



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:57 PM UTC

PDB ID : 5W6P / pdb_00005w6p
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 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:

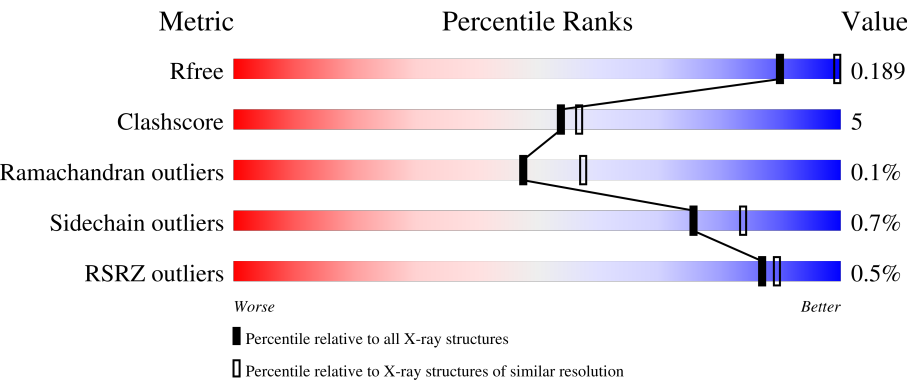
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.33 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}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 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	680	89%10%.
1	B	680	87%12%.
1	C	680	% 87%12%.
1	D	680	89%11%
1	E	680	89%11%.

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Mol	Chain	Length	Quality of chain
1	F	680	 89% 11%

2 Entry composition

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

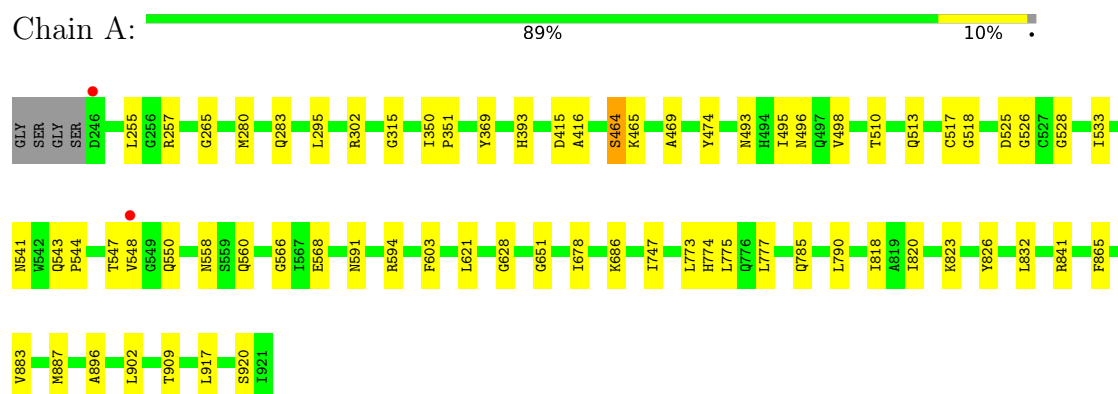
- Molecule 5 is water.

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

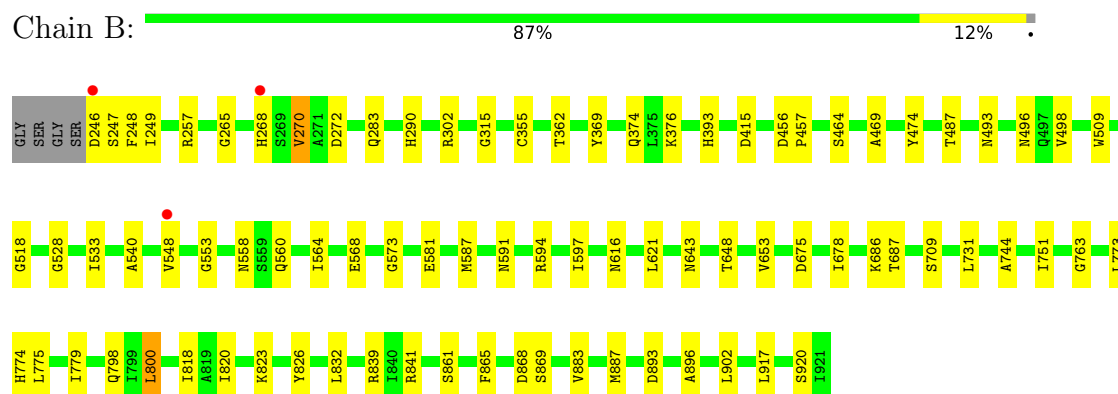
3 Residue-property plots [i](#)

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.

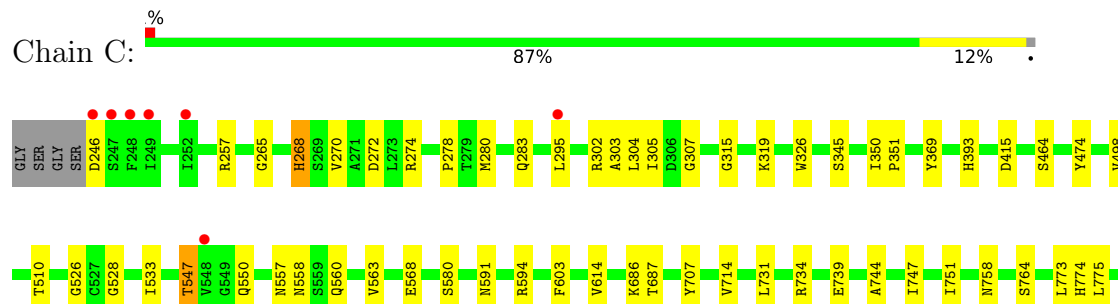
• Molecule 1: tailspike protein 2



• Molecule 1: tailspike protein 2



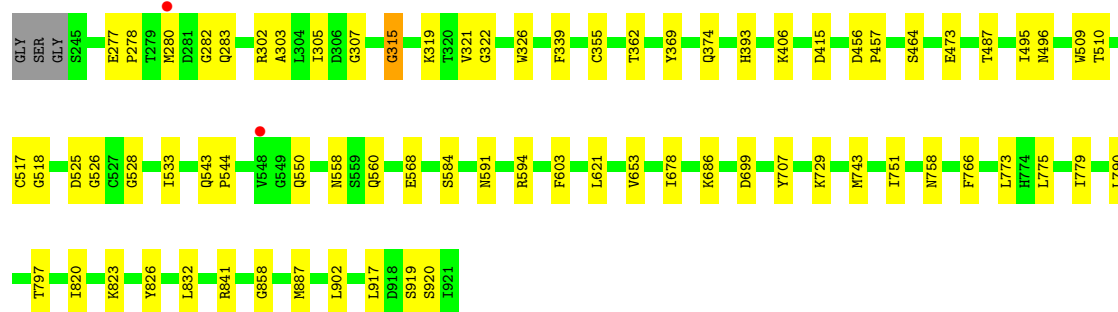
• Molecule 1: tailspike protein 2





- Molecule 1: tailspike protein 2

Chain D: 89% 11%



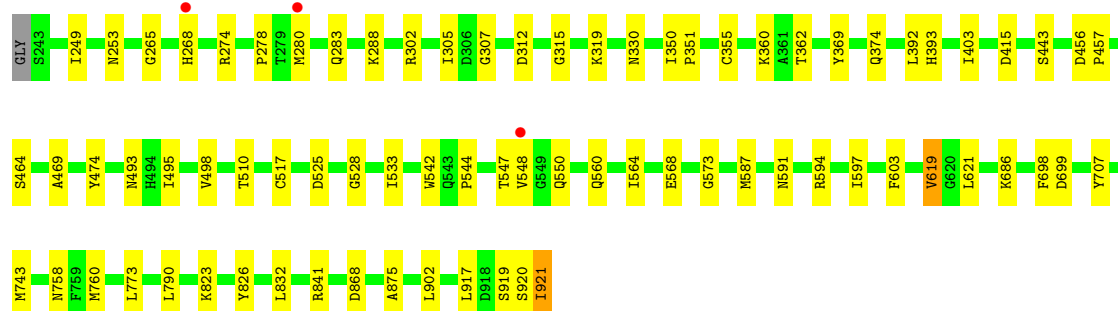
- Molecule 1: tailspike protein 2

Chain E: 89% 11%



- Molecule 1: tailspike protein 2

Chain F: 89% 11%



4 Data and refinement statistics

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 46.68 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.68-2.33) 99.1 (46.68-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_2666: ???)	Depositor
R, R_{free}	0.154 , 0.190 0.153 , 0.189	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 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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: 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	0.22	0/5150	0.44	0/7006
1	B	0.20	0/5159	0.43	0/7018
1	C	0.20	0/5150	0.43	0/7006
1	D	0.21	0/5165	0.44	0/7026
1	E	0.20	0/5150	0.44	0/7006
1	F	0.20	0/5166	0.43	0/7027
All	All	0.21	0/30940	0.43	0/42089

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5053	0	4909	42	0
1	B	5059	0	4917	57	0
1	C	5053	0	4909	63	0
1	D	5065	0	4922	48	0
1	E	5053	0	4910	50	0
1	F	5069	0	4922	55	0
2	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	11	0
5	C	319	0	0	7	0
5	D	339	0	0	8	1
5	E	330	0	0	10	0
5	F	317	0	0	9	0
All	All	32399	36	29525	292	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 (292) 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:E:887:MET:HE3	1:E:912:ILE:HG13	1.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:B:594:ARG:O	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:CG1	2.23	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:D:743:MET:HE3	1:D:820:ILE:HD11	1.74	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: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: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:D:773:LEU:C	1:D:773:LEU:HD23	2.28	0.58
1:C:547:THR:HG22	5:C:1177:HOH:O	2.03	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASP:CG	1:B:247:SER:H	2.12	0.57
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:HD12	1:B:249:ILE:H	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:E:887:MET:HG3	1:F:686:LYS:HA	1.91	0.53
1:E:887:MET:CE	1:E:912:ILE:HG13	2.32	0.53
1:F:875:ALA:HB1	5:F:1136:HOH:O	2.08	0.53
1:B:893:ASP:OD2	4:B:1007:EDO:O2	2.15	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:573:GLY:HA2	1:B:597:ILE:HG12	1.91	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:F:743:MET:HE2	1:F:760:MET:HB2	1.93	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:E:487:THR:HG1	1:E:509:TRP:CG	2.28	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: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:B:376:LYS:NZ	5:B:1108:HOH:O	2.44	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:B:773:LEU:C	1:B:773:LEU:HD23	2.37	0.50
1:F:917:LEU:HA	1:F:920:SER:O	2.12	0.50
1:C:773:LEU:HD23	1:C:773:LEU:C	2.37	0.49
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:F:773:LEU:C	1:F:773:LEU:HD23	2.39	0.48
1:A:469:ALA:HA	1:A:493:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:621:LEU:C	1:A:621:LEU:HD23	2.41	0.46
1:A:773:LEU:C	1:A:773:LEU:HD23	2.41	0.46
1:E:621:LEU:C	1:E:621:LEU:HD23	2.41	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:C:868:ASP:OD1	1:C:868:ASP:C	2.59	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:E:773:LEU:HD23	1:E:773:LEU:C	2.40	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: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:B:868:ASP:C	1:B:868:ASP:OD1	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:621:LEU:HD23	1:B:621:LEU:C	2.42	0.44
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
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:D:686:LYS:NZ	5:D:1117:HOH:O	2.50	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:HG	1:C:295:LEU:O	2.18	0.44
1:C:764:SER:HB3	1:C:869:SER:HG	1.83	0.44
1:D:307:GLY:O	1:D:319:LYS:NZ	2.49	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:F:456:ASP:CG	1:F:457:PRO:HD2	2.43	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:F:621:LEU:C	1:F:621:LEU:HD23	2.43	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:D:729:LYS:NZ	5:D:1122:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:621:LEU:HD23	1:D:621:LEU:C	2.43	0.43
1:B:751:ILE:HG23	1:B:779:ILE:HD13	2.01	0.43
1:B:456:ASP:CG	1:B:457:PRO:HD2	2.43	0.43
1:D:456:ASP:CG	1:D:457:PRO:HD2	2.44	0.42
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:487:THR:HG1	1:B:509:TRP:CG	2.38	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
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: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:A:651:GLY:HA2	1:C:614:VAL:HG11	2.01	0.41
1:A:823:LYS:HG2	1:A:826:TYR:HB3	2.01	0.41
1:A:350:ILE:HB	1:A:351:PRO:HD3	2.02	0.41
1:D:533:ILE:HG21	1:F:533:ILE:HG22	2.03	0.41
1:C:714:VAL:O	1:C:714:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:744:ALA:HA	1:C:818:ILE:O	2.21	0.41
1:E:487:THR:HG1	1:E:509:TRP:CD1	2.39	0.41
1:E:649:ILE:O	1:E:678:ILE:HA	2.20	0.41
1:F:369:TYR:HA	1:F:393:HIS:O	2.20	0.41
1:F:868:ASP:OD1	1:F:868:ASP:C	2.64	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:O	1:E:548:VAL:CG1	2.69	0.41
1:F:591:ASN:HA	1:F:619:VAL:HG12	2.03	0.41
1:D:487:THR:HG1	1:D:509:TRP:CG	2.38	0.40
1:B:548:VAL:HG13	1:B:548:VAL:O	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

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

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	674/680 (99%)	642 (95%)	31 (5%)	1 (0%)	48	57
1	B	675/680 (99%)	643 (95%)	31 (5%)	1 (0%)	48	57
1	C	674/680 (99%)	644 (96%)	29 (4%)	1 (0%)	48	57
1	D	676/680 (99%)	644 (95%)	31 (5%)	1 (0%)	48	57
1	E	674/680 (99%)	642 (95%)	31 (5%)	1 (0%)	48	57
1	F	677/680 (100%)	647 (96%)	29 (4%)	1 (0%)	48	57
All	All	4050/4080 (99%)	3862 (95%)	182 (4%)	6 (0%)	48	57

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

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%)	549 (99%)	5 (1%)	70	80
1	B	555/556 (100%)	552 (100%)	3 (0%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	554/556 (100%)	549 (99%)	5 (1%)	70	80
1	D	556/556 (100%)	554 (100%)	2 (0%)	84	89
1	E	554/556 (100%)	549 (99%)	5 (1%)	70	80
1	F	556/556 (100%)	552 (99%)	4 (1%)	76	84
All	All	3329/3336 (100%)	3305 (99%)	24 (1%)	76	84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LEU
1	A	464	SER
1	A	541	ASN
1	A	548	VAL
1	A	841	ARG
1	B	270	VAL
1	B	709	SER
1	B	800	LEU
1	C	268	HIS
1	C	270	VAL
1	C	345	SER
1	C	547	THR
1	C	841	ARG
1	D	321	VAL
1	D	841	ARG
1	E	268	HIS
1	E	548	VAL
1	E	594	ARG
1	E	697	THR
1	E	841	ARG
1	F	548	VAL
1	F	619	VAL
1	F	841	ARG
1	F	921	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	A	268	HIS
1	A	511	ASN

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Mol	Chain	Res	Type
1	A	776	GLN
1	B	372	ASN
1	B	425	GLN
1	B	570	GLN
1	B	593	ASN
1	B	776	GLN
1	B	806	ASN
1	C	513	GLN
1	C	557	ASN
1	C	558	ASN
1	C	570	GLN
1	C	593	ASN
1	C	690	GLN
1	C	776	GLN
1	D	570	GLN
1	D	593	ASN
1	D	598	ASN
1	D	670	ASN
1	D	690	GLN
1	D	776	GLN
1	E	374	GLN
1	E	425	GLN
1	E	616	ASN
1	E	670	ASN
1	E	690	GLN
1	E	758	ASN
1	E	776	GLN
1	F	425	GLN
1	F	515	ASN
1	F	541	ASN
1	F	570	GLN
1	F	593	ASN
1	F	690	GLN
1	F	776	GLN
1	F	806	ASN
1	F	904	ASN

5.3.3 RNA ⓘ

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 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	1012	-	3,3,3	0.51	0	2,2,2	0.32	0
4	EDO	E	1006	-	3,3,3	0.51	0	2,2,2	0.44	0
4	EDO	B	1007	-	3,3,3	0.44	0	2,2,2	0.31	0
4	EDO	C	1007	-	3,3,3	0.48	0	2,2,2	0.38	0
4	EDO	D	1013	-	3,3,3	0.53	0	2,2,2	0.33	0
4	EDO	A	1009	-	3,3,3	0.46	0	2,2,2	0.43	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	1012	-	-	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	-
4	EDO	D	1013	-	-	1/1/1/1	-
4	EDO	A	1009	-	-	0/1/1/1	-

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	1012	EDO	O1-C1-C2-O2
4	D	1013	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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(Å²)	Q<0.9	
1	A	676/680 (99%)	-0.65	2 (0%)	90	91	26, 37, 54, 122	0
1	B	676/680 (99%)	-0.58	3 (0%)	88	90	25, 39, 64, 125	1 (0%)
1	C	676/680 (99%)	-0.56	7 (1%)	79	82	25, 38, 69, 123	0
1	D	677/680 (99%)	-0.58	2 (0%)	90	91	22, 38, 60, 98	1 (0%)
1	E	676/680 (99%)	-0.57	2 (0%)	90	91	28, 39, 56, 94	0
1	F	679/680 (99%)	-0.47	3 (0%)	88	90	30, 41, 65, 113	0
All	All	4060/4080 (99%)	-0.57	19 (0%)	87	89	22, 39, 62, 125	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	246	ASP	4.9
1	D	548	VAL	4.0
1	E	548	VAL	3.6
1	B	246	ASP	3.3
1	B	548	VAL	3.2
1	C	548	VAL	3.2
1	F	268	HIS	3.2
1	C	295	LEU	3.1
1	E	246	ASP	3.0
1	D	280	MET	2.9
1	A	246	ASP	2.6
1	A	548	VAL	2.6
1	C	249	ILE	2.4
1	C	248	PHE	2.3
1	F	548	VAL	2.3
1	F	280	MET	2.1
1	B	268	HIS	2.1
1	C	252	ILE	2.1
1	C	247	SER	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
4	EDO	E	1006	4/4	0.71	0.18	53,63,71,71	0
2	ZN	D	1003	1/1	0.73	0.14	134,134,134,134	0
4	EDO	A	1009	4/4	0.74	0.17	53,64,69,69	0
4	EDO	D	1012	4/4	0.75	0.14	44,53,61,61	0
4	EDO	C	1007	4/4	0.75	0.22	47,56,67,67	0
2	ZN	C	1005	1/1	0.80	0.12	134,134,134,134	0
4	EDO	D	1013	4/4	0.80	0.16	42,52,63,63	0
2	ZN	D	1004	1/1	0.80	0.13	72,72,72,72	1
2	ZN	B	1003	1/1	0.81	0.11	135,135,135,135	0
2	ZN	F	1003	1/1	0.82	0.10	125,125,125,125	0
2	ZN	D	1002	1/1	0.84	0.11	135,135,135,135	0
2	ZN	C	1004	1/1	0.85	0.09	153,153,153,153	0
2	ZN	F	1006	1/1	0.86	0.12	117,117,117,117	0
2	ZN	E	1004	1/1	0.88	0.09	131,131,131,131	0
4	EDO	B	1007	4/4	0.88	0.12	38,57,69,69	0
2	ZN	A	1007	1/1	0.89	0.09	89,89,89,89	0
2	ZN	E	1005	1/1	0.91	0.08	117,117,117,117	0
2	ZN	D	1010	1/1	0.93	0.10	106,106,106,106	0
2	ZN	C	1006	1/1	0.94	0.09	118,118,118,118	0
2	ZN	B	1006	1/1	0.95	0.09	74,74,74,74	0
2	ZN	A	1002	1/1	0.95	0.10	84,84,84,84	0
2	ZN	A	1006	1/1	0.95	0.05	57,57,57,57	0
2	ZN	B	1004	1/1	0.96	0.24	57,57,57,57	1
2	ZN	D	1007	1/1	0.97	0.06	62,62,62,62	0
3	K	D	1011	1/1	0.97	0.08	35,35,35,35	0
2	ZN	D	1009	1/1	0.97	0.05	100,100,100,100	0
2	ZN	D	1001	1/1	0.97	0.05	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	1001	1/1	0.98	0.04	58,58,58,58	0
2	ZN	E	1001	1/1	0.98	0.06	67,67,67,67	0
2	ZN	C	1001	1/1	0.98	0.05	63,63,63,63	0
2	ZN	C	1003	1/1	0.98	0.07	80,80,80,80	0
2	ZN	F	1001	1/1	0.98	0.04	59,59,59,59	0
2	ZN	A	1004	1/1	0.98	0.05	65,65,65,65	0
2	ZN	F	1004	1/1	0.98	0.04	59,59,59,59	0
2	ZN	F	1005	1/1	0.98	0.06	82,82,82,82	0
2	ZN	A	1003	1/1	0.99	0.03	37,37,37,37	0
2	ZN	D	1008	1/1	0.99	0.09	65,65,65,65	0
2	ZN	C	1002	1/1	0.99	0.03	49,49,49,49	0
2	ZN	B	1001	1/1	0.99	0.02	45,45,45,45	1
3	K	A	1008	1/1	0.99	0.04	34,34,34,34	0
2	ZN	B	1005	1/1	0.99	0.03	62,62,62,62	0
2	ZN	E	1002	1/1	0.99	0.03	57,57,57,57	0
2	ZN	E	1003	1/1	0.99	0.03	46,46,46,46	0
2	ZN	B	1002	1/1	0.99	0.03	58,58,58,58	0
2	ZN	D	1005	1/1	0.99	0.07	46,46,46,46	0
2	ZN	D	1006	1/1	0.99	0.03	60,60,60,60	0
2	ZN	F	1002	1/1	0.99	0.03	60,60,60,60	0
2	ZN	A	1005	1/1	1.00	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.