:NH1	1:F:69:ILE:HD11	2.31	0.46
1:F:109:VAL:HG13	1:F:153:VAL:HG13	1.97	0.46
1:A:237:THR:O	1:A:240:HIS:HB3	2.16	0.46
1:B:48:ARG:HB3	1:B:49:GLU:H	1.46	0.46
1:B:107:VAL:HG11	1:B:244:ILE:HD12	1.98	0.46
1:C:162:PHE:HD1	1:C:163:TYR:CE1	2.33	0.46
1:F:9:LEU:CD1	1:F:81:LEU:HD12	2.46	0.46
1:A:197:MET:HG3	2:A:301:THM:O2	2.16	0.45
1:D:111:THR:HG22	1:D:137:THR:HG21	1.99	0.45
1:A:197:MET:HE1	1:B:76:ILE:HD11	1.98	0.45
1:E:166:GLN:OE1	1:E:168:ARG:NH1	2.50	0.45
1:F:38:MET:HE2	1:F:55:ALA:HB3	1.98	0.45
1:F:116:LEU:HB2	1:F:159:SER:HA	1.97	0.45
1:A:27:ASP:HB3	1:A:30:ARG:HG2	1.98	0.45
1:A:141:VAL:O	1:A:145:LYS:N	2.49	0.45
1:F:163:TYR:N	1:F:164:PRO:HD3	2.32	0.45
1:C:107:VAL:HG12	1:C:218:GLY:HA2	1.98	0.45
1:D:16:LEU:CB	1:D:17:GLN:HA	2.47	0.45
1:A:184:MET:HE1	1:A:223:ARG:HB3	1.98	0.45
1:E:234:MET:O	1:E:234:MET:SD	2.75	0.45
1:F:84:LEU:HD23	1:F:84:LEU:HA	1.53	0.45
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.98	0.45
1:B:84:LEU:HD12	1:B:84:LEU:HA	1.73	0.45
1:C:69:ILE:N	1:D:49:GLU:OE2	2.34	0.45
1:E:155:VAL:HG23	1:E:192:VAL:HA	1.98	0.45
1:B:108:LEU:HD13	1:B:152:HIS:HB2	1.99	0.45
1:C:198:GLU:N	1:C:198:GLU:OE1	2.50	0.45
1:C:229:PRO:HB2	1:C:234:MET:SD	2.57	0.45
1:F:163:TYR:HA	1:F:168:ARG:HD2	1.98	0.45
1:B:95:THR:OG1	1:B:96:GLY:N	2.49	0.45
1:C:234:MET:HG3	1:C:235:LYS:H	1.82	0.45
1:C:234:MET:HG3	1:C:235:LYS:N	2.32	0.45
1:D:196:GLU:OE2	1:D:199:SER:N	2.46	0.45
1:F:60:LYS:HB2	1:F:253:LEU:HD21	1.99	0.45
1:C:31:VAL:HG21	1:C:66:SER:HB2	1.99	0.45
1:C:163:TYR:H	1:C:164:PRO:CD	2.30	0.45
1:A:220:ILE:O	1:A:229:PRO:HG3	2.18	0.44
1:C:117:ASP:OD1	1:C:120:SER:CB	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:ILE:HB	1:F:64:VAL:HG22	1.99	0.44
1:E:56:GLU:HG3	1:E:61:ALA:HA	1.99	0.44
1:E:180:PHE:HA	1:E:183:SER:HB3	1.98	0.44
1:B:69:ILE:HD11	2:B:301:THM:H5'2	1.99	0.44
1:C:31:VAL:HG13	1:C:64:VAL:HG12	1.99	0.44
1:C:96:GLY:HA2	1:C:221:VAL:O	2.18	0.44
1:E:27:ASP:OD1	1:F:48:ARG:NH1	2.50	0.44
1:A:71:GLY:O	1:A:75:SER:N	2.39	0.44
1:D:165:GLY:HA2	1:D:180:PHE:CD1	2.52	0.44
1:C:57:LEU:HG	1:C:250:ARG:HG2	1.99	0.44
1:E:31:VAL:HG13	1:E:64:VAL:HG12	1.99	0.44
1:E:237:THR:O	1:E:240:HIS:HB2	2.18	0.44
1:B:141:VAL:HG11	1:C:134:PHE:CE2	2.53	0.44
1:C:43:LYS:HZ2	1:C:53:TRP:NE1	2.16	0.44
1:C:228:ILE:HG13	1:C:229:PRO:HD2	1.98	0.44
1:D:101:HIS:CD2	1:D:102:ILE:HG13	2.53	0.44
1:D:71:GLY:N	1:D:72:PRO:CD	2.80	0.44
1:E:43:LYS:HB2	1:E:53:TRP:CH2	2.53	0.44
1:E:235:LYS:C	1:E:237:THR:N	2.74	0.44
1:E:31:VAL:HG21	1:E:66:SER:HB3	1.99	0.44
1:E:161:THR:HB	1:E:164:PRO:HD2	2.00	0.44
1:E:250:ARG:O	1:E:253:LEU:CD1	2.53	0.44
1:A:21:LEU:HD12	1:A:252:LEU:HD22	1.99	0.44
1:A:115:ARG:NH1	1:A:128:PHE:O	2.50	0.44
1:B:9:LEU:HD23	1:B:11:LEU:HD12	1.99	0.44
1:A:86:ILE:HG22	1:A:87:ARG:N	2.33	0.43
1:B:146:SER:OG	1:B:251:ARG:NH2	2.51	0.43
1:C:117:ASP:CG	1:C:120:SER:OG	2.61	0.43
1:D:40:LYS:O	1:D:42:VAL:HG23	2.18	0.43
1:D:116:LEU:HB2	1:D:159:SER:HA	1.99	0.43
1:B:23:ILE:HD13	1:B:38:MET:HE1	1.99	0.43
1:C:126:MET:HE3	1:C:126:MET:HA	1.99	0.43
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.86	0.43
1:D:92:ILE:HG13	1:D:93:GLY:N	2.33	0.43
1:F:12:THR:HG22	1:F:15:ASP:CG	2.43	0.43
1:F:37:LEU:HD13	1:F:243:LYS:HG2	2.00	0.43
1:E:42:VAL:HG11	1:E:54:ARG:NH2	2.34	0.43
1:B:24:VAL:O	1:B:91:ARG:HD2	2.19	0.43
1:E:131:VAL:HG13	6:E:302:PG4:O5	2.19	0.43
1:E:13:LYS:H	1:E:13:LYS:HG2	1.22	0.43
1:E:57:LEU:HD12	1:E:57:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ALA:HA	1:B:232:GLU:HA	1.76	0.43
1:D:194:ASN:N	1:D:194:ASN:OD1	2.51	0.43
1:E:239:SER:O	1:E:243:LYS:HB2	2.19	0.43
1:C:220:ILE:HB	1:C:229:PRO:HB3	2.01	0.43
1:A:202:LEU:HA	1:A:205:MET:HE3	2.01	0.43
1:B:8:HIS:HB3	1:B:50:PHE:CE1	2.54	0.43
1:D:12:THR:OG1	1:D:13:LYS:N	2.52	0.43
1:D:111:THR:OG1	1:D:154:GLY:O	2.35	0.43
1:D:141:VAL:HG22	1:D:153:VAL:HG21	2.00	0.43
1:C:30:ARG:HG2	1:C:30:ARG:HH11	1.84	0.42
1:D:31:VAL:HG13	1:D:64:VAL:HG12	2.01	0.42
1:D:67:THR:OG1	1:D:91:ARG:NH1	2.52	0.42
1:E:86:ILE:HD13	1:E:86:ILE:H	1.80	0.42
1:E:221:VAL:HG21	1:E:228:ILE:HG13	2.00	0.42
1:A:16:LEU:HD11	1:A:84:LEU:C	2.44	0.42
1:A:106:ASP:H	1:A:219:VAL:HB	1.84	0.42
1:B:169:TYR:O	1:B:174:GLY:HA2	2.19	0.42
1:E:122:HIS:ND1	1:F:161:THR:OG1	2.47	0.42
1:D:153:VAL:HG12	1:D:154:GLY:N	2.33	0.42
1:E:27:ASP:HA	1:E:28:PRO:HD3	1.91	0.42
1:E:81:LEU:HB3	1:E:86:ILE:HG12	2.01	0.42
1:F:16:LEU:O	1:F:17:GLN:HB2	2.19	0.42
1:F:222:ASN:HB3	1:F:225:GLN:HB3	2.01	0.42
1:B:161:THR:HG22	1:B:164:PRO:HD2	2.00	0.42
1:C:27:ASP:HB3	1:C:30:ARG:HB3	2.02	0.42
1:C:34:ILE:HG13	1:C:242:VAL:HG13	2.02	0.42
1:D:32:GLU:HG3	1:D:53:TRP:CZ2	2.55	0.42
1:D:38:MET:HG3	1:D:56:GLU:O	2.19	0.42
1:D:44:LEU:HD11	1:D:54:ARG:HB2	2.01	0.42
1:E:80:GLU:HA	1:E:83:GLN:OE1	2.18	0.42
1:F:150:THR:HG22	1:F:152:HIS:HE1	1.85	0.42
1:A:92:ILE:HA	1:A:216:VAL:HG13	2.01	0.42
1:D:75:SER:OG	1:D:76:ILE:N	2.53	0.42
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.90	0.42
1:F:177:VAL:CG1	1:F:178:ARG:N	2.82	0.42
1:A:15:ASP:HB3	1:A:44:LEU:CD2	2.49	0.42
1:D:204:THR:O	1:D:208:SER:CB	2.68	0.42
1:D:205:MET:O	1:D:209:GLN:HG2	2.19	0.42
1:D:226:GLN:CD	1:D:226:GLN:H	2.27	0.42
1:F:15:ASP:OD1	1:F:44:LEU:HD22	2.19	0.42
1:A:119:ALA:N	1:B:160:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLU:HG3	1:B:251:ARG:HH11	1.83	0.42
1:B:223:ARG:NH1	1:B:223:ARG:CG	2.53	0.42
1:E:234:MET:C	1:E:236:GLN:N	2.71	0.42
1:A:16:LEU:HA	1:A:63:ILE:HD11	2.01	0.42
1:F:95:THR:CG2	1:F:196:GLU:HB2	2.44	0.42
1:F:222:ASN:HB3	1:F:225:GLN:CB	2.50	0.42
1:A:123:PHE:CZ	1:B:161:THR:HG21	2.55	0.42
1:D:38:MET:HE1	1:D:246:VAL:HG12	2.01	0.42
1:D:108:LEU:HD13	1:D:194:ASN:CG	2.45	0.42
1:A:147:ILE:HG21	1:A:240:HIS:CE1	2.55	0.41
1:E:38:MET:HG3	1:E:57:LEU:HD13	2.02	0.41
1:A:138:THR:HA	1:F:134:PHE:HZ	1.84	0.41
1:D:114:VAL:HA	1:E:129:PRO:HD3	2.02	0.41
1:D:248:ALA:O	1:D:252:LEU:HD12	2.20	0.41
1:E:26:GLY:HA2	1:E:68:GLY:H	1.85	0.41
1:E:37:LEU:HD13	1:E:37:LEU:HA	1.94	0.41
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.82	0.41
1:B:75:SER:HA	1:B:205:MET:SD	2.61	0.41
1:D:124:ALA:HB1	1:D:128:PHE:HB3	2.02	0.41
1:D:140:LEU:HD22	1:D:216:VAL:HB	2.02	0.41
1:F:99:GLN:NE2	1:F:192:VAL:O	2.49	0.41
1:A:31:VAL:HG13	1:A:64:VAL:HG12	2.03	0.41
1:B:142:GLU:HA	1:B:145:LYS:HB2	2.02	0.41
1:B:163:TYR:HB2	1:B:164:PRO:HD3	2.03	0.41
1:E:42:VAL:O	1:E:54:ARG:N	2.35	0.41
1:E:42:VAL:N	1:E:54:ARG:O	2.39	0.41
1:A:206:CYS:HA	1:A:211:LEU:HB2	2.03	0.41
1:B:82:ALA:O	1:B:85:GLY:HA3	2.20	0.41
1:B:161:THR:CG2	1:B:164:PRO:HD2	2.51	0.41
1:D:102:ILE:HD13	1:D:108:LEU:HD21	2.02	0.41
1:F:6:VAL:HG21	1:F:9:LEU:HB2	2.02	0.41
1:F:12:THR:N	1:F:15:ASP:OD2	2.49	0.41
1:B:187:TRP:HB3	1:B:192:VAL:HB	2.03	0.41
1:D:94:THR:HG21	1:D:220:ILE:HD11	2.02	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.91	0.40
1:D:87:ARG:N	1:D:87:ARG:HD3	2.36	0.40
1:B:220:ILE:HG22	1:B:235:LYS:HB3	2.03	0.40
1:C:201:THR:O	1:C:205:MET:HG2	2.21	0.40
1:D:169:TYR:O	1:D:174:GLY:HA2	2.22	0.40
1:D:235:LYS:O	1:D:238:GLU:HG2	2.21	0.40
1:A:228:ILE:H	1:A:228:ILE:HG13	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:TYR:H	1:F:164:PRO:CD	2.33	0.40
1:A:106:ASP:CG	1:A:150:THR:HG21	2.47	0.40
1:A:180:PHE:HA	1:A:183:SER:HB2	2.04	0.40
1:B:90:LEU:HD11	1:B:252:LEU:HD12	2.04	0.40
1:E:133:ASP:HA	6:E:302:PG4:C8	2.52	0.40
1:C:15:ASP:O	1:C:54:ARG:NH1	2.54	0.40
1:F:166:GLN:HB3	1:F:223:ARG:HH22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/253 (98%)	242 (98%)	6 (2%)	0	100	100
1	B	248/253 (98%)	241 (97%)	7 (3%)	0	100	100
1	C	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	30	43
1	D	248/253 (98%)	243 (98%)	5 (2%)	0	100	100
1	E	248/253 (98%)	234 (94%)	14 (6%)	0	100	100
1	F	241/253 (95%)	235 (98%)	6 (2%)	0	100	100
All	All	1481/1518 (98%)	1436 (97%)	44 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	163	TYR

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	199/202 (98%)	186 (94%)	13 (6%)	15	27
1	B	199/202 (98%)	179 (90%)	20 (10%)	7	11
1	C	199/202 (98%)	195 (98%)	4 (2%)	48	70
1	D	199/202 (98%)	188 (94%)	11 (6%)	19	34
1	E	199/202 (98%)	187 (94%)	12 (6%)	17	31
1	F	194/202 (96%)	188 (97%)	6 (3%)	35	57
All	All	1189/1212 (98%)	1123 (94%)	66 (6%)	19	33

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	30	ARG
1	A	32	GLU
1	A	44	LEU
1	A	62	VAL
1	A	88	THR
1	A	92	ILE
1	A	94	THR
1	A	145	LYS
1	A	170	ASP
1	A	197	MET
1	A	216	VAL
1	A	233	THR
1	B	20	GLN
1	B	29	GLU
1	B	39	ASP
1	B	43	LYS
1	B	49	GLU
1	B	62	VAL
1	B	84	LEU
1	B	153	VAL
1	B	167	GLU

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Mol	Chain	Res	Type
1	B	178	ARG
1	B	181	LYS
1	B	209	GLN
1	B	211	LEU
1	B	215	MET
1	B	223	ARG
1	B	228	ILE
1	B	234	MET
1	B	235	LYS
1	B	236	GLN
1	B	237	THR
1	C	30	ARG
1	C	38	MET
1	C	227	GLU
1	C	236	GLN
1	D	16	LEU
1	D	39	ASP
1	D	73	SER
1	D	90	LEU
1	D	92	ILE
1	D	94	THR
1	D	101	HIS
1	D	115	ARG
1	D	178	ARG
1	D	240	HIS
1	D	253	LEU
1	E	13	LYS
1	E	21	LEU
1	E	40	LYS
1	E	49	GLU
1	E	86	ILE
1	E	147	ILE
1	E	160	ASP
1	E	194	ASN
1	E	233	THR
1	E	237	THR
1	E	250	ARG
1	E	252	LEU
1	F	16	LEU
1	F	24	VAL
1	F	44	LEU
1	F	109	VAL

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Mol	Chain	Res	Type
1	F	176	VAL
1	F	196	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	240	HIS
1	B	101	HIS
1	B	222	ASN
1	B	236	GLN
1	C	222	ASN
1	C	230	ASN
1	D	8	HIS
1	D	101	HIS
1	D	209	GLN
1	E	8	HIS
1	E	222	ASN
1	F	225	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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
2	THM	D	301	-	18,18,18	2.01	8 (44%)	26,26,26	2.33	8 (30%)
2	THM	B	301	-	18,18,18	1.97	7 (38%)	26,26,26	2.36	6 (23%)
4	EDO	F	303	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	E	303	-	3,3,3	0.45	0	2,2,2	0.33	0
2	THM	E	301	-	18,18,18	2.24	5 (27%)	26,26,26	2.55	8 (30%)
6	PG4	E	302	-	12,12,12	0.73	0	11,11,11	0.97	0
2	THM	A	301	-	18,18,18	1.93	8 (44%)	26,26,26	2.39	8 (30%)
4	EDO	C	301	-	3,3,3	0.42	0	2,2,2	0.39	0
2	THM	F	301	-	18,18,18	1.97	8 (44%)	26,26,26	2.31	8 (30%)
5	PEG	D	302	-	6,6,6	0.64	0	5,5,5	0.76	0
3	IPA	A	302	-	3,3,3	0.53	0	3,3,3	0.20	0
4	EDO	A	303	-	3,3,3	0.34	0	2,2,2	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	THM	D	301	-	-	0/6/18/18	0/2/2/2
2	THM	B	301	-	-	0/6/18/18	0/2/2/2
4	EDO	F	303	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
2	THM	E	301	-	-	0/6/18/18	0/2/2/2
6	PG4	E	302	-	-	4/10/10/10	-
2	THM	A	301	-	-	2/6/18/18	0/2/2/2
4	EDO	C	301	-	-	0/1/1/1	-
2	THM	F	301	-	-	0/6/18/18	0/2/2/2
5	PEG	D	302	-	-	4/4/4/4	-
4	EDO	A	303	-	-	1/1/1/1	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	THM	C6-N1	-5.38	1.28	1.38
2	E	301	THM	C4-N3	-4.42	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	THM	C6-N1	3.92	1.44	1.38
2	B	301	THM	C6-N1	3.87	1.44	1.38
2	F	301	THM	C6-N1	3.83	1.44	1.38
2	E	301	THM	C2-N3	-3.82	1.31	1.38
2	A	301	THM	C6-N1	3.65	1.44	1.38
2	F	301	THM	C2-N1	3.39	1.43	1.38
2	D	301	THM	C2-N1	3.36	1.43	1.38
2	B	301	THM	C2-N1	3.24	1.43	1.38
2	A	301	THM	C2-N1	3.19	1.43	1.38
2	D	301	THM	O3'-C3'	-2.96	1.37	1.43
2	E	301	THM	C1'-N1	-2.95	1.40	1.48
2	B	301	THM	O3'-C3'	-2.91	1.37	1.43
2	A	301	THM	O3'-C3'	-2.86	1.37	1.43
2	F	301	THM	O3'-C3'	-2.82	1.37	1.43
2	E	301	THM	O4'-C4'	-2.67	1.39	1.45
2	B	301	THM	C2-N3	2.50	1.42	1.38
2	F	301	THM	C2-N3	2.50	1.42	1.38
2	D	301	THM	C2-N3	2.48	1.42	1.38
2	B	301	THM	C2'-C3'	-2.45	1.46	1.52
2	D	301	THM	C2'-C3'	-2.40	1.46	1.52
2	F	301	THM	C6-C5	2.36	1.38	1.34
2	A	301	THM	C4-C5	2.36	1.48	1.44
2	B	301	THM	C6-C5	2.35	1.38	1.34
2	F	301	THM	C2'-C3'	-2.29	1.47	1.52
2	A	301	THM	O4'-C4'	-2.27	1.39	1.45
2	A	301	THM	C2'-C3'	-2.23	1.47	1.52
2	A	301	THM	C2-N3	2.22	1.41	1.38
2	D	301	THM	O4'-C4'	-2.22	1.40	1.45
2	D	301	THM	C6-C5	2.20	1.38	1.34
2	F	301	THM	C4-C5	2.19	1.48	1.44
2	F	301	THM	O4'-C4'	-2.16	1.40	1.45
2	A	301	THM	C6-C5	2.14	1.38	1.34
2	B	301	THM	O4'-C4'	-2.10	1.40	1.45
2	D	301	THM	C4-C5	2.07	1.48	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	THM	C5-C4-N3	6.17	120.69	115.32
2	A	301	THM	C4-N3-C2	-6.00	119.47	127.34
2	B	301	THM	C4-N3-C2	-5.93	119.56	127.34
2	D	301	THM	C5-C4-N3	5.91	120.46	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	THM	C4-N3-C2	-5.84	119.68	127.34
2	A	301	THM	C5-C4-N3	5.82	120.38	115.32
2	D	301	THM	C4-N3-C2	-5.79	119.75	127.34
2	E	301	THM	O4-C4-C5	-5.78	118.30	124.92
2	F	301	THM	C5-C4-N3	5.60	120.19	115.32
2	E	301	THM	C4-N3-C2	-5.35	120.33	127.34
2	E	301	THM	C5-C6-N1	-5.04	117.84	123.31
2	B	301	THM	O4-C4-C5	-4.96	119.24	124.92
2	E	301	THM	N3-C2-N1	4.61	120.89	114.89
2	D	301	THM	O4-C4-C5	-4.58	119.67	124.92
2	F	301	THM	O4-C4-C5	-4.27	120.03	124.92
2	F	301	THM	N3-C2-N1	4.14	120.29	114.89
2	A	301	THM	N3-C2-N1	4.13	120.27	114.89
2	E	301	THM	C5-C4-N3	4.05	118.85	115.32
2	B	301	THM	N3-C2-N1	3.81	119.86	114.89
2	D	301	THM	N3-C2-N1	3.77	119.80	114.89
2	A	301	THM	O4-C4-C5	-3.61	120.79	124.92
2	A	301	THM	C5-C6-N1	-3.60	119.41	123.31
2	E	301	THM	O2-C2-N1	-3.42	118.35	122.80
2	D	301	THM	C5-C6-N1	-3.34	119.69	123.31
2	B	301	THM	C5-C6-N1	-3.32	119.71	123.31
2	F	301	THM	C5-C6-N1	-3.22	119.81	123.31
2	A	301	THM	O2-C2-N1	-2.64	119.36	122.80
2	B	301	THM	O2-C2-N1	-2.58	119.43	122.80
2	A	301	THM	C5M-C5-C6	-2.56	119.39	122.85
2	F	301	THM	O2-C2-N1	-2.55	119.48	122.80
2	F	301	THM	C6-C5-C4	2.30	119.92	118.02
2	D	301	THM	O2-C2-N1	-2.30	119.80	122.80
2	E	301	THM	O4'-C4'-C3'	-2.30	100.41	105.65
2	A	301	THM	C6-C5-C4	2.28	119.90	118.02
2	E	301	THM	C4'-O4'-C1'	-2.24	104.18	109.51
2	F	301	THM	C5M-C5-C6	-2.17	119.92	122.85
2	D	301	THM	C5'-C4'-C3'	-2.16	109.44	114.82
2	D	301	THM	C6-C5-C4	2.10	119.75	118.02

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	THM	C3'-C4'-C5'-O5'
4	A	303	EDO	O1-C1-C2-O2
2	A	301	THM	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	D	302	PEG	O1-C1-C2-O2
6	E	302	PG4	O2-C3-C4-O3
6	E	302	PG4	O4-C7-C8-O5
5	D	302	PEG	C1-C2-O2-C3
5	D	302	PEG	C4-C3-O2-C2
5	D	302	PEG	O2-C3-C4-O4
6	E	302	PG4	C6-C5-O3-C4
6	E	302	PG4	C3-C4-O3-C5

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	THM	1	0
2	E	301	THM	1	0
6	E	302	PG4	2	0
2	A	301	THM	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/253 (98%)	-1.35	0 100 100	37, 60, 61, 64	1 (0%)
1	B	250/253 (98%)	-1.30	0 100 100	34, 59, 60, 61	3 (1%)
1	C	250/253 (98%)	-1.30	0 100 100	34, 59, 61, 62	5 (2%)
1	D	250/253 (98%)	-1.34	0 100 100	34, 59, 61, 62	1 (0%)
1	E	250/253 (98%)	-1.33	0 100 100	32, 59, 60, 62	3 (1%)
1	F	245/253 (96%)	-1.31	0 100 100	45, 60, 61, 67	1 (0%)
All	All	1495/1518 (98%)	-1.32	0 100 100	32, 59, 61, 67	14 (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
4	EDO	C	301	4/4	0.92	0.07	62,62,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	F	303	4/4	0.94	0.06	65,67,69,69	0
6	PG4	E	302	13/13	0.96	0.06	60,64,68,68	0
3	IPA	A	302	4/4	0.97	0.06	60,60,60,60	0
5	PEG	D	302	7/7	0.97	0.06	67,67,68,68	0
4	EDO	E	303	4/4	0.97	0.04	58,58,58,59	0
2	THM	B	301	17/17	0.98	0.04	54,59,60,60	0
2	THM	D	301	17/17	0.99	0.04	63,64,67,67	0
2	THM	E	301	17/17	0.99	0.04	59,60,60,61	0
2	THM	F	301	17/17	0.99	0.04	59,63,67,68	0
2	THM	A	301	17/17	0.99	0.04	62,63,63,64	0
4	EDO	A	303	4/4	0.99	0.04	20,20,20,20	0
7	K	F	302	1/1	0.99	0.06	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.