



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:15 PM GMT

PDB ID : 4XXJ
Title : Crystal Structure of Escherichia coli-Expressed Halobacterium salinarum Bacteriorhodopsin in the Trimeric Form
Authors : Bratanov, D.; Balandin, T.; Round, E.; Gushchin, I.; Gordeliy, V.
Deposited on : 2015-01-30
Resolution : 1.90 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

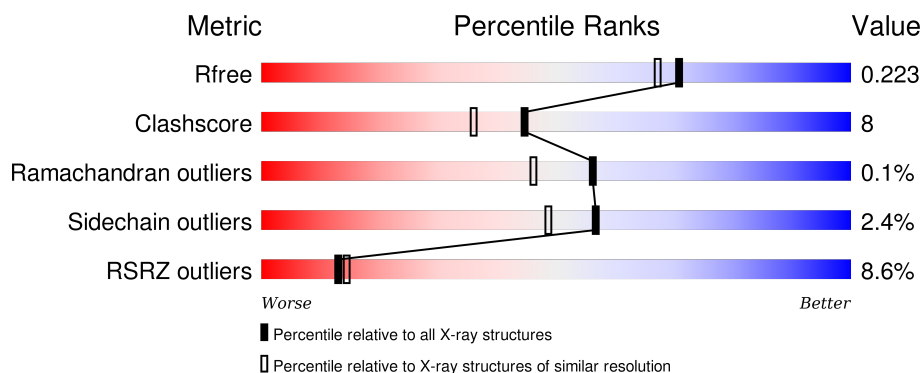
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	269	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	269	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	269	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</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
2	LFA	A	303	-	-	-	X
2	LFA	A	304	-	-	-	X
2	LFA	A	306	-	-	-	X
2	LFA	A	307	-	-	-	X
2	LFA	A	310	-	-	-	X
2	LFA	A	313	-	-	-	X
2	LFA	B	301	-	-	-	X
2	LFA	B	303	-	-	-	X
2	LFA	B	307	-	-	-	X
2	LFA	B	308	-	-	-	X
2	LFA	C	301	-	-	-	X
2	LFA	C	303	-	-	-	X
2	LFA	C	307	-	-	-	X
2	LFA	C	308	-	-	-	X
2	LFA	C	309	-	-	-	X
2	LFA	C	310	-	-	-	X
2	LFA	C	311	-	-	-	X
3	MPG	B	309	-	-	-	X
3	MPG	C	313	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5704 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	1	0
			1778	1206	263	299	10			
1	B	224	Total	C	N	O	S	0	1	0
			1746	1186	258	292	10			
1	C	228	Total	C	N	O	S	0	1	0
			1770	1201	262	297	10			

There are 60 discrepancies between the modelled and reference sequences:

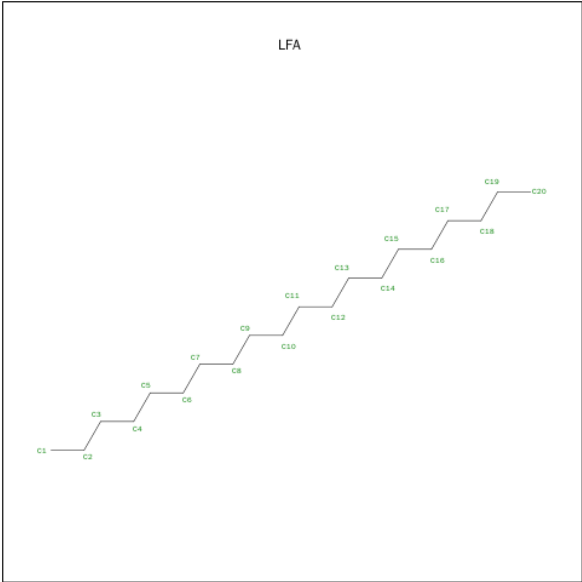
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P02945
A	250	GLY	-	expression tag	UNP P02945
A	251	SER	-	expression tag	UNP P02945
A	252	GLY	-	expression tag	UNP P02945
A	253	ILE	-	expression tag	UNP P02945
A	254	GLU	-	expression tag	UNP P02945
A	255	GLY	-	expression tag	UNP P02945
A	256	ARG	-	expression tag	UNP P02945
A	257	SER	-	expression tag	UNP P02945
A	258	GLY	-	expression tag	UNP P02945
A	259	ALA	-	expression tag	UNP P02945
A	260	PRO	-	expression tag	UNP P02945
A	261	HIS	-	expression tag	UNP P02945
A	262	HIS	-	expression tag	UNP P02945
A	263	HIS	-	expression tag	UNP P02945
A	264	HIS	-	expression tag	UNP P02945
A	265	HIS	-	expression tag	UNP P02945
A	266	HIS	-	expression tag	UNP P02945
A	267	HIS	-	expression tag	UNP P02945
A	268	HIS	-	expression tag	UNP P02945
B	0	MET	-	initiating methionine	UNP P02945
B	250	GLY	-	expression tag	UNP P02945
B	251	SER	-	expression tag	UNP P02945

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Chain	Residue	Modelled	Actual	Comment	Reference
B	252	GLY	-	expression tag	UNP P02945
B	253	ILE	-	expression tag	UNP P02945
B	254	GLU	-	expression tag	UNP P02945
B	255	GLY	-	expression tag	UNP P02945
B	256	ARG	-	expression tag	UNP P02945
B	257	SER	-	expression tag	UNP P02945
B	258	GLY	-	expression tag	UNP P02945
B	259	ALA	-	expression tag	UNP P02945
B	260	PRO	-	expression tag	UNP P02945
B	261	HIS	-	expression tag	UNP P02945
B	262	HIS	-	expression tag	UNP P02945
B	263	HIS	-	expression tag	UNP P02945
B	264	HIS	-	expression tag	UNP P02945
B	265	HIS	-	expression tag	UNP P02945
B	266	HIS	-	expression tag	UNP P02945
B	267	HIS	-	expression tag	UNP P02945
B	268	HIS	-	expression tag	UNP P02945
C	0	MET	-	initiating methionine	UNP P02945
C	250	GLY	-	expression tag	UNP P02945
C	251	SER	-	expression tag	UNP P02945
C	252	GLY	-	expression tag	UNP P02945
C	253	ILE	-	expression tag	UNP P02945
C	254	GLU	-	expression tag	UNP P02945
C	255	GLY	-	expression tag	UNP P02945
C	256	ARG	-	expression tag	UNP P02945
C	257	SER	-	expression tag	UNP P02945
C	258	GLY	-	expression tag	UNP P02945
C	259	ALA	-	expression tag	UNP P02945
C	260	PRO	-	expression tag	UNP P02945
C	261	HIS	-	expression tag	UNP P02945
C	262	HIS	-	expression tag	UNP P02945
C	263	HIS	-	expression tag	UNP P02945
C	264	HIS	-	expression tag	UNP P02945
C	265	HIS	-	expression tag	UNP P02945
C	266	HIS	-	expression tag	UNP P02945
C	267	HIS	-	expression tag	UNP P02945
C	268	HIS	-	expression tag	UNP P02945

- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: C₂₀H₄₂).



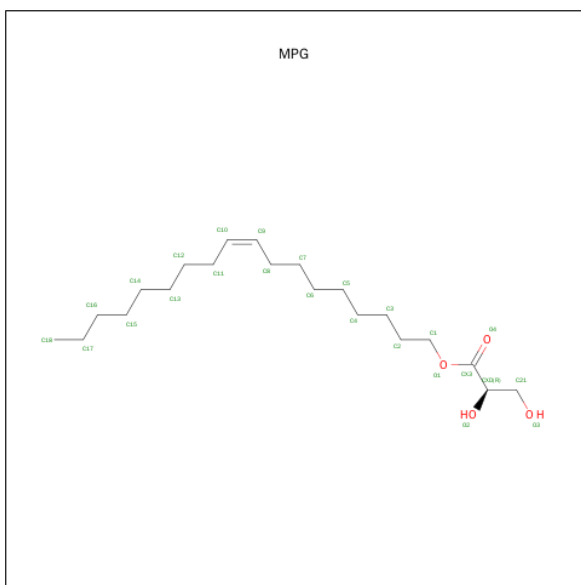
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			7	7		
2	A	1	Total	C	0	0
			5	5		
2	A	1	Total	C	0	0
			11	11		
2	A	1	Total	C	0	0
			10	10		
2	A	1	Total	C	0	0
			7	7		
2	A	1	Total	C	0	0
			7	7		
2	A	1	Total	C	0	0
			7	7		
2	A	1	Total	C	0	0
			6	6		
2	A	1	Total	C	0	0
			6	6		
2	A	1	Total	C	0	0
			10	10		
2	A	1	Total	C	0	0
			8	8		
2	A	1	Total	C	0	0
			10	10		
2	B	1	Total	C	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 6 6	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C 5 5	0	0

- Molecule 3 is 1-MONOOLEOYL-RAC-GLYCEROL (three-letter code: MPG) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 24	C 21	O 3	0	0
3	B	1	Total 24	C 21	O 3	0	0
3	C	1	Total 24	C 21	O 3	0	0

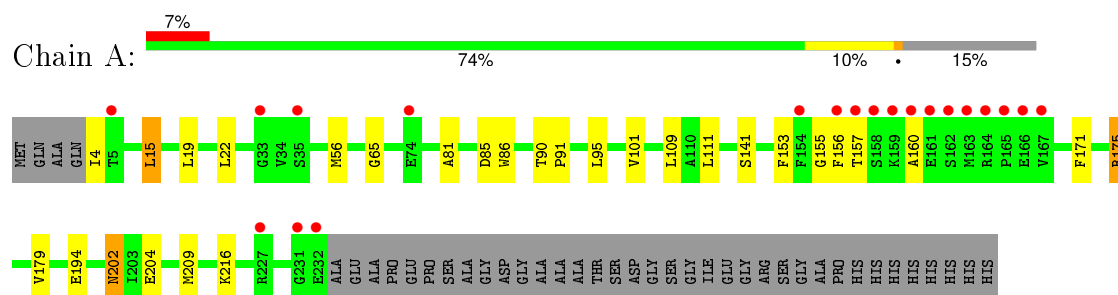
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	28	Total O 28 28	0	0
4	C	30	Total O 30 30	0	0

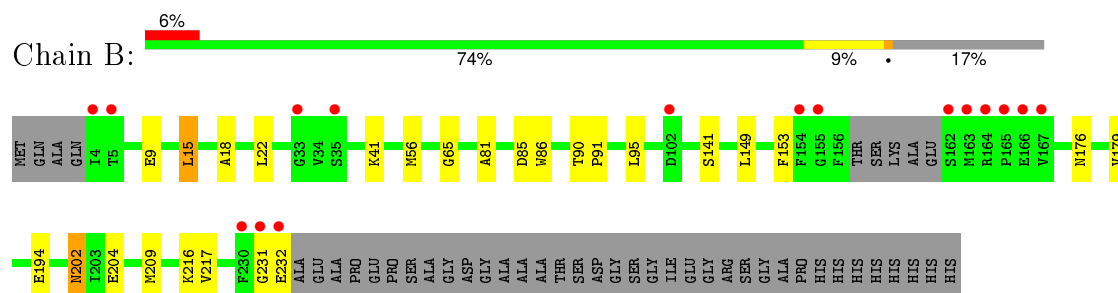
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

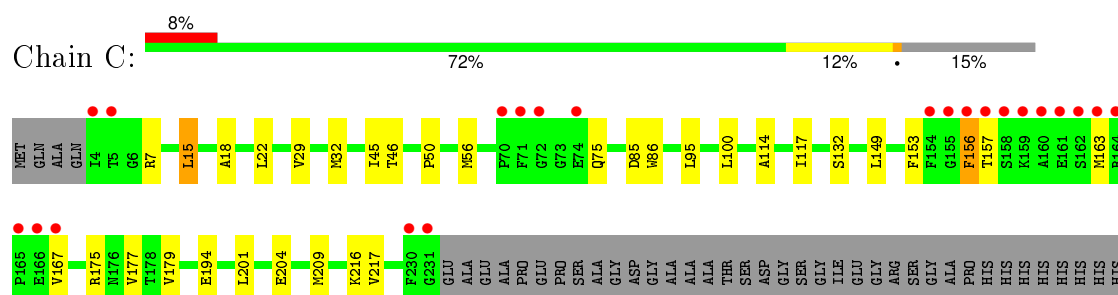
• Molecule 1: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin



• Molecule 1: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.84Å 60.76Å 113.36Å 90.00° 99.78° 90.00°	Depositor
Resolution (Å)	49.20 – 1.90 49.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.20-1.90) 98.8 (49.16-1.90)	Depositor EDS
R_{merge}	7.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.183 , 0.214 0.196 , 0.223	Depositor DCC
R_{free} test set	2770 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 55459 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5704	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPG, LFA, LYR

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	0.33	0/1799	0.46	0/2459
1	B	0.32	0/1766	0.46	0/2413
1	C	0.33	0/1791	0.45	0/2449
All	All	0.33	0/5356	0.46	0/7321

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	1778	0	1834	29	0
1	B	1746	0	1804	22	0
1	C	1770	0	1825	32	0
2	A	101	0	180	5	0
2	B	56	0	98	3	0
2	C	91	0	161	2	0
3	A	24	0	40	4	0
3	B	24	0	40	1	0
3	C	24	0	40	6	0
4	A	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	0	2	0
4	C	30	0	0	2	0
All	All	5704	0	6022	92	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 (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HG2	1:A:175:ARG:HH11	1.08	1.17
3:C:313:MPG:H121	3:C:313:MPG:H82C	1.09	1.07
1:A:216:LYR:H9	1:A:216:LYR:H192	1.42	1.01
3:C:313:MPG:C8	3:C:313:MPG:H121	1.92	0.95
3:C:313:MPG:C12	3:C:313:MPG:H82C	1.97	0.93
1:A:175:ARG:HH11	1:A:175:ARG:CG	1.85	0.89
1:B:216:LYR:H192	1:B:216:LYR:H9	1.53	0.89
1:C:216:LYR:H9	1:C:216:LYR:H192	1.56	0.87
1:C:157:THR:CG2	1:C:175:ARG:HH22	1.88	0.85
1:A:175:ARG:HG2	1:A:175:ARG:NH1	1.88	0.83
1:C:132:SER:OG	4:C:401:HOH:O	1.96	0.82
1:C:157:THR:OG1	1:C:175:ARG:NH2	2.15	0.79
1:A:216:LYR:H192	1:A:216:LYR:C9	2.14	0.78
1:C:157:THR:HG23	1:C:175:ARG:HH22	1.49	0.78
1:B:56[B]:MET:HE3	4:B:409:HOH:O	1.86	0.75
1:A:109:LEU:CD1	2:A:303:LFA:H11	2.18	0.73
1:C:153:PHE:CE2	1:C:179:VAL:HG21	2.24	0.72
1:B:216:LYR:H192	1:B:216:LYR:C9	2.23	0.68
1:B:153:PHE:CE2	1:B:179:VAL:HG21	2.30	0.67
1:C:216:LYR:C9	1:C:216:LYR:H192	2.27	0.65
1:B:194:GLU:OE1	1:B:204:GLU:OE2	2.19	0.61
3:A:314:MPG:H82C	3:A:314:MPG:C12	2.30	0.61
1:A:109:LEU:HD11	2:A:303:LFA:H11	1.83	0.60
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.37	0.60
1:C:117:ILE:HG21	3:C:313:MPG:H111	1.84	0.60
3:A:314:MPG:C8	3:A:314:MPG:C12	2.79	0.59
1:C:56[A]:MET:HG3	1:C:85:ASP:HB2	1.86	0.58
1:C:86:TRP:CD1	1:C:216:LYR:HC2	2.40	0.57
1:A:157:THR:OG1	1:A:175:ARG:NE	2.27	0.56
1:C:15:LEU:HB3	1:C:209:MET:HE2	1.88	0.55
1:B:217:VAL:HG11	2:B:307:LFA:H61	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG12	1:A:160:ALA:HB2	1.90	0.53
1:A:109:LEU:HD12	2:A:303:LFA:H11	1.91	0.53
1:C:194:GLU:OE1	4:C:425:HOH:O	2.18	0.53
1:B:15:LEU:HB3	1:B:209:MET:HE2	1.90	0.53
1:A:101:VAL:CG1	1:A:160:ALA:HB2	2.39	0.53
1:B:56[B]:MET:CE	4:B:409:HOH:O	2.49	0.52
1:A:157:THR:HG1	1:A:175:ARG:HE	1.55	0.51
1:B:65:GLY:HA3	1:B:81:ALA:HB2	1.92	0.51
1:A:56[B]:MET:HE3	4:A:410:HOH:O	2.10	0.51
1:A:175:ARG:NH1	1:A:175:ARG:CG	2.56	0.51
1:C:15:LEU:HD22	1:C:209:MET:HE1	1.93	0.50
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.48	0.49
1:C:29:VAL:HG13	1:C:32:MET:CE	2.43	0.49
3:A:314:MPG:H82C	3:A:314:MPG:H122	1.93	0.49
1:B:217:VAL:HG11	2:B:307:LFA:C6	2.43	0.48
1:A:141:SER:HB3	1:A:216:LYR:H142	1.96	0.48
3:C:313:MPG:C8	3:C:313:MPG:C12	2.69	0.47
1:A:216:LYR:C19	1:A:216:LYR:C9	2.86	0.47
3:A:314:MPG:H121	3:A:314:MPG:C8	2.45	0.47
1:A:56[A]:MET:HG3	1:A:85:ASP:HB2	1.98	0.46
1:A:111:LEU:HD11	1:A:156:PHE:CZ	2.50	0.46
1:B:231:GLY:O	1:B:232:GLU:C	2.53	0.46
2:A:311:LFA:H32	2:A:312:LFA:H41	1.97	0.46
1:C:156:PHE:C	1:C:156:PHE:HD1	2.18	0.46
1:A:194:GLU:OE2	1:A:204:GLU:OE2	2.34	0.45
1:C:29:VAL:HG13	1:C:32:MET:HE1	1.99	0.45
1:C:156:PHE:C	1:C:156:PHE:CD1	2.89	0.45
1:A:216:LYR:H10	1:A:216:LYR:H81	1.80	0.45
1:A:86:TRP:CD1	1:A:216:LYR:HC2	2.51	0.45
1:B:9:GLU:HB3	1:B:202:ASN:HA	1.99	0.44
1:B:18:ALA:O	1:B:22:LEU:HD13	2.18	0.44
1:C:157:THR:CB	1:C:175:ARG:HH22	2.30	0.43
1:C:194:GLU:OE2	1:C:204:GLU:OE2	2.35	0.43
1:A:19:LEU:HD22	2:A:313:LFA:H52	1.99	0.43
1:C:114:ALA:HB2	3:C:313:MPG:H61C	1.99	0.43
1:C:216:LYR:H10	1:C:216:LYR:H81	1.88	0.43
1:B:176:ASN:HB2	2:B:308:LFA:H22	2.01	0.43
1:B:41:LYS:HE3	1:B:41:LYS:HB2	1.79	0.43
1:B:15:LEU:HB3	1:B:209:MET:CE	2.48	0.43
1:B:56[A]:MET:HG3	1:B:85:ASP:HB2	2.00	0.43
1:B:141:SER:HB3	1:B:216:LYR:H142	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:VAL:HG11	2:C:311:LFA:H91	2.00	0.43
1:B:90:THR:N	1:B:91:PRO:CD	2.82	0.43
1:C:163:MET:HE2	1:C:167:VAL:HG11	2.00	0.43
1:C:149:LEU:HD22	1:C:179:VAL:HG22	2.01	0.43
1:C:18:ALA:O	1:C:22:LEU:HD13	2.18	0.42
1:B:149:LEU:HD22	1:B:179:VAL:HG22	2.00	0.42
3:B:309:MPG:H141	3:B:309:MPG:H112	1.76	0.42
1:A:65:GLY:HA3	1:A:81:ALA:HB2	2.02	0.42
1:C:46:THR:O	1:C:50:PRO:HD2	2.20	0.42
1:B:216:LYR:H81	1:B:216:LYR:H10	1.87	0.41
1:C:100:LEU:O	1:C:163:MET:HE2	2.19	0.41
1:C:163:MET:CE	1:C:167:VAL:HG11	2.51	0.41
1:A:202:ASN:H	1:A:202:ASN:HD22	1.67	0.41
1:A:109:LEU:CD2	1:C:45:ILE:HG13	2.50	0.41
1:A:90:THR:OG1	1:A:91:PRO:HD3	2.21	0.41
1:C:216:LYR:C19	1:C:216:LYR:C9	2.97	0.41
1:C:177:VAL:HA	2:C:312:LFA:H41	2.03	0.41
1:A:15:LEU:HB3	1:A:209:MET:HE2	2.02	0.40
1:B:86:TRP:CD1	1:B:216:LYR:HC2	2.56	0.40
1:C:7:ARG:HH11	1:C:201:LEU:HD23	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	227/269 (84%)	226 (100%)	0	1 (0%)	39	27
1	B	220/269 (82%)	219 (100%)	1 (0%)	0	100	100
1	C	226/269 (84%)	223 (99%)	3 (1%)	0	100	100
All	All	673/807 (83%)	668 (99%)	4 (1%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	GLY

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	179/209 (86%)	173 (97%)	6 (3%)	44	33
1	B	177/209 (85%)	174 (98%)	3 (2%)	68	64
1	C	178/209 (85%)	174 (98%)	4 (2%)	60	53
All	All	534/627 (85%)	521 (98%)	13 (2%)	57	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	15	LEU
1	A	22	LEU
1	A	95	LEU
1	A	175	ARG
1	A	202	ASN
1	B	15	LEU
1	B	95	LEU
1	B	202	ASN
1	C	15	LEU
1	C	75	GLN
1	C	95	LEU
1	C	156	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	202	ASN

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Mol	Chain	Res	Type
1	B	202	ASN
1	C	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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$
1	LYR	A	216	1	27,29,30	1.20	3 (11%)	33,37,39	1.72	7 (21%)
1	LYR	B	216	1	27,29,30	1.30	2 (7%)	33,37,39	1.62	6 (18%)
1	LYR	C	216	1	27,29,30	1.30	3 (11%)	33,37,39	1.63	5 (15%)

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
1	LYR	A	216	1	-	0/21/40/42	0/1/1/1
1	LYR	B	216	1	-	0/21/40/42	0/1/1/1
1	LYR	C	216	1	-	0/21/40/42	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	LYR	C5-C3	-2.33	1.40	1.45
1	C	216	LYR	C2-C3	2.03	1.39	1.33
1	B	216	LYR	C2-C3	2.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	LYR	C17-C11	2.18	1.56	1.53
1	A	216	LYR	C2-C3	2.33	1.40	1.33
1	A	216	LYR	C7-C80	2.65	1.39	1.35
1	B	216	LYR	C7-C80	2.78	1.39	1.35
1	C	216	LYR	C7-C80	3.17	1.40	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	LYR	C13-C12-C11	-4.57	119.76	124.62
1	C	216	LYR	C13-C12-C11	-4.37	119.97	124.62
1	A	216	LYR	C13-C12-C11	-4.32	120.02	124.62
1	A	216	LYR	C7-C6-C5	-3.88	111.11	123.11
1	A	216	LYR	C10-C9-C80	-3.75	120.55	126.21
1	C	216	LYR	C7-C6-C5	-3.57	112.09	123.11
1	B	216	LYR	C7-C6-C5	-3.36	112.72	123.11
1	A	216	LYR	C8-C80-C7	-2.50	119.25	122.89
1	B	216	LYR	C8-C80-C7	-2.43	119.35	122.89
1	C	216	LYR	C8-C80-C7	-2.41	119.38	122.89
1	C	216	LYR	C10-C9-C80	-2.31	122.72	126.21
1	C	216	LYR	C15-C14-C12	-2.13	110.33	113.87
1	B	216	LYR	O-C-CA	-2.08	120.15	125.72
1	B	216	LYR	C10-C9-C80	-2.07	123.07	126.21
1	A	216	LYR	C18-C17-C11	-2.07	107.17	110.33
1	A	216	LYR	O-C-CA	-2.02	120.30	125.72
1	A	216	LYR	C14-C12-C11	2.34	125.31	122.73
1	B	216	LYR	C14-C12-C11	2.50	125.48	122.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	216	LYR	6	0
1	B	216	LYR	5	0
1	C	216	LYR	5	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

36 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	LFA	A	301	-	6,6,19	0.25	0	5,5,18	0.42	0
2	LFA	A	302	-	4,4,19	0.30	0	3,3,18	0.42	0
2	LFA	A	303	-	10,10,19	0.25	0	9,9,18	0.55	0
2	LFA	A	304	-	9,9,19	0.25	0	8,8,18	0.51	0
2	LFA	A	305	-	6,6,19	0.26	0	5,5,18	0.43	0
2	LFA	A	306	-	6,6,19	0.24	0	5,5,18	0.44	0
2	LFA	A	307	-	6,6,19	0.26	0	5,5,18	0.45	0
2	LFA	A	308	-	6,6,19	0.25	0	5,5,18	0.43	0
2	LFA	A	309	-	5,5,19	0.27	0	4,4,18	0.33	0
2	LFA	A	310	-	5,5,19	0.27	0	4,4,18	0.34	0
2	LFA	A	311	-	9,9,19	0.27	0	8,8,18	0.53	0
2	LFA	A	312	-	7,7,19	0.29	0	6,6,18	0.45	0
2	LFA	A	313	-	9,9,19	0.24	0	8,8,18	0.52	0
3	MPG	A	314	-	23,23,24	0.36	0	23,23,25	0.94	1 (4%)
2	LFA	B	301	-	6,6,19	0.26	0	5,5,18	0.42	0
2	LFA	B	302	-	5,5,19	0.28	0	4,4,18	0.35	0
2	LFA	B	303	-	6,6,19	0.26	0	5,5,18	0.45	0
2	LFA	B	304	-	5,5,19	0.26	0	4,4,18	0.38	0
2	LFA	B	305	-	5,5,19	0.26	0	4,4,18	0.38	0
2	LFA	B	306	-	5,5,19	0.23	0	4,4,18	0.37	0
2	LFA	B	307	-	9,9,19	0.26	0	8,8,18	0.51	0
2	LFA	B	308	-	7,7,19	0.27	0	6,6,18	0.48	0
3	MPG	B	309	-	23,23,24	0.27	0	23,23,25	0.84	2 (8%)
2	LFA	C	301	-	6,6,19	0.29	0	5,5,18	0.40	0
2	LFA	C	302	-	6,6,19	0.28	0	5,5,18	0.39	0
2	LFA	C	303	-	10,10,19	0.18	0	9,9,18	0.62	0
2	LFA	C	304	-	9,9,19	0.25	0	8,8,18	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	C	305	-	6,6,19	0.24	0	5,5,18	0.40	0
2	LFA	C	306	-	5,5,19	0.26	0	4,4,18	0.34	0
2	LFA	C	307	-	5,5,19	0.26	0	4,4,18	0.35	0
2	LFA	C	308	-	5,5,19	0.28	0	4,4,18	0.33	0
2	LFA	C	309	-	5,5,19	0.26	0	4,4,18	0.38	0
2	LFA	C	310	-	5,5,19	0.28	0	4,4,18	0.32	0
2	LFA	C	311	-	13,13,19	0.28	0	12,12,18	0.49	0
2	LFA	C	312	-	4,4,19	0.28	0	3,3,18	0.40	0
3	MPG	C	313	-	23,23,24	0.33	0	23,23,25	0.89	2 (8%)

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	LFA	A	301	-	-	0/4/4/17	0/0/0/0
2	LFA	A	302	-	-	0/2/2/17	0/0/0/0
2	LFA	A	303	-	-	0/8/8/17	0/0/0/0
2	LFA	A	304	-	-	0/7/7/17	0/0/0/0
2	LFA	A	305	-	-	0/4/4/17	0/0/0/0
2	LFA	A	306	-	-	0/4/4/17	0/0/0/0
2	LFA	A	307	-	-	0/4/4/17	0/0/0/0
2	LFA	A	308	-	-	0/4/4/17	0/0/0/0
2	LFA	A	309	-	-	0/3/3/17	0/0/0/0
2	LFA	A	310	-	-	0/3/3/17	0/0/0/0
2	LFA	A	311	-	-	0/7/7/17	0/0/0/0
2	LFA	A	312	-	-	0/5/5/17	0/0/0/0
2	LFA	A	313	-	-	0/7/7/17	0/0/0/0
3	MPG	A	314	-	-	0/22/22/25	0/0/0/0
2	LFA	B	301	-	-	0/4/4/17	0/0/0/0
2	LFA	B	302	-	-	0/3/3/17	0/0/0/0
2	LFA	B	303	-	-	0/4/4/17	0/0/0/0
2	LFA	B	304	-	-	0/3/3/17	0/0/0/0
2	LFA	B	305	-	-	0/3/3/17	0/0/0/0
2	LFA	B	306	-	-	0/3/3/17	0/0/0/0
2	LFA	B	307	-	-	0/7/7/17	0/0/0/0
2	LFA	B	308	-	-	0/5/5/17	0/0/0/0
3	MPG	B	309	-	-	0/22/22/25	0/0/0/0
2	LFA	C	301	-	-	0/4/4/17	0/0/0/0
2	LFA	C	302	-	-	0/4/4/17	0/0/0/0
2	LFA	C	303	-	-	0/8/8/17	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	304	-	-	0/7/7/17	0/0/0/0
2	LFA	C	305	-	-	0/4/4/17	0/0/0/0
2	LFA	C	306	-	-	0/3/3/17	0/0/0/0
2	LFA	C	307	-	-	0/3/3/17	0/0/0/0
2	LFA	C	308	-	-	0/3/3/17	0/0/0/0
2	LFA	C	309	-	-	0/3/3/17	0/0/0/0
2	LFA	C	310	-	-	0/3/3/17	0/0/0/0
2	LFA	C	311	-	-	0/11/11/17	0/0/0/0
2	LFA	C	312	-	-	0/2/2/17	0/0/0/0
3	MPG	C	313	-	-	0/22/22/25	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	313	MPG	C1-O1-CX3	2.03	119.96	113.42
3	B	309	MPG	O1-CX3-CXD	2.16	116.86	109.65
3	B	309	MPG	C1-O1-CX3	2.33	120.92	113.42
3	C	313	MPG	O1-CX3-CXD	2.93	119.44	109.65
3	A	314	MPG	O1-CX3-CXD	3.49	121.29	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	LFA	3	0
2	A	311	LFA	1	0
2	A	312	LFA	1	0
2	A	313	LFA	1	0
3	A	314	MPG	4	0
2	B	307	LFA	2	0
2	B	308	LFA	1	0
3	B	309	MPG	1	0
2	C	311	LFA	1	0
2	C	312	LFA	1	0
3	C	313	MPG	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	228/269 (84%)	0.28	20 (8%) 12 14	20, 30, 60, 86	0
1	B	223/269 (82%)	0.26	16 (7%) 18 20	20, 30, 57, 81	0
1	C	227/269 (84%)	0.41	22 (9%) 10 11	20, 32, 63, 96	0
All	All	678/807 (84%)	0.32	58 (8%) 13 14	20, 31, 62, 96	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	MET	8.0
1	A	163	MET	7.4
1	C	160	ALA	6.9
1	B	4	ILE	6.8
1	C	162	SER	6.7
1	C	163	MET	6.5
1	A	162	SER	6.4
1	C	158	SER	5.9
1	A	165	PRO	5.8
1	C	155	GLY	5.8
1	C	154	PHE	5.7
1	B	165	PRO	5.6
1	A	164	ARG	5.4
1	B	162	SER	5.4
1	C	161	GLU	5.3
1	A	232	GLU	5.2
1	B	166	GLU	5.2
1	B	164	ARG	5.2
1	A	160	ALA	5.2
1	A	158	SER	4.9
1	C	159	LYS	4.7
1	B	231	GLY	4.6
1	A	159	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	161	GLU	4.3
1	C	165	PRO	4.2
1	B	5	THR	4.2
1	C	164	ARG	4.1
1	A	156	PHE	4.1
1	B	230	PHE	4.1
1	A	166	GLU	4.0
1	A	231	GLY	3.8
1	A	157	THR	3.7
1	C	5	THR	3.6
1	C	4	ILE	3.3
1	B	35	SER	3.2
1	C	74	GLU	3.2
1	B	232	GLU	3.0
1	B	33	GLY	2.9
1	B	154	PHE	2.9
1	A	227	ARG	2.8
1	A	33	GLY	2.7
1	A	167	VAL	2.7
1	B	167	VAL	2.6
1	C	156	PHE	2.5
1	C	70	PRO	2.4
1	C	167	VAL	2.4
1	C	231	GLY	2.4
1	B	155	GLY	2.3
1	C	72	GLY	2.3
1	A	154	PHE	2.2
1	C	230	PHE	2.2
1	B	102	ASP	2.2
1	A	35	SER	2.2
1	A	5	THR	2.1
1	C	166	GLU	2.1
1	C	71	PHE	2.0
1	A	74	GLU	2.0
1	C	157	THR	2.0

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

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
1	LYR	A	216	29/30	0.91	0.12	-	20,25,29,30	0
1	LYR	C	216	29/30	0.91	0.14	-	23,25,29,32	0
1	LYR	B	216	29/30	0.91	0.13	-	20,25,30,31	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	LFA	C	310	6/20	0.51	0.21	13.11	45,51,56,56	0
2	LFA	A	303	11/20	0.89	0.26	8.56	44,46,49,52	0
2	LFA	C	303	11/20	0.89	0.23	7.52	44,45,53,54	0
2	LFA	A	304	10/20	0.86	0.20	6.56	36,42,47,48	0
2	LFA	B	303	7/20	0.77	0.17	6.34	40,46,57,59	0
2	LFA	C	301	7/20	0.68	0.28	6.30	52,54,56,57	0
2	LFA	C	307	6/20	0.81	0.21	5.73	34,43,47,53	0
2	LFA	A	307	7/20	0.71	0.19	5.30	36,39,43,46	0
2	LFA	C	308	6/20	0.71	0.22	4.97	41,43,46,48	0
2	LFA	B	301	7/20	0.85	0.16	4.76	36,43,46,53	0
2	LFA	B	307	10/20	0.76	0.16	4.41	48,55,59,61	0
2	LFA	C	311	14/20	0.64	0.18	4.10	44,54,60,61	0
3	MPG	C	313	24/25	0.84	0.17	3.77	41,50,59,69	0
2	LFA	A	306	7/20	0.85	0.15	3.09	39,43,53,56	0
2	LFA	A	313	10/20	0.90	0.14	2.99	51,53,59,64	0
3	MPG	B	309	24/25	0.86	0.14	2.57	39,46,54,67	0
2	LFA	B	308	8/20	0.61	0.21	2.37	49,50,60,62	0
2	LFA	C	309	6/20	0.85	0.20	2.10	58,59,61,64	0
2	LFA	A	310	6/20	0.76	0.19	2.01	49,53,57,58	0
3	MPG	A	314	24/25	0.89	0.13	1.55	37,49,57,60	0
2	LFA	A	308	7/20	0.77	0.17	1.45	45,48,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LFA	C	312	5/20	0.84	0.17	0.76	50,51,55,61	0
2	LFA	C	305	7/20	0.88	0.13	0.26	40,45,50,52	0
2	LFA	A	309	6/20	0.89	0.11	0.02	42,46,50,51	0
2	LFA	B	305	6/20	0.86	0.14	-0.01	42,44,47,48	0
2	LFA	C	304	10/20	0.82	0.12	-0.38	44,47,57,59	0
2	LFA	C	302	7/20	0.84	0.22	-	35,41,54,54	0
2	LFA	B	304	6/20	0.83	0.14	-	53,55,60,63	0
2	LFA	C	306	6/20	0.74	0.17	-	53,54,57,59	0
2	LFA	A	305	7/20	0.77	0.15	-	51,53,58,61	0
2	LFA	A	312	8/20	0.78	0.20	-	51,58,59,59	0
2	LFA	B	306	6/20	0.82	0.17	-	45,48,49,58	0
2	LFA	A	302	5/20	0.91	0.22	-	46,49,52,54	0
2	LFA	B	302	6/20	0.93	0.17	-	56,57,59,66	0
2	LFA	A	301	7/20	0.84	0.19	-	39,43,47,47	0
2	LFA	A	311	10/20	0.70	0.21	-	55,59,63,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.