



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:16 PM GMT

PDB ID : 4HRU
Title : Molecular tweezers modulate 14-3-3 protein-protein interactions
Authors : Bier, D.; Ottmann, C.
Deposited on : 2012-10-28
Resolution : 3.15 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

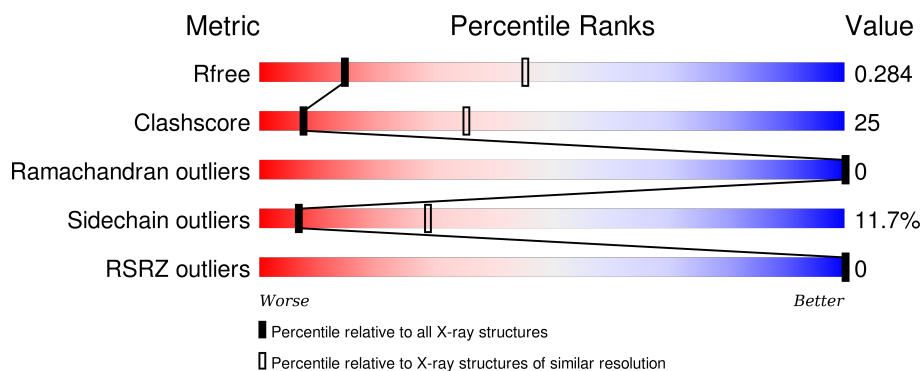
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.15 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	234	 61% 26% 8% .

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.

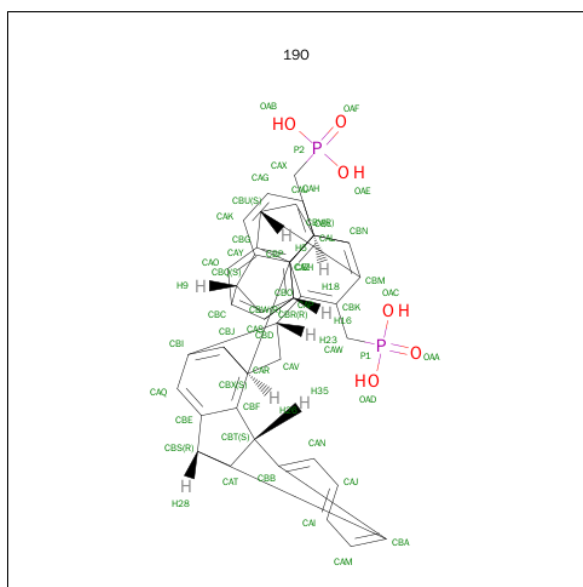
- Molecule 1 is a protein called 14-3-3 protein sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1769	1108	299	351	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P31947
A	-1	GLY	-	EXPRESSION TAG	UNP P31947
A	0	SER	-	EXPRESSION TAG	UNP P31947

- Molecule 2 is NARIUM-(5,7 ,9 ,11 ,16 ,18 ,20 ,22)-5,7,9,11,16,18,20,22-OCTAHYDRO-5,22:7,20:9,18:11,16-TETRAMETHANONONACEN-8,19-BISPHOSPHATE (three-letter code: 19O) (formula: $C_{44}H_{36}O_6P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			52	44	6	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

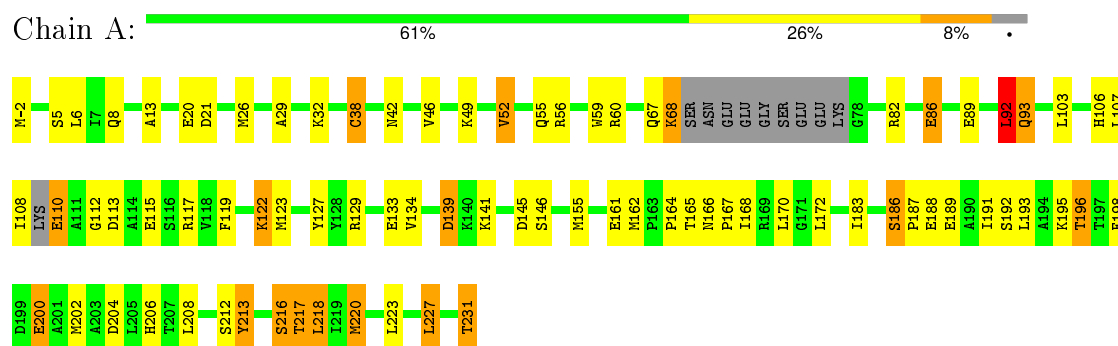
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total	O	0	0
			180	180		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 14-3-3 protein sigma



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	63.50 Å 154.71 Å 77.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.58 – 3.15 19.58 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.58-3.15) 99.9 (19.58-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 3.15 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.299 0.187 , 0.284	Depositor DCC
R_{free} test set	342 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 6825 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2003	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 19O, CL

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	0.66	0/1796	0.73	1/2414 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	92	LEU	CA-CB-CG	5.71	128.44	115.30

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	1769	0	1755	92	0
2	A	52	0	34	1	0
3	A	1	0	0	0	1
4	A	1	0	0	0	0
5	A	180	0	0	50	1
All	All	2003	0	1789	92	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 25.

All (92) 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:67:GLN:HG3	5:A:550:HOH:O	1.41	1.20
1:A:5:SER:HA	5:A:456:HOH:O	1.41	1.16
1:A:113:ASP:HB3	5:A:473:HOH:O	1.49	1.11
1:A:107:LEU:HD12	5:A:466:HOH:O	1.55	1.06
1:A:21:ASP:HB2	5:A:439:HOH:O	1.59	1.01
1:A:68:LYS:HD2	5:A:550:HOH:O	1.62	0.98
1:A:213:TYR:O	1:A:217:THR:HG23	1.62	0.97
1:A:29:ALA:HB3	5:A:449:HOH:O	1.62	0.97
1:A:103:LEU:HA	5:A:466:HOH:O	1.65	0.94
1:A:191:ILE:HB	5:A:539:HOH:O	1.69	0.91
1:A:26:MET:HA	5:A:449:HOH:O	1.71	0.88
1:A:108:ILE:O	1:A:110:GLU:N	2.07	0.88
1:A:196:THR:HG22	1:A:200:GLU:OE1	1.74	0.86
1:A:115:GLU:HG2	5:A:409:HOH:O	1.75	0.86
1:A:172:LEU:HA	5:A:446:HOH:O	1.76	0.84
1:A:108:ILE:O	1:A:110:GLU:HG3	1.76	0.84
1:A:223:LEU:HD12	5:A:450:HOH:O	1.76	0.84
1:A:191:ILE:HA	5:A:464:HOH:O	1.78	0.83
1:A:122:LYS:HE2	5:A:446:HOH:O	1.77	0.82
1:A:122:LYS:HG3	5:A:446:HOH:O	1.78	0.81
1:A:198:PHE:CD2	1:A:220:MET:HE3	2.22	0.75
1:A:49:LYS:HG2	5:A:407:HOH:O	1.89	0.72
1:A:13:ALA:HB2	5:A:439:HOH:O	1.91	0.70
1:A:220:MET:HA	5:A:450:HOH:O	1.91	0.70
1:A:-2:MET:HB2	5:A:514:HOH:O	1.91	0.70
1:A:13:ALA:CB	5:A:439:HOH:O	2.40	0.70
1:A:139:ASP:HB2	5:A:416:HOH:O	1.92	0.70
1:A:68:LYS:HD3	5:A:519:HOH:O	1.94	0.67
1:A:42:ASN:O	1:A:46:VAL:HG23	1.96	0.66
1:A:172:LEU:CA	5:A:446:HOH:O	2.42	0.63
1:A:113:ASP:HB2	5:A:419:HOH:O	1.99	0.63
1:A:55:GLN:HB2	5:A:434:HOH:O	1.98	0.62
1:A:6:LEU:HD11	1:A:32:LYS:HE3	1.81	0.61
1:A:162:MET:HE1	1:A:168:ILE:HB	1.84	0.60
1:A:187:PRO:HD3	5:A:433:HOH:O	2.02	0.59
1:A:164:PRO:HD2	5:A:463:HOH:O	2.02	0.58
1:A:52:VAL:O	1:A:56:ARG:HG3	2.05	0.56
1:A:59:TRP:CE2	1:A:134:VAL:HG12	2.40	0.56
1:A:227:LEU:O	1:A:231:THR:N	2.26	0.55
1:A:82:ARG:NH2	5:A:560:HOH:O	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLU:O	1:A:191:ILE:HG22	2.05	0.55
1:A:165:THR:HB	5:A:465:HOH:O	2.06	0.55
1:A:13:ALA:HB2	5:A:457:HOH:O	2.08	0.54
1:A:60:ARG:HD3	5:A:504:HOH:O	2.07	0.54
1:A:198:PHE:CE2	1:A:220:MET:HE3	2.42	0.54
1:A:67:GLN:HG3	1:A:68:LYS:H	1.73	0.54
1:A:141:LYS:HG2	5:A:431:HOH:O	2.07	0.53
1:A:204:ASP:OD1	1:A:206:HIS:HE1	1.91	0.53
1:A:112:GLY:H	1:A:117:ARG:HD2	1.74	0.52
1:A:188:GLU:CG	1:A:189:GLU:H	2.22	0.52
1:A:82:ARG:NH1	1:A:86:GLU:OE1	2.44	0.51
1:A:119:PHE:HE1	1:A:123:MET:CE	2.23	0.51
1:A:129:ARG:HG3	1:A:183:ILE:HG13	1.92	0.51
1:A:208:LEU:HD22	5:A:465:HOH:O	2.10	0.50
1:A:212:SER:O	1:A:216:SER:HB2	2.12	0.50
1:A:82:ARG:O	1:A:86:GLU:HB2	2.12	0.50
1:A:186:SER:C	1:A:188:GLU:H	2.14	0.49
1:A:86:GLU:HG3	5:A:422:HOH:O	2.12	0.49
1:A:112:GLY:HA3	5:A:424:HOH:O	2.13	0.48
1:A:186:SER:C	1:A:188:GLU:N	2.65	0.48
1:A:155:MET:CE	1:A:193:LEU:HD11	2.44	0.47
1:A:213:TYR:CD2	2:A:301:19O:H35	2.49	0.47
1:A:155:MET:HE2	1:A:193:LEU:HD11	1.98	0.46
1:A:89:GLU:O	1:A:93:GLN:HG3	2.16	0.46
1:A:133:GLU:HA	5:A:498:HOH:O	2.16	0.46
1:A:119:PHE:CE1	1:A:123:MET:CE	2.99	0.46
1:A:188:GLU:HG2	1:A:189:GLU:H	1.81	0.45
1:A:13:ALA:HB1	5:A:439:HOH:O	2.09	0.45
1:A:198:PHE:CD2	1:A:220:MET:CE	2.98	0.45
1:A:110:GLU:HG2	5:A:495:HOH:O	2.15	0.45
1:A:20:GLU:HA	5:A:462:HOH:O	2.16	0.45
1:A:191:ILE:HD12	1:A:227:LEU:HD23	1.99	0.44
1:A:106:HIS:HB3	5:A:458:HOH:O	2.18	0.44
1:A:20:GLU:CA	5:A:462:HOH:O	2.66	0.44
1:A:195:LYS:HB3	1:A:195:LYS:HE2	1.79	0.44
1:A:103:LEU:HD23	5:A:466:HOH:O	2.18	0.44
1:A:8:GLN:HB2	5:A:456:HOH:O	2.17	0.43
1:A:103:LEU:CA	5:A:466:HOH:O	2.44	0.43
1:A:192:SER:O	1:A:196:THR:OG1	2.26	0.43
1:A:161:GLU:OE1	1:A:161:GLU:HA	2.18	0.43
1:A:164:PRO:O	1:A:170:LEU:HD21	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:MET:O	1:A:127:TYR:HD2	2.02	0.42
1:A:108:ILE:C	5:A:549:HOH:O	2.56	0.42
1:A:204:ASP:HB3	5:A:463:HOH:O	2.20	0.42
1:A:188:GLU:CG	1:A:189:GLU:N	2.82	0.42
1:A:218:LEU:O	1:A:218:LEU:HD22	2.20	0.42
1:A:6:LEU:CD1	1:A:32:LYS:HE3	2.48	0.41
1:A:38:CYS:HB2	5:A:438:HOH:O	2.19	0.41
1:A:166:ASN:HA	1:A:167:PRO:HD3	1.80	0.41
1:A:198:PHE:CE2	1:A:220:MET:CE	3.03	0.40
1:A:92:LEU:HD13	5:A:434:HOH:O	2.21	0.40
1:A:107:LEU:HB2	5:A:466:HOH:O	2.22	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)
3:A:302:CL:CL	5:A:469:HOH:O[3_456]	1.54	0.66

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	219/234 (94%)	197 (90%)	22 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	189/198 (96%)	167 (88%)	22 (12%)	7	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	CYS
1	A	52	VAL
1	A	68	LYS
1	A	86	GLU
1	A	92	LEU
1	A	93	GLN
1	A	110	GLU
1	A	122	LYS
1	A	139	ASP
1	A	145	ASP
1	A	146	SER
1	A	186	SER
1	A	196	THR
1	A	200	GLU
1	A	202	MET
1	A	213	TYR
1	A	216	SER
1	A	217	THR
1	A	218	LEU
1	A	220	MET
1	A	227	LEU
1	A	231	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	206	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
2	19O	A	301	-	64,64,64	5.18	56 (87%)	100,108,108	1.93	21 (21%)

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	19O	A	301	-	-	0/10/90/90	0/0/13/13

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	19O	P1-CAW	-10.14	1.65	1.79
2	A	301	19O	CBO-CBW	-9.60	1.40	1.52
2	A	301	19O	CBN-CBV	-9.58	1.41	1.52
2	A	301	19O	CBM-CBU	-9.37	1.41	1.52
2	A	301	19O	CBF-CBT	-8.03	1.38	1.52
2	A	301	19O	CBP-CBX	-8.01	1.42	1.52
2	A	301	19O	CBJ-CBX	-7.52	1.39	1.52
2	A	301	19O	CBG-CBU	-7.51	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	19O	CAY-CBQ	-7.43	1.39	1.52
2	A	301	19O	CBI-CBW	-7.38	1.39	1.52
2	A	301	19O	CBE-CBS	-7.31	1.40	1.52
2	A	301	19O	CBB-CBT	-7.20	1.40	1.52
2	A	301	19O	CBA-CBS	-7.03	1.40	1.52
2	A	301	19O	CAT-CBS	-6.97	1.47	1.55
2	A	301	19O	CAT-CBT	-6.66	1.48	1.55
2	A	301	19O	CBD-CBR	-6.52	1.41	1.52
2	A	301	19O	CAZ-CBR	-6.50	1.41	1.52
2	A	301	19O	CBC-CBQ	-6.43	1.41	1.52
2	A	301	19O	CAW-CBK	-6.27	1.39	1.52
2	A	301	19O	CAU-CBV	-6.24	1.48	1.55
2	A	301	19O	CBH-CBV	-6.23	1.41	1.52
2	A	301	19O	CAV-CBX	-6.17	1.48	1.55
2	A	301	19O	CAS-CBR	-6.14	1.48	1.55
2	A	301	19O	CAU-CBU	-5.63	1.49	1.55
2	A	301	19O	CAX-CBL	-5.49	1.41	1.52
2	A	301	19O	CAS-CBQ	-5.34	1.49	1.55
2	A	301	19O	CAV-CBW	-5.25	1.49	1.55
2	A	301	19O	CAM-CBA	-4.19	1.34	1.39
2	A	301	19O	CAN-CBB	-4.01	1.34	1.39
2	A	301	19O	CAK-CAY	-3.83	1.34	1.39
2	A	301	19O	CAL-CAZ	-3.56	1.34	1.39
2	A	301	19O	CBO-CBP	-3.52	1.35	1.41
2	A	301	19O	CBM-CBN	-3.27	1.35	1.41
2	A	301	19O	CAR-CBJ	-3.27	1.34	1.39
2	A	301	19O	P2-CAX	-3.17	1.75	1.79
2	A	301	19O	CAR-CBF	-3.17	1.34	1.39
2	A	301	19O	CBE-CBF	-3.11	1.34	1.40
2	A	301	19O	CBA-CBB	-3.10	1.34	1.40
2	A	301	19O	CBO-CBK	-3.08	1.33	1.39
2	A	301	19O	CAQ-CBE	-3.05	1.34	1.39
2	A	301	19O	CAQ-CBI	-2.93	1.34	1.39
2	A	301	19O	CAO-CBG	-2.92	1.34	1.39
2	A	301	19O	CBI-CBJ	-2.91	1.34	1.40
2	A	301	19O	P2-OAB	-2.84	1.48	1.54
2	A	301	19O	CAO-CBC	-2.77	1.34	1.39
2	A	301	19O	CBG-CBH	-2.73	1.35	1.40
2	A	301	19O	CAP-CBH	-2.72	1.35	1.39
2	A	301	19O	CBC-CBD	-2.72	1.35	1.40
2	A	301	19O	CBM-CBK	-2.62	1.34	1.39
2	A	301	19O	CAY-CAZ	-2.58	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	19O	CAP-CBD	-2.55	1.35	1.39
2	A	301	19O	CBN-CBL	-2.51	1.35	1.39
2	A	301	19O	P2-OAE	2.23	1.60	1.54
2	A	301	19O	P1-OAC	3.73	1.64	1.54
2	A	301	19O	P1-OAD	4.44	1.65	1.54
2	A	301	19O	P2-OAF	4.52	1.60	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	19O	CBW-CAV-CBX	-5.74	91.41	94.42
2	A	301	19O	CBQ-CAS-CBR	-4.72	91.95	94.42
2	A	301	19O	CBU-CAU-CBV	-4.12	92.26	94.42
2	A	301	19O	OAE-P2-OAF	-4.02	102.12	112.40
2	A	301	19O	CBS-CAT-CBT	-3.99	92.33	94.42
2	A	301	19O	CBM-CBN-CBL	-2.24	119.90	122.95
2	A	301	19O	CBP-CBO-CBK	-2.13	120.06	122.95
2	A	301	19O	CBI-CAQ-CBE	-2.01	119.37	123.19
2	A	301	19O	CAO-CBC-CBQ	2.01	133.45	131.54
2	A	301	19O	CAQ-CBI-CBW	2.41	133.82	131.54
2	A	301	19O	CAQ-CBE-CBS	2.42	133.84	131.54
2	A	301	19O	CAZ-CBR-CBD	2.70	108.14	105.33
2	A	301	19O	CAY-CBQ-CBC	2.82	108.26	105.33
2	A	301	19O	CAP-CBH-CBV	2.82	134.22	131.54
2	A	301	19O	CAP-CBD-CBR	2.85	134.24	131.54
2	A	301	19O	OAA-P1-CAW	2.87	118.17	111.05
2	A	301	19O	CBN-CBV-CBH	4.45	108.15	104.46
2	A	301	19O	CBP-CBX-CBJ	4.50	108.19	104.46
2	A	301	19O	CBM-CBU-CBG	4.53	108.22	104.46
2	A	301	19O	CBO-CBW-CBI	4.69	108.35	104.46
2	A	301	19O	OAB-P2-CAX	5.67	119.74	107.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	19O	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	224/234 (95%)	-0.52	0 100 100	17, 31, 54, 67	0

There are no RSRZ outliers to report.

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	19O	A	301	52/52	0.91	0.24	1.51	47,54,57,57	0
3	CL	A	302	1/1	0.97	0.14	-0.31	60,60,60,60	0
4	MG	A	303	1/1	0.85	0.20	-	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.