Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2020 – 11:23 AM EST

PDB ID	:	5W6P
Title	:	Crystal structure of Bacteriophage CBA120 tailspike protein 2 enzymatically active domain (TSP2dN, orf211)
Authors	:	Plattner, M.; Shneider, M.M.; Leiman, P.G.
Deposited on	:	2017-06-16
Resolution	:	2.33 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 following versions of software and data (see references ⓘ) were used in the production of this report:

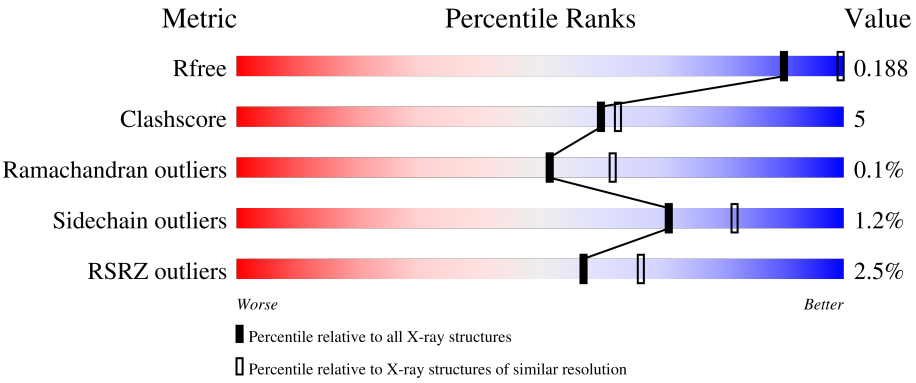
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.33 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	680	89% 10%
1	B	680	3% 88% 11%
1	C	680	3% 87% 12%
1	D	680	2% 90% 9%
1	E	680	89% 10%

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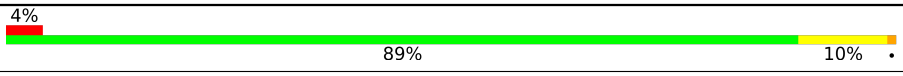
Mol	Chain	Length	Quality of chain
1	F	680	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32435 atoms, of which 36 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 tailspike protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	676	Total	C	N	O	S	0	0	0
			5053	3162	867	1003	21			
1	B	676	Total	C	N	O	S	0	1	0
			5059	3166	868	1004	21			
1	C	676	Total	C	N	O	S	0	0	0
			5053	3162	867	1003	21			
1	D	677	Total	C	N	O	S	0	1	0
			5065	3169	869	1006	21			
1	E	676	Total	C	N	O	S	0	0	0
			5053	3162	867	1003	21			
1	F	679	Total	C	N	O	S	0	0	0
			5069	3170	870	1008	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP G3M190
A	243	SER	-	expression tag	UNP G3M190
A	244	GLY	-	expression tag	UNP G3M190
A	245	SER	-	expression tag	UNP G3M190
B	242	GLY	-	expression tag	UNP G3M190
B	243	SER	-	expression tag	UNP G3M190
B	244	GLY	-	expression tag	UNP G3M190
B	245	SER	-	expression tag	UNP G3M190
C	242	GLY	-	expression tag	UNP G3M190
C	243	SER	-	expression tag	UNP G3M190
C	244	GLY	-	expression tag	UNP G3M190
C	245	SER	-	expression tag	UNP G3M190
D	242	GLY	-	expression tag	UNP G3M190
D	243	SER	-	expression tag	UNP G3M190
D	244	GLY	-	expression tag	UNP G3M190
D	245	SER	-	expression tag	UNP G3M190
E	242	GLY	-	expression tag	UNP G3M190

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Chain	Residue	Modelled	Actual	Comment	Reference
E	243	SER	-	expression tag	UNP G3M190
E	244	GLY	-	expression tag	UNP G3M190
E	245	SER	-	expression tag	UNP G3M190
F	242	GLY	-	expression tag	UNP G3M190
F	243	SER	-	expression tag	UNP G3M190
F	244	GLY	-	expression tag	UNP G3M190
F	245	SER	-	expression tag	UNP G3M190

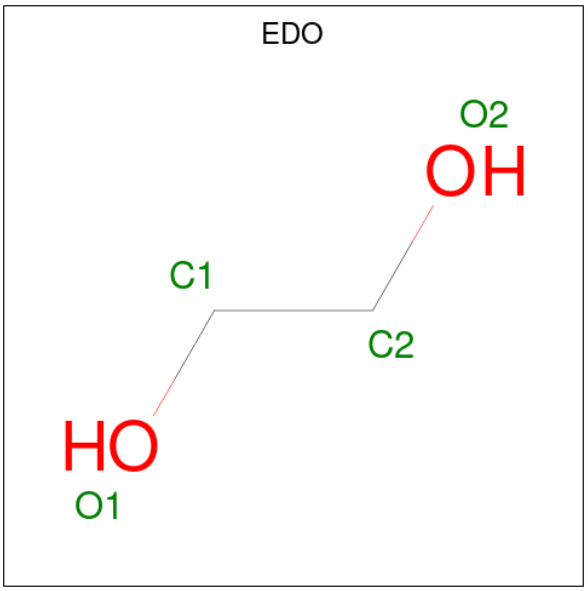
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	10	Total Zn 10 10	0	0
2	E	5	Total Zn 5 5	0	0
2	B	6	Total Zn 6 6	0	0
2	C	6	Total Zn 6 6	0	0
2	A	7	Total Zn 7 7	0	0
2	F	6	Total Zn 6 6	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	D	1	Total C H O 10 2 6 2	0	0
4	D	1	Total C H O 10 2 6 2	0	0
4	E	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is water.

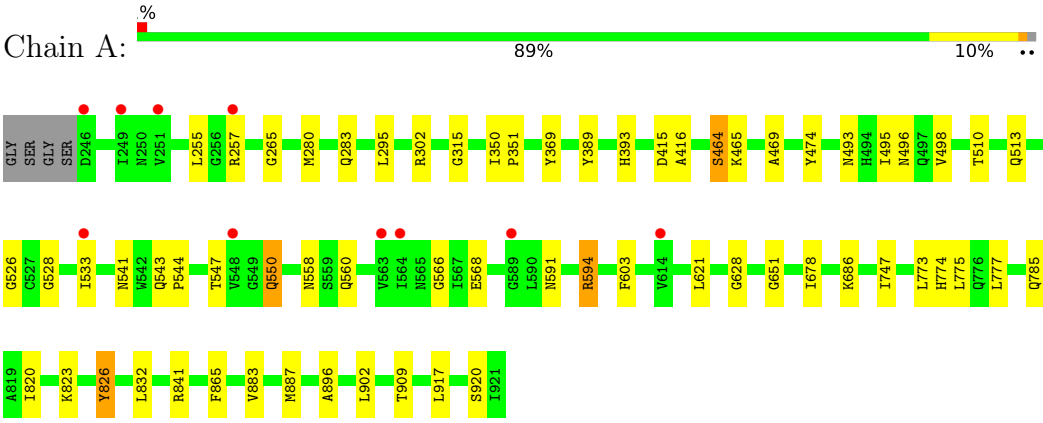
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	353	Total O 353 353	0	0
5	B	323	Total O 323 323	0	0
5	C	319	Total O 319 319	0	0
5	D	339	Total O 339 339	0	0
5	E	330	Total O 330 330	0	0
5	F	317	Total O 317 317	0	0

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.

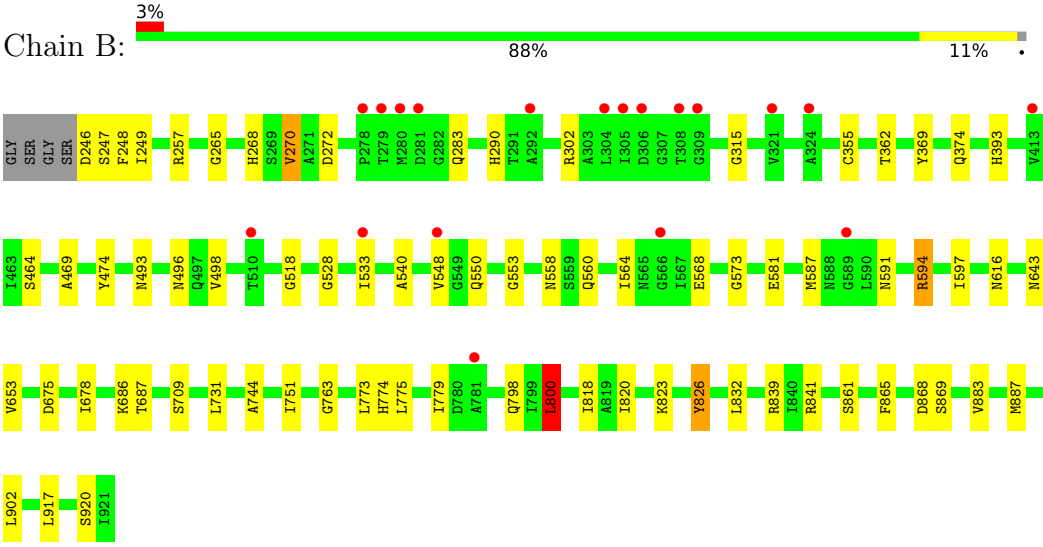
• Molecule 1: tailspike protein 2

Chain A:



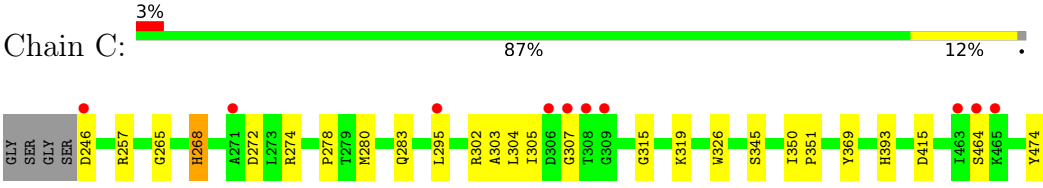
• Molecule 1: tailspike protein 2

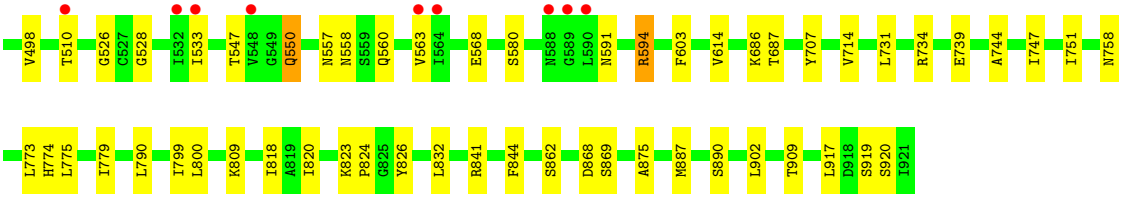
Chain B:



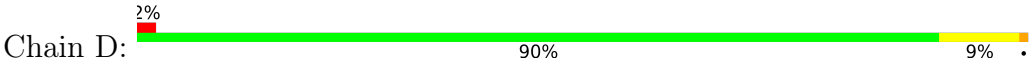
• Molecule 1: tailspike protein 2

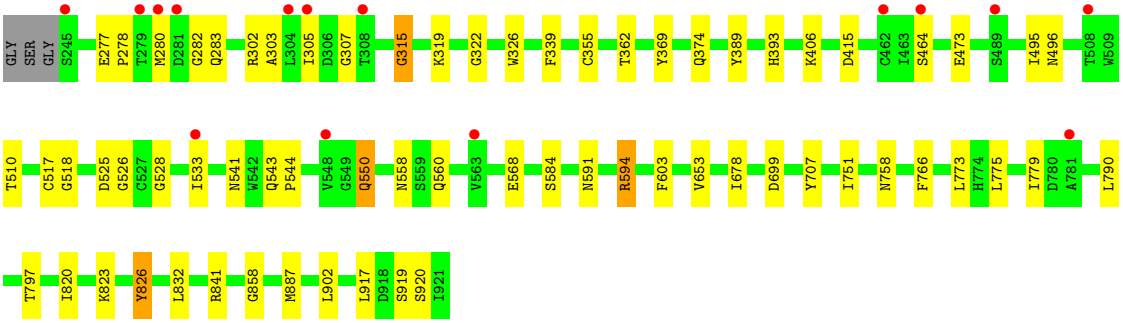
Chain C:



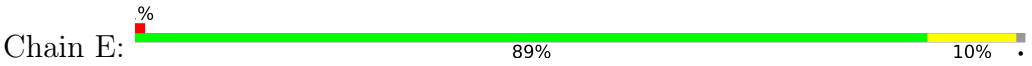


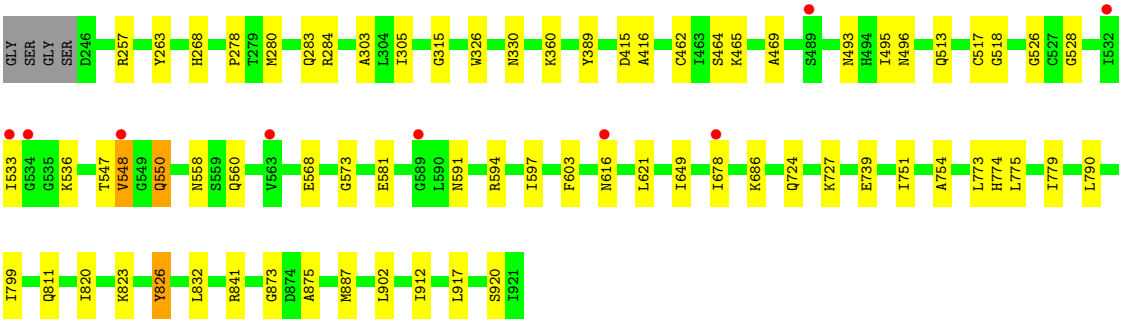
• Molecule 1: tailspike protein 2



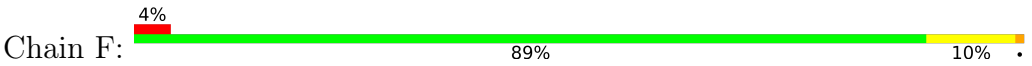


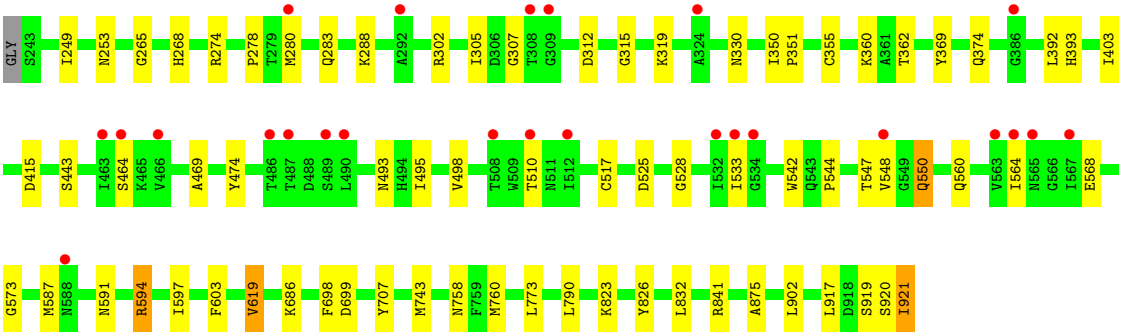
• Molecule 1: tailspike protein 2





• Molecule 1: tailspike protein 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.52Å 303.23Å 113.21Å 90.00° 90.38° 90.00°	Depositor
Resolution (Å)	46.68 – 2.33 49.93 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.68-2.33) 99.1 (49.93-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_2666: ???)	Depositor
R, R_{free}	0.154 , 0.190 0.151 , 0.188	Depositor DCC
R_{free} test set	9750 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32435	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, EDO

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	0.32	0/5150	0.53	0/7006
1	B	0.31	0/5159	0.53	1/7018 (0.0%)
1	C	0.31	0/5150	0.53	0/7006
1	D	0.31	0/5165	0.53	0/7026
1	E	0.32	0/5150	0.53	0/7006
1	F	0.32	0/5166	0.52	0/7027
All	All	0.32	0/30940	0.53	1/42089 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	800	LEU	CA-CB-CG	5.41	127.75	115.30

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	5053	0	4909	42	0
1	B	5059	0	4917	53	0
1	C	5053	0	4909	63	0
1	D	5065	0	4922	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5053	0	4910	47	0
1	F	5069	0	4922	52	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	6	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	6	6	0	0
4	B	4	6	6	1	0
4	C	4	6	6	0	0
4	D	8	12	12	0	0
4	E	4	6	6	0	0
5	A	353	0	0	3	1
5	B	323	0	0	10	0
5	C	319	0	0	8	0
5	D	339	0	0	6	1
5	E	330	0	0	10	0
5	F	317	0	0	9	0
All	All	32399	36	29525	276	1

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 5.

All (276) 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:584:SER:HB2	1:F:619:VAL:CG2	1.87	1.04
1:B:374[B]:GLN:OE1	5:B:1101:HOH:O	1.82	0.95
1:D:525:ASP:OD2	5:D:1101:HOH:O	1.93	0.86
1:C:790:LEU:HD22	1:C:799:ILE:HG12	1.58	0.86
1:E:518:GLY:O	1:E:547:THR:HG21	1.78	0.82
1:E:616:ASN:ND2	5:E:1102:HOH:O	2.07	0.82
1:F:443:SER:OG	5:F:1101:HOH:O	1.96	0.81
1:B:246:ASP:OD1	5:B:1102:HOH:O	2.00	0.80
1:B:246:ASP:N	5:B:1105:HOH:O	2.16	0.79
1:C:268:HIS:ND1	1:C:272:ASP:OD2	2.16	0.78
1:D:584:SER:HB2	1:F:619:VAL:HG22	1.65	0.78
1:A:513:GLN:NE2	5:A:1102:HOH:O	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:LEU:HD21	1:C:902:LEU:HD22	1.65	0.77
1:C:278:PRO:HG2	1:C:305:ILE:HD13	1.67	0.77
1:C:246:ASP:OD1	5:C:1101:HOH:O	2.03	0.76
1:E:739:GLU:OE1	5:E:1101:HOH:O	2.04	0.75
1:F:698:PHE:HB2	1:F:921:ILE:HD12	1.69	0.74
1:B:594:ARG:O	1:B:594:ARG:HD3	1.88	0.73
1:A:594:ARG:O	1:A:594:ARG:HD3	1.88	0.73
1:E:832:LEU:HD21	1:E:902:LEU:HD22	1.69	0.73
1:D:758:ASN:ND2	5:D:1104:HOH:O	2.22	0.72
1:F:253:ASN:ND2	5:F:1105:HOH:O	2.22	0.71
1:C:758:ASN:ND2	5:C:1102:HOH:O	2.21	0.71
1:F:594:ARG:O	1:F:594:ARG:HD3	1.92	0.70
5:B:1299:HOH:O	1:C:739:GLU:HG3	1.92	0.69
1:B:528:GLY:HA2	1:B:560:GLN:O	1.91	0.69
1:A:628:GLY:O	5:A:1101:HOH:O	2.09	0.69
1:E:887:MET:HE3	1:E:912:ILE:HG13	1.74	0.69
1:F:525:ASP:OD2	5:F:1102:HOH:O	2.11	0.68
1:D:594:ARG:O	1:D:594:ARG:HD3	1.94	0.67
1:B:616:ASN:OD1	5:B:1104:HOH:O	2.13	0.67
1:C:594:ARG:O	1:C:594:ARG:HD3	1.95	0.67
1:D:832:LEU:HD21	1:D:902:LEU:HD22	1.77	0.66
1:B:832:LEU:HD21	1:B:902:LEU:HD22	1.77	0.65
1:D:699:ASP:OD1	5:D:1102:HOH:O	2.14	0.65
1:E:536:LYS:HG2	5:E:1266:HOH:O	1.97	0.64
1:B:893:ASP:OD2	4:B:1007:EDO:O2	2.15	0.63
1:B:648:THR:HG22	5:B:1191:HOH:O	1.99	0.62
1:C:528:GLY:HA2	1:C:560:GLN:O	2.00	0.62
1:F:528:GLY:HA2	1:F:560:GLN:O	2.00	0.61
1:F:832:LEU:HD21	1:F:902:LEU:HD22	1.82	0.61
1:E:528:GLY:HA2	1:E:560:GLN:O	2.00	0.61
1:E:775:LEU:HD22	1:E:820:ILE:CG2	2.31	0.61
1:E:513:GLN:NE2	5:E:1105:HOH:O	2.33	0.60
1:B:775:LEU:HD22	1:B:820:ILE:CG2	2.32	0.59
1:E:526:GLY:HA2	1:E:558:ASN:O	2.02	0.59
1:B:270:VAL:HG22	1:B:290:HIS:O	2.02	0.59
1:C:747:ILE:HD12	1:C:818:ILE:HD12	1.85	0.59
1:E:887:MET:CE	1:E:912:ILE:HG13	2.32	0.59
1:F:568:GLU:HA	1:F:591:ASN:O	2.03	0.59
1:A:525:ASP:OD2	5:A:1103:HOH:O	2.17	0.59
1:D:528:GLY:HA2	1:D:560:GLN:O	2.01	0.59
1:C:547:THR:HG22	5:C:1177:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:374:GLN:HG2	5:F:1366:HOH:O	2.03	0.58
1:F:698:PHE:HB2	1:F:921:ILE:CD1	2.33	0.58
1:C:303:ALA:HB2	1:C:326:TRP:CZ3	2.40	0.57
1:F:547:THR:OG1	5:F:1103:HOH:O	2.14	0.57
1:C:774:HIS:HD2	5:C:1172:HOH:O	1.88	0.57
1:F:278:PRO:HG2	1:F:305:ILE:HD13	1.86	0.57
1:D:653:VAL:HG21	1:D:678:ILE:HD11	1.87	0.56
1:B:774:HIS:HD2	5:B:1154:HOH:O	1.87	0.56
1:B:249:ILE:H	1:B:249:ILE:HD12	1.70	0.56
1:C:307:GLY:O	1:C:319:LYS:NZ	2.34	0.55
1:A:528:GLY:HA2	1:A:560:GLN:O	2.06	0.55
1:D:775:LEU:HD22	1:D:820:ILE:CG2	2.37	0.55
1:D:374[B]:GLN:NE2	1:D:406:LYS:HD3	2.22	0.55
1:C:823:LYS:CG	1:C:824:PRO:HD2	2.37	0.54
1:A:510:THR:HA	1:A:533:ILE:O	2.08	0.53
1:B:823:LYS:HG2	1:B:826:TYR:HB3	1.90	0.53
1:D:584:SER:HB2	1:F:619:VAL:HG23	1.83	0.53
1:D:773:LEU:HD23	1:D:773:LEU:C	2.28	0.53
1:E:887:MET:HG3	1:F:686:LYS:HA	1.91	0.53
1:F:875:ALA:HB1	5:F:1136:HOH:O	2.08	0.53
1:E:774:HIS:HD2	5:E:1251:HOH:O	1.91	0.53
1:D:550:GLN:HG3	1:D:603:PHE:CE1	2.44	0.52
1:B:246:ASP:CG	1:B:247:SER:H	2.12	0.52
1:B:573:GLY:HA2	1:B:597:ILE:HG12	1.91	0.52
1:C:494:HIS:NE2	5:C:1107:HOH:O	2.34	0.52
1:A:777:LEU:HD11	1:A:785:GLN:HB3	1.92	0.52
1:B:917:LEU:HA	1:B:920:SER:O	2.09	0.52
1:B:839:ARG:NH1	1:B:841:ARG:HD2	2.24	0.52
1:D:496:ASN:O	1:D:518:GLY:HA3	2.10	0.52
1:E:568:GLU:HA	1:E:591:ASN:O	2.10	0.52
1:A:415:ASP:HA	1:A:464:SER:O	2.09	0.51
1:C:568:GLU:HA	1:C:591:ASN:O	2.10	0.51
1:A:369:TYR:HA	1:A:393:HIS:O	2.10	0.51
1:A:774:HIS:HB2	1:A:790:LEU:HB2	1.92	0.51
1:B:268:HIS:HB3	5:B:1403:HOH:O	2.10	0.51
1:E:469:ALA:HA	1:E:493:ASN:O	2.10	0.51
1:A:775:LEU:HD22	1:A:820:ILE:CG2	2.40	0.51
1:E:917:LEU:HA	1:E:920:SER:O	2.10	0.51
1:C:278:PRO:HG2	1:C:305:ILE:CD1	2.38	0.51
1:D:415:ASP:HA	1:D:464:SER:O	2.11	0.51
1:E:875:ALA:HB1	5:E:1282:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ILE:CG2	1:A:896:ALA:HB1	2.41	0.51
1:C:774:HIS:HB2	1:C:790:LEU:HB2	1.92	0.51
1:E:811:GLN:HA	5:E:1276:HOH:O	2.11	0.51
1:E:257:ARG:NH2	1:E:263:TYR:OH	2.44	0.50
1:F:743:MET:HE2	1:F:760:MET:HB2	1.94	0.50
1:A:865:PHE:CZ	1:A:883:VAL:HG13	2.46	0.50
1:F:330:ASN:O	1:F:360:LYS:NZ	2.44	0.50
1:B:474:TYR:HA	1:B:498:VAL:O	2.11	0.50
1:E:303:ALA:HB2	1:E:326:TRP:CZ3	2.46	0.50
1:F:699:ASP:OD2	5:F:1104:HOH:O	2.20	0.50
1:A:832:LEU:HD21	1:A:902:LEU:HD22	1.93	0.50
1:B:369:TYR:HA	1:B:393:HIS:O	2.11	0.50
1:F:917:LEU:HA	1:F:920:SER:O	2.12	0.50
1:E:284:ARG:NH1	5:E:1111:HOH:O	2.40	0.49
1:B:653:VAL:HG21	1:B:678:ILE:HD11	1.95	0.49
1:E:257:ARG:O	1:F:265:GLY:HA3	2.13	0.49
1:D:766:PHE:CZ	1:D:797:THR:OG1	2.66	0.49
1:E:790:LEU:HG	1:E:799:ILE:HG12	1.95	0.49
1:F:823:LYS:HG2	1:F:826:TYR:HB3	1.95	0.49
1:C:775:LEU:HD22	1:C:820:ILE:CG2	2.43	0.49
1:F:274:ARG:HG2	1:F:319:LYS:O	2.12	0.49
1:B:265:GLY:HA3	1:C:257:ARG:O	2.11	0.49
1:F:469:ALA:HA	1:F:493:ASN:O	2.12	0.49
1:C:274:ARG:HG2	1:C:319:LYS:O	2.12	0.48
1:C:875:ALA:HB1	5:C:1110:HOH:O	2.12	0.48
1:D:303:ALA:HB2	1:D:326:TRP:CZ3	2.48	0.48
1:A:568:GLU:HA	1:A:591:ASN:O	2.14	0.48
1:B:355:CYS:HB3	1:B:362:THR:OG1	2.12	0.48
1:E:280:MET:HG3	1:E:283:GLN:HB2	1.95	0.48
1:B:686:LYS:HA	1:C:887:MET:HG3	1.95	0.48
1:E:415:ASP:HA	1:E:464:SER:O	2.13	0.48
1:F:573:GLY:HA2	1:F:597:ILE:HG12	1.96	0.48
1:B:415:ASP:HA	1:B:464:SER:O	2.14	0.48
1:D:751:ILE:HD12	1:D:779:ILE:HD11	1.95	0.48
1:E:774:HIS:HB2	1:E:790:LEU:HB2	1.95	0.48
1:A:543:GLN:HB3	1:A:544:PRO:HD3	1.96	0.48
1:C:823:LYS:HG2	1:C:824:PRO:N	2.28	0.48
1:A:469:ALA:HA	1:A:493:ASN:O	2.15	0.47
1:C:268:HIS:HB2	5:C:1393:HOH:O	2.14	0.47
1:C:823:LYS:HG3	1:C:824:PRO:HD2	1.95	0.47
1:C:734:ARG:O	1:C:862:SER:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:ASN:O	1:E:518:GLY:HA3	2.14	0.47
1:A:474:TYR:HA	1:A:498:VAL:O	2.15	0.47
1:A:773:LEU:HA	1:A:790:LEU:O	2.15	0.47
1:C:707:TYR:CD1	1:C:919:SER:HA	2.50	0.47
1:D:278:PRO:HG2	1:D:305:ILE:HD13	1.97	0.47
1:C:557:ASN:ND2	1:C:558:ASN:OD1	2.44	0.47
1:D:369:TYR:HA	1:D:393:HIS:O	2.15	0.47
1:D:315:GLY:HA3	1:D:339:PHE:CD2	2.49	0.46
1:F:415:ASP:HA	1:F:464:SER:O	2.14	0.46
1:A:257:ARG:O	1:C:265:GLY:HA3	2.15	0.46
1:A:280:MET:HG3	1:A:283:GLN:HB2	1.97	0.46
1:A:416:ALA:HA	1:A:465:LYS:O	2.16	0.46
1:B:678:ILE:HG12	1:B:896:ALA:HB1	1.97	0.46
1:D:568:GLU:HA	1:D:591:ASN:O	2.16	0.46
1:F:564:ILE:O	1:F:587:MET:HA	2.16	0.46
1:B:687:THR:HA	1:C:909:THR:O	2.15	0.46
1:C:731:LEU:CD2	1:C:869:SER:HA	2.46	0.46
1:B:268:HIS:CE1	1:B:272:ASP:OD2	2.69	0.45
1:A:518:GLY:O	1:A:547:THR:HG21	2.16	0.45
1:D:280:MET:HG3	1:D:283:GLN:HB2	1.97	0.45
1:B:469:ALA:HA	1:B:493:ASN:O	2.16	0.45
1:B:568:GLU:HA	1:B:591:ASN:O	2.16	0.45
1:C:350:ILE:HB	1:C:351:PRO:HD3	1.98	0.45
1:D:473:GLU:OE1	5:D:1103:HOH:O	2.21	0.45
1:D:526:GLY:HA2	1:D:558:ASN:O	2.16	0.45
1:E:823:LYS:HG2	1:E:826:TYR:HB3	1.99	0.45
1:B:773:LEU:HD23	1:B:773:LEU:C	2.37	0.45
1:D:277:GLU:OE1	1:D:322:GLY:N	2.43	0.45
1:E:727:LYS:HE2	1:E:873:GLY:O	2.17	0.45
1:C:773:LEU:C	1:C:773:LEU:HD23	2.37	0.45
1:D:355:CYS:HB3	1:D:362:THR:OG1	2.17	0.45
1:A:909:THR:O	1:C:687:THR:HA	2.17	0.45
1:C:268:HIS:CE1	1:C:272:ASP:OD2	2.70	0.45
1:C:280:MET:HG3	1:C:283:GLN:HB2	1.97	0.45
1:A:550:GLN:HG3	1:A:603:PHE:CE1	2.52	0.45
1:C:510:THR:HA	1:C:533:ILE:O	2.17	0.45
1:E:278:PRO:HG2	1:E:305:ILE:HD13	1.98	0.45
1:E:416:ALA:HA	1:E:465:LYS:O	2.17	0.45
1:E:550:GLN:HG3	1:E:603:PHE:CE1	2.51	0.45
1:E:547:THR:HB	5:E:1138:HOH:O	2.17	0.44
1:A:887:MET:HG3	1:C:686:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASP:HA	1:C:464:SER:O	2.17	0.44
1:C:800:LEU:HD22	1:C:844:PHE:CD1	2.52	0.44
1:D:543:GLN:HB3	1:D:544:PRO:HD3	2.00	0.44
1:C:369:TYR:HA	1:C:393:HIS:O	2.17	0.44
1:A:526:GLY:HA2	1:A:558:ASN:O	2.18	0.44
1:A:566:GLY:HA2	1:C:563:VAL:HG11	1.99	0.44
1:F:268:HIS:HA	1:F:288:LYS:HB3	2.00	0.44
1:F:355:CYS:HB3	1:F:362:THR:OG1	2.17	0.44
1:F:392:LEU:HD12	1:F:403:ILE:HD11	1.99	0.44
1:C:295:LEU:O	1:C:295:LEU:HG	2.18	0.44
1:F:773:LEU:HA	1:F:790:LEU:O	2.18	0.44
1:D:282:GLY:O	1:D:302:ARG:NH1	2.47	0.43
1:D:307:GLY:O	1:D:319:LYS:NZ	2.49	0.43
1:F:474:TYR:HA	1:F:498:VAL:O	2.18	0.43
1:B:564:ILE:O	1:B:587:MET:HA	2.19	0.43
1:D:887:MET:HG3	1:E:686:LYS:HA	1.99	0.43
1:E:724:GLN:O	1:E:727:LYS:HG2	2.18	0.43
1:B:823:LYS:CG	1:B:826:TYR:HB3	2.48	0.43
1:C:751:ILE:HG23	1:C:779:ILE:HD13	1.99	0.43
1:D:858:GLY:HA3	5:D:1238:HOH:O	2.18	0.43
1:F:312:ASP:HB2	1:F:319:LYS:CG	2.48	0.43
1:A:295:LEU:HD11	1:C:302:ARG:HD3	1.99	0.43
1:B:496:ASN:O	1:B:518:GLY:HA3	2.18	0.43
5:D:1411:HOH:O	1:E:462:CYS:HB3	2.18	0.43
1:B:798:GLN:HG2	1:B:800:LEU:HD22	1.99	0.43
1:C:550:GLN:HG3	1:C:603:PHE:CE1	2.54	0.43
1:C:809:LYS:HE3	5:C:1228:HOH:O	2.18	0.43
1:D:707:TYR:CG	1:D:919:SER:HA	2.53	0.43
1:A:533:ILE:HG21	1:B:533:ILE:HG22	1.99	0.43
1:C:917:LEU:HA	1:C:920:SER:O	2.18	0.43
1:F:307:GLY:HA3	1:F:319:LYS:NZ	2.33	0.43
1:B:643:ASN:O	1:C:823:LYS:HE3	2.18	0.43
1:B:751:ILE:HG23	1:B:779:ILE:HD13	2.01	0.43
1:F:773:LEU:HD23	1:F:773:LEU:C	2.39	0.43
1:D:510:THR:HA	1:D:533:ILE:O	2.19	0.42
1:D:773:LEU:HA	1:D:790:LEU:O	2.18	0.42
1:D:917:LEU:HA	1:D:920:SER:O	2.19	0.42
1:E:495:ILE:O	1:E:517:CYS:HA	2.19	0.42
1:A:265:GLY:HA3	1:B:257:ARG:O	2.20	0.42
1:B:865:PHE:CZ	1:B:883:VAL:HG13	2.53	0.42
1:D:495:ILE:O	1:D:517:CYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:LYS:HA	1:B:887:MET:HG3	2.01	0.42
1:F:350:ILE:HB	1:F:351:PRO:HD3	2.01	0.42
1:F:550:GLN:HG3	1:F:603:PHE:CE1	2.55	0.42
1:F:743:MET:CE	1:F:760:MET:HB2	2.50	0.42
1:B:248:PHE:HB3	5:B:1105:HOH:O	2.19	0.42
1:F:280:MET:HG3	1:F:283:GLN:HB2	2.02	0.42
1:B:731:LEU:CD2	1:B:869:SER:HA	2.50	0.42
1:C:823:LYS:HG2	1:C:824:PRO:HD2	2.01	0.42
1:F:495:ILE:O	1:F:517:CYS:HA	2.19	0.42
1:F:542:TRP:CD2	1:F:544:PRO:HD2	2.55	0.42
1:A:917:LEU:HA	1:A:920:SER:O	2.19	0.42
1:C:304:LEU:HD23	1:C:304:LEU:HA	1.92	0.42
1:D:823:LYS:HG2	1:D:826:TYR:HB3	2.02	0.42
1:A:495:ILE:O	1:A:517:CYS:HA	2.20	0.42
1:A:773:LEU:HD23	1:A:773:LEU:C	2.41	0.41
1:B:675:ASP:OD2	1:C:890:SER:HB3	2.19	0.41
1:B:744:ALA:HA	1:B:818:ILE:O	2.19	0.41
1:E:573:GLY:HA2	1:E:597:ILE:HG12	2.02	0.41
1:E:621:LEU:HD23	1:E:621:LEU:C	2.41	0.41
1:A:621:LEU:HD23	1:A:621:LEU:C	2.41	0.41
1:A:823:LYS:HG2	1:A:826:TYR:HB3	2.01	0.41
1:A:651:GLY:HA2	1:C:614:VAL:HG11	2.01	0.41
1:A:350:ILE:HB	1:A:351:PRO:HD3	2.02	0.41
1:C:868:ASP:C	1:C:868:ASP:OD1	2.59	0.41
1:D:533:ILE:HG21	1:F:533:ILE:HG22	2.03	0.41
1:C:714:VAL:HG12	1:C:714:VAL:O	2.21	0.41
1:B:558:ASN:HA	1:B:581:GLU:O	2.21	0.41
1:C:474:TYR:HA	1:C:498:VAL:O	2.20	0.41
1:D:533:ILE:HG22	1:E:533:ILE:HG21	2.02	0.41
1:F:283:GLN:O	1:F:302:ARG:HA	2.20	0.41
1:F:758:ASN:ND2	5:F:1108:HOH:O	2.40	0.41
1:A:283:GLN:O	1:A:302:ARG:HA	2.20	0.41
1:A:496:ASN:O	1:A:518:GLY:HA3	2.21	0.41
1:C:526:GLY:HA2	1:C:558:ASN:O	2.21	0.41
1:E:581:GLU:OE2	5:E:1103:HOH:O	2.22	0.41
1:E:751:ILE:HD12	1:E:779:ILE:HD11	2.01	0.41
1:C:278:PRO:HG3	1:C:303:ALA:HB1	2.02	0.41
1:C:557:ASN:HA	1:C:580:SER:O	2.21	0.41
1:E:773:LEU:C	1:E:773:LEU:HD23	2.40	0.41
1:E:754:ALA:HA	1:E:779:ILE:O	2.20	0.41
1:F:249:ILE:HG22	5:F:1105:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:510:THR:HA	1:F:533:ILE:O	2.21	0.41
1:F:707:TYR:CG	1:F:919:SER:HA	2.55	0.41
1:B:249:ILE:HD11	5:B:1228:HOH:O	2.20	0.41
1:E:649:ILE:O	1:E:678:ILE:HA	2.20	0.41
1:C:744:ALA:HA	1:C:818:ILE:O	2.21	0.41
1:F:369:TYR:HA	1:F:393:HIS:O	2.20	0.41
1:B:283:GLN:O	1:B:302:ARG:HA	2.21	0.41
1:B:540:ALA:CB	1:B:553:GLY:HA2	2.51	0.41
1:E:548:VAL:CG1	1:E:548:VAL:O	2.69	0.41
1:F:591:ASN:HA	1:F:619:VAL:HG12	2.03	0.41
1:B:548:VAL:O	1:B:548:VAL:HG13	2.21	0.40
1:B:763:GLY:CA	1:B:861:SER:HB3	2.51	0.40
1:C:707:TYR:CG	1:C:919:SER:HA	2.56	0.40
1:F:312:ASP:HB2	1:F:319:LYS:HG2	2.04	0.40
1:E:330:ASN:O	1:E:360:LYS:NZ	2.55	0.40
1:A:747:ILE:HD12	1:A:818:ILE:HD12	2.03	0.40
1:D:584:SER:HB2	1:F:619:VAL:HG21	1.92	0.40
1:B:868:ASP:C	1:B:868:ASP:OD1	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1435:HOH:O	5:D:1413:HOH:O[1_554]	1.83	0.37

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	674/680 (99%)	642 (95%)	31 (5%)	1 (0%)	51 62
1	B	675/680 (99%)	643 (95%)	31 (5%)	1 (0%)	51 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	674/680 (99%)	644 (96%)	29 (4%)	1 (0%)	51 62
1	D	676/680 (99%)	644 (95%)	31 (5%)	1 (0%)	51 62
1	E	674/680 (99%)	642 (95%)	31 (5%)	1 (0%)	51 62
1	F	677/680 (100%)	647 (96%)	29 (4%)	1 (0%)	51 62
All	All	4050/4080 (99%)	3862 (95%)	182 (4%)	6 (0%)	51 62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLY
1	D	315	GLY
1	E	315	GLY
1	B	315	GLY
1	C	315	GLY
1	F	315	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	554/556 (100%)	546 (99%)	8 (1%)	67 78
1	B	555/556 (100%)	549 (99%)	6 (1%)	73 83
1	C	554/556 (100%)	548 (99%)	6 (1%)	73 83
1	D	556/556 (100%)	550 (99%)	6 (1%)	73 83
1	E	554/556 (100%)	547 (99%)	7 (1%)	69 79
1	F	556/556 (100%)	550 (99%)	6 (1%)	73 83
All	All	3329/3336 (100%)	3290 (99%)	39 (1%)	71 82

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LEU

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Mol	Chain	Res	Type
1	A	389	TYR
1	A	464	SER
1	A	541	ASN
1	A	550	GLN
1	A	594	ARG
1	A	826	TYR
1	A	841	ARG
1	B	270	VAL
1	B	550	GLN
1	B	594	ARG
1	B	709	SER
1	B	800	LEU
1	B	826	TYR
1	C	268	HIS
1	C	345	SER
1	C	550	GLN
1	C	594	ARG
1	C	826	TYR
1	C	841	ARG
1	D	389	TYR
1	D	541	ASN
1	D	550	GLN
1	D	594	ARG
1	D	826	TYR
1	D	841	ARG
1	E	268	HIS
1	E	389	TYR
1	E	548	VAL
1	E	550	GLN
1	E	594	ARG
1	E	826	TYR
1	E	841	ARG
1	F	548	VAL
1	F	550	GLN
1	F	594	ARG
1	F	619	VAL
1	F	841	ARG
1	F	921	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 42 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	EDO	D	1013	-	3,3,3	0.56	0	2,2,2	0.28	0
4	EDO	E	1006	-	3,3,3	0.54	0	2,2,2	0.42	0
4	EDO	B	1007	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	C	1007	-	3,3,3	0.51	0	2,2,2	0.34	0
4	EDO	A	1009	-	3,3,3	0.50	0	2,2,2	0.39	0
4	EDO	D	1012	-	3,3,3	0.54	0	2,2,2	0.28	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
4	EDO	D	1013	-	-	1/1/1/1	-
4	EDO	E	1006	-	-	0/1/1/1	-
4	EDO	B	1007	-	-	0/1/1/1	-
4	EDO	C	1007	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1009	-	-	0/1/1/1	-
4	EDO	D	1012	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1013	EDO	O1-C1-C2-O2
4	D	1012	EDO	O1-C1-C2-O2
4	C	1007	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1007	EDO	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, 95^{th} 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	676/680 (99%)	-0.38	10 (1%)	73	81	26, 37, 54, 122	0
1	B	676/680 (99%)	-0.22	21 (3%)	49	59	26, 39, 64, 125	0
1	C	676/680 (99%)	-0.14	20 (2%)	50	60	25, 38, 69, 123	0
1	D	677/680 (99%)	-0.26	15 (2%)	62	71	27, 38, 60, 98	0
1	E	676/680 (99%)	-0.36	9 (1%)	77	83	28, 39, 56, 94	0
1	F	679/680 (99%)	-0.04	25 (3%)	41	52	30, 41, 65, 113	0
All	All	4060/4080 (99%)	-0.23	100 (2%)	57	66	25, 39, 62, 125	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	548	VAL	5.2
1	C	548	VAL	5.2
1	B	548	VAL	4.0
1	C	533	ILE	3.8
1	B	280	MET	3.8
1	D	781	ALA	3.7
1	D	280	MET	3.7
1	F	533	ILE	3.6
1	B	305	ILE	3.6
1	F	309	GLY	3.3
1	C	308	THR	3.3
1	E	548	VAL	3.3
1	C	464	SER	3.1
1	F	308	THR	3.1
1	F	548	VAL	3.0
1	B	281	ASP	3.0
1	F	324	ALA	3.0
1	F	463	ILE	2.9
1	B	308	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	279	THR	2.9
1	A	533	ILE	2.9
1	E	533	ILE	2.9
1	E	563	VAL	2.9
1	D	533	ILE	2.8
1	D	305	ILE	2.8
1	C	564	ILE	2.8
1	F	532	ILE	2.8
1	D	279	THR	2.8
1	C	309	GLY	2.7
1	F	466	VAL	2.7
1	F	487	THR	2.7
1	C	532	ILE	2.7
1	D	245	SER	2.7
1	F	490	LEU	2.7
1	F	563	VAL	2.7
1	E	532	ILE	2.6
1	B	321	VAL	2.6
1	A	563	VAL	2.6
1	C	307	GLY	2.6
1	E	534	GLY	2.6
1	F	564	ILE	2.5
1	A	548	VAL	2.5
1	C	589	GLY	2.5
1	B	533	ILE	2.5
1	E	489	SER	2.5
1	F	292	ALA	2.5
1	D	563	VAL	2.5
1	B	304	LEU	2.5
1	B	413	VAL	2.4
1	B	292	ALA	2.4
1	B	781	ALA	2.4
1	A	249	ILE	2.3
1	C	463	ILE	2.3
1	D	304	LEU	2.3
1	B	510	THR	2.3
1	F	510	THR	2.3
1	D	462	CYS	2.3
1	F	512	ILE	2.3
1	F	486	THR	2.3
1	E	616	ASN	2.3
1	B	278	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	588	ASN	2.3
1	F	489	SER	2.3
1	D	508	THR	2.2
1	C	563	VAL	2.2
1	C	295	LEU	2.2
1	C	306	ASP	2.2
1	C	590	LEU	2.2
1	D	489	SER	2.2
1	E	589	GLY	2.2
1	A	246	ASP	2.2
1	C	271	ALA	2.2
1	F	534	GLY	2.2
1	B	649	ILE	2.2
1	A	251	VAL	2.1
1	C	246	ASP	2.1
1	B	462	CYS	2.1
1	D	308	THR	2.1
1	D	464	SER	2.1
1	E	678	ILE	2.1
1	C	465	LYS	2.1
1	A	564	ILE	2.1
1	D	281	ASP	2.1
1	B	324	ALA	2.1
1	B	309	GLY	2.1
1	F	386	GLY	2.1
1	F	464	SER	2.1
1	B	306	ASP	2.0
1	F	280	MET	2.0
1	F	565	ASN	2.0
1	C	510	THR	2.0
1	F	508	THR	2.0
1	B	589	GLY	2.0
1	C	489	SER	2.0
1	A	589	GLY	2.0
1	B	566	GLY	2.0
1	A	614	VAL	2.0
1	C	588	ASN	2.0
1	F	567	ILE	2.0
1	A	257	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	ZN	B	1003	1/1	0.25	0.19	135,135,135,135	0
2	ZN	D	1003	1/1	0.45	0.17	134,134,134,134	0
2	ZN	D	1004	1/1	0.65	0.15	72,72,72,72	1
2	ZN	C	1004	1/1	0.66	0.18	153,153,153,153	0
2	ZN	A	1007	1/1	0.78	0.13	89,89,89,89	0
2	ZN	F	1006	1/1	0.79	0.10	117,117,117,117	0
2	ZN	F	1003	1/1	0.82	0.28	125,125,125,125	0
4	EDO	E	1006	4/4	0.82	0.17	53,63,71,71	0
2	ZN	D	1002	1/1	0.83	0.07	135,135,135,135	0
2	ZN	C	1005	1/1	0.86	0.06	134,134,134,134	0
4	EDO	A	1009	4/4	0.86	0.19	53,64,69,69	0
2	ZN	E	1005	1/1	0.87	0.07	117,117,117,117	0
4	EDO	C	1007	4/4	0.89	0.20	47,56,67,67	0
4	EDO	D	1012	4/4	0.90	0.12	44,53,61,61	0
4	EDO	B	1007	4/4	0.90	0.31	38,57,69,69	0
2	ZN	E	1004	1/1	0.92	0.06	131,131,131,131	0
2	ZN	C	1006	1/1	0.92	0.20	118,118,118,118	0
2	ZN	B	1004	1/1	0.93	0.28	57,57,57,57	1
4	EDO	D	1013	4/4	0.94	0.14	42,52,63,63	0
2	ZN	D	1010	1/1	0.95	0.20	106,106,106,106	0
2	ZN	A	1002	1/1	0.95	0.04	84,84,84,84	0
2	ZN	D	1008	1/1	0.96	0.12	65,65,65,65	0
2	ZN	D	1007	1/1	0.96	0.06	62,62,62,62	0
2	ZN	A	1006	1/1	0.97	0.06	57,57,57,57	0
2	ZN	F	1004	1/1	0.97	0.04	59,59,59,59	0
2	ZN	D	1009	1/1	0.97	0.04	100,100,100,100	0
2	ZN	B	1006	1/1	0.97	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	1001	1/1	0.97	0.04	58,58,58,58	0
2	ZN	D	1001	1/1	0.97	0.03	79,79,79,79	0
2	ZN	A	1004	1/1	0.98	0.05	65,65,65,65	0
2	ZN	C	1001	1/1	0.98	0.07	63,63,63,63	0
2	ZN	D	1006	1/1	0.98	0.04	60,60,60,60	0
2	ZN	B	1002	1/1	0.98	0.03	58,58,58,58	0
2	ZN	F	1005	1/1	0.98	0.07	82,82,82,82	0
2	ZN	A	1003	1/1	0.98	0.07	37,37,37,37	0
2	ZN	C	1003	1/1	0.98	0.09	80,80,80,80	0
3	K	D	1011	1/1	0.98	0.18	35,35,35,35	0
2	ZN	F	1001	1/1	0.98	0.06	59,59,59,59	0
2	ZN	C	1002	1/1	0.98	0.06	49,49,49,49	0
2	ZN	F	1002	1/1	0.98	0.05	60,60,60,60	0
2	ZN	E	1001	1/1	0.99	0.06	67,67,67,67	0
2	ZN	D	1005	1/1	0.99	0.19	46,46,46,46	0
2	ZN	E	1003	1/1	0.99	0.05	46,46,46,46	0
3	K	A	1008	1/1	0.99	0.19	34,34,34,34	0
2	ZN	A	1005	1/1	0.99	0.10	32,32,32,32	0
2	ZN	B	1001	1/1	0.99	0.03	45,45,45,45	1
2	ZN	E	1002	1/1	0.99	0.04	57,57,57,57	0
2	ZN	B	1005	1/1	0.99	0.04	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.