



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2022 – 12:16 PM JST

PDB ID : 7VGV  
Title : Anion free form of light-driven chloride ion-pumping rhodopsin, NM-R3, structure determined by serial femtosecond crystallography at SACLA  
Authors : Hosaka, T.; Nango, E.; Nakane, T.; Luo, F.; Kimura-Someya, T.; Shirouzu, M.  
Deposited on : 2021-09-18  
Resolution : 2.30 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
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)	:	2.26

**i**

## X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
--------	-----------------	-------

 $R_{free}$ 

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.

1

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DD9	A	304	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6440 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.

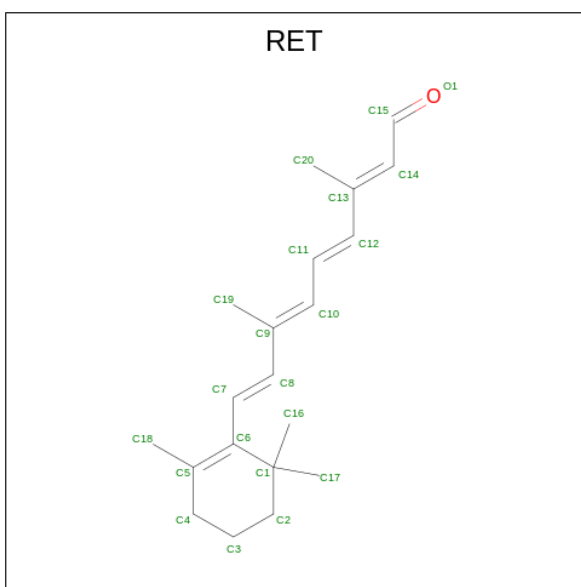
- Molecule 1 is a protein called Chloride pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2067	1374	320	359	14			
1	B	263	Total	C	N	O	S	0	0	0
			2057	1367	318	358	14			
1	C	264	Total	C	N	O	S	0	0	0
			2069	1375	321	359	14			

There are 21 discrepancies between the modelled and reference sequences:

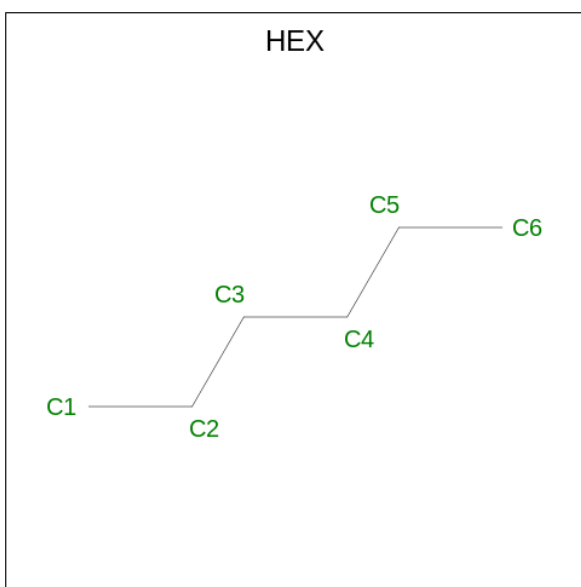
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP W8VZW3
A	-5	SER	-	expression tag	UNP W8VZW3
A	-4	SER	-	expression tag	UNP W8VZW3
A	-3	GLY	-	expression tag	UNP W8VZW3
A	-2	SER	-	expression tag	UNP W8VZW3
A	-1	SER	-	expression tag	UNP W8VZW3
A	0	GLY	-	expression tag	UNP W8VZW3
B	-6	GLY	-	expression tag	UNP W8VZW3
B	-5	SER	-	expression tag	UNP W8VZW3
B	-4	SER	-	expression tag	UNP W8VZW3
B	-3	GLY	-	expression tag	UNP W8VZW3
B	-2	SER	-	expression tag	UNP W8VZW3
B	-1	SER	-	expression tag	UNP W8VZW3
B	0	GLY	-	expression tag	UNP W8VZW3
C	-6	GLY	-	expression tag	UNP W8VZW3
C	-5	SER	-	expression tag	UNP W8VZW3
C	-4	SER	-	expression tag	UNP W8VZW3
C	-3	GLY	-	expression tag	UNP W8VZW3
C	-2	SER	-	expression tag	UNP W8VZW3
C	-1	SER	-	expression tag	UNP W8VZW3
C	0	GLY	-	expression tag	UNP W8VZW3

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



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 HEXANE (three-letter code: HEX) (formula: C<sub>6</sub>H<sub>14</sub>).



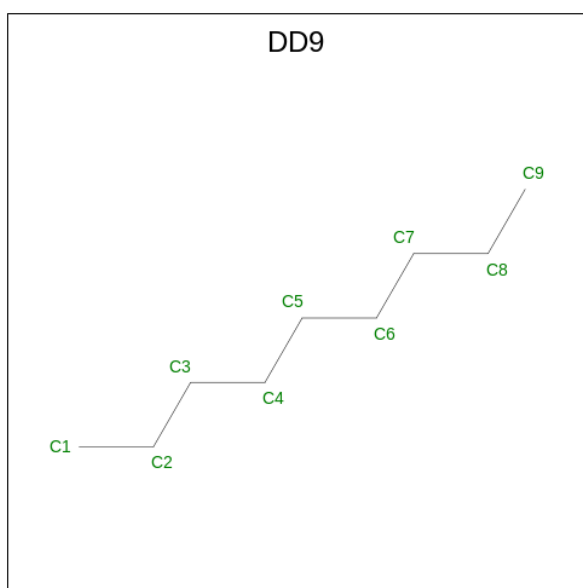
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0

*Continued on next page...*

Continued from previous page...

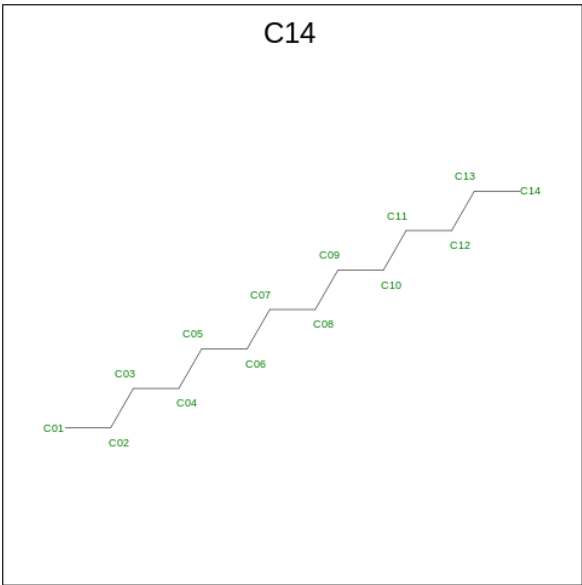
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	C	1	Total C 6 6	0	0

- Molecule 4 is nonane (three-letter code: DD9) (formula: C<sub>9</sub>H<sub>20</sub>).



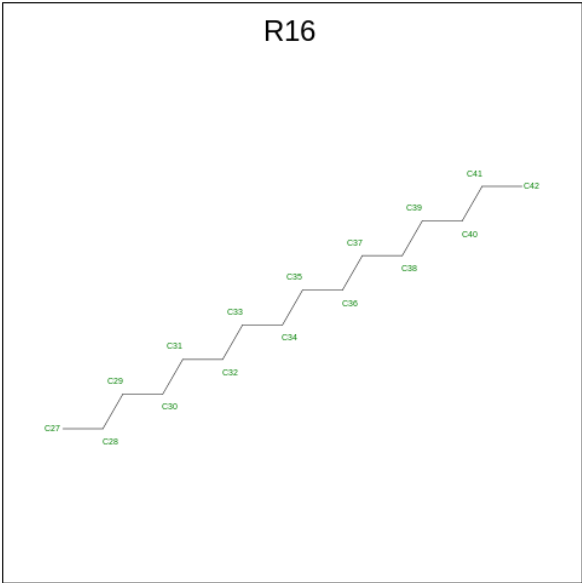
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 9 9	0	0
4	A	1	Total C 9 9	0	0
4	B	1	Total C 9 9	0	0

- Molecule 5 is TETRADECANE (three-letter code: C14) (formula: C<sub>14</sub>H<sub>30</sub>).



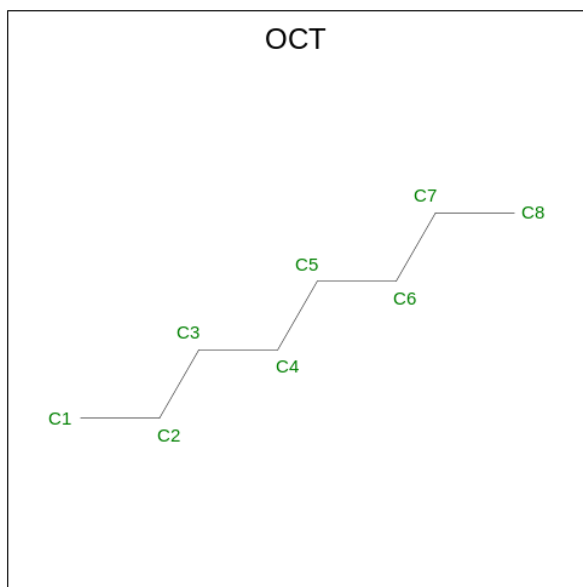
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			14	14		
5	B	1	Total	C	0	0
			14	14		

- Molecule 6 is HEXADECANE (three-letter code: R16) (formula: C<sub>16</sub>H<sub>34</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C	0	0
			16	16		

- Molecule 7 is N-OCTANE (three-letter code: OCT) (formula: C<sub>8</sub>H<sub>18</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C 8 8	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	2	Total Cl 2 2	0	0

- Molecule 9 is water.

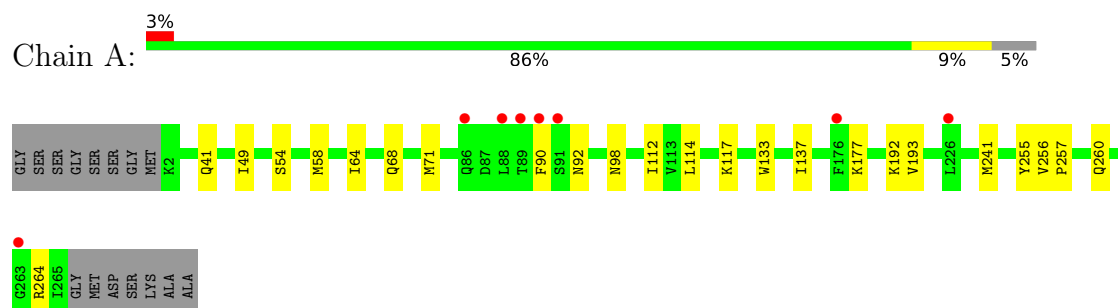
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	25	Total O 25 25	0	0
9	B	15	Total O 15 15	0	0
9	C	30	Total O 30 30	0	0



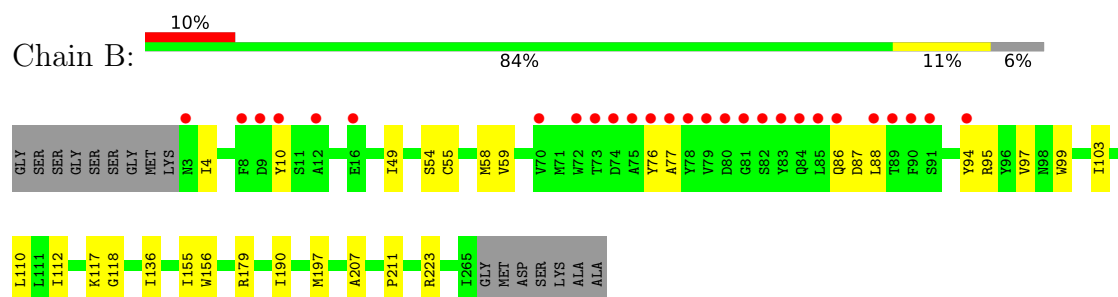
### 3 Residue-property plots [i](#)

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.

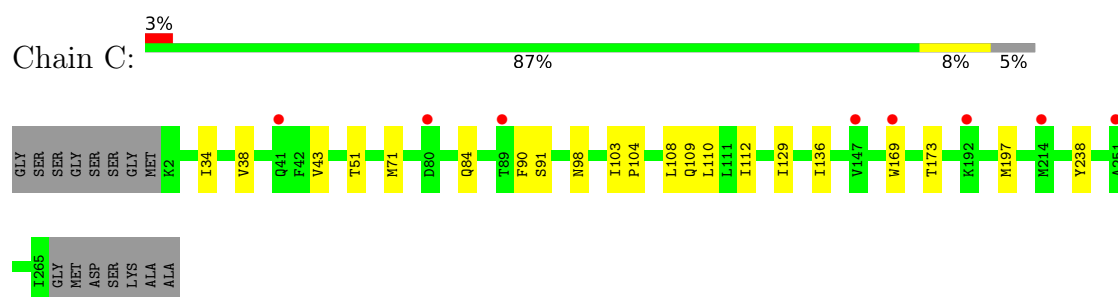
- Molecule 1: Chloride pumping rhodopsin



- Molecule 1: Chloride pumping rhodopsin



- Molecule 1: Chloride pumping rhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.40Å 69.50Å 231.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.46 – 2.30 47.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.46-2.30) 100.0 (47.70-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.210 , 0.241 0.210 , 0.222	Depositor DCC
$R_{free}$ test set	2806 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 78.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7037e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: R16, RET, HEX, C14, DD9, OCT, 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	0.25	0/2119	0.39	0/2890
1	B	0.26	0/2109	0.40	0/2878
1	C	0.25	0/2121	0.38	0/2892
All	All	0.25	0/6349	0.39	0/8660

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 [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	2067	0	2089	11	0
1	B	2057	0	2074	16	0
1	C	2069	0	2096	12	0
2	A	20	0	27	1	0
2	B	20	0	27	2	0
2	C	20	0	27	1	0
3	A	12	0	28	0	0
3	B	18	0	42	1	0
3	C	6	0	14	0	0
4	A	18	0	40	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	9	0	20	1	0
5	A	14	0	30	1	0
5	B	14	0	30	0	0
6	A	16	0	34	0	0
7	B	8	0	18	0	0
8	C	2	0	0	1	0
9	A	25	0	0	2	0
9	B	15	0	0	0	0
9	C	30	0	0	0	0
All	All	6440	0	6596	43	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 3.

All (43) 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:98:ASN:ND2	8:C:302:CL:CL	2.54	0.78
1:B:103:ILE:HD12	1:B:136:ILE:HD11	1.74	0.69
1:A:193:VAL:HG22	1:A:241:MET:HE3	1.75	0.67
1:C:103:ILE:HD12	1:C:136:ILE:HD11	1.82	0.62
1:C:43:VAL:HG21	1:C:51:THR:HG21	1.84	0.60
1:B:94:TYR:HA	1:B:97:VAL:HG22	1.86	0.57
1:A:68:GLN:NE2	9:A:402:HOH:O	2.29	0.57
1:B:55:CYS:O	1:B:59:VAL:HG23	2.05	0.56
1:A:64:ILE:HD13	1:A:98:ASN:HB2	1.87	0.56
1:B:4:ILE:HD13	1:B:211:PRO:HG3	1.89	0.55
1:A:71:MET:HE3	1:A:90:PHE:HA	1.89	0.53
1:A:255:TYR:CE2	1:A:257:PRO:HG2	2.45	0.52
1:B:110:LEU:HD22	1:B:197:MET:HE1	1.91	0.52
1:C:71:MET:HE3	1:C:90:PHE:HA	1.92	0.51
1:A:92:ASN:HB2	9:A:420:HOH:O	2.12	0.50
1:C:110:LEU:HD22	1:C:197:MET:HE1	1.93	0.50
2:B:301:RET:H8	2:B:301:RET:H161	1.94	0.50
1:C:169:TRP:O	1:C:173:THR:HG23	2.11	0.49
2:A:301:RET:H8	2:A:301:RET:H161	1.93	0.49
1:B:155:ILE:HG13	1:B:156:TRP:N	2.27	0.49
1:B:207:ALA:HB1	1:B:223:ARG:HG3	1.96	0.48
1:C:108:LEU:O	1:C:112:ILE:HG13	2.14	0.47
3:B:303:HEX:H63	4:B:305:DD9:H9	1.96	0.47
1:B:99:TRP:CD1	2:B:301:RET:H14	2.51	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ILE:O	1:C:38:VAL:HG13	2.15	0.46
1:A:133:TRP:O	1:A:137:ILE:HG22	2.16	0.46
2:C:301:RET:H161	2:C:301:RET:H8	1.98	0.45
1:B:10:TYR:HE2	1:B:76:TYR:CE2	2.35	0.45
1:B:49:ILE:HG23	1:B:112:ILE:HD13	1.99	0.45
1:A:49:ILE:HG23	1:A:112:ILE:HD13	1.98	0.44
1:B:87:ASP:OD1	1:B:88:LEU:N	2.51	0.44
1:B:190:ILE:HD12	1:B:190:ILE:HA	1.92	0.43
1:C:104:PRO:HB3	1:C:129:ILE:HG12	2.00	0.42
1:B:95:ARG:HG2	1:B:95:ARG:HH11	1.84	0.42
1:A:117:LYS:HE2	1:C:84:GLN:NE2	2.35	0.42
1:A:54:SER:O	1:A:58:MET:HG2	2.19	0.42
1:A:256:VAL:HG12	1:A:260:GLN:NE2	2.34	0.41
1:C:109:GLN:HE21	1:C:238:TYR:HE2	1.69	0.41
5:A:306:C14:H092	5:A:306:C14:H121	1.89	0.41
1:B:54:SER:O	1:B:58:MET:HG2	2.21	0.41
1:B:77:ALA:HB3	1:B:86:GLN:NE2	2.36	0.40
1:C:197:MET:HE2	1:C:197:MET:HB2	1.77	0.40
1:B:117:LYS:HD2	1:B:118:GLY:H	1.86	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	262/279 (94%)	260 (99%)	2 (1%)	0	100	100
1	B	261/279 (94%)	260 (100%)	1 (0%)	0	100	100
1	C	262/279 (94%)	259 (99%)	3 (1%)	0	100	100
All	All	785/837 (94%)	779 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/226 (95%)	210 (98%)	5 (2%)	50	67
1	B	214/226 (95%)	213 (100%)	1 (0%)	88	95
1	C	216/226 (96%)	215 (100%)	1 (0%)	88	95
All	All	645/678 (95%)	638 (99%)	7 (1%)	73	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	114	LEU
1	A	177	LYS
1	A	192	LYS
1	A	264	ARG
1	B	179	ARG
1	C	91	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	86	GLN
1	A	260	GLN
1	B	84	GLN
1	C	84	GLN
1	C	98	ASN
1	C	109	GLN
1	C	248	GLN

### 5.3.3 RNA

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	HEX	B	302	-	5,5,5	0.31	0	4,4,4	0.58	0
6	R16	A	307	-	15,15,15	0.29	0	14,14,14	0.87	0
2	RET	B	301	1	20,20,21	0.84	0	27,27,28	0.77	0
4	DD9	A	304	-	8,8,8	0.30	0	7,7,7	0.78	0
5	C14	A	306	-	13,13,13	0.30	0	12,12,12	0.86	0
2	RET	C	301	1	20,20,21	0.85	0	27,27,28	0.74	0
2	RET	A	301	1	20,20,21	0.84	0	27,27,28	0.76	0
3	HEX	B	303	-	5,5,5	0.31	0	4,4,4	0.59	0
4	DD9	B	305	-	8,8,8	0.29	0	7,7,7	0.81	0
3	HEX	C	304	-	5,5,5	0.31	0	4,4,4	0.58	0
7	OCT	B	307	-	7,7,7	0.30	0	6,6,6	0.74	0
5	C14	B	306	-	13,13,13	0.30	0	12,12,12	0.84	0
3	HEX	B	304	-	5,5,5	0.32	0	4,4,4	0.57	0
3	HEX	A	303	-	5,5,5	0.31	0	4,4,4	0.57	0
3	HEX	A	302	-	5,5,5	0.32	0	4,4,4	0.57	0
4	DD9	A	305	-	8,8,8	0.30	0	7,7,7	0.80	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
3	HEX	B	302	-	-	1/3/3/3	-
6	R16	A	307	-	-	5/13/13/13	-
2	RET	B	301	1	-	0/13/30/31	0/1/1/1
4	DD9	A	304	-	-	0/6/6/6	-
5	C14	A	306	-	-	1/11/11/11	-
2	RET	C	301	1	-	0/13/30/31	0/1/1/1
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	HEX	B	303	-	-	0/3/3/3	-
4	DD9	B	305	-	-	2/6/6/6	-
3	HEX	C	304	-	-	1/3/3/3	-
7	OCT	B	307	-	-	3/5/5/5	-
5	C14	B	306	-	-	3/11/11/11	-
3	HEX	B	304	-	-	1/3/3/3	-
3	HEX	A	303	-	-	2/3/3/3	-
3	HEX	A	302	-	-	1/3/3/3	-
4	DD9	A	305	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	307	OCT	C4-C5-C6-C7
6	A	307	R16	C38-C39-C40-C41
6	A	307	R16	C35-C36-C37-C38
6	A	307	R16	C29-C30-C31-C32
5	B	306	C14	C08-C09-C10-C11
3	A	302	HEX	C2-C3-C4-C5
5	B	306	C14	C03-C04-C05-C06
5	A	306	C14	C07-C08-C09-C10
6	A	307	R16	C39-C40-C41-C42
3	A	303	HEX	C1-C2-C3-C4
3	B	304	HEX	C1-C2-C3-C4
3	A	303	HEX	C2-C3-C4-C5
7	B	307	OCT	C5-C6-C7-C8
3	C	304	HEX	C3-C4-C5-C6
4	B	305	DD9	C2-C3-C4-C5
5	B	306	C14	C02-C03-C04-C05
7	B	307	OCT	C1-C2-C3-C4
6	A	307	R16	C33-C34-C35-C36

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	305	DD9	C5-C6-C7-C8
3	B	302	HEX	C3-C4-C5-C6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	RET	2	0
5	A	306	C14	1	0
2	C	301	RET	1	0
2	A	301	RET	1	0
3	B	303	HEX	1	0
4	B	305	DD9	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/279 (94%)	0.16	8 (3%) 50 57	32, 45, 73, 96	0
1	B	263/279 (94%)	0.51	27 (10%) 6 9	33, 49, 89, 122	0
1	C	264/279 (94%)	0.11	8 (3%) 50 57	43, 55, 72, 89	0
All	All	791/837 (94%)	0.26	43 (5%) 25 32	32, 51, 77, 122	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	ASP	8.5
1	B	78	TYR	8.2
1	B	89	THR	7.1
1	A	89	THR	7.0
1	B	79	VAL	6.8
1	B	81	GLY	6.4
1	B	90	PHE	5.7
1	B	83	TYR	5.1
1	B	12	ALA	5.0
1	B	91	SER	4.3
1	B	82	SER	4.3
1	B	75	ALA	4.3
1	B	85	LEU	4.2
1	A	90	PHE	4.1
1	A	88	LEU	4.1
1	B	70	VAL	4.1
1	B	76	TYR	4.0
1	B	73	THR	3.8
1	A	176	PHE	3.4
1	B	84	GLN	3.3
1	B	10	TYR	3.3
1	B	8	PHE	3.2
1	B	72	TRP	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	41	GLN	3.0
1	B	86	GLN	3.0
1	B	3	ASN	3.0
1	A	86	GLN	2.8
1	B	74	ASP	2.7
1	B	88	LEU	2.7
1	C	147	VAL	2.6
1	B	16	GLU	2.6
1	A	263	GLY	2.5
1	C	214	MET	2.2
1	A	91	SER	2.2
1	C	169	TRP	2.2
1	C	89	THR	2.2
1	B	77	ALA	2.2
1	C	80	ASP	2.1
1	B	9	ASP	2.1
1	A	226	LEU	2.1
1	B	94	TYR	2.1
1	C	192	LYS	2.0
1	C	251	ALA	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	HEX	B	304	6/6	0.57	0.18	70,80,84,86	0
3	HEX	A	303	6/6	0.65	0.17	60,65,66,68	0
3	HEX	B	302	6/6	0.76	0.19	49,54,60,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DD9	A	304	9/9	0.77	0.42	50,56,65,71	0
8	CL	C	303	1/1	0.79	0.14	92,92,92,92	0
5	C14	B	306	14/14	0.80	0.21	47,62,73,73	0
4	DD9	B	305	9/9	0.80	0.29	54,60,69,70	0
5	C14	A	306	14/14	0.81	0.20	55,65,76,76	0
6	R16	A	307	16/16	0.82	0.27	44,55,61,62	0
7	OCT	B	307	8/8	0.84	0.46	48,59,62,63	0
3	HEX	C	304	6/6	0.86	0.17	57,67,68,74	0
3	HEX	B	303	6/6	0.87	0.36	38,47,55,61	0
4	DD9	A	305	9/9	0.88	0.21	53,59,65,69	0
3	HEX	A	302	6/6	0.92	0.22	58,65,69,78	0
2	RET	C	301	20/21	0.94	0.16	37,48,57,57	0
2	RET	A	301	20/21	0.94	0.17	29,36,43,44	0
2	RET	B	301	20/21	0.94	0.16	31,38,46,46	0
8	CL	C	302	1/1	0.97	0.14	51,51,51,51	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.