Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 06:14 AM EDT

PDB ID	:	6DTD
Title	:	High-resolution crystal structure of Cas13b from Prevotella buccae
Authors	:	Slaymaker, I.M.S.; Zhang, F.Z.
Deposited on	:	2018-06-15
Resolution	:	1.65 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 (i) 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 (i)) were used in the production of this report:

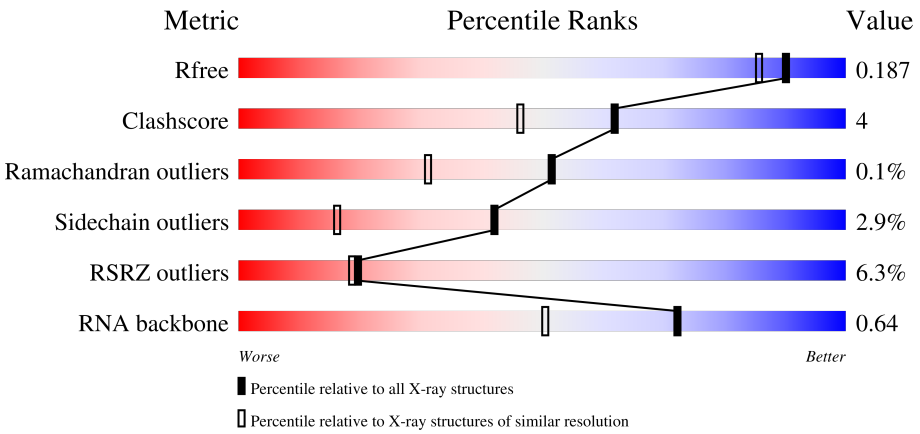
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)
RNA backbone	3102	1011 (2.36-0.96)

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	1127	6% 84% 8% • 7%
2	C	37	65% 35%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	C	101	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19079 atoms, of which 8732 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.

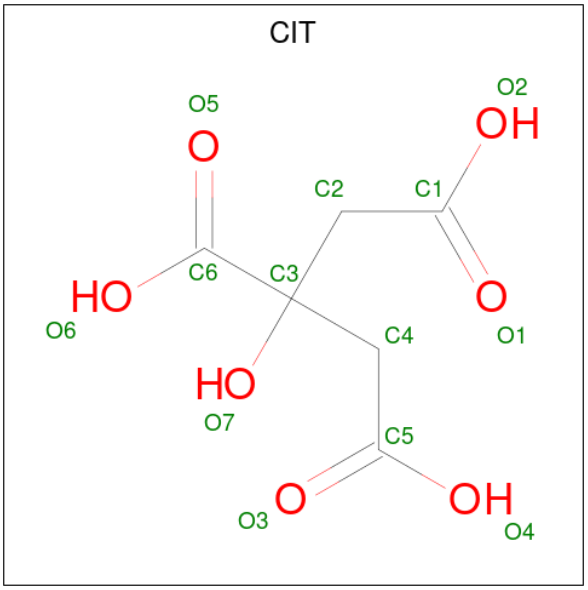
- Molecule 1 is a protein called nuclease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1053	16792	5514	8235	1461	1549	33	0	13	0

- Molecule 2 is a RNA chain called RNA (37-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	C	37	1175	350	395	132	261	37	0	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	18	6	5	7	0	0
			Total	C	H	O		
3	A	1	18	6	5	7	0	0

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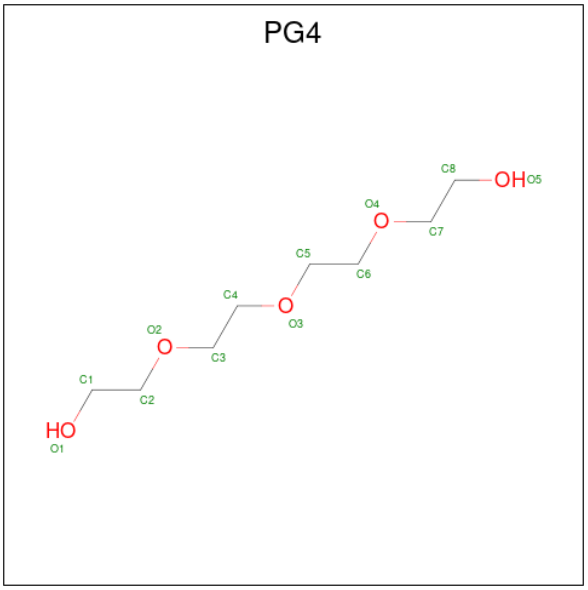
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	18	6	5	7	0	0
			Total	C	H	O		
3	A	1	18	6	5	7	0	0
			Total	C	H	O		
3	A	1	18	6	5	7	0	0
			Total	C	H	O		
3	A	1	18	6	5	7	0	0
			Total	C	H	O		
3	A	1	18	6	5	7	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	31	8	18	5	0	0
			Total	C	H	O		
5	A	1	31	8	18	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	23	6	13	4	0	0
			Total	C	H	O		
5	C	1	31	8	18	5	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	C	2	2	2	0	0

- Molecule 7 is water.

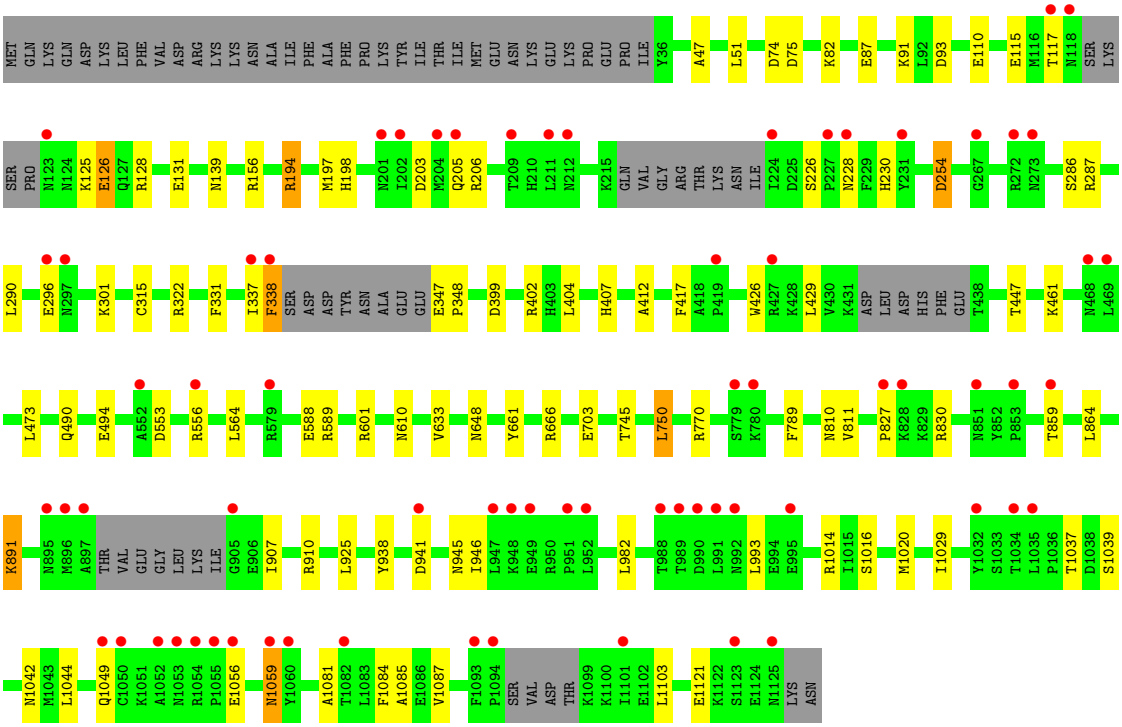
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	695	695	695	0	0
			Total	O		
7	C	171	171	171	0	0

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.

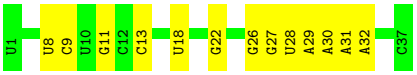
- Molecule 1: nuclease

Chain A:



- Molecule 2: RNA (37-MER)

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.82Å 124.65Å 140.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.65 – 1.65 46.65 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.65-1.65) 86.6 (46.65-1.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.22 (at 1.60Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.153 , 0.185 0.156 , 0.187	Depositor DCC
R_{free} test set	10468 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19079	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, PG4, CL, NA

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	0.61	2/8782 (0.0%)	0.67	7/11876 (0.1%)
2	C	1.17	0/870	1.34	4/1351 (0.3%)
All	All	0.68	2/9652 (0.0%)	0.76	11/13227 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	GLU	CB-CG	-6.14	1.40	1.52
1	A	87	GLU	CD-OE2	-5.16	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	322	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	C	26	G	O5'-P-OP2	-5.77	100.50	105.70
1	A	287	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	750	LEU	CB-CG-CD1	5.61	120.53	111.00
1	A	156	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	C	32	A	N1-C6-N6	5.30	121.78	118.60
1	A	322	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	C	29	A	O4'-C1'-N9	5.28	112.42	108.20
1	A	750	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	589	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	C	8	U	P-O3'-C3'	5.07	125.79	119.70

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	8557	8235	8192	67	0
2	C	780	395	395	8	0
3	A	91	35	35	7	0
4	A	1	0	0	0	0
4	C	1	0	0	6	0
5	A	36	49	49	9	0
5	C	13	18	18	5	0
6	C	2	0	0	0	0
7	A	695	0	0	18	0
7	C	171	0	0	3	0
All	All	10347	8732	8689	80	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 4.

All (80) 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:206:ARG:N	7:A:1301:HOH:O	1.62	1.26
1:A:205:GLN:C	7:A:1301:HOH:O	1.78	1.10
1:A:139:ASN:OD1	7:A:1302:HOH:O	1.74	1.02
1:A:810:ASN:ND2	7:A:1305:HOH:O	1.94	1.01
1:A:407:HIS:ND1	7:A:1306:HOH:O	1.96	0.98
1:A:126:GLU:OE1	7:A:1303:HOH:O	1.81	0.96
1:A:601:ARG:HH22	5:A:1210:PG4:H61	1.30	0.96
1:A:494:GLU:OE1	7:A:1304:HOH:O	1.85	0.93
1:A:206:ARG:CA	7:A:1301:HOH:O	2.07	0.91
2:C:13:C:O2'	5:C:102:PG4:H21	1.81	0.80
4:C:101:CL:CL	7:C:312:HOH:O	2.39	0.77
1:A:402:ARG:NH2	3:A:1205:CIT:O1	2.18	0.76
1:A:941:ASP:OD1	1:A:945:ASN:N	2.19	0.76
2:C:11:G:O6	4:C:101:CL:CL	2.41	0.75
2:C:27:G:O6	4:C:101:CL:CL	2.42	0.74
1:A:490:GLN:OE1	7:A:1307:HOH:O	2.06	0.73
4:C:101:CL:CL	7:C:224:HOH:O	2.46	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:OE2	7:A:1308:HOH:O	2.08	0.71
1:A:588:GLU:OE2	7:A:1309:HOH:O	2.09	0.70
4:C:101:CL:CL	7:C:308:HOH:O	2.47	0.68
1:A:230:HIS:ND1	3:A:1204:CIT:O1	2.26	0.68
1:A:203:ASP:OD2	1:A:206:ARG:N	2.28	0.66
1:A:347:GLU:CB	1:A:348:PRO:CD	2.73	0.66
1:A:601:ARG:HH22	5:A:1210:PG4:C6	2.08	0.64
1:A:198:HIS:NE2	3:A:1206:CIT:O1	2.31	0.64
2:C:28:U:O4	4:C:101:CL:CL	2.53	0.64
1:A:286:SER:OG	5:A:1211:PG4:H71	1.98	0.64
1:A:429:LEU:HD12	1:A:473[B]:LEU:HD13	1.80	0.63
1:A:337:ILE:HG22	1:A:337:ILE:O	1.99	0.62
1:A:1121:GLU:OE2	7:A:1310:HOH:O	2.16	0.61
1:A:194:ARG:HD3	3:A:1206:CIT:O3	2.02	0.59
1:A:93[B]:ASP:OD1	1:A:666:ARG:NE	2.36	0.58
2:C:30:A:N6	5:C:102:PG4:H71	2.19	0.58
2:C:30:A:C6	5:C:102:PG4:H71	2.39	0.58
1:A:407:HIS:CG	7:A:1306:HOH:O	2.52	0.56
1:A:338:PHE:CD2	1:A:338:PHE:N	2.72	0.56
1:A:633[B]:VAL:HG12	1:A:661:TYR:CE2	2.41	0.56
2:C:27:G:H21	5:C:102:PG4:H61	1.71	0.56
1:A:1056:GLU:O	1:A:1059:ASN:ND2	2.38	0.55
1:A:226:SER:OG	1:A:228:ASN:OD1	2.27	0.53
1:A:827:PRO:O	1:A:830:ARG:HG3	2.10	0.51
1:A:461:LYS:NZ	7:A:1327:HOH:O	2.43	0.51
1:A:206:ARG:HA	7:A:1301:HOH:O	1.95	0.50
1:A:553:ASP:OD1	1:A:556:ARG:NH2	2.45	0.50
1:A:811:VAL:O	7:A:1305:HOH:O	2.20	0.50
1:A:315:CYS:HB2	1:A:331:PHE:CZ	2.46	0.50
1:A:117:THR:HG23	1:A:131:GLU:OE2	2.14	0.48
1:A:938:TYR:HB2	1:A:946:ILE:HG23	1.95	0.48
1:A:402:ARG:HH21	3:A:1205:CIT:C1	2.26	0.48
3:A:1206:CIT:O3	3:A:1206:CIT:O7	2.32	0.48
1:A:891:LYS:HD3	1:A:907:ILE:HD11	1.96	0.47
1:A:315:CYS:HB2	1:A:331:PHE:CE1	2.50	0.47
1:A:1016:SER:O	1:A:1020:MET:HG3	2.14	0.47
1:A:128:ARG:NH1	1:A:610:ASN:OD1	2.39	0.47
1:A:1084:PHE:O	1:A:1087:VAL:HG22	2.15	0.47
1:A:286:SER:CB	5:A:1211:PG4:H71	2.46	0.46
1:A:125:LYS:HE3	1:A:610:ASN:HD21	1.81	0.45
1:A:601:ARG:NH2	5:A:1210:PG4:H71	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:GLU:HG2	7:A:1316:HOH:O	2.16	0.45
1:A:301:LYS:NZ	5:A:1209:PG4:H82	2.31	0.45
1:A:301:LYS:HZ2	5:A:1209:PG4:H82	1.82	0.44
1:A:347:GLU:CB	1:A:348:PRO:HD3	2.45	0.44
1:A:1081:ALA:O	1:A:1085:ALA:HB2	2.17	0.44
1:A:601:ARG:NH2	5:A:1210:PG4:H61	2.13	0.44
1:A:1039:SER:HB3	1:A:1042:ASN:HB2	2.00	0.44
2:C:13:C:H1'	5:C:102:PG4:H61	1.99	0.43
1:A:1029:ILE:HD12	1:A:1037:THR:HG22	2.00	0.43
1:A:426:TRP:CE3	1:A:473[A]:LEU:HD21	2.54	0.42
1:A:347:GLU:N	7:A:1342:HOH:O	2.52	0.42
1:A:770:ARG:NH2	1:A:789:PHE:O	2.52	0.42
1:A:982:LEU:HD21	1:A:1103:LEU:HD23	2.02	0.41
1:A:412:ALA:HB3	1:A:417:PHE:CE2	2.56	0.41
1:A:601:ARG:HH22	5:A:1210:PG4:H71	1.85	0.41
3:A:1202:CIT:C6	3:A:1202:CIT:O3	2.68	0.41
1:A:47:ALA:HB1	1:A:1014[A]:ARG:HD2	2.02	0.41
1:A:197:MET:SD	1:A:830:ARG:NH2	2.94	0.41
1:A:254:ASP:OD2	1:A:290:LEU:HD12	2.21	0.40
1:A:337:ILE:HD13	1:A:337:ILE:HA	1.92	0.40
1:A:1044:LEU:HD23	1:A:1044:LEU:HA	1.90	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	1052/1127 (93%)	1030 (98%)	21 (2%)	1 (0%)	51 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	GLU

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	876/1039 (84%)	851 (97%)	25 (3%)	42 16

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	74	ASP
1	A	75	ASP
1	A	82	LYS
1	A	91	LYS
1	A	115	GLU
1	A	126	GLU
1	A	194	ARG
1	A	254	ASP
1	A	338	PHE
1	A	399	ASP
1	A	404	LEU
1	A	447	THR
1	A	564	LEU
1	A	648	ASN
1	A	745	THR
1	A	750	LEU
1	A	859	THR
1	A	864	LEU
1	A	891	LYS
1	A	910	ARG
1	A	925	LEU
1	A	993	LEU
1	A	1049	GLN
1	A	1059	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	36/37 (97%)	4 (11%)	1 (2%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	9	C
2	C	18	U
2	C	22	G
2	C	31	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	31	A

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	PG4	A	1211	-	9,9,12	0.56	0	8,8,11	0.38	0
3	CIT	A	1204	-	12,12,12	1.21	0	17,17,17	1.58	3 (17%)
3	CIT	A	1202	-	12,12,12	1.04	1 (8%)	17,17,17	1.63	4 (23%)
5	PG4	A	1209	-	12,12,12	0.58	0	11,11,11	0.54	0
3	CIT	A	1206	-	12,12,12	1.16	0	17,17,17	1.56	3 (17%)
3	CIT	A	1201	-	12,12,12	1.06	0	17,17,17	1.63	3 (17%)
3	CIT	A	1207	-	12,12,12	1.09	0	17,17,17	1.54	3 (17%)
3	CIT	A	1205	-	12,12,12	1.15	0	17,17,17	1.72	3 (17%)
3	CIT	A	1203	-	12,12,12	1.11	0	17,17,17	1.44	3 (17%)
5	PG4	A	1210	-	12,12,12	0.57	0	11,11,11	0.50	0
5	PG4	C	102	-	12,12,12	0.55	0	11,11,11	0.96	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
5	PG4	A	1211	-	-	4/7/7/10	-
3	CIT	A	1204	-	-	5/16/16/16	-
3	CIT	A	1202	-	-	0/16/16/16	-
5	PG4	A	1209	-	-	5/10/10/10	-
3	CIT	A	1206	-	-	8/16/16/16	-
3	CIT	A	1201	-	-	0/16/16/16	-
3	CIT	A	1207	-	-	4/16/16/16	-
3	CIT	A	1205	-	-	3/16/16/16	-
3	CIT	A	1203	-	-	0/16/16/16	-
5	PG4	A	1210	-	-	6/10/10/10	-
5	PG4	C	102	-	-	5/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	CIT	C3-C6	2.10	1.55	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1205	CIT	O6-C6-C3	4.51	121.79	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1201	CIT	O6-C6-C3	3.71	120.25	113.14
3	A	1204	CIT	O6-C6-C3	3.64	120.12	113.14
3	A	1202	CIT	O6-C6-C3	3.50	119.86	113.14
3	A	1207	CIT	O6-C6-C3	3.16	119.21	113.14
3	A	1206	CIT	C3-C4-C5	-2.96	105.84	113.92
3	A	1206	CIT	O6-C6-C3	2.93	118.75	113.14
3	A	1204	CIT	C3-C2-C1	-2.86	106.09	113.92
3	A	1207	CIT	C2-C3-C6	-2.72	104.02	110.03
3	A	1203	CIT	O6-C6-C3	2.69	118.29	113.14
3	A	1206	CIT	C3-C2-C1	-2.56	106.91	113.92
3	A	1207	CIT	C4-C3-C2	2.52	115.78	109.31
3	A	1205	CIT	C3-C2-C1	-2.43	107.27	113.92
3	A	1203	CIT	O7-C3-C6	2.35	112.29	108.96
3	A	1205	CIT	O2-C1-C2	2.33	121.72	114.35
3	A	1202	CIT	O3-C5-C4	-2.30	116.44	122.95
3	A	1201	CIT	O7-C3-C6	-2.27	105.73	108.96
3	A	1202	CIT	C4-C3-C2	-2.21	103.65	109.31
3	A	1203	CIT	C2-C3-C6	-2.19	105.18	110.03
3	A	1204	CIT	O2-C1-C2	2.17	121.22	114.35
3	A	1202	CIT	O2-C1-C2	2.07	120.91	114.35
3	A	1201	CIT	O7-C3-C4	2.06	114.08	109.38

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	CIT	C2-C3-C4-C5
3	A	1205	CIT	C2-C3-C4-C5
3	A	1205	CIT	O7-C3-C4-C5
3	A	1206	CIT	C2-C3-C6-O5
3	A	1206	CIT	C2-C3-C6-O6
3	A	1206	CIT	O7-C3-C6-O5
3	A	1206	CIT	O7-C3-C6-O6
5	C	102	PG4	C4-C3-O2-C2
3	A	1204	CIT	C6-C3-C4-C5
5	C	102	PG4	C6-C5-O3-C4
5	A	1210	PG4	O3-C5-C6-O4
5	A	1210	PG4	C4-C3-O2-C2
5	A	1211	PG4	O2-C3-C4-O3
5	A	1210	PG4	O2-C3-C4-O3
5	A	1209	PG4	O1-C1-C2-O2
3	A	1205	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	A	1210	PG4	O4-C7-C8-O5
3	A	1204	CIT	O7-C3-C4-C5
5	C	102	PG4	O4-C7-C8-O5
5	A	1209	PG4	C6-C5-O3-C4
5	A	1210	PG4	C8-C7-O4-C6
5	A	1210	PG4	C6-C5-O3-C4
5	A	1209	PG4	O3-C5-C6-O4
3	A	1206	CIT	O2-C1-C2-C3
5	A	1211	PG4	C3-C4-O3-C5
3	A	1206	CIT	O1-C1-C2-C3
5	A	1209	PG4	C1-C2-O2-C3
3	A	1206	CIT	O7-C3-C4-C5
3	A	1207	CIT	C3-C4-C5-O4
3	A	1207	CIT	C1-C2-C3-C4
3	A	1207	CIT	C3-C4-C5-O3
3	A	1206	CIT	C2-C3-C4-C5
3	A	1207	CIT	O7-C3-C4-C5
5	C	102	PG4	C8-C7-O4-C6
5	C	102	PG4	O3-C5-C6-O4
5	A	1211	PG4	O4-C7-C8-O5
3	A	1204	CIT	O1-C1-C2-C3
5	A	1211	PG4	O3-C5-C6-O4
3	A	1204	CIT	O2-C1-C2-C3
5	A	1209	PG4	C8-C7-O4-C6

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1211	PG4	2	0
3	A	1204	CIT	1	0
3	A	1202	CIT	1	0
5	A	1209	PG4	2	0
3	A	1206	CIT	3	0
3	A	1205	CIT	2	0
5	A	1210	PG4	5	0
5	C	102	PG4	5	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	1053/1127 (93%)	0.05	69 (6%) 18 17	24, 39, 77, 96	0
2	C	37/37 (100%)	-0.47	0 100 100	25, 30, 44, 57	0
All	All	1090/1164 (93%)	0.03	69 (6%) 20 19	24, 39, 77, 96	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PHE	8.0
1	A	991	LEU	6.2
1	A	1093	PHE	6.1
1	A	227	PRO	5.5
1	A	905	GLY	5.4
1	A	224	ILE	5.0
1	A	779	SER	5.0
1	A	827	PRO	4.9
1	A	990	ASP	4.7
1	A	123	ASN	4.6
1	A	896	MET	4.4
1	A	228	ASN	4.4
1	A	851	ASN	4.3
1	A	897	ALA	4.2
1	A	296	GLU	4.1
1	A	205	GLN	4.1
1	A	117	THR	4.0
1	A	1094	PRO	4.0
1	A	204	MET	3.9
1	A	337	ILE	3.7
1	A	947	LEU	3.7
1	A	988	THR	3.5
1	A	297	ASN	3.3
1	A	828	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	859	THR	3.1
1	A	209	THR	3.0
1	A	201	ASN	3.0
1	A	992	ASN	3.0
1	A	853	PRO	2.9
1	A	895	ASN	2.8
1	A	948	LYS	2.8
1	A	469	LEU	2.8
1	A	273	ASN	2.7
1	A	952	LEU	2.7
1	A	1101	ILE	2.7
1	A	272	ARG	2.7
1	A	468	ASN	2.7
1	A	780	LYS	2.7
1	A	202	ILE	2.6
1	A	552	ALA	2.6
1	A	579	ARG	2.6
1	A	1052	ALA	2.5
1	A	212	ASN	2.5
1	A	1123	SER	2.5
1	A	556	ARG	2.5
1	A	1082	THR	2.5
1	A	1054	ARG	2.4
1	A	989	THR	2.4
1	A	1125	ASN	2.4
1	A	1032	TYR	2.3
1	A	949	GLU	2.3
1	A	941	ASP	2.3
1	A	211	LEU	2.3
1	A	1056	GLU	2.2
1	A	118	ASN	2.2
1	A	1060	TYR	2.2
1	A	267	GLY	2.2
1	A	231	TYR	2.2
1	A	427	ARG	2.1
1	A	1035	LEU	2.1
1	A	1059	ASN	2.1
1	A	951	PRO	2.1
1	A	995	GLU	2.1
1	A	1050	CYS	2.1
1	A	1049	GLN	2.0
1	A	1053	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1034	THR	2.0
1	A	419	PRO	2.0
1	A	1055	PRO	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
5	PG4	A	1211	10/13	0.50	0.27	97,117,119,121	0
3	CIT	A	1205	13/13	0.59	0.25	101,103,124,124	0
3	CIT	A	1206	13/13	0.65	0.26	95,97,115,118	0
5	PG4	A	1209	13/13	0.70	0.25	89,108,121,122	0
5	PG4	A	1210	13/13	0.71	0.21	83,100,112,113	0
3	CIT	A	1203	13/13	0.76	0.14	63,72,85,86	0
3	CIT	A	1207	13/13	0.81	0.20	69,91,111,111	0
3	CIT	A	1204	13/13	0.85	0.34	76,85,103,103	0
6	NA	C	104	1/1	0.88	0.10	53,53,53,53	0
5	PG4	C	102	13/13	0.90	0.14	65,82,99,99	0
6	NA	C	103	1/1	0.93	0.18	60,60,60,60	0
3	CIT	A	1201	13/13	0.94	0.07	43,50,60,60	0
3	CIT	A	1202	13/13	0.98	0.06	38,41,48,48	0
4	CL	A	1208	1/1	0.99	0.10	40,40,40,40	0
4	CL	C	101	1/1	0.99	0.04	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.