



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 11:25 AM EST

PDB ID : 1ACC
Title : ANTHRAX PROTECTIVE ANTIGEN
Authors : Petosa, C.; Liddington, R.C.
Deposited on : 1997-02-05
Resolution : 2.10 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

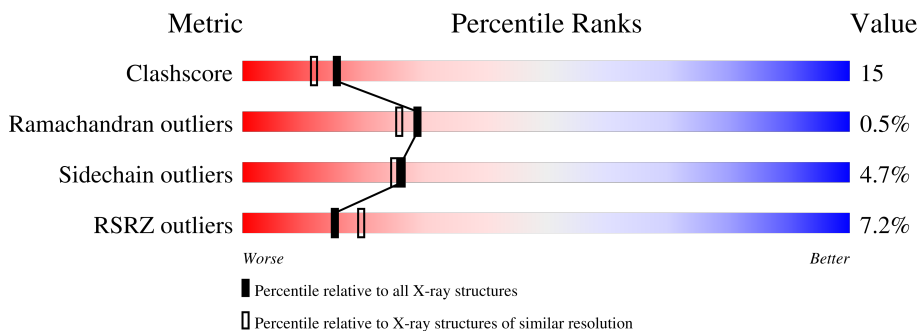
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	735	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5672 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 ANTHRAX PROTECTIVE ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	665	5282	3317	898	1060	7	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	388	Total	O	0	0
			388	388		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.30Å 93.70Å 82.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10 19.63 – 1.89	Depositor EDS
% Data completeness (in resolution range)	93.4 (6.00-2.10) 92.2 (19.63-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 1.89Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.223 , 0.296 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5672	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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	0.37	0/5371	0.72	0/7271

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	712	GLU	Mainchain

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	5282	0	5223	155	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	388	0	0	22	0
All	All	5672	0	5223	155	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 15.

All (155) 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:A:409:ASN:HD22	1:A:410:TYR:H	0.98	0.92
1:A:326:ASN:HD21	1:A:504:ARG:HH21	1.20	0.87
1:A:352:LEU:HD12	1:A:356:ASP:HB2	1.59	0.84
1:A:352:LEU:CD1	1:A:356:ASP:HB2	2.09	0.82
1:A:240:THR:HG21	1:A:242:ARG:HH11	1.44	0.82
1:A:298:THR:OG1	1:A:601:ASN:HB3	1.78	0.82
1:A:199:LYS:HG3	1:A:200:ARG:HG3	1.62	0.82
1:A:326:ASN:ND2	1:A:504:ARG:HH21	1.81	0.79
1:A:253:HIS:HD2	1:A:255:LEU:H	1.29	0.78
1:A:231:ASP:HB2	1:A:232:PRO:HD2	1.66	0.75
1:A:409:ASN:HD22	1:A:410:TYR:N	1.79	0.74
1:A:76:GLU:HB3	1:A:105:LYS:HD3	1.71	0.72
1:A:710:PRO:HG3	1:A:716:THR:HG22	1.72	0.71
1:A:17:GLN:O	1:A:39:THR:HA	1.90	0.71
1:A:409:ASN:ND2	1:A:410:TYR:H	1.82	0.70
1:A:629:LEU:HD12	1:A:631:ILE:HD11	1.72	0.70
1:A:404:ILE:HG12	3:A:1136:HOH:O	1.91	0.69
1:A:263:HIS:HE1	3:A:920:HOH:O	1.76	0.69
1:A:361:ASN:HD21	1:A:422:ASN:H	1.42	0.67
1:A:643:ILE:HD12	1:A:723:LYS:HD3	1.76	0.67
1:A:633:LYS:HE3	3:A:1162:HOH:O	1.94	0.67
1:A:357:THR:CG2	1:A:433:THR:HG23	2.24	0.66
1:A:326:ASN:HD21	1:A:504:ARG:NH2	1.91	0.66
1:A:263:HIS:HD2	3:A:867:HOH:O	1.78	0.65
1:A:691:ASN:ND2	1:A:692:PRO:HD2	2.13	0.64
1:A:69:ILE:HG12	1:A:116:ILE:HD11	1.80	0.63
1:A:352:LEU:HG	1:A:436:TYR:HD1	1.62	0.63
1:A:244:ASP:HB3	1:A:247:VAL:HG23	1.82	0.62
1:A:357:THR:HG23	1:A:433:THR:HG23	1.81	0.61
1:A:70:LYS:HB3	1:A:113:LEU:HD23	1.81	0.61
1:A:226:TRP:CE2	1:A:234:SER:HB3	2.36	0.60
1:A:341:ALA:HB2	3:A:878:HOH:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:O	1:A:153:LEU:HD12	2.01	0.60
1:A:159:LYS:HD2	1:A:180:ASN:HB2	1.84	0.60
1:A:271:LEU:HD23	1:A:439:PHE:HE1	1.69	0.58
1:A:449:ARG:HD2	1:A:451:ASP:OD1	2.04	0.57
1:A:98:ASN:O	1:A:98:ASN:ND2	2.35	0.57
1:A:660:TYR:HB2	1:A:707:ILE:HG13	1.86	0.56
1:A:29:PHE:CE1	1:A:62:SER:HB2	2.41	0.56
1:A:140:GLN:HG2	3:A:1092:HOH:O	2.05	0.56
1:A:232:PRO:HD3	1:A:480:VAL:HG11	1.87	0.56
1:A:352:LEU:HD12	1:A:356:ASP:CB	2.34	0.55
1:A:265:ASP:OD1	1:A:295:THR:HB	2.07	0.55
1:A:352:LEU:HD11	1:A:356:ASP:HB2	1.87	0.55
1:A:249:PRO:HA	1:A:252:ARG:HD2	1.89	0.55
1:A:712:GLU:O	1:A:712:GLU:HG2	2.08	0.54
1:A:635:ILE:O	1:A:638:ILE:HG13	2.09	0.53
1:A:380:THR:HG23	1:A:395:LYS:HG2	1.89	0.53
1:A:198:ASN:HD22	1:A:199:LYS:N	2.07	0.53
1:A:636:ARG:NH1	1:A:674:THR:HG23	2.23	0.53
1:A:76:GLU:HB3	1:A:105:LYS:CD	2.39	0.52
1:A:541:GLN:NE2	1:A:544:GLY:H	2.07	0.52
1:A:123:GLU:C	1:A:125:PRO:HD3	2.30	0.52
1:A:684:LYS:HD2	1:A:684:LYS:N	2.25	0.52
1:A:96:VAL:O	1:A:103:SER:HA	2.10	0.51
1:A:18:GLY:HA3	1:A:38:SER:O	2.11	0.51
1:A:298:THR:HG23	3:A:951:HOH:O	2.10	0.51
1:A:238:LYS:HD2	3:A:945:HOH:O	2.11	0.51
1:A:122:ARG:HG2	3:A:1000:HOH:O	2.10	0.51
1:A:85:ASN:HD22	1:A:85:ASN:N	2.08	0.50
1:A:385:LEU:HD12	3:A:833:HOH:O	2.10	0.50
1:A:365:ARG:NH2	1:A:413:SER:O	2.44	0.50
1:A:54:PRO:HG2	1:A:57:ASN:OD1	2.11	0.50
1:A:240:THR:HG23	1:A:242:ARG:HG3	1.92	0.50
1:A:468:ARG:HG2	3:A:1074:HOH:O	2.11	0.50
1:A:645:GLU:OE2	1:A:653:LYS:HG2	2.11	0.50
1:A:125:PRO:HG3	3:A:1000:HOH:O	2.12	0.49
1:A:636:ARG:HG3	3:A:941:HOH:O	2.13	0.49
1:A:352:LEU:CD1	1:A:356:ASP:CB	2.87	0.49
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.39	0.49
1:A:691:ASN:OD1	1:A:693:ASN:HB2	2.13	0.49
1:A:92:ASP:O	1:A:93:ASP:HB2	2.13	0.48
1:A:583:LEU:C	1:A:584:ASN:HD22	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ILE:HG22	1:A:98:ASN:N	2.28	0.48
1:A:539:ASN:HB3	3:A:1110:HOH:O	2.12	0.48
1:A:397:LYS:HE3	1:A:400:GLN:OE1	2.13	0.48
1:A:76:GLU:HB3	1:A:105:LYS:CG	2.43	0.48
1:A:488:THR:HG22	1:A:506:ALA:HA	1.96	0.48
1:A:85:ASN:H	1:A:85:ASN:ND2	2.12	0.48
1:A:68:PHE:HB2	1:A:152:GLN:HG2	1.96	0.48
1:A:246:ASN:HB2	1:A:373:PRO:HG3	1.96	0.47
1:A:387:LYS:O	1:A:449:ARG:NH2	2.46	0.47
1:A:46:PRO:HB2	1:A:48:SER:OG	2.15	0.47
1:A:76:GLU:CB	1:A:105:LYS:HD3	2.42	0.47
1:A:91:VAL:O	1:A:94:GLN:HB3	2.15	0.47
1:A:523:LEU:O	1:A:527:LEU:HD13	2.15	0.47
1:A:85:ASN:N	1:A:85:ASN:ND2	2.61	0.47
1:A:159:LYS:CD	1:A:180:ASN:HB2	2.45	0.47
1:A:352:LEU:HG	1:A:436:TYR:CD1	2.47	0.47
1:A:354:THR:HA	1:A:436:TYR:CG	2.50	0.47
1:A:623:SER:HB2	3:A:803:HOH:O	2.14	0.47
1:A:659:ARG:HD3	1:A:662:MET:SD	2.55	0.47
1:A:137:THR:HA	1:A:142:LYS:O	2.16	0.46
1:A:533:PHE:CE2	1:A:542:TYR:HB2	2.50	0.46
1:A:463:ASN:OD1	1:A:465:GLU:HB2	2.15	0.46
1:A:662:MET:HE3	1:A:681:TYR:CD1	2.51	0.46
1:A:74:SER:OG	1:A:109:GLU:HA	2.14	0.46
1:A:395:LYS:HA	3:A:885:HOH:O	2.15	0.46
1:A:78:THR:O	1:A:136:TRP:HA	2.16	0.46
1:A:399:ASN:ND2	3:A:1143:HOH:O	2.49	0.45
1:A:324:PHE:HD1	1:A:588:ASN:ND2	2.15	0.45
1:A:62:SER:HA	1:A:120:TYR:O	2.17	0.45
1:A:636:ARG:HH12	1:A:666:SER:HB2	1.82	0.45
1:A:357:THR:HG21	1:A:433:THR:HG23	1.96	0.44
1:A:405:LEU:HD13	1:A:411:TYR:HB2	1.98	0.44
1:A:74:SER:HB3	1:A:107:ARG:NH2	2.32	0.44
1:A:361:ASN:HD21	1:A:422:ASN:N	2.13	0.44
1:A:123:GLU:O	1:A:125:PRO:HD3	2.17	0.44
1:A:240:THR:CG2	1:A:242:ARG:HH11	2.24	0.44
1:A:293:THR:HG22	1:A:334:ILE:HA	2.00	0.44
1:A:69:ILE:HG12	1:A:116:ILE:CG1	2.48	0.44
1:A:69:ILE:HG12	1:A:116:ILE:CD1	2.46	0.44
1:A:191:GLY:HA2	1:A:219:TYR:O	2.18	0.44
1:A:29:PHE:CZ	1:A:119:GLN:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLN:O	1:A:32:PRO:HD3	2.18	0.43
1:A:262:VAL:HA	1:A:367:VAL:O	2.18	0.43
1:A:614:GLU:OE2	1:A:617:ARG:HD2	2.18	0.43
1:A:576:THR:HG22	1:A:577:VAL:HG13	2.01	0.43
1:A:619:VAL:HG22	1:A:629:LEU:HD22	2.00	0.43
1:A:636:ARG:HG2	3:A:939:HOH:O	2.17	0.43
1:A:70:LYS:HB3	1:A:113:LEU:CD2	2.45	0.43
1:A:78:THR:HA	3:A:1002:HOH:O	2.19	0.43
1:A:85:ASN:ND2	1:A:86:HIS:ND1	2.67	0.43
1:A:178:ARG:HH21	1:A:223:PRO:CG	2.32	0.43
1:A:384:VAL:HG11	1:A:449:ARG:NH2	2.34	0.43
1:A:460:ALA:HA	1:A:471:VAL:HA	2.00	0.43
1:A:403:GLN:HE22	1:A:413:SER:H	1.67	0.42
1:A:299:HIS:HB2	3:A:850:HOH:O	2.19	0.42
1:A:699:TYR:HB3	1:A:723:LYS:HB2	2.02	0.42
1:A:133:LYS:HE3	3:A:1010:HOH:O	2.19	0.42
1:A:267:GLU:OE2	1:A:365:ARG:HD2	2.19	0.42
1:A:558:THR:O	1:A:562:ILE:HG12	2.19	0.42
1:A:205:PRO:O	1:A:211:HIS:HE1	2.02	0.42
1:A:524:LYS:O	1:A:528:LYS:HG3	2.20	0.42
1:A:338:LEU:HG	1:A:661:ASP:OD2	2.19	0.41
1:A:19:LEU:HD21	1:A:116:ILE:HD12	2.01	0.41
1:A:271:LEU:HD23	1:A:439:PHE:CE1	2.52	0.41
1:A:70:LYS:HD3	1:A:152:GLN:NE2	2.34	0.41
1:A:87:VAL:CG1	1:A:88:THR:N	2.82	0.41
1:A:378:LEU:HB2	1:A:396:ALA:HB3	2.02	0.41
1:A:645:GLU:CD	1:A:653:LYS:HG2	2.41	0.41
1:A:397:LYS:HB2	1:A:400:GLN:HB2	2.02	0.41
1:A:609:GLU:HG2	1:A:724:ILE:HG12	2.02	0.41
1:A:194:VAL:HA	1:A:202:PHE:O	2.21	0.41
1:A:236:PHE:O	1:A:240:THR:HB	2.21	0.41
1:A:50:LEU:HA	1:A:50:LEU:HD23	1.83	0.41
1:A:86:HIS:CD2	1:A:122:ARG:HD2	2.56	0.41
1:A:240:THR:HG21	1:A:242:ARG:NH1	2.24	0.41
1:A:497:ASP:O	1:A:498:LEU:HB2	2.20	0.41
1:A:595:ARG:HD2	3:A:998:HOH:O	2.19	0.41
1:A:253:HIS:CD2	1:A:255:LEU:H	2.20	0.40
1:A:240:THR:HG21	1:A:242:ARG:HD2	2.04	0.40
1:A:601:ASN:HD22	1:A:601:ASN:HA	1.72	0.40
1:A:220:LYS:HB3	1:A:220:LYS:NZ	2.36	0.40
1:A:194:VAL:HG21	1:A:239:VAL:O	2.22	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	651/735 (89%)	617 (95%)	31 (5%)	3 (0%)	29 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	THR
1	A	426	ASP
1	A	713	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	600/661 (91%)	572 (95%)	28 (5%)	26 25

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	69	ILE
1	A	85	ASN
1	A	98	ASN
1	A	110	LYS

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	136	TRP
1	A	148	SER
1	A	152	GLN
1	A	198	ASN
1	A	240	THR
1	A	298	THR
1	A	353	ASN
1	A	354	THR
1	A	361	ASN
1	A	388	ASN
1	A	409	ASN
1	A	428	SER
1	A	429	SER
1	A	470	ARG
1	A	511	SER
1	A	517	THR
1	A	535	GLU
1	A	553	ASN
1	A	583	LEU
1	A	629	LEU
1	A	659	ARG
1	A	713	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	30	GLN
1	A	85	ASN
1	A	94	GLN
1	A	124	ASN
1	A	150	ASN
1	A	152	GLN
1	A	180	ASN
1	A	198	ASN
1	A	253	HIS
1	A	263	HIS
1	A	326	ASN
1	A	361	ASN
1	A	388	ASN
1	A	403	GLN

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Mol	Chain	Res	Type
1	A	409	ASN
1	A	424	GLN
1	A	541	GLN
1	A	584	ASN
1	A	601	ASN
1	A	697	ASN
1	A	705	ASN
1	A	709	ASN
1	A	713	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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	665/735 (90%)	0.21	48 (7%) 15 19	6, 24, 57, 87	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	713	ASN	11.2
1	A	124	ASN	8.5
1	A	712	GLU	6.1
1	A	15	SER	5.3
1	A	14	SER	5.1
1	A	303	VAL	4.8
1	A	424	GLN	4.3
1	A	320	VAL	4.2
1	A	324	PHE	4.0
1	A	427	PHE	3.8
1	A	425	ASP	3.8
1	A	340	LEU	3.7
1	A	351	GLY	3.4
1	A	510	PRO	3.2
1	A	511	SER	3.2
1	A	354	THR	3.2
1	A	714	GLY	3.0
1	A	341	ALA	3.0
1	A	17	GLN	3.0
1	A	104	ASN	2.9
1	A	198	ASN	2.9
1	A	16	SER	2.9
1	A	103	SER	2.7
1	A	516	THR	2.7
1	A	400	GLN	2.7
1	A	69	ILE	2.7
1	A	127	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	600	ARG	2.5
1	A	73	LYS	2.4
1	A	352	LEU	2.4
1	A	112	ARG	2.4
1	A	302	GLU	2.3
1	A	126	THR	2.3
1	A	275	GLU	2.3
1	A	468	ARG	2.3
1	A	326	ASN	2.3
1	A	570	ASN	2.3
1	A	140	GLN	2.3
1	A	470	ARG	2.3
1	A	208	SER	2.3
1	A	339	SER	2.2
1	A	338	LEU	2.2
1	A	51	GLU	2.2
1	A	670	GLN	2.2
1	A	355	ALA	2.1
1	A	436	TYR	2.1
1	A	288	THR	2.0
1	A	342	GLY	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(Å ²)	Q<0.9
2	CA	A	801	1/1	0.99	0.05	13,13,13,13	0
2	CA	A	800	1/1	1.00	0.05	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.