



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 10:18 pm GMT

PDB ID : 1OLP
Title : Alpha Toxin from Clostridium Absonum
Authors : Briggs, D.C.; Basak, A.K.
Deposited on : 2003-08-11
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

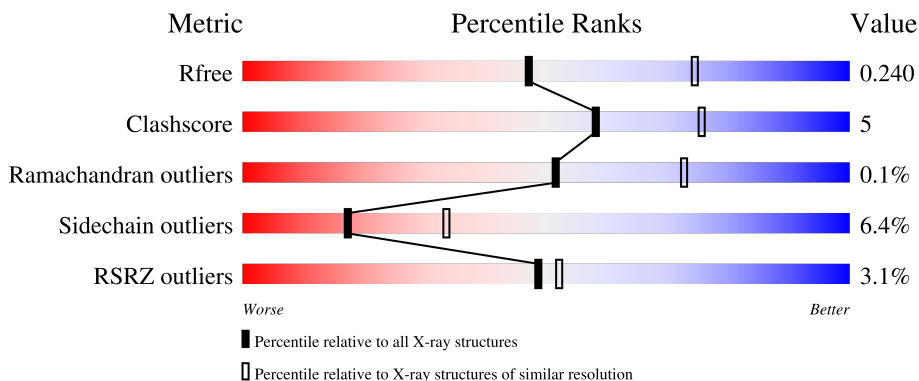
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	 2% 84% 13% .
1	B	370	 % 86% 13% .
1	C	370	 6% 83% 16% .
1	D	370	 3% 79% 17% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12292 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 ALPHA-TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	Total 3014	C 1910	N 498	O 600	S 6	0	0	0
1	B	370	Total 2976	C 1887	N 490	O 593	S 6	0	0	0
1	C	370	Total 2968	C 1884	N 485	O 593	S 6	0	0	0
1	D	365	Total 2952	C 1870	N 484	O 592	S 6	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ca 2	0	0
2	B	2	Total 2	Ca 2	0	0
2	C	2	Total 2	Ca 2	0	0
2	D	2	Total 2	Ca 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Zn 3	0	0
3	B	3	Total 3	Zn 3	0	0
3	C	3	Total 3	Zn 3	0	0
3	D	3	Total 3	Zn 3	0	0

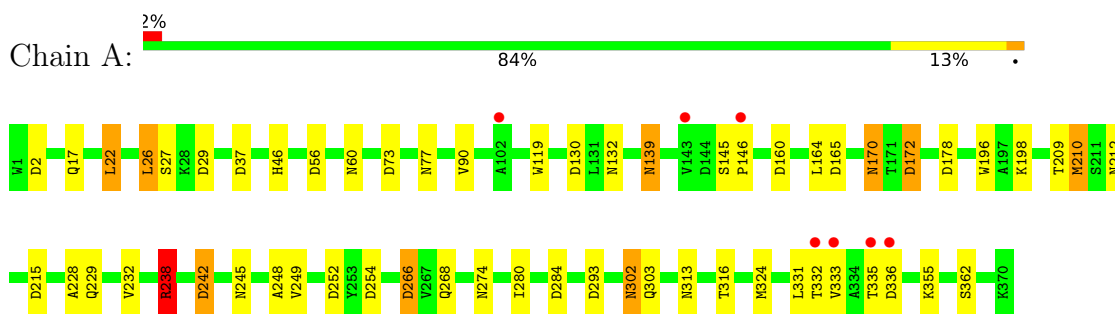
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total 125	O 125	0	0
4	B	104	Total 104	O 104	0	0
4	C	52	Total 52	O 52	0	0
4	D	81	Total 81	O 81	0	0

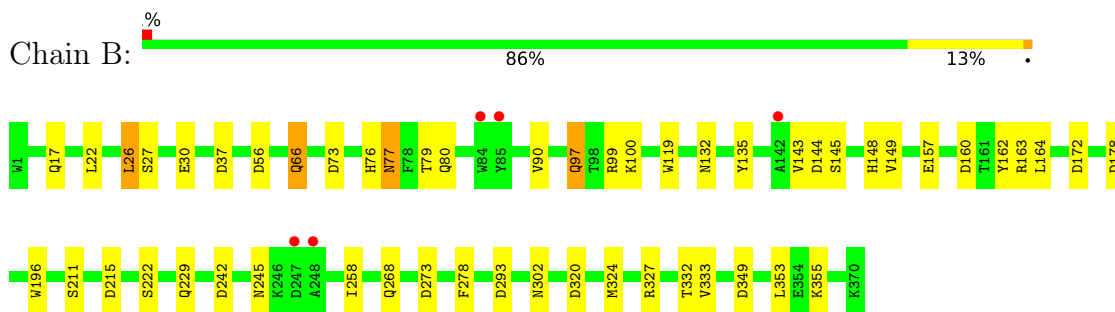
3 Residue-property plots [i](#)

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.

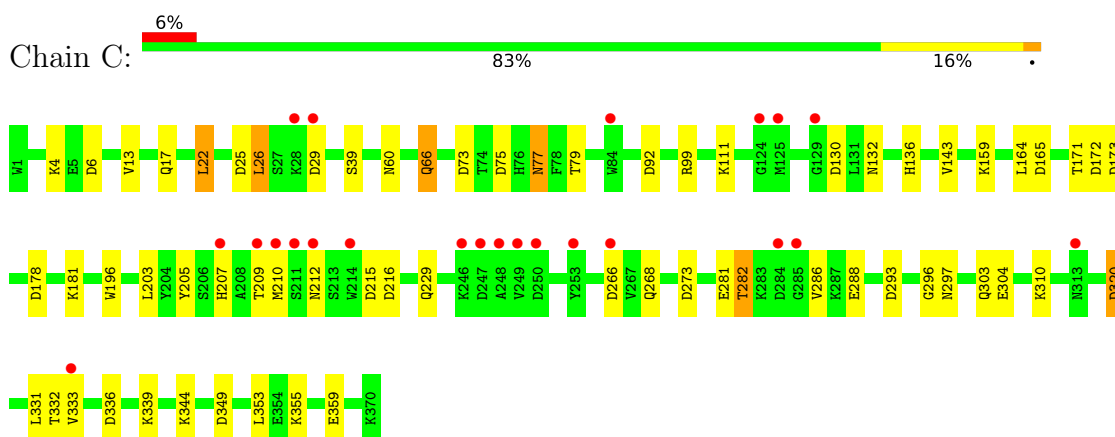
- Molecule 1: ALPHA-TOXIN



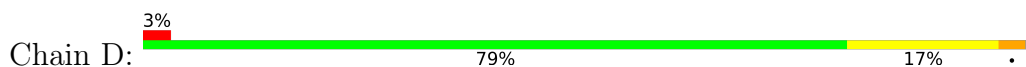
- Molecule 1: ALPHA-TOXIN

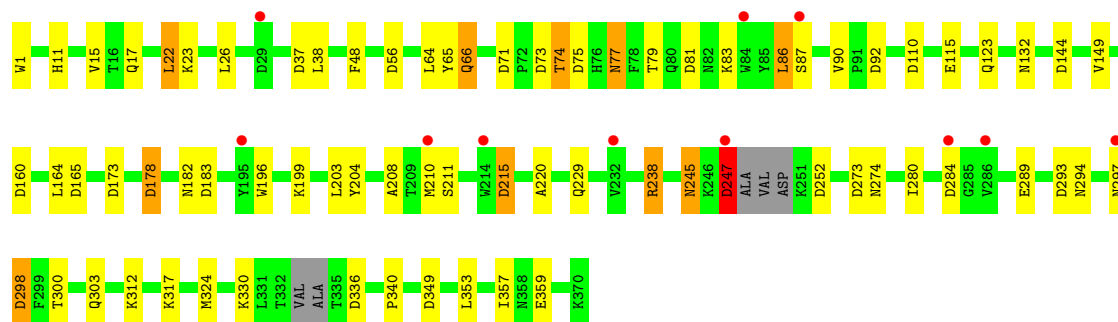


- Molecule 1: ALPHA-TOXIN



- Molecule 1: ALPHA-TOXIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.96Å 193.59Å 92.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.50 29.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.75-2.50) 95.7 (29.71-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.178 , 0.237 0.185 , 0.240	Depositor DCC
R_{free} test set	2840 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtrriage
Anisotropy	0.096	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.020 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: CA, ZN

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	0.53	0/3097	0.82	18/4207 (0.4%)
1	B	0.50	0/3059	0.79	12/4163 (0.3%)
1	C	0.48	0/3051	0.81	18/4154 (0.4%)
1	D	0.48	0/3033	0.83	19/4125 (0.5%)
All	All	0.50	0/12240	0.81	67/16649 (0.4%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	293	ASP	CB-CG-OD1	7.26	124.84	118.30
1	D	215	ASP	CB-CG-OD1	7.22	124.80	118.30
1	C	165	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	178	ASP	CB-CG-OD1	7.04	124.64	118.30
1	D	173	ASP	CB-CG-OD2	7.00	124.60	118.30
1	C	336	ASP	CB-CG-OD1	6.73	124.35	118.30
1	A	238	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	C	75	ASP	CB-CG-OD1	6.56	124.20	118.30
1	D	284	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	293	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	349	ASP	CB-CG-OD1	6.30	123.97	118.30
1	D	75	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C	178	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	29	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	172	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	215	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	183	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	92	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	144	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	238	ARG	NE-CZ-NH1	6.09	123.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	ASP	CB-CG-OD2	6.05	123.75	118.30
1	C	349	ASP	CB-CG-OD1	6.03	123.72	118.30
1	D	178	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	165	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	92	ASP	CB-CG-OD1	5.89	123.61	118.30
1	D	247	ASP	CB-CG-OD2	5.86	123.58	118.30
1	D	349	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	29	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	293	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	266	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	6	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	37	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	273	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	298	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	130	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	172	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	215	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	73	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	178	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	215	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	254	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	242	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	25	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	320	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	73	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	56	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	216	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	165	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	110	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	284	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	273	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	37	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	73	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	273	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	173	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	242	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	293	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	172	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	56	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	252	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	144	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	73	ASP	CB-CG-OD2	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	320	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	160	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	56	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	37	ASP	CB-CG-OD2	5.03	122.82	118.30

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	3014	0	2797	23	0
1	B	2976	0	2712	23	0
1	C	2968	0	2691	31	0
1	D	2952	0	2685	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	125	0	0	1	0
4	B	104	0	0	2	0
4	C	52	0	0	0	0
4	D	81	0	0	3	0
All	All	12292	0	10885	110	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 5.

All (110) 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:66:GLN:H	1:B:66:GLN:HE21	1.10	0.97
1:C:66:GLN:H	1:C:66:GLN:HE21	1.29	0.80
1:D:74:THR:HG21	1:D:81:ASP:OD2	1.84	0.77
1:A:22:LEU:HD22	1:A:26:LEU:HD13	1.68	0.74
1:D:164:LEU:H	1:D:229:GLN:HE22	1.38	0.71
1:D:65:TYR:CZ	4:D:2016:HOH:O	2.43	0.70
1:B:135:TYR:HB2	4:B:2047:HOH:O	1.93	0.68
1:C:207:HIS:HE2	1:D:297:ASN:HA	1.59	0.68
1:D:77:ASN:HD22	1:D:79:THR:H	1.42	0.67
1:D:66:GLN:HE21	1:D:66:GLN:H	1.44	0.66
1:A:170:ASN:HD22	1:A:170:ASN:C	2.01	0.63
1:C:207:HIS:NE2	1:D:297:ASN:HA	2.14	0.63
1:A:274:ASN:ND2	1:A:336:ASP:OD1	2.34	0.60
1:C:164:LEU:H	1:C:229:GLN:HE22	1.48	0.60
1:A:209:THR:HB	1:A:212:ASN:HD22	1.66	0.60
1:B:164:LEU:H	1:B:229:GLN:HE22	1.48	0.59
1:C:26:LEU:HD12	1:C:171:THR:HG21	1.83	0.58
1:B:324:MET:CE	1:B:353:LEU:HD13	2.35	0.57
1:A:46:HIS:CD2	4:A:2017:HOH:O	2.58	0.57
1:A:164:LEU:H	1:A:229:GLN:HE22	1.52	0.57
1:B:77:ASN:HD22	1:B:79:THR:H	1.52	0.57
1:A:170:ASN:HD22	1:A:172:ASP:H	1.52	0.56
1:D:64:LEU:H	1:D:66:GLN:HE22	1.51	0.56
1:D:65:TYR:CE2	4:D:2016:HOH:O	2.59	0.56
1:A:170:ASN:ND2	1:A:172:ASP:H	2.04	0.56
1:B:66:GLN:H	1:B:66:GLN:NE2	1.93	0.55
1:C:207:HIS:HE1	1:D:297:ASN:CB	2.20	0.54
1:C:207:HIS:CE1	1:D:297:ASN:HB3	2.42	0.54
1:C:207:HIS:CE1	1:D:297:ASN:HA	2.42	0.54
1:D:280:ILE:HG22	1:D:324:MET:HG2	1.90	0.54
1:B:97:GLN:HA	1:B:97:GLN:HE21	1.72	0.54
1:D:17:GLN:HB3	1:D:229:GLN:HE21	1.73	0.54
1:C:207:HIS:HE1	1:D:297:ASN:HB3	1.73	0.54
1:A:228:ALA:O	1:A:232:VAL:HG23	2.08	0.53
1:A:17:GLN:HB3	1:A:229:GLN:HE21	1.74	0.53
1:B:17:GLN:NE2	1:B:163:ARG:HE	2.06	0.53
1:C:77:ASN:C	1:C:77:ASN:HD22	2.12	0.53
1:D:83:LYS:HA	1:D:86:LEU:HD22	1.91	0.52
1:A:245:ASN:ND2	1:A:248:ALA:HB2	2.25	0.52
1:D:1:TRP:HB2	1:D:11:HIS:CD2	2.45	0.52
1:A:146:PRO:HD2	1:A:210:MET:SD	2.50	0.52
1:D:132:ASN:HD21	1:D:196:TRP:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLN:NE2	1:D:164:LEU:O	2.43	0.51
1:C:132:ASN:HD21	1:C:196:TRP:HB3	1.75	0.51
1:B:132:ASN:HD21	1:B:196:TRP:HB3	1.76	0.50
1:C:332:THR:HG22	1:C:333:VAL:N	2.27	0.50
1:A:170:ASN:HD21	1:A:172:ASP:HB2	1.76	0.50
1:C:13:VAL:HG21	1:C:159:LYS:HD2	1.93	0.50
1:C:22:LEU:HD22	1:C:26:LEU:HD13	1.94	0.50
1:C:17:GLN:NE2	1:C:164:LEU:O	2.45	0.50
1:A:245:ASN:HD22	1:A:248:ALA:HB2	1.77	0.49
1:B:148:HIS:CD2	4:B:2047:HOH:O	2.65	0.49
1:D:252:ASP:OD2	1:D:317:LYS:HB3	2.13	0.49
1:C:17:GLN:HB3	1:C:229:GLN:HE21	1.78	0.48
1:B:66:GLN:HE21	1:B:66:GLN:N	1.93	0.48
1:A:280:ILE:HG22	1:A:324:MET:HG2	1.96	0.48
1:C:77:ASN:HD22	1:C:79:THR:H	1.60	0.48
1:A:238:ARG:HD2	1:A:242:ASP:OD2	2.14	0.47
1:C:207:HIS:CE1	1:D:297:ASN:CB	2.97	0.47
1:B:76:HIS:HB3	1:B:80:GLN:HB2	1.96	0.47
1:B:332:THR:HG22	1:B:333:VAL:H	1.79	0.47
1:C:164:LEU:H	1:C:229:GLN:NE2	2.13	0.47
1:D:74:THR:CG2	1:D:81:ASP:OD2	2.60	0.47
1:D:123:GLN:NE2	4:D:2036:HOH:O	2.47	0.47
1:A:268:GLN:NE2	1:B:119:TRP:HE1	2.13	0.46
1:A:60:ASN:HD21	1:A:303:GLN:HA	1.80	0.46
1:C:60:ASN:ND2	1:C:304:GLU:H	2.14	0.46
1:D:203:LEU:HD12	1:D:220:ALA:HA	1.98	0.46
1:D:245:ASN:HD22	1:D:247:ASP:H	1.64	0.46
1:D:77:ASN:ND2	1:D:79:THR:H	2.13	0.46
1:D:164:LEU:H	1:D:229:GLN:NE2	2.09	0.46
1:D:15:VAL:HB	1:D:48:PHE:CE2	2.52	0.45
1:C:26:LEU:CD1	1:C:171:THR:HG21	2.46	0.45
1:D:340:PRO:HG2	1:D:357:ILE:HG21	1.99	0.45
1:D:204:TYR:HA	1:D:208:ALA:HB3	1.99	0.45
1:D:17:GLN:CB	1:D:229:GLN:HE21	2.30	0.45
1:D:199:LYS:O	1:D:203:LEU:HD23	2.17	0.45
1:C:60:ASN:HD21	1:C:303:GLN:HA	1.81	0.44
1:C:282:THR:HA	1:C:320:ASP:O	2.16	0.44
1:D:71:ASP:HB3	1:D:74:THR:CG2	2.48	0.44
1:D:182:ASN:O	1:D:238:ARG:NH2	2.51	0.43
1:A:313:ASN:ND2	1:A:316:THR:OG1	2.52	0.43
1:B:162:TYR:CE1	1:B:222:SER:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HD21	1:A:196:TRP:HB3	1.84	0.42
1:C:130:ASP:O	1:C:136:HIS:HB2	2.20	0.42
1:D:71:ASP:CG	1:D:74:THR:HG22	2.40	0.42
1:C:205:TYR:CD2	1:D:87:SER:HB3	2.54	0.42
1:D:297:ASN:O	1:D:300:THR:HG23	2.19	0.42
1:D:22:LEU:HD22	1:D:26:LEU:HD13	2.01	0.42
1:D:245:ASN:HD22	1:D:247:ASP:N	2.17	0.42
1:B:77:ASN:ND2	1:B:79:THR:OG1	2.52	0.42
1:B:258:ILE:HD11	1:B:278:PHE:CE1	2.55	0.42
1:C:26:LEU:HD12	1:C:26:LEU:HA	1.96	0.41
1:C:77:ASN:C	1:C:77:ASN:ND2	2.74	0.41
1:D:1:TRP:HB2	1:D:11:HIS:NE2	2.35	0.41
1:B:164:LEU:H	1:B:229:GLN:NE2	2.15	0.41
1:D:132:ASN:ND2	1:D:196:TRP:HB3	2.35	0.41
1:C:203:LEU:O	1:C:207:HIS:HB2	2.20	0.41
1:C:344:LYS:HA	1:C:353:LEU:O	2.20	0.41
1:D:274:ASN:ND2	1:D:336:ASP:OD1	2.40	0.41
1:B:211:SER:HA	1:C:296:GLY:HA2	2.03	0.41
1:A:266:ASP:HB2	1:A:302:ASN:ND2	2.36	0.41
1:D:22:LEU:HD13	1:D:38:LEU:HD22	2.03	0.41
1:B:97:GLN:HE22	1:B:100:LYS:NZ	2.19	0.40
1:A:119:TRP:HE1	1:B:268:GLN:NE2	2.19	0.40
1:A:139:ASN:HD22	1:A:139:ASN:HA	1.66	0.40
1:D:298:ASP:HA	1:D:303:GLN:HE22	1.86	0.40
1:B:26:LEU:HD12	1:B:30:GLU:HG3	2.02	0.40
1:B:149:VAL:CG2	1:C:143:VAL:HG22	2.52	0.40
1:D:77:ASN:ND2	1:D:79:THR:OG1	2.53	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	368/370 (100%)	363 (99%)	5 (1%)	0	100	100
1	B	368/370 (100%)	357 (97%)	11 (3%)	0	100	100
1	C	368/370 (100%)	358 (97%)	9 (2%)	1 (0%)	41	61
1	D	359/370 (97%)	347 (97%)	11 (3%)	1 (0%)	41	61
All	All	1463/1480 (99%)	1425 (97%)	36 (2%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	286	VAL
1	D	294	ASN

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	316/319 (99%)	296 (94%)	20 (6%)	18	34
1	B	304/319 (95%)	288 (95%)	16 (5%)	22	43
1	C	301/319 (94%)	279 (93%)	22 (7%)	14	27
1	D	305/319 (96%)	284 (93%)	21 (7%)	15	30
All	All	1226/1276 (96%)	1147 (94%)	79 (6%)	17	33

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	22	LEU
1	A	26	LEU
1	A	27	SER
1	A	77	ASN
1	A	90	VAL
1	A	139	ASN
1	A	145	SER
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	198	LYS
1	A	210	MET
1	A	238	ARG
1	A	249	VAL
1	A	302	ASN
1	A	331	LEU
1	A	332	THR
1	A	333	VAL
1	A	335	THR
1	A	355	LYS
1	A	362	SER
1	B	22	LEU
1	B	26	LEU
1	B	27	SER
1	B	66	GLN
1	B	77	ASN
1	B	90	VAL
1	B	97	GLN
1	B	99	ARG
1	B	143	VAL
1	B	145	SER
1	B	157	GLU
1	B	160	ASP
1	B	245	ASN
1	B	302	ASN
1	B	327	ARG
1	B	355	LYS
1	C	4	LYS
1	C	22	LEU
1	C	26	LEU
1	C	39	SER
1	C	66	GLN
1	C	77	ASN
1	C	99	ARG
1	C	111	LYS
1	C	181	LYS
1	C	209	THR
1	C	210	MET
1	C	212	ASN
1	C	268	GLN
1	C	281	GLU
1	C	282	THR

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Mol	Chain	Res	Type
1	C	288	GLU
1	C	297	ASN
1	C	310	LYS
1	C	331	LEU
1	C	339	LYS
1	C	355	LYS
1	C	359	GLU
1	D	22	LEU
1	D	23	LYS
1	D	66	GLN
1	D	74	THR
1	D	77	ASN
1	D	86	LEU
1	D	90	VAL
1	D	115	GLU
1	D	149	VAL
1	D	178	ASP
1	D	210	MET
1	D	211	SER
1	D	215	ASP
1	D	238	ARG
1	D	245	ASN
1	D	247	ASP
1	D	289	GLU
1	D	312	LYS
1	D	330	LYS
1	D	353	LEU
1	D	359	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	77	ASN
1	A	132	ASN
1	A	139	ASN
1	A	170	ASN
1	A	186	ASN
1	A	212	ASN
1	A	229	GLN
1	A	245	ASN
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	302	ASN
1	A	313	ASN
1	B	17	GLN
1	B	60	ASN
1	B	66	GLN
1	B	77	ASN
1	B	97	GLN
1	B	123	GLN
1	B	132	ASN
1	B	186	ASN
1	B	212	ASN
1	B	227	ASN
1	B	229	GLN
1	B	268	GLN
1	B	302	ASN
1	C	60	ASN
1	C	66	GLN
1	C	77	ASN
1	C	123	GLN
1	C	132	ASN
1	C	139	ASN
1	C	186	ASN
1	C	229	GLN
1	C	297	ASN
1	C	302	ASN
1	C	303	GLN
1	D	49	GLN
1	D	60	ASN
1	D	66	GLN
1	D	77	ASN
1	D	123	GLN
1	D	132	ASN
1	D	186	ASN
1	D	212	ASN
1	D	229	GLN
1	D	245	ASN
1	D	303	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	370/370 (100%)	-0.18	7 (1%) 66 69	18, 28, 44, 56	0
1	B	370/370 (100%)	-0.10	5 (1%) 75 77	18, 31, 49, 66	0
1	C	370/370 (100%)	0.22	23 (6%) 20 21	25, 38, 59, 76	0
1	D	365/370 (98%)	0.08	11 (3%) 50 53	22, 37, 57, 67	0
All	All	1475/1480 (99%)	0.01	46 (3%) 49 52	18, 33, 55, 76	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	ALA	4.6
1	C	247	ASP	4.6
1	C	249	VAL	4.2
1	D	297	ASN	3.7
1	D	247	ASP	3.7
1	A	335	THR	3.6
1	C	212	ASN	3.4
1	B	248	ALA	3.3
1	D	29	ASP	3.3
1	B	84	TRP	3.2
1	C	246	LYS	3.2
1	B	247	ASP	3.2
1	D	84	TRP	3.0
1	D	210	MET	2.9
1	A	143	VAL	2.9
1	D	214	TRP	2.9
1	D	87	SER	2.8
1	A	333	VAL	2.8
1	C	250	ASP	2.8
1	C	207	HIS	2.8
1	C	333	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	210	MET	2.7
1	C	124	GLY	2.7
1	A	332	THR	2.7
1	C	253	TYR	2.6
1	C	129	GLY	2.5
1	C	285	GLY	2.5
1	C	211	SER	2.5
1	B	85	TYR	2.5
1	C	214	TRP	2.4
1	C	125	MET	2.4
1	C	28	LYS	2.4
1	B	142	ALA	2.4
1	C	84	TRP	2.3
1	A	336	ASP	2.2
1	C	209	THR	2.2
1	A	146	PRO	2.2
1	C	313	ASN	2.2
1	D	286	VAL	2.2
1	C	29	ASP	2.2
1	D	195	TYR	2.1
1	D	232	VAL	2.1
1	C	266	ASP	2.1
1	C	284	ASP	2.1
1	D	284	ASP	2.0
1	A	102	ALA	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, 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(\AA^2)	Q<0.9
2	CA	D	1371	1/1	0.71	0.16	69,69,69,69	0
2	CA	D	1372	1/1	0.86	0.19	83,83,83,83	0
2	CA	A	1372	1/1	0.89	0.20	69,69,69,69	0
2	CA	B	1371	1/1	0.92	0.09	67,67,67,67	0
2	CA	C	1372	1/1	0.92	0.19	77,77,77,77	0
2	CA	C	1371	1/1	0.94	0.06	80,80,80,80	0
2	CA	A	1371	1/1	0.96	0.18	51,51,51,51	0
3	ZN	B	1374	1/1	0.97	0.07	46,46,46,46	0
3	ZN	A	1374	1/1	0.98	0.06	43,43,43,43	0
2	CA	B	1372	1/1	0.98	0.15	52,52,52,52	0
3	ZN	C	1373	1/1	0.98	0.15	29,29,29,29	0
3	ZN	C	1375	1/1	0.98	0.15	32,32,32,32	0
3	ZN	D	1375	1/1	0.98	0.14	28,28,28,28	0
3	ZN	B	1375	1/1	0.99	0.12	26,26,26,26	0
3	ZN	A	1375	1/1	0.99	0.16	23,23,23,23	0
3	ZN	C	1374	1/1	0.99	0.13	36,36,36,36	0
3	ZN	B	1373	1/1	0.99	0.11	23,23,23,23	0
3	ZN	D	1373	1/1	0.99	0.13	27,27,27,27	0
3	ZN	A	1373	1/1	0.99	0.11	24,24,24,24	0
3	ZN	D	1374	1/1	1.00	0.11	29,29,29,29	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.