



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2017 – 01:19 pm GMT

PDB ID : 5ITC
Title : 2.2-Angstrom in meso crystal structure of Haloquadratum Walsbyi Bacteriorhodopsin (HwBR) from Styrene Maleic Acid (SMA) Polymer Nanodiscs
Authors : Broecker, J.; Eger, B.T.; Ernst, O.P.
Deposited on : 2016-03-16
Resolution : 2.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	recalc29047
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc29047

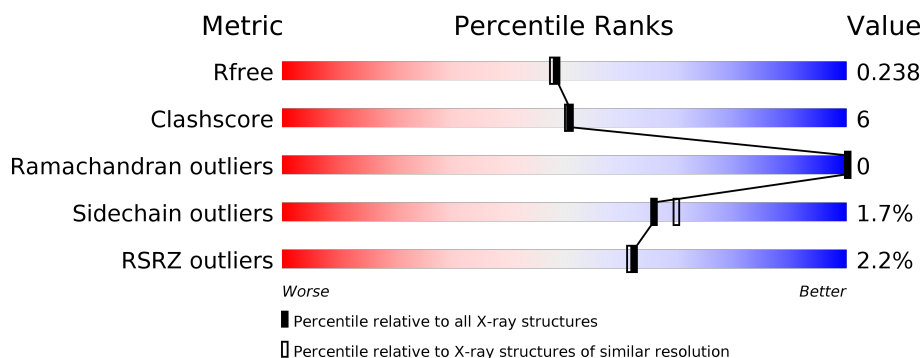
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	268	<div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	268	<div> <div> <div></div> <div>74%</div> <div>11%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	268	<div> <div> <div></div> <div>74%</div> <div>10%</div> <div>15%</div> </div> </div>

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
3	OLC	A	302	-	-	-	X
3	OLC	A	304	-	-	-	X
3	OLC	C	303	-	-	-	X
4	OLB	A	303	-	-	-	X
4	OLB	A	305	-	-	-	X
4	OLB	A	306	-	-	-	X
4	OLB	B	302	-	-	-	X
4	OLB	C	302	-	-	-	X
4	OLB	C	304	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5831 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 Bacteriorhodopsin-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	5	0
			1788	1191	274	316	7			
1	B	228	Total	C	N	O	S	0	5	0
			1780	1189	270	314	7			
1	C	228	Total	C	N	O	S	0	6	0
			1792	1195	275	315	7			

There are 48 discrepancies between the modelled and reference sequences:

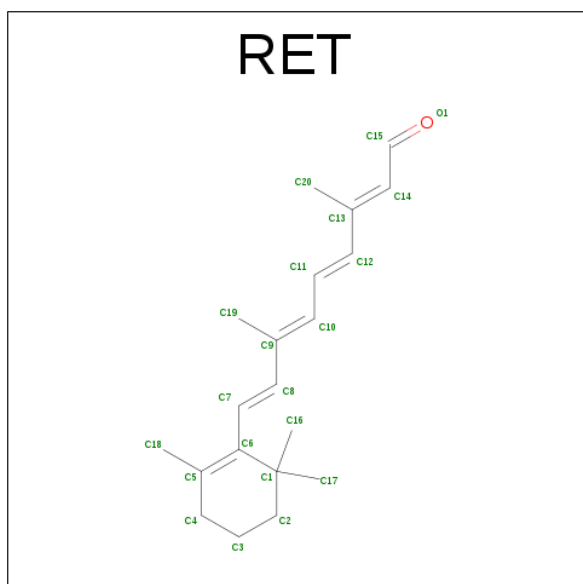
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q18DH8
A	2	ALA	-	expression tag	UNP Q18DH8
A	255	HIS	-	expression tag	UNP Q18DH8
A	256	HIS	-	expression tag	UNP Q18DH8
A	257	HIS	-	expression tag	UNP Q18DH8
A	258	HIS	-	expression tag	UNP Q18DH8
A	259	HIS	-	expression tag	UNP Q18DH8
A	260	HIS	-	expression tag	UNP Q18DH8
A	261	LEU	-	expression tag	UNP Q18DH8
A	262	GLU	-	expression tag	UNP Q18DH8
A	263	HIS	-	expression tag	UNP Q18DH8
A	264	HIS	-	expression tag	UNP Q18DH8
A	265	HIS	-	expression tag	UNP Q18DH8
A	266	HIS	-	expression tag	UNP Q18DH8
A	267	HIS	-	expression tag	UNP Q18DH8
A	268	HIS	-	expression tag	UNP Q18DH8
B	1	MET	-	initiating methionine	UNP Q18DH8
B	2	ALA	-	expression tag	UNP Q18DH8
B	255	HIS	-	expression tag	UNP Q18DH8
B	256	HIS	-	expression tag	UNP Q18DH8
B	257	HIS	-	expression tag	UNP Q18DH8
B	258	HIS	-	expression tag	UNP Q18DH8
B	259	HIS	-	expression tag	UNP Q18DH8

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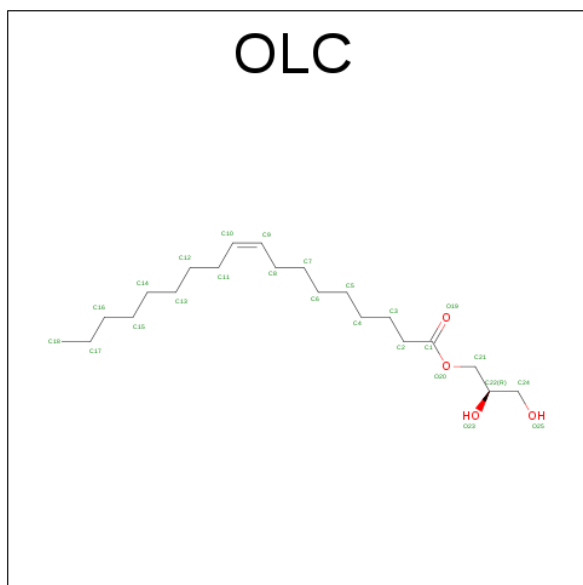
Chain	Residue	Modelled	Actual	Comment	Reference
B	260	HIS	-	expression tag	UNP Q18DH8
B	261	LEU	-	expression tag	UNP Q18DH8
B	262	GLU	-	expression tag	UNP Q18DH8
B	263	HIS	-	expression tag	UNP Q18DH8
B	264	HIS	-	expression tag	UNP Q18DH8
B	265	HIS	-	expression tag	UNP Q18DH8
B	266	HIS	-	expression tag	UNP Q18DH8
B	267	HIS	-	expression tag	UNP Q18DH8
B	268	HIS	-	expression tag	UNP Q18DH8
C	1	MET	-	initiating methionine	UNP Q18DH8
C	2	ALA	-	expression tag	UNP Q18DH8
C	255	HIS	-	expression tag	UNP Q18DH8
C	256	HIS	-	expression tag	UNP Q18DH8
C	257	HIS	-	expression tag	UNP Q18DH8
C	258	HIS	-	expression tag	UNP Q18DH8
C	259	HIS	-	expression tag	UNP Q18DH8
C	260	HIS	-	expression tag	UNP Q18DH8
C	261	LEU	-	expression tag	UNP Q18DH8
C	262	GLU	-	expression tag	UNP Q18DH8
C	263	HIS	-	expression tag	UNP Q18DH8
C	264	HIS	-	expression tag	UNP Q18DH8
C	265	HIS	-	expression tag	UNP Q18DH8
C	266	HIS	-	expression tag	UNP Q18DH8
C	267	HIS	-	expression tag	UNP Q18DH8
C	268	HIS	-	expression tag	UNP Q18DH8

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



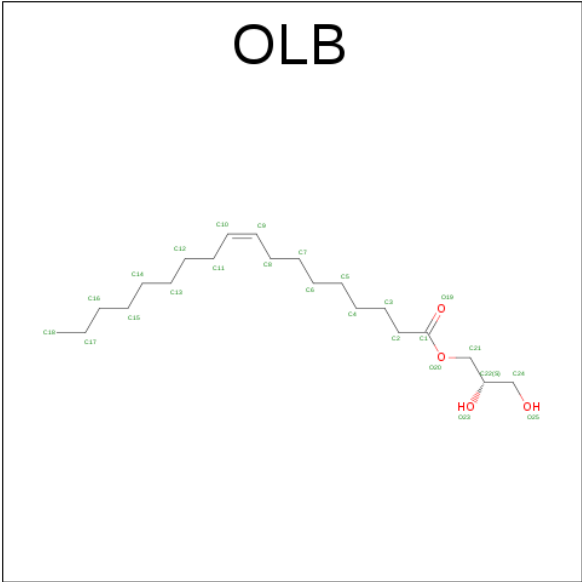
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 20 20	0	0
2	B	1	Total C 20 20	0	0
2	C	1	Total C 20 20	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	C	1	Total C O 25 21 4	0	0

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	B	1	Total	C	O	0	0
			25	21	4		
4	B	1	Total	C	O	0	0
			25	21	4		
4	C	1	Total	C	O	0	0
			25	21	4		
4	C	1	Total	C	O	0	0
			25	21	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	52	Total	O	0	0
			52	52		
5	C	52	Total	O	0	0
			52	52		

- Molecule 1: Bacteriorhodopsin-I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 61.59Å 119.09Å 90.00° 116.16° 90.00°	Depositor
Resolution (Å)	33.43 – 2.00 33.43 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.43-2.00) 93.9 (33.43-2.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.200 , 0.239 0.201 , 0.238	Depositor DCC
R_{free} test set	2298 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5831	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLB, OLC, RET

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	0.75	0/1839	0.84	2/2509 (0.1%)
1	B	0.71	0/1834	0.83	0/2504
1	C	0.74	0/1846	0.87	1/2519 (0.0%)
All	All	0.73	0/5519	0.85	3/7532 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLY	N-CA-C	6.55	129.47	113.10
1	A	93	ASP	CB-CG-OD1	5.79	123.52	118.30
1	C	93	ASP	CB-CG-OD1	5.47	123.22	118.30

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	1788	0	1841	24	0
1	B	1780	0	1840	23	0
1	C	1792	0	1852	22	0
2	A	20	0	27	3	0
2	B	20	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	27	3	0
3	A	50	0	80	2	0
3	C	25	0	40	6	0
4	A	75	0	120	11	0
4	B	50	0	80	5	0
4	C	50	0	80	6	0
5	A	57	0	0	1	0
5	B	52	0	0	0	0
5	C	52	0	0	0	0
All	All	5831	0	6014	76	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 6.

All (76) 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:C:114:ARG:HB3	3:C:303:OLC:H21A	1.53	0.90
1:A:128:VAL:HG11	4:C:302:OLB:H31	1.58	0.86
1:C:13:VAL:HG12	1:C:14:GLU:HG3	1.63	0.80
4:A:306:OLB:H32	1:B:95:LEU:HD11	1.68	0.75
4:A:306:OLB:H37	1:B:95:LEU:HD21	1.68	0.73
4:A:306:OLB:H17	1:B:99:PRO:HB2	1.72	0.70
1:A:48:GLU:OE1	4:A:305:OLB:H22	1.93	0.69
1:B:174:ASP:OD2	1:B:235:ARG:NH1	2.27	0.67
4:B:303:OLB:H3A	1:C:155:PHE:HE2	1.64	0.63
1:B:119:LEU:HD22	1:B:156:LEU:HD12	1.81	0.62
1:C:72:GLY:HA2	1:C:88:TRP:CE2	2.36	0.61
2:A:301:RET:H161	2:A:301:RET:H8	1.79	0.61
1:A:113:GLN:HG3	4:A:303:OLB:H2A	1.81	0.60
1:A:100:LEU:HD21	4:A:305:OLB:H18	1.84	0.60
1:A:94:TRP:CD1	2:A:301:RET:H14	2.37	0.59
1:B:119:LEU:HD22	1:B:156:LEU:CD1	2.34	0.57
1:B:47:LYS:HE2	4:B:303:OLB:O23	2.05	0.57
1:A:152:SER:HB3	4:C:304:OLB:H221	1.88	0.55
1:C:114:ARG:HB3	3:C:303:OLC:C21	2.32	0.55
1:B:94:TRP:CD1	2:B:301:RET:H14	2.41	0.55
1:A:114:ARG:NH1	5:A:401:HOH:O	2.28	0.54
1:C:72:GLY:HA2	1:C:88:TRP:CZ2	2.43	0.54
1:C:146:TRP:CE2	1:C:198:LEU:HD13	2.44	0.53
1:C:119:LEU:HG	1:C:159:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235[B]:ARG:HA	1:A:238:MET:HE2	1.92	0.52
1:A:235[A]:ARG:HA	1:A:238:MET:HE2	1.91	0.52
2:B:301:RET:H161	2:B:301:RET:H8	1.91	0.52
1:A:13:VAL:HG12	1:A:14:GLU:HG3	1.92	0.51
1:A:107:LEU:HD21	4:A:303:OLB:H21	1.92	0.51
1:A:47:LYS:NZ	3:A:302:OLC:O25	2.44	0.51
1:B:185:ILE:O	1:B:189:THR:HG23	2.12	0.50
4:A:306:OLB:H32	1:B:95:LEU:HD21	1.93	0.49
1:C:218:VAL:O	1:C:222:VAL:HG12	2.13	0.49
1:C:55:LEU:HD21	4:C:302:OLB:H19	1.94	0.49
1:A:63[B]:SER:OG	1:A:93:ASP:HB2	2.13	0.48
1:B:119:LEU:HG	1:B:159:TYR:CE1	2.48	0.48
1:B:80:ASN:HB3	1:B:82:ARG:H	1.78	0.48
1:C:146:TRP:CD1	1:C:197:TRP:CE3	3.02	0.48
1:C:118:ALA:HA	3:C:303:OLC:H2A	1.96	0.48
1:B:38:GLY:HA3	4:B:303:OLB:H24	1.95	0.47
1:B:132:VAL:O	1:B:136[B]:THR:HG23	2.14	0.47
1:C:94:TRP:CD1	2:C:301:RET:H14	2.49	0.47
1:A:121:GLY:HA2	4:C:302:OLB:H18	1.95	0.47
2:C:301:RET:H8	2:C:301:RET:H161	1.97	0.47
1:A:158:TYR:HD1	3:A:304:OLC:H3A	1.80	0.46
1:A:122:ILE:HG12	4:C:304:OLB:H5	1.98	0.46
1:B:59:ILE:HG23	3:C:303:OLC:H15A	1.97	0.46
1:C:80:ASN:HB3	1:C:82:ARG:H	1.80	0.46
1:C:128:VAL:HG11	3:C:303:OLC:H16A	1.98	0.45
1:A:96:PHE:CZ	4:A:306:OLB:H35	2.51	0.45
4:B:303:OLB:H241	4:B:303:OLB:H20	1.71	0.45
1:A:73:LEU:HB2	1:A:87:TYR:CE1	2.52	0.45
2:A:301:RET:H7	2:A:301:RET:H181	1.73	0.45
1:B:11:LEU:HB3	1:B:12:GLY:H	1.46	0.44
2:C:301:RET:H181	2:C:301:RET:H7	1.76	0.44
1:A:108:LEU:HD22	1:A:182:LEU:HD12	1.99	0.44
1:C:119:LEU:HA	1:C:119:LEU:HD23	1.80	0.44
4:A:305:OLB:H34	1:B:128:VAL:HG11	2.00	0.43
1:C:48:GLU:OE1	4:C:302:OLB:H21	2.18	0.43
1:B:160:LEU:O	1:B:164:PHE:HB2	2.17	0.43
4:B:302:OLB:H18	4:B:302:OLB:H4A	1.76	0.43
1:A:11:LEU:HD23	1:A:68:PHE:CE1	2.54	0.42
1:C:118:ALA:HB3	1:C:159:TYR:OH	2.18	0.42
1:C:84:VAL:HG13	1:C:201[A]:THR:HG23	2.01	0.42
1:C:160:LEU:O	1:C:164:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:O	1:A:189:THR:HG23	2.19	0.42
1:C:128:VAL:CG1	3:C:303:OLC:H16A	2.49	0.42
1:A:159:TYR:C	1:A:159:TYR:CD1	2.94	0.41
1:B:146:TRP:CD1	1:B:197:TRP:CE3	3.09	0.41
1:A:78:LEU:HD12	1:A:82:ARG:HB3	2.02	0.41
1:B:53:THR:O	1:B:57:PRO:HD2	2.21	0.41
1:B:40:ASP:O	1:B:42:GLN:NE2	2.54	0.41
1:A:43:ASP:HA	1:A:44:PRO:HD3	1.87	0.41
1:B:118:ALA:HB3	1:B:159:TYR:OH	2.21	0.41
1:C:43:ASP:HA	1:C:44:PRO:HD3	1.92	0.40
4:A:306:OLB:H24	1:B:113:GLN:HA	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	231/268 (86%)	231 (100%)	0	0	100	100
1	B	231/268 (86%)	230 (100%)	1 (0%)	0	100	100
1	C	232/268 (87%)	232 (100%)	0	0	100	100
All	All	694/804 (86%)	693 (100%)	1 (0%)	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	186/213 (87%)	183 (98%)	3 (2%)	68	72
1	B	186/213 (87%)	183 (98%)	3 (2%)	68	72
1	C	187/213 (88%)	184 (98%)	3 (2%)	68	72
All	All	559/639 (88%)	550 (98%)	9 (2%)	66	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	104	ASP
1	A	159	TYR
1	B	47	LYS
1	B	104	ASP
1	B	159	TYR
1	C	104	ASP
1	C	156	LEU
1	C	159	TYR

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	RET	A	301	1	19,20,21	0.73	1 (5%)	27,27,28	1.40	4 (14%)
3	OLC	A	302	-	24,24,24	0.94	1 (4%)	25,25,25	1.04	1 (4%)
4	OLB	A	303	-	24,24,24	0.92	1 (4%)	25,25,25	1.10	1 (4%)
3	OLC	A	304	-	24,24,24	0.90	1 (4%)	25,25,25	1.06	1 (4%)
4	OLB	A	305	-	24,24,24	0.97	1 (4%)	25,25,25	1.21	1 (4%)
4	OLB	A	306	-	24,24,24	0.94	1 (4%)	25,25,25	1.05	1 (4%)
2	RET	B	301	1	19,20,21	0.77	1 (5%)	27,27,28	1.56	4 (14%)
4	OLB	B	302	-	24,24,24	0.92	1 (4%)	25,25,25	1.13	1 (4%)
4	OLB	B	303	-	24,24,24	0.95	1 (4%)	25,25,25	0.94	1 (4%)
2	RET	C	301	1	19,20,21	0.84	1 (5%)	27,27,28	1.78	7 (25%)
4	OLB	C	302	-	24,24,24	0.96	1 (4%)	25,25,25	0.99	1 (4%)
3	OLC	C	303	-	24,24,24	0.99	1 (4%)	25,25,25	1.14	1 (4%)
4	OLB	C	304	-	24,24,24	0.89	1 (4%)	25,25,25	0.85	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	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	OLC	A	302	-	-	0/24/24/24	0/0/0/0
4	OLB	A	303	-	-	0/24/24/24	0/0/0/0
3	OLC	A	304	-	-	0/24/24/24	0/0/0/0
4	OLB	A	305	-	-	0/24/24/24	0/0/0/0
4	OLB	A	306	-	-	0/24/24/24	0/0/0/0
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
4	OLB	B	302	-	-	0/24/24/24	0/0/0/0
4	OLB	B	303	-	-	0/24/24/24	0/0/0/0
2	RET	C	301	1	-	0/13/30/31	0/1/1/1
4	OLB	C	302	-	-	0/24/24/24	0/0/0/0
3	OLC	C	303	-	-	0/24/24/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLB	C	304	-	-	0/24/24/24	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C11-C10	-2.47	1.36	1.43
2	C	301	RET	C11-C10	-2.45	1.36	1.43
2	B	301	RET	C11-C10	-2.36	1.36	1.43
4	C	304	OLB	O20-C1	3.37	1.43	1.33
4	A	303	OLB	O20-C1	3.43	1.43	1.33
3	A	304	OLC	O20-C1	3.44	1.43	1.33
4	B	302	OLB	O20-C1	3.48	1.43	1.33
3	A	302	OLC	O20-C1	3.50	1.43	1.33
4	A	306	OLB	O20-C1	3.51	1.43	1.33
4	B	303	OLB	O20-C1	3.53	1.43	1.33
4	C	302	OLB	O20-C1	3.54	1.43	1.33
3	C	303	OLC	O20-C1	3.70	1.44	1.33
4	A	305	OLB	O20-C1	3.70	1.44	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	RET	C18-C5-C6	-4.57	119.40	124.51
2	C	301	RET	C3-C4-C5	-3.85	107.17	113.78
2	A	301	RET	C18-C5-C6	-3.62	120.46	124.51
2	B	301	RET	C3-C4-C5	-2.95	108.71	113.78
2	C	301	RET	C7-C6-C5	-2.38	115.87	121.54
2	B	301	RET	C18-C5-C6	-2.31	121.93	124.51
2	C	301	RET	C10-C11-C12	-2.30	116.18	123.23
2	B	301	RET	C2-C3-C4	-2.14	106.26	111.34
2	A	301	RET	C2-C1-C6	2.06	113.70	110.48
4	B	303	OLB	O20-C1-C2	2.15	118.17	111.90
2	C	301	RET	C1-C6-C7	2.24	122.01	115.73
2	A	301	RET	C1-C6-C7	2.37	122.38	115.73
4	C	302	OLB	O20-C1-C2	2.43	118.96	111.90
2	C	301	RET	C19-C9-C8	2.43	121.97	118.10
2	C	301	RET	C20-C13-C12	2.52	122.11	118.10
2	A	301	RET	C20-C13-C12	2.94	122.78	118.10
3	A	302	OLC	O20-C1-C2	2.95	120.48	111.90
3	A	304	OLC	O20-C1-C2	3.01	120.67	111.90
4	A	306	OLB	O20-C1-C2	3.21	121.24	111.90
3	C	303	OLC	C21-O20-C1	3.34	127.19	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	OLB	O20-C1-C2	3.42	121.86	111.90
4	B	302	OLB	O20-C1-C2	3.60	122.36	111.90
4	A	305	OLB	C21-O20-C1	3.98	129.11	117.13
2	B	301	RET	C20-C13-C12	4.17	124.75	118.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	3	0
3	A	302	OLC	1	0
4	A	303	OLB	2	0
3	A	304	OLC	1	0
4	A	305	OLB	3	0
4	A	306	OLB	6	0
2	B	301	RET	2	0
4	B	302	OLB	1	0
4	B	303	OLB	4	0
2	C	301	RET	3	0
4	C	302	OLB	4	0
3	C	303	OLC	6	0
4	C	304	OLB	2	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	228/268 (85%)	0.02	4 (1%) 69 68	15, 22, 37, 60	0
1	B	228/268 (85%)	0.05	4 (1%) 69 68	16, 23, 39, 56	0
1	C	228/268 (85%)	0.05	7 (3%) 49 49	16, 22, 36, 59	0
All	All	684/804 (85%)	0.04	15 (2%) 62 61	15, 22, 38, 60	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	LEU	6.1
1	B	11	LEU	5.3
1	B	42	GLN	4.2
1	C	12	GLY	4.2
1	A	40	ASP	3.8
1	C	40	ASP	3.8
1	C	170[A]	ASP	3.1
1	A	11	LEU	2.8
1	A	12	GLY	2.7
1	B	13	VAL	2.5
1	C	42[A]	GLN	2.4
1	C	155	PHE	2.4
1	B	235	ARG	2.3
1	A	42	GLN	2.2
1	C	127	ILE	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 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
4	OLB	A	303	25/25	0.61	0.29	10.05	45,50,60,61	0
4	OLB	A	305	25/25	0.59	0.28	9.17	41,49,63,63	0
4	OLB	A	306	25/25	0.64	0.29	8.89	49,56,58,59	0
4	OLB	C	302	25/25	0.66	0.29	8.75	47,50,61,61	0
3	OLC	C	303	25/25	0.44	0.31	7.96	46,47,53,56	0
4	OLB	B	302	25/25	0.72	0.24	6.39	45,57,62,64	0
3	OLC	A	304	25/25	0.66	0.21	4.72	47,49,59,59	0
3	OLC	A	302	25/25	0.77	0.18	2.65	43,49,56,58	0
4	OLB	C	304	25/25	0.84	0.18	2.59	39,47,52,54	0
4	OLB	B	303	25/25	0.75	0.18	1.98	34,46,53,55	0
2	RET	A	301	20/21	0.93	0.11	0.41	13,16,20,23	0
2	RET	C	301	20/21	0.93	0.12	0.39	13,17,20,21	0
2	RET	B	301	20/21	0.92	0.10	-0.14	8,19,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.