Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:46 AM UTC

PDB ID	:	4A1T / pdb_00004a1t
Title	:	Co-Complex of the of NS3-4A protease with the inhibitory peptide CP5- 46-A (in-House data)
Authors	:	Schmelz, S.; Kuegler, J.; Collins, J.; Heinz, D.W.
Deposited on	:	2011-09-19
Resolution	:	2.05 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:

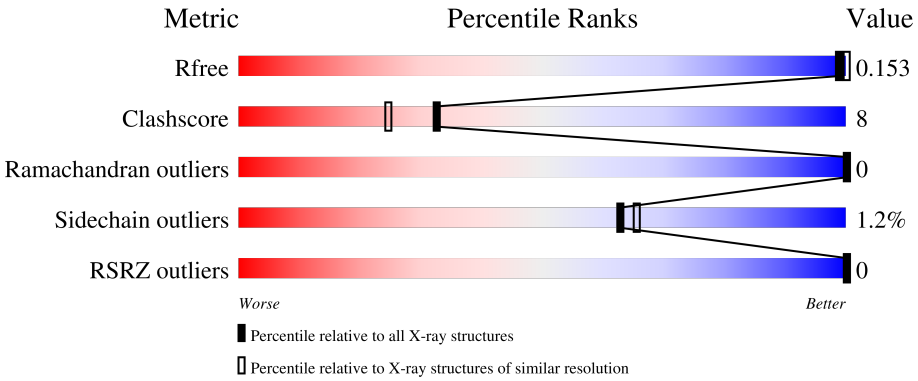
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 <=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	203	76% 19% 5%
1	B	203	85% 10% .
2	C	21	76% 5% 19%
2	D	21	71% 14% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	1182	-	-	X	-
6	GOL	A	1190	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3456 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 NONSTRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	6	0
			1453	904	264	274	11			
1	B	194	Total	C	N	O	S	0	8	0
			1462	910	264	276	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LYS	-	linker	UNP P26662
A	0	GLY	-	linker	UNP P26662
A	1	GLY	-	linker	UNP P26662
A	181	GLY	-	expression tag	UNP P26662
A	182	SER	-	expression tag	UNP P26662
A	183	HIS	-	expression tag	UNP P26662
A	184	HIS	-	expression tag	UNP P26662
A	185	HIS	-	expression tag	UNP P26662
A	186	HIS	-	expression tag	UNP P26662
A	187	HIS	-	expression tag	UNP P26662
A	188	HIS	-	expression tag	UNP P26662
A	26	ARG	LYS	SEE REMARK 999	UNP P26662
A	30	GLU	ASP	SEE REMARK 999	UNP P26662
A	36	VAL	LEU	SEE REMARK 999	UNP P26662
A	86	GLN	PRO	SEE REMARK 999	UNP P26662
A	94	LEU	MET	SEE REMARK 999	UNP P26662
A	114	ILE	VAL	variant	UNP P26662
A	132	VAL	ILE	variant	UNP P26662
A	150	ALA	VAL	SEE REMARK 999	UNP P26662
A	170	VAL	ILE	SEE REMARK 999	UNP P26662
B	-1	LYS	-	linker	UNP P26662
B	0	GLY	-	linker	UNP P26662
B	1	GLY	-	linker	UNP P26662
B	181	GLY	-	expression tag	UNP P26662

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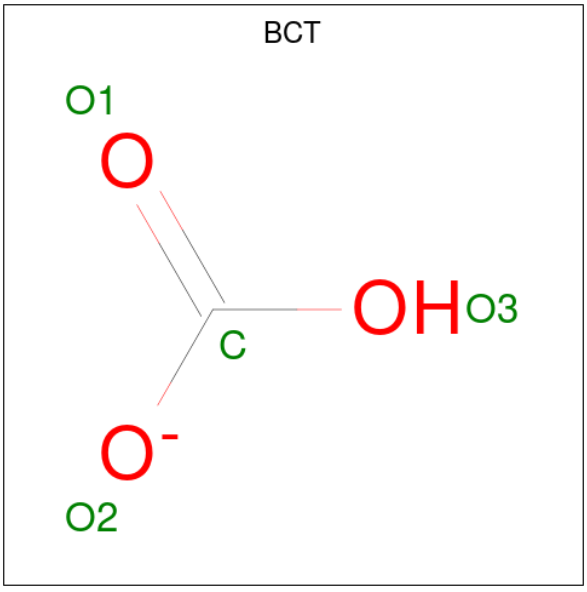
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Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	expression tag	UNP P26662
B	183	HIS	-	expression tag	UNP P26662
B	184	HIS	-	expression tag	UNP P26662
B	185	HIS	-	expression tag	UNP P26662
B	186	HIS	-	expression tag	UNP P26662
B	187	HIS	-	expression tag	UNP P26662
B	188	HIS	-	expression tag	UNP P26662
B	26	ARG	LYS	SEE REMARK 999	UNP P26662
B	30	GLU	ASP	SEE REMARK 999	UNP P26662
B	36	VAL	LEU	SEE REMARK 999	UNP P26662
B	86	GLN	PRO	SEE REMARK 999	UNP P26662
B	94	LEU	MET	SEE REMARK 999	UNP P26662
B	114	ILE	VAL	variant	UNP P26662
B	132	VAL	ILE	variant	UNP P26662
B	150	ALA	VAL	SEE REMARK 999	UNP P26662
B	170	VAL	ILE	SEE REMARK 999	UNP P26662

- Molecule 2 is a protein called CP5-46-A PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	S	0	0	0
			132	86	22	23	1			
2	D	18	Total	C	N	O	S	0	0	0
			141	90	23	27	1			

- Molecule 3 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 1 3	0	0

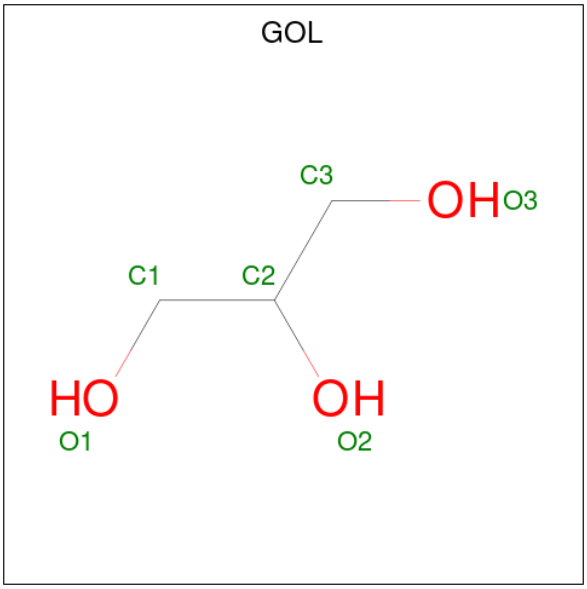
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Cl 5 5	0	0
5	B	4	Total Cl 4 4	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

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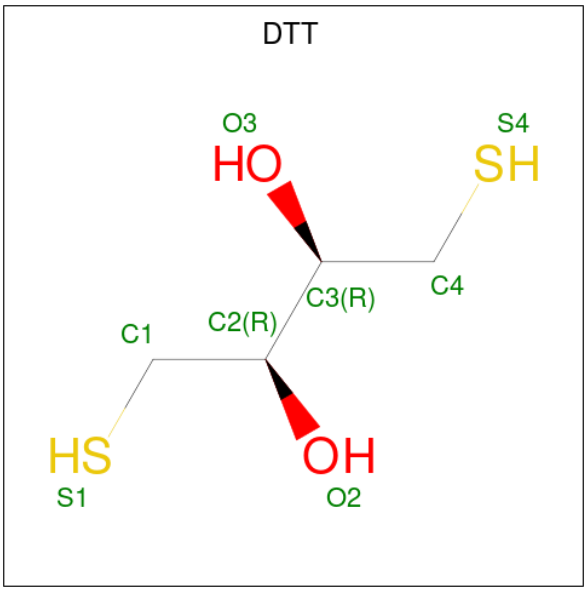
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 6 6	0	1

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0
7	B	1	Total Zn 1 1	0	0

- Molecule 8 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O S 8 4 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	92	Total O 92 92	0	0
9	B	109	Total O 109 109	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	9	Total O 9 9	0	0
9	D	7	Total O 7 7	0	0

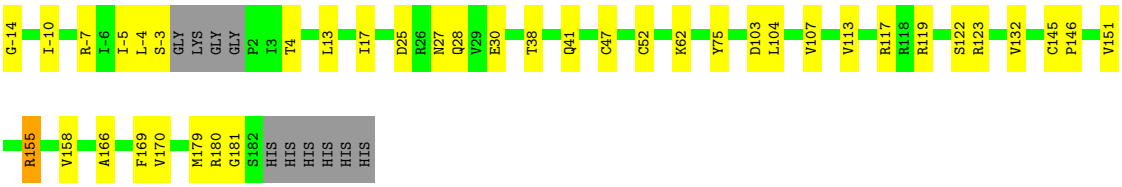
3 Residue-property plots (i)

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: NONSTRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3

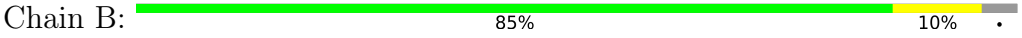
Chain A:





• Molecule 1: NONSTRUCTURAL PROTEIN 4A, SERINE PROTEASE NS3

Chain B:

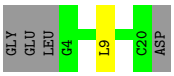




• Molecule 2: CP5-46-A PEPTIDE

Chain C:

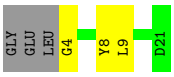




• Molecule 2: CP5-46-A PEPTIDE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	93.25Å 93.25Å 83.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.71 – 2.05 19.71 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.71-2.05) 100.0 (19.71-2.05)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.48 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.245 (Not available) , 0.153	Depositor DCC
R_{free} test set	1288 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.257 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3456	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CL, DTT, K, ZN, BCT

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	0.79	0/1479	0.90	0/2011
1	B	0.77	0/1492	0.92	0/2030
2	C	0.84	0/136	0.85	0/185
2	D	0.91	0/145	0.91	0/196
All	All	0.79	0/3252	0.90	0/4422

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

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	1453	0	1469	32	0
1	B	1462	0	1482	18	0
2	C	132	0	126	1	0
2	D	141	0	130	6	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
5	A	5	0	0	0	0
5	B	4	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	24	0	32	8	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	8	0	10	0	0
9	A	92	0	0	1	0
9	B	109	0	0	3	0
9	C	9	0	0	0	0
9	D	7	0	0	0	0
All	All	3456	0	3249	51	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 8.

All (51) 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:38:THR:HB	6:A:1191:GOL:H11	1.34	1.09
1:A:180:ARG:HB3	1:A:181:GLY:HA3	1.62	0.81
1:A:104:LEU:HD22	1:A:151[B]:VAL:HG11	1.74	0.69
5:B:1182:CL:CL	9:B:2048:HOH:O	2.49	0.67
1:A:-5[B]:ILE:C	1:A:-5[B]:ILE:HD13	2.20	0.67
1:B:154:PHE:CZ	2:D:9:LEU:HD12	2.30	0.66
1:A:104:LEU:HD22	1:A:151[A]:VAL:HG21	1.79	0.65
1:B:-3:SER:HB3	1:B:4:THR:OG1	1.96	0.65
1:A:180:ARG:HB3	1:A:181:GLY:CA	2.27	0.64
1:B:132:VAL:HG12	5:B:1183:CL:CL	2.38	0.60
1:A:-10:ILE:HB	6:A:1190:GOL:H12	1.86	0.58
1:A:25:ASP:OD2	6:A:1190:GOL:C1	2.53	0.57
1:A:-14:GLY:N	6:A:1191:GOL:O2	2.32	0.57
1:B:178:THR:O	1:B:179:MET:HB2	2.05	0.57
1:B:148:GLY:O	9:B:2105:HOH:O	2.17	0.56
1:B:175:MET:O	1:B:179:MET:N	2.34	0.56
1:A:27:ASN:HB2	6:A:1190:GOL:H11	1.86	0.56
1:A:75:TYR:CZ	1:A:179:MET:HG2	2.43	0.54
1:A:-3:SER:HB3	1:A:4:THR:OG1	2.07	0.53
1:A:158:VAL:HB	1:A:166:ALA:HB3	1.91	0.53
1:A:-10:ILE:HG22	6:A:1190:GOL:H2	1.92	0.52
1:A:-5[B]:ILE:HD13	1:A:-5[B]:ILE:O	2.10	0.52
1:B:154:PHE:CZ	2:D:9:LEU:CD1	2.93	0.52
1:B:149:HIS:CD2	5:B:1185:CL:CL	3.00	0.52
1:B:154:PHE:CE2	2:D:9:LEU:HD12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:CB	1:A:181:GLY:CA	2.89	0.50
1:B:38:THR:HB	5:B:1182:CL:CL	2.49	0.50
1:B:173:GLU:O	1:B:176:GLU:HG2	2.12	0.50
1:B:110:HIS:HD2	9:B:2084:HOH:O	1.94	0.49
1:A:-4:LEU:HD21	1:A:107:VAL:HG21	1.93	0.49
1:A:41:GLN:HE22	6:A:1192[A]:GOL:H32	1.78	0.49
1:A:28:GLN:NE2	1:A:30:GLU:OE2	2.46	0.49
1:A:123:ARG:NH2	9:A:2077:HOH:O	2.46	0.49
1:B:116:VAL:HG22	1:B:126:LEU:HD23	1.95	0.48
1:A:180:ARG:CB	1:A:181:GLY:HA3	2.32	0.47
1:A:145:CYS:HB2	1:A:146:PRO:HD2	1.97	0.46
1:A:13:LEU:O	1:A:17:ILE:HG12	2.16	0.45
1:A:47:CYS:HA	1:A:52[B]:CYS:HA	1.98	0.45
1:A:122:SER:HB2	1:A:169:PHE:O	2.16	0.45
1:B:154:PHE:HZ	2:D:9:LEU:CD1	2.31	0.44
1:B:32:GLU:HA	1:B:92:ARG:O	2.18	0.43
1:B:155:ARG:NH2	2:D:8:TYR:OH	2.51	0.43
1:A:103:ASP:O	1:A:146:PRO:HD3	2.19	0.43
1:B:178:THR:O	1:B:179:MET:CB	2.66	0.43
1:A:117:ARG:HE	1:A:119:ARG:NH2	2.17	0.42
1:B:159:CYS:O	2:D:4:GLY:HA3	2.19	0.42
1:A:145:CYS:HB2	1:A:146:PRO:CD	2.50	0.42
1:A:107:VAL:HG22	1:A:113:VAL:HG22	2.00	0.41
1:A:155:ARG:HG3	1:A:170:VAL:HG23	2.02	0.41
1:A:62:LYS:HE2	6:A:1191:GOL:H2	2.03	0.41
1:A:132:VAL:HG22	2:C:9:LEU:HD21	2.03	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	195/203 (96%)	191 (98%)	4 (2%)	0	100	100
1	B	200/203 (98%)	199 (100%)	1 (0%)	0	100	100
2	C	15/21 (71%)	15 (100%)	0	0	100	100
2	D	16/21 (76%)	16 (100%)	0	0	100	100
All	All	426/448 (95%)	421 (99%)	5 (1%)	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	162/164 (99%)	160 (99%)	2 (1%)	63	65
1	B	163/164 (99%)	161 (99%)	2 (1%)	63	65
2	C	14/17 (82%)	14 (100%)	0	100	100
2	D	15/17 (88%)	15 (100%)	0	100	100
All	All	354/362 (98%)	350 (99%)	4 (1%)	63	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-7	ARG
1	A	155	ARG
1	B	-7	ARG
1	B	63	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	B	28	GLN
1	B	34	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 15 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	$\#\|Z\| > 2$
3	BCT	A	1183	-	3,3,3	0.49	0	2,3,3	0.86	0
6	GOL	A	1192[B]	-	5,5,5	0.44	0	5,5,5	0.32	0
6	GOL	A	1190	-	5,5,5	0.20	0	5,5,5	0.83	0
6	GOL	A	1191	-	5,5,5	0.23	0	5,5,5	0.34	0
8	DTT	B	1186	-	7,7,7	0.52	0	4,8,8	1.30	0
6	GOL	A	1192[A]	-	5,5,5	0.31	0	5,5,5	0.29	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
6	GOL	A	1192[B]	-	-	1/4/4/4	-
6	GOL	A	1190	-	-	2/4/4/4	-
6	GOL	A	1191	-	-	2/4/4/4	-
8	DTT	B	1186	-	-	2/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1192[A]	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1190	GOL	C1-C2-C3-O3
6	A	1191	GOL	C1-C2-C3-O3
6	A	1192[A]	GOL	O1-C1-C2-C3
8	B	1186	DTT	C2-C3-C4-S4
8	B	1186	DTT	O3-C3-C4-S4
6	A	1190	GOL	O2-C2-C3-O3
6	A	1191	GOL	O2-C2-C3-O3
6	A	1192[A]	GOL	O1-C1-C2-O2
6	A	1192[A]	GOL	C1-C2-C3-O3
6	A	1192[B]	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1190	GOL	4	0
6	A	1191	GOL	3	0
6	A	1192[A]	GOL	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

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, 95^{th} 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	193/203 (95%)	-1.46	0	100	100	7, 20, 36, 65	6 (3%)
1	B	194/203 (95%)	-1.46	0	100	100	8, 21, 40, 66	8 (4%)
2	C	17/21 (80%)	-1.30	0	100	100	15, 27, 50, 55	0
2	D	18/21 (85%)	-1.26	0	100	100	14, 29, 55, 56	0
All	All	422/448 (94%)	-1.45	0	100	100	7, 21, 43, 66	14 (3%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
6	GOL	A	1192[A]	6/6	0.91	0.07	28,29,30,31	6
6	GOL	A	1192[B]	6/6	0.91	0.07	23,25,26,27	6
6	GOL	A	1190	6/6	0.97	0.14	23,25,27,29	0
3	BCT	A	1183	4/4	0.97	0.06	30,30,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	B	1184	1/1	0.97	0.08	58,58,58,58	0
6	GOL	A	1191	6/6	0.98	0.13	28,29,30,31	0
5	CL	B	1182	1/1	0.98	0.04	45,45,45,45	0
5	CL	B	1183	1/1	0.98	0.05	47,47,47,47	0
5	CL	A	1185	1/1	0.99	0.07	43,43,43,43	0
5	CL	B	1185	1/1	0.99	0.03	28,28,28,28	0
8	DTT	B	1186	8/8	0.99	0.09	38,40,43,49	0
4	K	B	1181	1/1	1.00	0.03	28,28,28,28	0
4	K	B	1188	1/1	1.00	0.02	26,26,26,26	0
4	K	A	1184	1/1	1.00	0.03	23,23,23,23	0
5	CL	A	1186	1/1	1.00	0.02	12,12,12,12	0
5	CL	A	1187	1/1	1.00	0.03	23,23,23,23	0
5	CL	A	1188	1/1	1.00	0.06	33,33,33,33	0
5	CL	A	1189	1/1	1.00	0.03	25,25,25,25	0
7	ZN	A	1193	1/1	1.00	0.01	34,34,34,34	0
7	ZN	B	1187	1/1	1.00	0.01	31,31,31,31	0
4	K	B	1180	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.