



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 AM UTC

PDB ID : 1Q31 / pdb_00001q31
Title : Crystal Structure of the Tobacco Etch Virus Protease C151A mutant
Authors : Nunn, C.M.; Djordjevic, S.; George, R.R.; Urquhart, G.T.; Chao, L.H.;
Tsuchiya, Y.
Deposited on : 2003-07-28
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

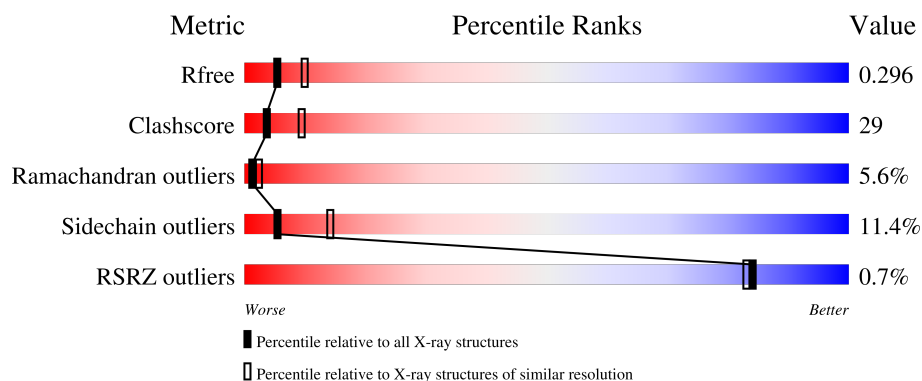
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	242	46% 36% 11% 6%
1	B	242	46% 37% 10% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3680 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.

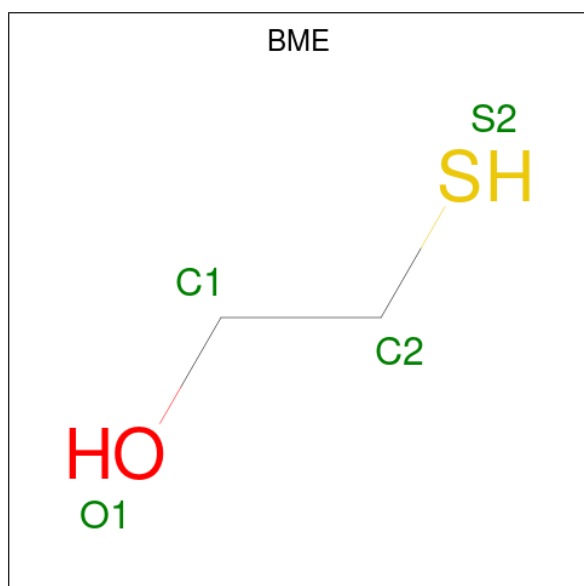
- Molecule 1 is a protein called Nuclear inclusion protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1822	1158	318	336	10			
1	B	226	Total	C	N	O	S	0	0	0
			1813	1153	317	333	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ALA	CYS	engineered mutation	UNP P04517
B	151	ALA	CYS	engineered mutation	UNP P04517

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

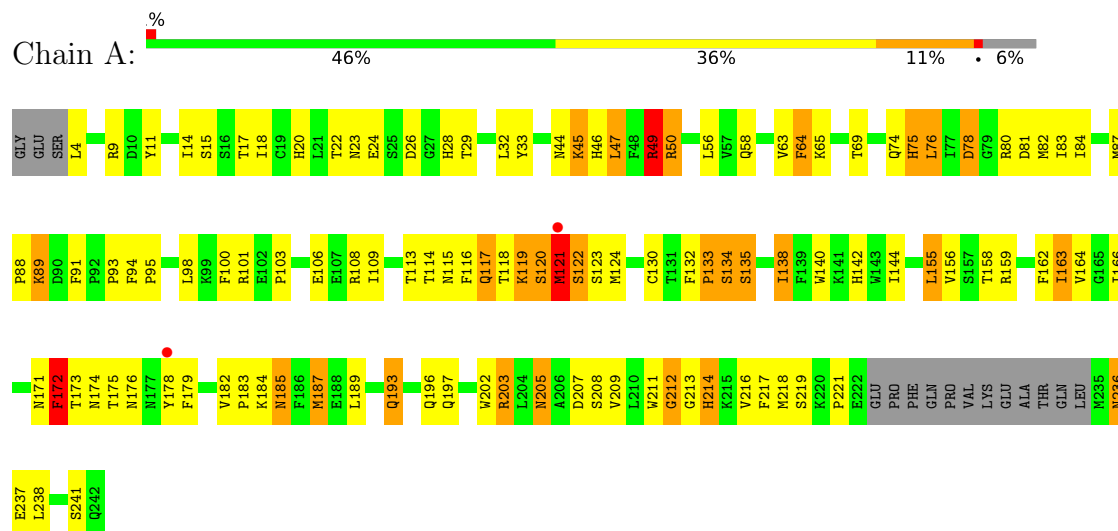
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	24	Total	O	0	0
			24	24		

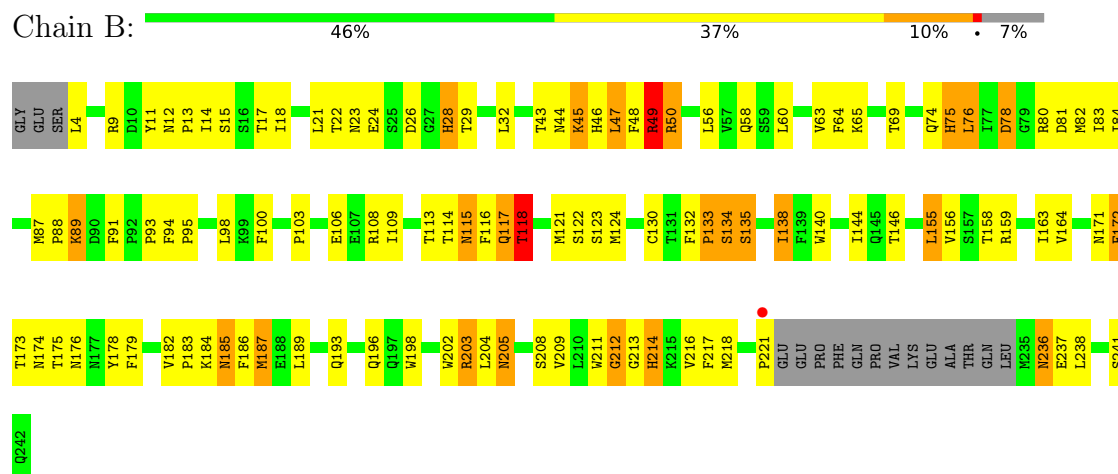
3 Residue-property plots [i](#)

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: Nuclear inclusion protein A



• Molecule 1: Nuclear inclusion protein A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.59Å 41.54Å 96.06Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	36.58 – 2.70 36.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.58-2.70) 92.8 (36.58-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.302 0.237 , 0.296	Depositor DCC
R_{free} test set	1364 reflections (8.94%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.982	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3680	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BME

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	0.67	1/1870 (0.1%)	1.13	15/2530 (0.6%)
1	B	0.68	0/1861	1.11	11/2518 (0.4%)
All	All	0.67	1/3731 (0.0%)	1.12	26/5048 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	MET	SD-CE	5.72	1.93	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ASN	N-CA-C	7.69	119.87	110.41
1	B	172	PHE	N-CA-C	7.37	120.37	111.82
1	A	172	PHE	N-CA-C	6.85	119.77	111.82
1	B	236	ASN	N-CA-C	6.73	119.01	110.33
1	B	49	ARG	N-CA-C	-6.50	104.23	111.71
1	A	122	SER	N-CA-C	6.36	124.35	110.80
1	A	49	ARG	N-CA-C	-6.24	104.76	112.38
1	B	163	ILE	N-CA-C	-6.08	99.82	108.58
1	B	237	GLU	N-CA-C	6.07	119.05	110.50
1	B	94	PHE	N-CA-C	-5.99	99.75	109.82
1	A	163	ILE	N-CA-C	-5.94	100.03	108.58
1	B	47	LEU	N-CA-C	-5.75	105.53	112.54
1	A	119	LYS	N-CA-C	-5.69	98.69	110.80
1	A	237	GLU	N-CA-C	5.63	118.81	110.48
1	A	94	PHE	N-CA-C	-5.63	100.37	109.82
1	A	78	ASP	N-CA-C	5.62	118.39	110.23
1	A	156	VAL	N-CA-C	5.61	116.02	108.17
1	B	78	ASP	N-CA-C	5.55	118.37	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	VAL	N-CA-C	5.54	115.93	108.17
1	B	115	ASN	N-CA-C	-5.24	106.57	113.17
1	A	47	LEU	N-CA-C	-5.12	106.29	112.54
1	A	117	GLN	N-CA-C	-5.09	107.04	113.20
1	A	121	MET	N-CA-C	-5.07	102.28	110.14
1	A	50	ARG	N-CA-C	-5.05	101.61	109.24
1	A	64	PHE	N-CA-C	-5.05	102.59	110.42
1	B	198	TRP	N-CA-C	5.00	117.56	110.50

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	1822	0	1780	108	0
1	B	1813	0	1774	102	0
2	A	4	0	5	0	0
2	B	4	0	5	0	0
3	A	13	0	0	1	0
3	B	24	0	0	0	0
All	All	3680	0	3564	209	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 29.

All (209) 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:118:THR:HG22	1:A:119:LYS:H	1.26	0.96
1:B:171:ASN:HD22	1:B:176:ASN:HB2	1.28	0.95
1:A:171:ASN:HD22	1:A:176:ASN:HB2	1.33	0.94
1:A:113:THR:HG22	1:A:114:THR:H	1.33	0.93
1:A:49:ARG:HD3	1:A:218:MET:HG3	1.55	0.87
1:A:106:GLU:HG2	1:A:132:PHE:HE2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PHE:CD1	1:A:172:PHE:N	2.40	0.86
1:A:172:PHE:H	1:A:172:PHE:HD1	1.23	0.85
1:B:106:GLU:HG2	1:B:132:PHE:HE2	1.41	0.84
1:B:49:ARG:HD3	1:B:218:MET:HG3	1.60	0.83
1:A:172:PHE:CE2	1:A:238:LEU:HB2	2.13	0.83
1:B:28:HIS:CE1	1:B:50:ARG:HG3	2.17	0.79
1:B:28:HIS:HE1	1:B:50:ARG:HG3	1.46	0.79
1:A:118:THR:HG22	1:A:119:LYS:N	2.01	0.76
1:B:114:THR:CG2	1:B:116:PHE:H	1.98	0.75
1:A:118:THR:CG2	1:A:119:LYS:H	1.99	0.75
1:A:172:PHE:HE2	1:A:238:LEU:HD12	1.50	0.75
1:B:24:GLU:HG3	1:B:29:THR:HG22	1.69	0.74
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.52	0.73
1:B:89:LYS:H	1:B:89:LYS:HD3	1.53	0.73
1:A:89:LYS:N	1:A:89:LYS:HD3	2.04	0.73
1:B:89:LYS:HD3	1:B:89:LYS:N	2.03	0.73
1:A:89:LYS:HD3	1:A:89:LYS:H	1.54	0.72
1:A:49:ARG:CD	1:A:218:MET:HG3	2.21	0.71
1:A:138:ILE:HB	1:A:212:GLY:HA3	1.73	0.71
1:A:24:GLU:HG3	1:A:29:THR:HG22	1.72	0.71
1:B:172:PHE:HE2	1:B:221:PRO:HG3	1.54	0.71
1:B:114:THR:HG22	1:B:116:PHE:H	1.55	0.70
1:B:49:ARG:CD	1:B:218:MET:HG3	2.21	0.70
1:B:138:ILE:HB	1:B:212:GLY:HA3	1.73	0.70
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.55	0.70
1:B:75:HIS:C	1:B:75:HIS:CD2	2.71	0.69
1:A:193:GLN:HA	1:A:196:GLN:CD	2.19	0.68
1:B:193:GLN:HA	1:B:196:GLN:CD	2.19	0.68
1:B:171:ASN:ND2	1:B:176:ASN:HB2	2.07	0.67
1:A:164:VAL:C	1:A:182:VAL:HG23	2.20	0.66
1:B:60:LEU:CD2	1:B:116:PHE:HA	2.25	0.66
1:B:100:PHE:HD1	1:B:187:MET:HE3	1.61	0.66
1:A:184:LYS:HG2	1:A:185:ASN:ND2	2.10	0.66
1:A:89:LYS:H	1:A:89:LYS:CD	2.09	0.65
1:A:75:HIS:C	1:A:75:HIS:CD2	2.75	0.65
1:B:89:LYS:H	1:B:89:LYS:CD	2.09	0.64
1:B:164:VAL:C	1:B:182:VAL:HG23	2.22	0.64
1:A:100:PHE:HD1	1:A:187:MET:HE3	1.64	0.63
1:A:106:GLU:CG	1:A:132:PHE:HE2	2.10	0.63
1:A:211:TRP:O	1:A:213:GLY:N	2.32	0.63
1:B:109:ILE:HD12	1:B:155:LEU:HD22	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:HG2	1:B:185:ASN:ND2	2.12	0.63
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.13	0.63
1:A:185:ASN:N	1:A:185:ASN:HD22	1.98	0.61
1:A:171:ASN:ND2	1:A:176:ASN:HB2	2.11	0.61
1:A:45:LYS:HE3	1:A:82:MET:O	2.00	0.61
1:A:173:THR:O	1:A:174:ASN:HB2	1.99	0.61
1:A:44:ASN:O	1:A:46:HIS:N	2.34	0.60
1:A:172:PHE:CZ	1:A:238:LEU:HB2	2.36	0.60
1:B:173:THR:O	1:B:174:ASN:HB2	2.01	0.60
1:A:113:THR:HG22	1:A:114:THR:N	2.12	0.60
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.16	0.60
1:B:211:TRP:O	1:B:213:GLY:N	2.34	0.60
1:B:74:GLN:OE1	1:B:202:TRP:N	2.34	0.60
1:B:171:ASN:C	1:B:171:ASN:OD1	2.45	0.59
1:B:172:PHE:CE2	1:B:221:PRO:HG3	2.34	0.59
1:A:109:ILE:HD12	1:A:155:LEU:HD22	1.84	0.59
1:A:171:ASN:OD1	1:A:171:ASN:C	2.45	0.59
1:A:172:PHE:CE2	1:A:238:LEU:HD12	2.36	0.58
1:B:171:ASN:HD22	1:B:176:ASN:CB	2.10	0.58
1:B:185:ASN:N	1:B:185:ASN:HD22	2.00	0.58
1:A:74:GLN:OE1	1:A:202:TRP:N	2.35	0.58
1:B:116:PHE:O	1:B:117:GLN:HB2	2.03	0.58
1:A:193:GLN:HA	1:A:196:GLN:NE2	2.19	0.57
1:B:116:PHE:O	1:B:117:GLN:CB	2.52	0.57
1:B:24:GLU:HG3	1:B:29:THR:CG2	2.35	0.57
1:B:106:GLU:HG2	1:B:132:PHE:CE2	2.32	0.57
1:B:193:GLN:HA	1:B:196:GLN:NE2	2.20	0.57
1:A:106:GLU:HG2	1:A:132:PHE:CE2	2.30	0.57
1:B:106:GLU:CG	1:B:132:PHE:HE2	2.14	0.56
1:B:60:LEU:HD21	1:B:116:PHE:HA	1.87	0.56
1:A:214:HIS:N	1:A:214:HIS:CD2	2.73	0.56
1:B:189:LEU:HD12	1:B:189:LEU:O	2.06	0.56
1:A:172:PHE:N	1:A:172:PHE:HD1	1.91	0.56
1:A:121:MET:O	1:A:121:MET:SD	2.64	0.55
1:B:114:THR:HG22	1:B:116:PHE:N	2.19	0.55
1:A:9:ARG:HG2	1:A:11:TYR:CZ	2.42	0.55
1:A:118:THR:C	1:A:120:SER:H	2.15	0.55
1:B:214:HIS:N	1:B:214:HIS:CD2	2.75	0.55
1:B:185:ASN:ND2	1:B:185:ASN:N	2.52	0.54
1:B:114:THR:HG23	1:B:116:PHE:H	1.70	0.54
1:A:4:LEU:N	1:A:4:LEU:HD23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:HG2	1:B:11:TYR:CZ	2.42	0.54
1:A:121:MET:O	1:A:122:SER:HB3	2.08	0.54
1:A:117:GLN:HA	1:A:117:GLN:NE2	2.22	0.54
1:A:185:ASN:ND2	1:A:185:ASN:N	2.50	0.54
1:B:75:HIS:C	1:B:75:HIS:HD2	2.14	0.54
1:A:103:PRO:HG2	1:A:140:TRP:CZ2	2.43	0.54
1:A:142:HIS:HD2	1:A:144:ILE:H	1.55	0.54
1:A:118:THR:O	1:A:119:LYS:HB3	2.09	0.53
1:B:140:TRP:O	1:B:178:TYR:HA	2.09	0.53
1:B:103:PRO:HG2	1:B:140:TRP:CZ2	2.43	0.53
1:A:134:SER:O	1:A:135:SER:HB2	2.09	0.53
1:A:217:PHE:HE1	1:A:238:LEU:HD22	1.74	0.52
1:B:113:THR:HG23	1:B:124:MET:HB2	1.92	0.52
1:B:217:PHE:HE1	1:B:238:LEU:HD22	1.73	0.52
1:A:140:TRP:O	1:A:178:TYR:HA	2.09	0.52
1:A:118:THR:O	1:A:119:LYS:CB	2.57	0.52
1:A:76:LEU:N	1:A:76:LEU:HD23	2.25	0.51
1:A:115:ASN:HB3	1:A:122:SER:OG	2.10	0.51
1:A:138:ILE:CB	1:A:212:GLY:HA3	2.40	0.51
1:B:4:LEU:N	1:B:4:LEU:HD23	2.25	0.51
1:B:44:ASN:O	1:B:46:HIS:N	2.44	0.51
1:B:138:ILE:CB	1:B:212:GLY:HA3	2.40	0.51
1:B:45:LYS:HE3	1:B:82:MET:O	2.11	0.51
1:B:17:THR:HG21	1:B:98:LEU:HD11	1.92	0.50
1:B:43:THR:OG1	1:B:44:ASN:N	2.44	0.50
1:A:64:PHE:CD2	1:A:65:LYS:N	2.79	0.50
1:A:17:THR:HG21	1:A:98:LEU:HD11	1.92	0.50
1:A:24:GLU:HG3	1:A:29:THR:CG2	2.39	0.50
1:B:103:PRO:O	1:B:140:TRP:CH2	2.65	0.50
1:B:159:ARG:HG2	1:B:159:ARG:HH11	1.77	0.50
1:A:193:GLN:HG3	1:A:193:GLN:O	2.12	0.49
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.77	0.49
1:A:173:THR:OG1	1:A:175:THR:HG23	2.11	0.49
1:A:189:LEU:HD12	1:A:189:LEU:O	2.13	0.49
1:B:60:LEU:HD23	1:B:116:PHE:HD2	1.77	0.49
1:A:23:ASN:ND2	1:A:69:THR:HG21	2.28	0.49
1:B:173:THR:OG1	1:B:175:THR:HG23	2.13	0.49
1:A:75:HIS:C	1:A:75:HIS:HD2	2.19	0.49
1:A:171:ASN:HD22	1:A:176:ASN:CB	2.15	0.49
1:A:166:ILE:HG13	1:A:166:ILE:O	2.13	0.48
1:B:134:SER:O	1:B:135:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LEU:HD13	1:B:179:PHE:CG	2.48	0.48
1:A:44:ASN:C	1:A:46:HIS:N	2.70	0.48
1:B:64:PHE:CD2	1:B:65:LYS:N	2.82	0.48
1:B:171:ASN:ND2	1:B:176:ASN:N	2.61	0.48
1:A:205:ASN:H	1:A:205:ASN:HD22	1.61	0.48
1:A:103:PRO:O	1:A:140:TRP:CH2	2.66	0.48
1:A:116:PHE:C	1:A:118:THR:H	2.20	0.48
1:B:44:ASN:C	1:B:46:HIS:N	2.72	0.47
1:B:117:GLN:C	1:B:118:THR:HG23	2.40	0.47
1:B:172:PHE:CE2	1:B:221:PRO:CG	2.97	0.47
1:B:217:PHE:CE1	1:B:238:LEU:HD22	2.49	0.47
1:B:56:LEU:HD23	1:B:56:LEU:C	2.39	0.47
1:B:100:PHE:CD1	1:B:187:MET:HE3	2.46	0.47
1:B:193:GLN:O	1:B:193:GLN:HG3	2.15	0.47
1:A:155:LEU:HD13	1:A:179:PHE:CG	2.50	0.47
1:A:100:PHE:CD1	1:A:187:MET:HE3	2.48	0.47
1:A:217:PHE:CE1	1:A:238:LEU:HD22	2.50	0.47
1:B:76:LEU:N	1:B:76:LEU:HD23	2.29	0.46
1:A:15:SER:HA	1:A:18:ILE:HG13	1.97	0.46
1:A:208:SER:HA	1:A:216:VAL:O	2.14	0.46
1:A:87:MET:HE2	1:A:91:PHE:CE1	2.51	0.46
1:B:203:ARG:HD2	1:B:205:ASN:HB3	1.99	0.45
1:B:23:ASN:ND2	1:B:69:THR:HG21	2.32	0.45
1:B:89:LYS:N	1:B:89:LYS:CD	2.73	0.45
1:B:205:ASN:HD22	1:B:205:ASN:H	1.65	0.45
1:A:133:PRO:HG3	1:A:140:TRP:CZ2	2.52	0.45
1:B:83:ILE:HG12	1:B:84:ILE:N	2.32	0.44
1:A:44:ASN:O	1:A:45:LYS:C	2.58	0.44
1:A:114:THR:HA	1:A:122:SER:O	2.17	0.44
1:A:197:GLN:HG3	1:B:203:ARG:CZ	2.47	0.44
1:B:15:SER:HA	1:B:18:ILE:HG13	2.00	0.44
1:A:217:PHE:N	1:A:217:PHE:CD1	2.85	0.44
1:A:46:HIS:CE1	1:A:241:SER:HB3	2.52	0.44
1:B:172:PHE:CE2	1:B:221:PRO:CD	3.00	0.44
1:A:56:LEU:C	1:A:56:LEU:HD23	2.43	0.43
1:A:219:SER:N	3:A:915:HOH:O	2.50	0.43
1:A:121:MET:O	1:A:122:SER:CB	2.65	0.43
1:A:159:ARG:HG2	1:A:159:ARG:NH1	2.33	0.43
1:B:217:PHE:CD1	1:B:217:PHE:N	2.85	0.43
1:A:101:ARG:HD3	1:A:162:PHE:CD1	2.53	0.43
1:B:58:GLN:HG3	1:B:63:VAL:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ASN:N	1:B:13:PRO:CD	2.82	0.43
1:B:202:TRP:CG	1:B:203:ARG:N	2.87	0.43
1:B:203:ARG:HG3	1:B:204:LEU:N	2.33	0.43
1:A:58:GLN:HG3	1:A:63:VAL:HG22	2.00	0.43
1:A:171:ASN:ND2	1:A:176:ASN:N	2.67	0.43
1:B:80:ARG:C	1:B:82:MET:H	2.27	0.43
1:A:115:ASN:CB	1:A:122:SER:OG	2.67	0.43
1:B:208:SER:HA	1:B:216:VAL:O	2.18	0.43
1:B:48:PHE:C	1:B:50:ARG:N	2.75	0.42
1:A:83:ILE:HG12	1:A:84:ILE:N	2.34	0.42
1:A:123:SER:O	1:A:124:MET:CG	2.67	0.42
1:A:101:ARG:HG3	1:A:101:ARG:HH11	1.84	0.42
1:B:15:SER:HB2	1:B:114:THR:OG1	2.19	0.42
1:B:46:HIS:CE1	1:B:241:SER:HB3	2.54	0.42
1:B:81:ASP:O	1:B:81:ASP:CG	2.62	0.42
1:A:116:PHE:C	1:A:118:THR:N	2.78	0.42
1:A:185:ASN:HD22	1:A:185:ASN:H	1.66	0.42
1:B:133:PRO:HG3	1:B:140:TRP:CZ2	2.54	0.42
1:A:98:LEU:HD23	1:A:163:ILE:CD1	2.50	0.42
1:B:22:THR:HB	1:B:56:LEU:HB3	2.02	0.42
1:B:44:ASN:O	1:B:45:LYS:C	2.62	0.42
1:B:123:SER:O	1:B:124:MET:CG	2.68	0.42
1:B:115:ASN:OD1	1:B:122:SER:HA	2.20	0.42
1:A:178:TYR:CD1	1:A:178:TYR:N	2.88	0.42
1:A:80:ARG:HH11	1:A:80:ARG:HG3	1.85	0.41
1:A:81:ASP:CG	1:A:81:ASP:O	2.61	0.41
1:A:22:THR:HB	1:A:56:LEU:HB3	2.02	0.41
1:B:87:MET:HE2	1:B:91:PHE:CE1	2.55	0.41
1:A:203:ARG:HD2	1:A:205:ASN:HB3	2.01	0.41
1:B:103:PRO:HB3	1:B:164:VAL:HB	2.03	0.41
1:A:44:ASN:C	1:A:46:HIS:H	2.28	0.41
1:B:159:ARG:HG2	1:B:159:ARG:NH1	2.35	0.41
1:B:186:PHE:O	1:B:189:LEU:HB3	2.20	0.41
1:B:134:SER:OG	1:B:214:HIS:NE2	2.51	0.41
1:A:80:ARG:C	1:A:82:MET:H	2.29	0.40
1:B:144:ILE:O	1:B:146:THR:HG23	2.22	0.40
1:A:20:HIS:HD2	1:A:33:TYR:CZ	2.39	0.40
1:A:123:SER:C	1:A:124:MET:HG3	2.47	0.40
1:B:121:MET:O	1:B:121:MET:HG2	2.21	0.40

There are no symmetry-related clashes.

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	223/242 (92%)	178 (80%)	32 (14%)	13 (6%)	1	2
1	B	222/242 (92%)	179 (81%)	31 (14%)	12 (5%)	1	2
All	All	445/484 (92%)	357 (80%)	63 (14%)	25 (6%)	1	2

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	GLY
1	B	118	THR
1	B	212	GLY
1	A	26	ASP
1	A	45	LYS
1	A	134	SER
1	B	26	ASP
1	B	45	LYS
1	A	120	SER
1	A	133	PRO
1	A	135	SER
1	B	133	PRO
1	B	134	SER
1	A	93	PRO
1	B	135	SER
1	A	95	PRO
1	A	193	GLN
1	B	88	PRO
1	B	93	PRO
1	B	95	PRO
1	A	221	PRO
1	B	117	GLN
1	A	88	PRO
1	B	138	ILE
1	A	138	ILE

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	207/220 (94%)	183 (88%)	24 (12%)	5	13
1	B	206/220 (94%)	183 (89%)	23 (11%)	6	15
All	All	413/440 (94%)	366 (89%)	47 (11%)	5	14

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	28	HIS
1	A	32	LEU
1	A	47	LEU
1	A	49	ARG
1	A	50	ARG
1	A	75	HIS
1	A	76	LEU
1	A	78	ASP
1	A	89	LYS
1	A	121	MET
1	A	130	CYS
1	A	155	LEU
1	A	158	THR
1	A	172	PHE
1	A	183	PRO
1	A	185	ASN
1	A	187	MET
1	A	203	ARG
1	A	205	ASN
1	A	207	ASP
1	A	209	VAL
1	A	214	HIS
1	A	236	ASN
1	B	14	ILE
1	B	21	LEU
1	B	28	HIS

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Mol	Chain	Res	Type
1	B	32	LEU
1	B	47	LEU
1	B	49	ARG
1	B	50	ARG
1	B	75	HIS
1	B	76	LEU
1	B	78	ASP
1	B	89	LYS
1	B	118	THR
1	B	130	CYS
1	B	155	LEU
1	B	158	THR
1	B	183	PRO
1	B	185	ASN
1	B	187	MET
1	B	203	ARG
1	B	205	ASN
1	B	209	VAL
1	B	214	HIS
1	B	236	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	44	ASN
1	A	75	HIS
1	A	117	GLN
1	A	142	HIS
1	A	185	ASN
1	A	197	GLN
1	A	205	ASN
1	B	20	HIS
1	B	28	HIS
1	B	44	ASN
1	B	58	GLN
1	B	75	HIS
1	B	117	GLN
1	B	185	ASN
1	B	197	GLN
1	B	205	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BME	B	901	1	3,3,3	0.78	0	2,2,2	0.17	0
2	BME	A	902	1	3,3,3	0.70	0	2,2,2	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	B	901	1	-	1/1/1/1	-
2	BME	A	902	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	BME	O1-C1-C2-S2
2	B	901	BME	O1-C1-C2-S2

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/242 (93%)	0.08	2 (0%) 81 80	34, 68, 116, 145	0
1	B	226/242 (93%)	0.11	1 (0%) 88 87	36, 66, 98, 147	0
All	All	453/484 (93%)	0.10	3 (0%) 84 83	34, 68, 112, 147	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	TYR	2.6
1	A	121	MET	2.4
1	B	221	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BME	B	901	4/4	0.62	0.22	72,72,72,72	0
2	BME	A	902	4/4	0.79	0.15	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.