



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:44 PM GMT

PDB ID : 1GZM
Title : STRUCTURE OF BOVINE RHODOPSIN IN A TRIGONAL CRYSTAL FORM
Authors : Li, J.
Deposited on : 2002-05-24
Resolution : 2.65 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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

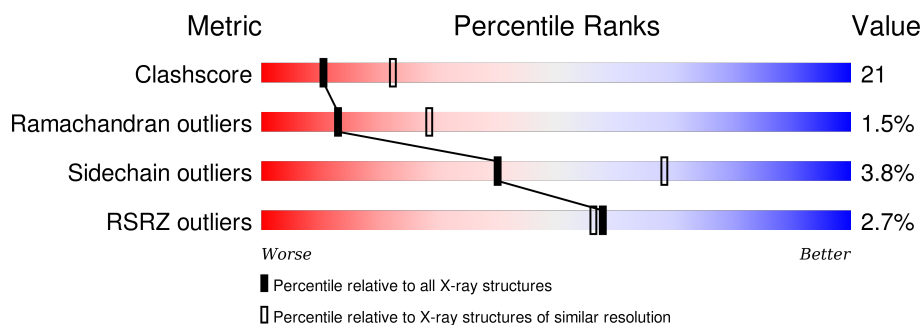
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	349	
1	B	349	

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	PLM	A	1333	-	-	-	X
3	PLM	A	1334	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLM	B	1333	-	-	-	X
3	PLM	B	1334	-	-	-	X
4	NAG	B	1335	-	-	X	-
5	PEF	A	1341	-	-	-	X
5	PEF	B	1342	-	-	-	X
6	LDA	B	1343	-	-	X	X
6	LDA	B	1348	-	-	X	-
7	C8E	A	1343	-	-	-	X
7	C8E	A	1345	-	-	-	X
7	C8E	A	1346	-	-	-	X
7	C8E	A	1347	-	-	-	X
7	C8E	A	1348	-	-	-	X
7	C8E	B	1340	-	-	-	X
7	C8E	B	1341	-	-	-	X
7	C8E	B	1344	-	-	-	X
7	C8E	B	1345	-	-	-	X
7	C8E	B	1346	-	-	-	X
7	C8E	B	1347	-	-	-	X

2 Entry composition [i](#)

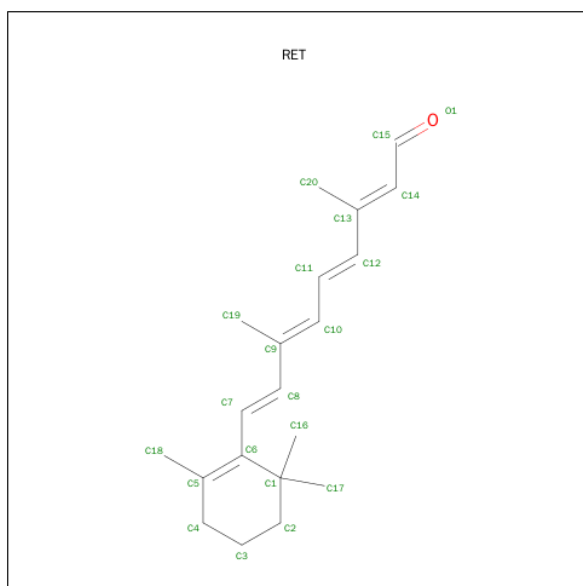
There are 9 unique types of molecules in this entry. The entry contains 5792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RHODOPSIN.

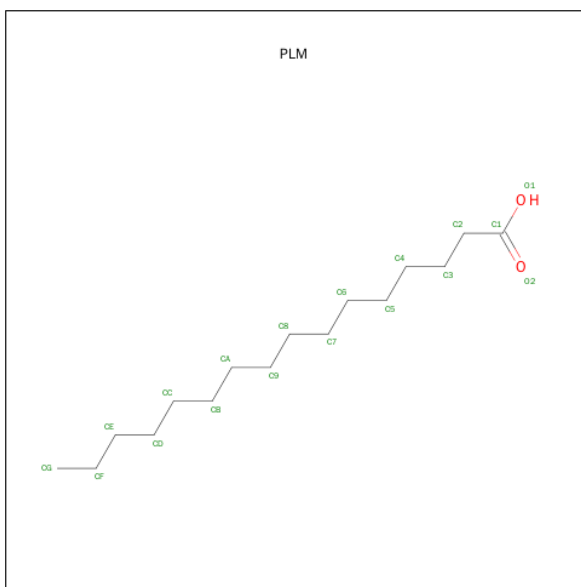
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	1
			2606	1733	403	444	26			
1	B	330	Total	C	N	O	S	0	0	1
			2606	1733	403	444	26			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



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

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).

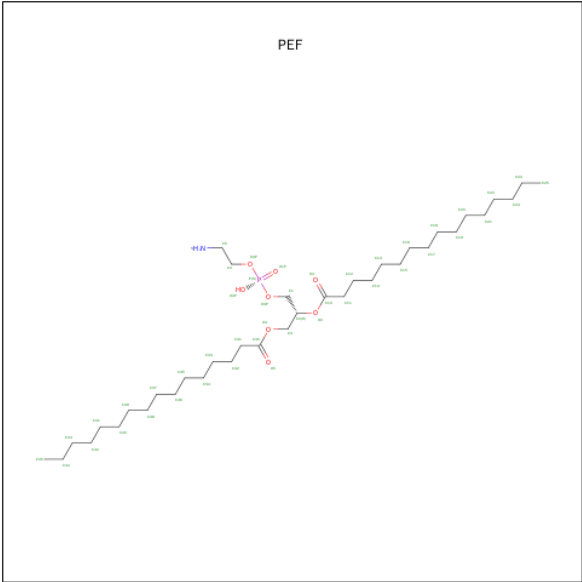


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

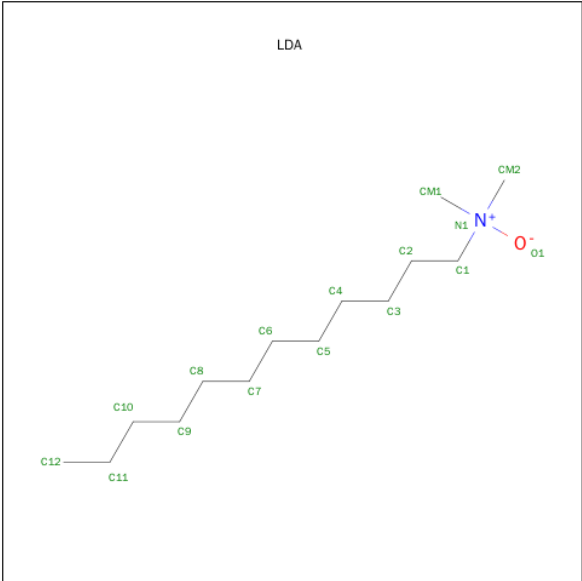
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C₃₇H₇₄NO₈P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C		0	0
			20	20			
5	B	1	Total	C		0	0
			24	24			

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



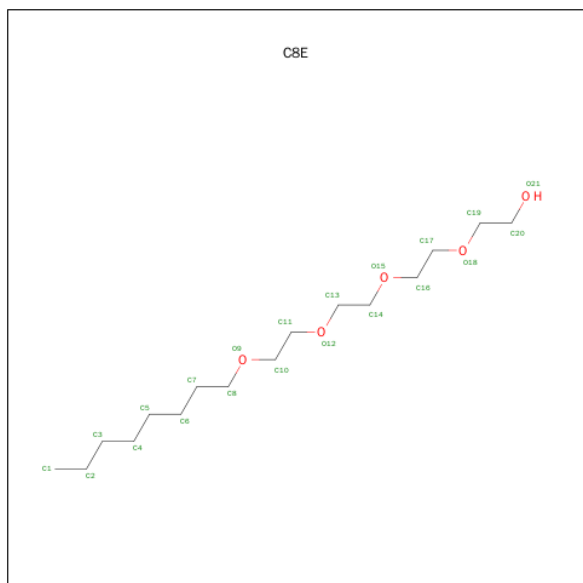
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			16	14	1	1		
6	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			17	14	3		
7	A	1	Total	C	O	0	0
			15	12	3		
7	A	1	Total	C	O	0	0
			10	9	1		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			21	16	5		
7	A	1	Total	C	O	0	0
			12	10	2		
7	B	1	Total	C	O	0	0
			21	16	5		
7	B	1	Total	C	O	0	0
			12	10	2		
7	B	1	Total	C	O	0	0
			14	11	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			14	12	2		
7	B	1	Total	C	O	0	0
			10	9	1		
7	B	1	Total	C	O	0	0
			18	14	4		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

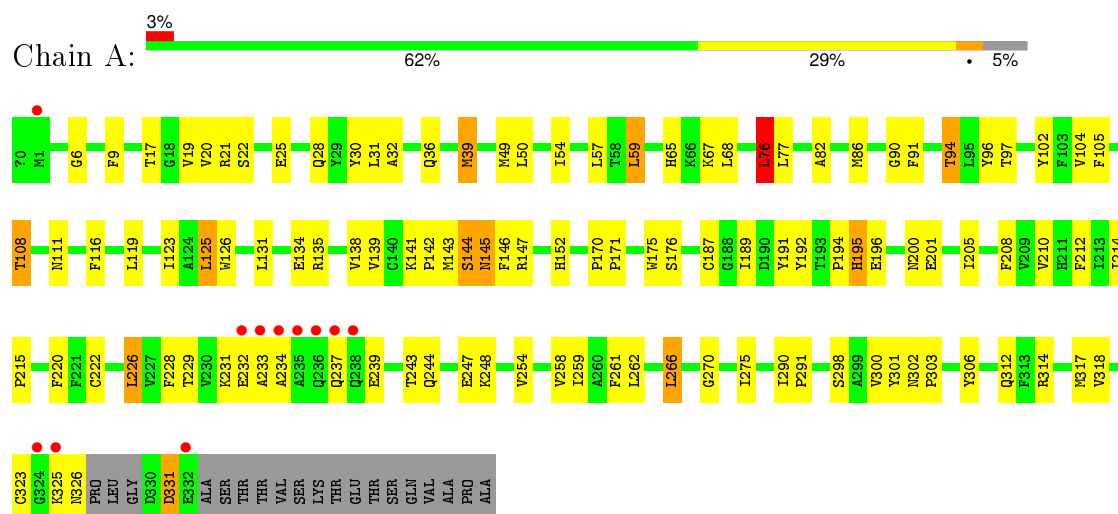
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	20	Total	O	0	0
			20	20		
9	B	20	Total	O	0	0
			20	20		

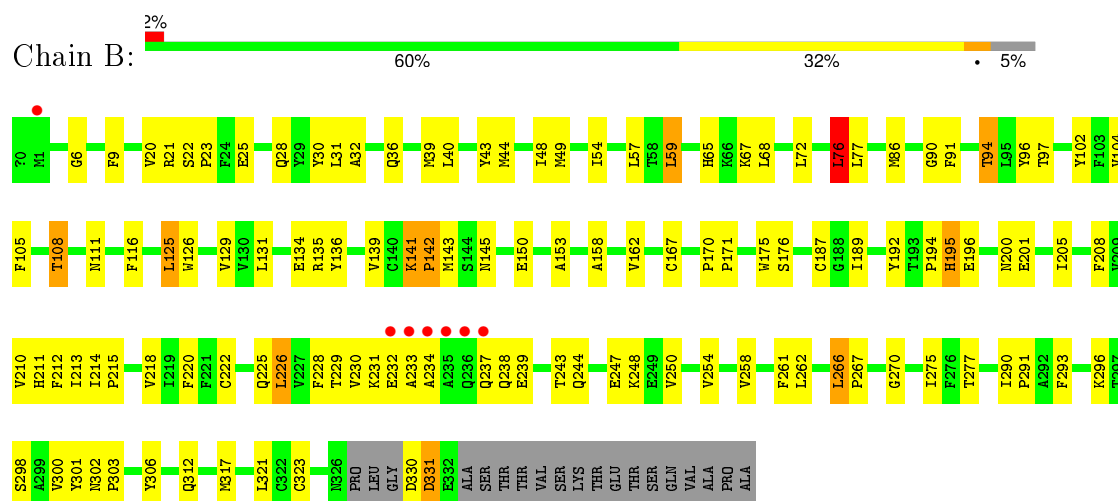
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: RHODOPSIN



• Molecule 1: RHODOPSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	103.82Å 103.82Å 76.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.65 44.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.00-2.65) 96.8 (44.96-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.235 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.9	EDS
Estimated twinning fraction	0.468 for -h,-k,l 0.047 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26063 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5792	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, ACE, LDA, RET, C8E, PEF, PLM

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	0.43	0/2685	0.61	1/3658 (0.0%)
1	B	0.44	0/2685	0.62	1/3658 (0.0%)
All	All	0.44	0/5370	0.61	2/7316 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	LEU	CA-CB-CG	-5.82	101.91	115.30
1	B	76	LEU	CA-CB-CG	-5.27	103.18	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2606	0	2569	113	0
1	B	2606	0	2569	116	0
2	A	20	0	27	1	0
2	B	20	0	27	1	0
3	A	34	0	62	2	0
3	B	34	0	62	2	0
4	A	78	0	68	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	78	0	68	7	0
5	A	20	0	32	0	0
5	B	24	0	40	0	0
6	A	16	0	31	3	0
6	B	32	0	49	26	0
7	A	93	0	153	6	0
7	B	89	0	142	9	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	20	0	0	2	0
9	B	20	0	0	2	0
All	All	5792	0	5899	249	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 21.

All (249) 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)
6:B:1343:LDA:H22	6:B:1348:LDA:C9	1.33	1.35
6:B:1343:LDA:C2	6:B:1348:LDA:H92	1.78	1.12
6:B:1343:LDA:HM23	6:B:1348:LDA:HM21	1.21	1.12
6:B:1343:LDA:C2	6:B:1348:LDA:C9	2.29	1.10
6:B:1343:LDA:H22	6:B:1348:LDA:H92	0.97	0.96
6:B:1343:LDA:H22	6:B:1348:LDA:H91	1.48	0.96
1:B:270:GLY:HA3	6:B:1343:LDA:H12	1.49	0.94
6:B:1343:LDA:H12	6:B:1348:LDA:H31	1.49	0.91
1:B:91:PHE:HA	1:B:94:THR:CG2	2.00	0.90
6:B:1343:LDA:HM23	6:B:1348:LDA:CM2	2.05	0.87
1:B:67:LYS:HG2	1:B:331:ASP:CB	2.06	0.86
1:A:91:PHE:HA	1:A:94:THR:CG2	2.07	0.84
1:B:28:GLN:HB3	1:B:31:LEU:HD12	1.61	0.82
6:B:1343:LDA:CM2	6:B:1348:LDA:HM21	2.11	0.76
1:A:28:GLN:HB3	1:A:31:LEU:HD12	1.67	0.76
1:B:111:ASN:HD22	7:B:1345:C8E:H71	1.50	0.75
1:A:239:GLU:HB2	1:A:244:GLN:HE21	1.53	0.73
1:B:239:GLU:HB2	1:B:244:GLN:HE21	1.54	0.73
1:B:201:GLU:HB2	9:B:2014:HOH:O	1.88	0.72
1:B:108:THR:HA	7:B:1345:C8E:H82	1.73	0.71
6:B:1343:LDA:HM13	6:B:1348:LDA:C3	1.77	0.70
1:B:67:LYS:HE2	1:B:330:ASP:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:HB3	6:B:1348:LDA:H82	1.75	0.69
1:B:111:ASN:HD22	7:B:1345:C8E:C7	2.06	0.68
1:A:232:GLU:HG2	1:A:232:GLU:O	1.92	0.68
1:B:302:ASN:HB2	9:B:2019:HOH:O	1.94	0.67
1:B:91:PHE:HA	1:B:94:THR:HG23	1.76	0.66
1:A:76:LEU:HD22	1:A:306:TYR:CG	2.30	0.66
1:A:143:MET:HE2	1:A:144:SER:H	1.59	0.66
6:B:1343:LDA:H12	6:B:1348:LDA:C3	2.19	0.66
1:B:76:LEU:HD22	1:B:306:TYR:CG	2.31	0.66
1:A:50:LEU:HD23	3:A:1333:PLM:HG1	1.76	0.65
1:A:67:LYS:HG2	1:A:331:ASP:CB	2.27	0.65
1:A:234:ALA:HB1	1:A:239:GLU:OE1	1.98	0.64
1:B:234:ALA:HB1	1:B:239:GLU:OE1	1.98	0.64
1:A:32:ALA:HB1	1:A:36:GLN:OE1	1.98	0.64
1:B:57:LEU:HD11	1:B:317:MET:HG3	1.80	0.63
1:A:229:THR:HA	1:A:233:ALA:HB3	1.80	0.63
1:B:68:LEU:HD23	1:B:312:GLN:NE2	2.14	0.63
1:A:318:VAL:CG1	1:A:326:ASN:HB2	2.28	0.63
1:A:290:ILE:HB	1:A:291:PRO:HD3	1.81	0.63
1:A:65:HIS:HB2	1:A:68:LEU:HD22	1.81	0.63
1:B:262:LEU:O	1:B:266:LEU:HB2	1.99	0.63
1:A:143:MET:HA	1:A:143:MET:HE3	1.79	0.62
1:A:259:ILE:HG23	7:B:1340:C8E:H41	1.81	0.62
1:B:102:TYR:CZ	1:B:104:VAL:HG12	2.35	0.62
1:A:102:TYR:CZ	1:A:104:VAL:HG12	2.34	0.62
6:B:1343:LDA:C1	6:B:1348:LDA:C3	2.78	0.62
1:A:318:VAL:HG12	1:A:326:ASN:HB2	1.81	0.62
1:B:105:PHE:O	1:B:108:THR:HG23	1.99	0.62
1:B:32:ALA:HB1	1:B:36:GLN:OE1	2.00	0.61
1:A:228:PHE:O	1:A:231:LYS:HB3	2.01	0.61
1:A:91:PHE:HA	1:A:94:THR:HG23	1.82	0.61
1:A:54:ILE:CD1	1:A:300:VAL:HG13	2.31	0.61
1:A:143:MET:CE	1:A:144:SER:H	2.14	0.61
4:B:1335:NAG:H4	4:B:1336:NAG:H82	1.83	0.60
1:A:111:ASN:HB3	7:A:1344:C8E:H61	1.82	0.60
1:A:232:GLU:CB	1:B:196:GLU:HG3	2.31	0.60
4:B:1335:NAG:H4	4:B:1336:NAG:N2	2.17	0.60
1:A:57:LEU:HD11	1:A:317:MET:HG3	1.83	0.59
1:B:290:ILE:HB	1:B:291:PRO:HD3	1.85	0.59
1:B:141:LYS:HE3	1:B:237:GLN:OE1	2.01	0.59
1:A:105:PHE:O	1:A:108:THR:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:ND2	7:B:1345:C8E:H71	2.16	0.59
1:A:262:LEU:O	1:A:266:LEU:HB2	2.03	0.59
1:B:96:TYR:HE1	1:B:104:VAL:HG21	1.67	0.58
1:B:54:ILE:CD1	1:B:300:VAL:HG13	2.33	0.58
1:B:90:GLY:O	1:B:94:THR:HG22	2.04	0.58
1:A:111:ASN:CB	7:A:1344:C8E:H61	2.34	0.57
1:A:244:GLN:O	1:A:248:LYS:HB2	2.04	0.57
1:A:220:PHE:CZ	1:B:205:ILE:HD13	2.40	0.57
1:B:270:GLY:HA3	6:B:1348:LDA:H31	1.87	0.57
1:A:298:SER:HA	1:A:301:TYR:CE2	2.40	0.57
1:B:244:GLN:O	1:B:248:LYS:HB2	2.04	0.56
1:B:76:LEU:HD22	1:B:306:TYR:CD2	2.39	0.56
1:A:90:GLY:O	1:A:94:THR:HG22	2.05	0.56
1:A:68:LEU:HD12	1:A:312:GLN:NE2	2.20	0.56
1:B:20:VAL:HA	1:B:30:TYR:CZ	2.40	0.56
1:A:59:LEU:HD13	1:A:77:LEU:HD11	1.87	0.56
1:A:205:ILE:HD13	1:B:220:PHE:CZ	2.41	0.56
6:B:1343:LDA:CM1	6:B:1348:LDA:H31	2.33	0.56
1:A:229:THR:HG23	1:A:234:ALA:HB2	1.88	0.56
1:A:229:THR:CG2	1:A:234:ALA:HB2	2.35	0.55
1:A:146:PHE:HZ	1:A:152:HIS:NE2	2.04	0.55
1:B:229:THR:CG2	1:B:234:ALA:HB2	2.37	0.55
1:B:228:PHE:O	1:B:231:LYS:HB3	2.06	0.55
1:A:76:LEU:HD22	1:A:306:TYR:CD2	2.43	0.54
1:A:96:TYR:HE1	1:A:104:VAL:HG21	1.72	0.54
1:A:232:GLU:HB3	1:B:196:GLU:HG3	1.90	0.53
1:B:266:LEU:HB3	6:B:1348:LDA:C8	2.39	0.53
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.89	0.53
1:B:270:GLY:CA	6:B:1348:LDA:H31	2.39	0.53
1:A:20:VAL:HA	1:A:30:TYR:CZ	2.44	0.53
1:B:229:THR:HG23	1:B:234:ALA:HB2	1.91	0.53
1:A:170:PRO:N	1:A:171:PRO:HD2	2.24	0.53
1:A:91:PHE:HA	1:A:94:THR:HG22	1.91	0.53
1:A:325:LYS:N	1:A:325:LYS:HD2	2.24	0.52
1:A:192:TYR:CE1	1:A:275:ILE:HD13	2.44	0.52
1:A:49:MET:HE3	1:A:49:MET:HA	1.91	0.52
1:A:325:LYS:H	1:A:325:LYS:HD2	1.75	0.52
1:B:22:SER:HB3	1:B:25:GLU:HG2	1.91	0.52
1:A:22:SER:HB3	1:A:25:GLU:HG2	1.92	0.51
6:B:1343:LDA:C1	6:B:1348:LDA:H92	2.38	0.51
1:A:68:LEU:CD1	1:A:312:GLN:HE21	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PRO:HG3	7:A:1343:C8E:H52	1.92	0.51
1:B:170:PRO:N	1:B:171:PRO:HD2	2.26	0.51
1:B:192:TYR:CE1	1:B:275:ILE:HD13	2.44	0.51
1:A:220:PHE:CE2	1:B:205:ILE:HD13	2.45	0.51
1:B:91:PHE:HA	1:B:94:THR:HG22	1.91	0.51
1:B:68:LEU:HD23	1:B:312:GLN:HE21	1.74	0.51
1:B:194:PRO:O	1:B:200:ASN:HB2	2.10	0.51
1:A:314:ARG:HD2	7:A:1346:C8E:H82	1.91	0.50
1:B:187:CYS:O	2:B:1332:RET:H12	2.11	0.50
1:B:59:LEU:C	1:B:59:LEU:HD12	2.32	0.50
1:A:229:THR:C	1:A:231:LYS:N	2.64	0.50
1:B:54:ILE:HD11	1:B:300:VAL:HG13	1.92	0.50
1:A:229:THR:C	1:A:231:LYS:H	2.15	0.50
1:A:142:PRO:HG2	1:A:143:MET:H	1.76	0.50
1:A:254:VAL:O	1:A:258:VAL:HG23	2.12	0.50
1:B:229:THR:C	1:B:231:LYS:H	2.14	0.49
1:A:68:LEU:HD12	1:A:312:GLN:HE21	1.76	0.49
1:A:187:CYS:O	2:A:1332:RET:H12	2.11	0.49
6:B:1343:LDA:C1	6:B:1348:LDA:H31	2.29	0.49
1:A:262:LEU:HB3	1:A:266:LEU:HD22	1.95	0.49
1:B:6:GLY:HA3	1:B:9:PHE:CZ	2.47	0.49
1:A:54:ILE:HD11	1:A:300:VAL:HG13	1.94	0.49
1:A:146:PHE:CZ	1:A:152:HIS:NE2	2.80	0.49
1:A:302:ASN:HB2	9:A:2019:HOH:O	2.11	0.49
1:A:270:GLY:HA2	6:A:1342:LDA:H71	1.95	0.49
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.95	0.49
1:B:96:TYR:CE1	1:B:104:VAL:HG21	2.47	0.49
1:B:65:HIS:HB3	1:B:331:ASP:CB	2.43	0.48
1:A:59:LEU:O	1:A:59:LEU:HD12	2.13	0.48
1:B:59:LEU:HD13	1:B:77:LEU:HD11	1.94	0.48
1:B:136:TYR:HE1	1:B:225:GLN:HE21	1.61	0.48
1:A:171:PRO:HA	1:A:175:TRP:O	2.12	0.48
1:A:59:LEU:C	1:A:59:LEU:HD12	2.34	0.48
1:B:298:SER:HA	1:B:301:TYR:CE2	2.47	0.48
1:B:303:PRO:O	1:B:306:TYR:HB3	2.14	0.48
1:B:222:CYS:O	1:B:226:LEU:HD12	2.14	0.48
1:A:205:ILE:HD13	1:B:220:PHE:CE2	2.49	0.48
1:B:229:THR:C	1:B:231:LYS:N	2.66	0.47
1:A:232:GLU:HB2	1:B:196:GLU:HG3	1.96	0.47
4:B:1335:NAG:O3	4:B:1335:NAG:H83	2.14	0.47
1:A:86:MET:HG2	1:A:116:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:HG22	1:A:247:GLU:HG3	1.95	0.47
1:B:139:VAL:HG12	1:B:139:VAL:O	2.15	0.47
4:A:1335:NAG:H83	4:A:1335:NAG:O3	2.15	0.47
1:B:210:VAL:HA	1:B:214:ILE:HD12	1.96	0.47
1:B:136:TYR:CZ	1:B:142:PRO:HG3	2.48	0.47
6:B:1343:LDA:C2	6:B:1348:LDA:H91	2.23	0.47
1:B:67:LYS:H	1:B:331:ASP:CB	2.28	0.47
1:A:54:ILE:HD13	1:A:300:VAL:HG13	1.96	0.47
1:A:65:HIS:HB3	1:A:331:ASP:CB	2.44	0.47
4:B:1335:NAG:H4	4:B:1336:NAG:C8	2.45	0.47
1:B:175:TRP:O	1:B:176:SER:HB3	2.14	0.47
1:A:194:PRO:O	1:A:195:HIS:C	2.53	0.47
1:B:208:PHE:O	1:B:213:ILE:HG12	2.15	0.46
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.50	0.46
1:A:196:GLU:HG3	1:B:232:GLU:HB2	1.96	0.46
1:A:208:PHE:O	1:A:212:PHE:HB3	2.15	0.46
1:A:143:MET:HG3	1:A:144:SER:N	2.30	0.46
1:B:59:LEU:O	1:B:59:LEU:HD12	2.15	0.46
1:B:158:ALA:O	1:B:162:VAL:HG23	2.15	0.46
1:B:96:TYR:HE1	1:B:104:VAL:CG2	2.28	0.46
1:A:97:THR:HG23	1:A:102:TYR:C	2.36	0.46
1:B:291:PRO:HG3	7:B:1344:C8E:C4	2.46	0.46
1:A:125:LEU:HG	1:A:261:PHE:CZ	2.51	0.45
1:B:111:ASN:HD22	7:B:1345:C8E:C8	2.28	0.45
1:A:270:GLY:HA3	6:A:1342:LDA:H42	1.98	0.45
1:B:293:PHE:HA	1:B:296:LYS:HE2	1.98	0.45
1:B:262:LEU:HB3	1:B:266:LEU:HD22	1.98	0.45
6:B:1343:LDA:H122	6:B:1343:LDA:H91	1.85	0.45
1:B:229:THR:HA	1:B:233:ALA:HB3	1.99	0.45
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.82	0.45
1:A:196:GLU:OE2	1:B:232:GLU:HB3	2.17	0.45
1:A:303:PRO:O	1:A:306:TYR:HB3	2.17	0.45
1:A:146:PHE:HZ	1:A:152:HIS:CD2	2.35	0.45
6:A:1342:LDA:H51	6:A:1342:LDA:H22	1.76	0.45
1:A:134:GLU:OE1	1:A:135:ARG:HD2	2.17	0.45
1:B:266:LEU:C	6:B:1348:LDA:H81	2.37	0.45
1:B:97:THR:HG23	1:B:102:TYR:C	2.37	0.45
1:A:96:TYR:CE1	1:A:104:VAL:HG21	2.52	0.45
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.52	0.45
1:B:208:PHE:O	1:B:212:PHE:HB3	2.16	0.45
1:B:321:LEU:O	3:B:1334:PLM:H31	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1343:LDA:CM1	6:B:1348:LDA:C3	2.51	0.44
1:A:126:TRP:CZ2	1:A:215:PRO:HG3	2.53	0.44
1:A:131:LEU:O	1:A:135:ARG:HG2	2.17	0.44
1:A:17:THR:OG1	1:A:19:VAL:HG12	2.17	0.44
1:A:139:VAL:HG12	1:A:139:VAL:O	2.16	0.44
4:B:1335:NAG:H61	4:B:1336:NAG:C8	2.47	0.44
1:B:167:CYS:HB2	1:B:211:HIS:CD2	2.53	0.44
1:A:39:MET:CE	1:A:39:MET:HA	2.48	0.44
1:B:270:GLY:HA3	6:B:1343:LDA:C1	2.35	0.44
1:B:49:MET:HA	1:B:49:MET:CE	2.48	0.44
1:A:201:GLU:HB2	9:A:2012:HOH:O	2.16	0.44
1:A:175:TRP:O	1:A:176:SER:HB3	2.17	0.43
1:B:194:PRO:O	1:B:195:HIS:C	2.56	0.43
7:A:1345:C8E:H82	1:B:277:THR:HB	1.98	0.43
1:B:230:VAL:O	1:B:230:VAL:HG12	2.17	0.43
1:A:210:VAL:HA	1:A:214:ILE:HD12	2.01	0.43
1:A:233:ALA:O	1:A:237:GLN:HG2	2.19	0.43
1:A:49:MET:CE	1:A:49:MET:HA	2.48	0.43
1:A:147:ARG:O	1:A:147:ARG:HG3	2.19	0.43
1:B:68:LEU:CD2	1:B:312:GLN:HE21	2.32	0.43
1:B:76:LEU:HD22	1:B:306:TYR:HB2	2.01	0.42
7:B:1340:C8E:H192	7:B:1340:C8E:H71	2.01	0.42
1:A:189:ILE:HB	1:A:191:TYR:CE1	2.53	0.42
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.53	0.42
1:B:86:MET:HG2	1:B:116:PHE:O	2.19	0.42
1:B:189:ILE:HA	1:B:189:ILE:HD13	1.89	0.42
1:A:232:GLU:HB3	1:B:196:GLU:OE2	2.19	0.42
1:B:233:ALA:O	1:B:237:GLN:NE2	2.53	0.42
1:B:54:ILE:HG22	3:B:1333:PLM:HE2	2.02	0.42
1:A:291:PRO:HG3	7:A:1343:C8E:H32	2.00	0.42
1:B:54:ILE:HD13	1:B:300:VAL:HG13	2.02	0.42
1:B:22:SER:HA	1:B:23:PRO:HD3	1.94	0.42
1:A:222:CYS:O	1:A:226:LEU:HD12	2.19	0.42
1:B:266:LEU:N	1:B:267:PRO:CD	2.83	0.42
7:B:1340:C8E:H192	7:B:1340:C8E:H51	2.02	0.42
1:B:171:PRO:HA	1:B:175:TRP:O	2.20	0.42
1:B:129:VAL:HG13	1:B:218:VAL:HG11	2.02	0.42
4:B:1335:NAG:H4	4:B:1336:NAG:C7	2.50	0.41
1:B:126:TRP:CZ2	1:B:215:PRO:HG3	2.54	0.41
1:B:40:LEU:O	1:B:43:TYR:HB3	2.20	0.41
1:B:239:GLU:CB	1:B:244:GLN:HE21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLU:OE2	1:A:138:VAL:HG21	2.19	0.41
1:B:91:PHE:O	1:B:94:THR:HG23	2.20	0.41
1:A:54:ILE:HG22	3:A:1333:PLM:HF2	2.01	0.41
1:B:72:LEU:HD22	1:B:250:VAL:HG13	2.03	0.41
6:B:1343:LDA:CM2	6:B:1348:LDA:CM2	2.80	0.41
1:A:194:PRO:O	1:A:200:ASN:HB2	2.21	0.41
4:B:1335:NAG:H61	4:B:1336:NAG:C7	2.50	0.41
1:B:254:VAL:O	1:B:258:VAL:HG23	2.21	0.41
1:A:141:LYS:HE2	1:A:237:GLN:OE1	2.20	0.41
1:B:243:THR:HG22	1:B:247:GLU:HG3	2.02	0.41
1:B:131:LEU:O	1:B:135:ARG:HG2	2.21	0.41
1:B:125:LEU:HG	1:B:261:PHE:CZ	2.55	0.41
1:A:82:ALA:HB2	1:A:123:ILE:HG21	2.03	0.41
1:A:96:TYR:HE1	1:A:104:VAL:CG2	2.33	0.40
1:A:189:ILE:HD13	1:A:189:ILE:HA	1.87	0.40
1:B:266:LEU:HA	1:B:266:LEU:HD12	1.88	0.40
1:B:141:LYS:HE3	1:B:141:LYS:HB2	1.95	0.40
1:A:119:LEU:HG	1:A:123:ILE:HD12	2.04	0.40
1:A:145:ASN:HD22	1:A:145:ASN:HA	1.65	0.40
1:B:134:GLU:OE1	1:B:135:ARG:HD2	2.22	0.40
1:B:150:GLU:O	1:B:153:ALA:HB3	2.22	0.40
1:B:44:MET:O	1:B:48:ILE:HG13	2.21	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	326/349 (93%)	301 (92%)	21 (6%)	4 (1%)	16	35
1	B	326/349 (93%)	303 (93%)	17 (5%)	6 (2%)	11	23
All	All	652/698 (93%)	604 (93%)	38 (6%)	10 (2%)	13	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	B	142	PRO
1	B	143	MET
1	A	331	ASP
1	B	238	GLN
1	B	331	ASP
1	A	195	HIS
1	A	323	CYS
1	B	323	CYS
1	B	195	HIS

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	278/296 (94%)	268 (96%)	10 (4%)	42	70
1	B	278/296 (94%)	267 (96%)	11 (4%)	38	66
All	All	556/592 (94%)	535 (96%)	21 (4%)	40	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	39	MET
1	A	59	LEU
1	A	76	LEU
1	A	94	THR
1	A	108	THR
1	A	125	LEU
1	A	145	ASN
1	A	226	LEU
1	A	266	LEU
1	B	21	ARG
1	B	39	MET
1	B	59	LEU

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Mol	Chain	Res	Type
1	B	76	LEU
1	B	94	THR
1	B	108	THR
1	B	125	LEU
1	B	141	LYS
1	B	145	ASN
1	B	226	LEU
1	B	266	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	244	GLN
1	A	312	GLN
1	A	315	ASN
1	B	111	ASN
1	B	145	ASN
1	B	225	GLN
1	B	244	GLN
1	B	312	GLN
1	B	315	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 carbohydrates 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	$\# Z > 2$
4	NAG	A	1335	1,4	14,14,15	0.67	0	15,19,21	0.70	0
4	NAG	A	1336	4	14,14,15	0.63	0	15,19,21	0.83	1 (6%)
4	BMA	A	1337	4	11,11,12	0.51	0	14,15,17	0.33	0
4	NAG	A	1338	1,4	14,14,15	0.54	0	15,19,21	0.86	0
4	NAG	A	1339	4	14,14,15	0.57	0	15,19,21	0.97	1 (6%)
4	BMA	A	1340	4	11,11,12	0.47	0	14,15,17	0.45	0
4	NAG	B	1335	1,4	14,14,15	0.62	0	15,19,21	0.64	0
4	NAG	B	1336	4	14,14,15	0.64	0	15,19,21	0.75	1 (6%)
4	NAG	B	1337	1,4	14,14,15	0.60	0	15,19,21	0.70	0
4	NAG	B	1338	4	14,14,15	0.71	0	15,19,21	0.71	0
4	BMA	B	1339	4	11,11,12	0.53	0	14,15,17	0.43	0
4	BMA	B	1350	4	11,11,12	0.56	0	14,15,17	0.42	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
4	NAG	A	1335	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1336	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1337	4	-	0/2/19/22	0/1/1/1
4	NAG	A	1338	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1339	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1340	4	-	0/2/19/22	0/1/1/1
4	NAG	B	1335	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1336	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1337	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1338	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1339	4	-	0/2/19/22	0/1/1/1
4	BMA	B	1350	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1339	NAG	C2-N2-C7	-2.86	119.37	123.04
4	B	1336	NAG	C2-N2-C7	-2.18	120.24	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1336	NAG	C2-N2-C7	-2.09	120.36	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1335	NAG	1	0
4	B	1335	NAG	7	0
4	B	1336	NAG	6	0

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z > 2$
2	RET	A	1332	1	19,20,21	0.99	1 (5%)	27,27,28	1.56	8 (29%)
3	PLM	A	1333	1	16,16,17	0.89	1 (6%)	15,15,17	0.63	0
3	PLM	A	1334	1	16,16,17	0.87	1 (6%)	15,15,17	0.64	0
5	PEF	A	1341	-	18,18,46	0.33	0	16,16,51	0.43	0
6	LDA	A	1342	-	15,15,15	1.09	2 (13%)	16,17,17	2.12	4 (25%)
7	C8E	A	1343	-	16,16,20	0.31	0	15,15,19	0.33	0
7	C8E	A	1344	-	14,14,20	0.18	0	13,13,19	0.48	0
7	C8E	A	1345	-	9,9,20	0.25	0	8,8,19	0.51	0
7	C8E	A	1346	-	17,17,20	0.29	0	16,16,19	0.40	0
7	C8E	A	1347	-	20,20,20	0.32	0	19,19,19	0.40	0
7	C8E	A	1348	-	11,11,20	0.23	0	10,10,19	0.47	0
2	RET	B	1332	1	19,20,21	0.96	1 (5%)	27,27,28	1.57	9 (33%)
3	PLM	B	1333	1	16,16,17	0.88	1 (6%)	15,15,17	0.64	0
3	PLM	B	1334	1	16,16,17	0.94	1 (6%)	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	C8E	B	1340	-	20,20,20	0.20	0	19,19,19	0.33	0
7	C8E	B	1341	-	11,11,20	0.25	0	10,10,19	0.39	0
5	PEF	B	1342	-	22,22,46	0.28	0	20,20,51	0.46	0
6	LDA	B	1343	-	15,15,15	0.70	0	16,17,17	2.04	3 (18%)
7	C8E	B	1344	-	13,13,20	0.27	0	12,12,19	0.36	0
7	C8E	B	1345	-	13,13,20	0.23	0	12,12,19	0.40	0
7	C8E	B	1346	-	9,9,20	0.30	0	8,8,19	0.41	0
7	C8E	B	1347	-	17,17,20	0.30	0	16,16,19	0.38	0
6	LDA	B	1348	-	15,15,15	0.85	1 (6%)	16,17,17	1.87	3 (18%)

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	1332	1	-	0/13/30/31	0/1/1/1
3	PLM	A	1333	1	-	0/14/14/15	0/0/0/0
3	PLM	A	1334	1	-	0/14/14/15	0/0/0/0
5	PEF	A	1341	-	-	0/14/14/50	0/0/0/0
6	LDA	A	1342	-	-	0/13/13/13	0/0/0/0
7	C8E	A	1343	-	-	0/14/14/18	0/0/0/0
7	C8E	A	1344	-	-	0/12/12/18	0/0/0/0
7	C8E	A	1345	-	-	0/7/7/18	0/0/0/0
7	C8E	A	1346	-	-	0/15/15/18	0/0/0/0
7	C8E	A	1347	-	-	0/18/18/18	0/0/0/0
7	C8E	A	1348	-	-	0/9/9/18	0/0/0/0
2	RET	B	1332	1	-	0/13/30/31	0/1/1/1
3	PLM	B	1333	1	-	0/14/14/15	0/0/0/0
3	PLM	B	1334	1	-	0/14/14/15	0/0/0/0
7	C8E	B	1340	-	-	0/18/18/18	0/0/0/0
7	C8E	B	1341	-	-	0/9/9/18	0/0/0/0
5	PEF	B	1342	-	-	0/18/18/50	0/0/0/0
6	LDA	B	1343	-	-	0/13/13/13	0/0/0/0
7	C8E	B	1344	-	-	0/11/11/18	0/0/0/0
7	C8E	B	1345	-	-	0/11/11/18	0/0/0/0
7	C8E	B	1346	-	-	0/7/7/18	0/0/0/0
7	C8E	B	1347	-	-	0/15/15/18	0/0/0/0
6	LDA	B	1348	-	-	0/13/13/13	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1333	PLM	O1-C1	-3.45	1.23	1.42
3	B	1333	PLM	O1-C1	-3.42	1.23	1.42
3	A	1334	PLM	O1-C1	-3.37	1.23	1.42
3	B	1334	PLM	O1-C1	-3.37	1.23	1.42
2	B	1332	RET	C1-C6	2.13	1.56	1.53
6	B	1348	LDA	C1-N1	2.27	1.55	1.51
6	A	1342	LDA	CM1-N1	2.47	1.53	1.49
2	A	1332	RET	C1-C6	2.57	1.57	1.53
6	A	1342	LDA	C1-N1	2.73	1.56	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1342	LDA	O1-N1-CM1	-5.32	101.95	109.05
6	B	1348	LDA	CM1-N1-C1	-4.22	96.16	109.77
6	B	1343	LDA	CM2-N1-C1	-3.52	98.43	109.77
6	A	1342	LDA	CM2-N1-CM1	-3.52	104.86	108.83
2	A	1332	RET	C8-C9-C10	-2.60	114.79	118.98
2	B	1332	RET	C8-C9-C10	-2.39	115.13	118.98
2	B	1332	RET	C18-C5-C4	-2.02	109.60	113.43
2	A	1332	RET	C19-C9-C10	2.02	125.89	122.90
6	B	1348	LDA	O1-N1-CM2	2.10	111.87	109.05
6	A	1342	LDA	O1-N1-C1	2.15	112.70	110.27
2	A	1332	RET	C10-C11-C12	2.20	129.85	123.13
2	B	1332	RET	C19-C9-C10	2.24	126.20	122.90
2	B	1332	RET	C10-C11-C12	2.35	130.29	123.13
2	B	1332	RET	C2-C1-C6	2.36	114.09	110.36
2	A	1332	RET	C7-C8-C9	2.41	129.89	126.22
2	A	1332	RET	C2-C1-C6	2.46	114.27	110.36
6	B	1343	LDA	O1-N1-CM2	2.52	112.43	109.05
2	B	1332	RET	C11-C12-C13	2.66	134.13	126.32
2	A	1332	RET	C11-C12-C13	2.72	134.33	126.32
2	B	1332	RET	C7-C8-C9	2.72	130.37	126.22
2	B	1332	RET	C20-C13-C12	3.03	123.14	118.10
2	A	1332	RET	C18-C5-C6	3.06	127.61	124.61
2	A	1332	RET	C20-C13-C12	3.11	123.28	118.10
2	B	1332	RET	C18-C5-C6	3.18	127.72	124.61
6	A	1342	LDA	O1-N1-CM2	4.73	115.37	109.05
6	B	1348	LDA	O1-N1-C1	4.75	115.61	110.27
6	B	1343	LDA	O1-N1-C1	6.47	117.56	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1332	RET	1	0
3	A	1333	PLM	2	0
6	A	1342	LDA	3	0
7	A	1343	C8E	2	0
7	A	1344	C8E	2	0
7	A	1345	C8E	1	0
7	A	1346	C8E	1	0
2	B	1332	RET	1	0
3	B	1333	PLM	1	0
3	B	1334	PLM	1	0
7	B	1340	C8E	3	0
6	B	1343	LDA	21	0
7	B	1344	C8E	1	0
7	B	1345	C8E	5	0
6	B	1348	LDA	23	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	329/349 (94%)	-0.11	11 (3%) 50 48	29, 45, 115, 173	0
1	B	329/349 (94%)	-0.18	7 (2%) 67 66	30, 45, 116, 174	0
All	All	658/698 (94%)	-0.15	18 (2%) 58 56	29, 45, 116, 174	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	10.9
1	A	238	GLN	9.3
1	A	234	ALA	9.1
1	A	235	ALA	9.0
1	B	236	GLN	6.8
1	B	234	ALA	5.6
1	B	235	ALA	5.1
1	A	232	GLU	5.0
1	A	324	GLY	4.3
1	A	236	GLN	4.1
1	A	332	GLU	2.9
1	B	233	ALA	2.9
1	B	237	GLN	2.6
1	A	325	LYS	2.5
1	A	1	MET	2.4
1	B	1	MET	2.4
1	A	237	GLN	2.4
1	B	232	GLU	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 ⓘ

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	NAG	B	1335	14/15	0.97	0.10	-1.20	72,80,90,97	0
4	NAG	A	1335	14/15	0.96	0.10	-1.22	74,82,86,92	0
4	NAG	A	1339	14/15	0.80	0.18	-	100,107,110,112	0
4	NAG	A	1338	14/15	0.90	0.18	-	72,77,81,91	0
4	NAG	B	1336	14/15	0.89	0.13	-	105,112,114,115	0
4	BMA	A	1337	11/12	0.90	0.15	-	117,119,120,120	0
4	BMA	B	1339	11/12	0.82	0.16	-	109,110,111,112	0
4	BMA	B	1350	11/12	0.89	0.16	-	116,117,118,118	0
4	NAG	B	1337	14/15	0.88	0.20	-	68,73,77,87	0
4	NAG	A	1336	14/15	0.88	0.13	-	100,107,109,113	0
4	BMA	A	1340	11/12	0.85	0.12	-	114,114,114,115	0
4	NAG	B	1338	14/15	0.91	0.18	-	97,105,108,109	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
7	C8E	A	1348	12/21	0.56	0.61	18.39	79,83,85,86	0
3	PLM	B	1333	17/18	0.92	0.64	15.32	53,59,76,78	0
7	C8E	B	1341	12/21	0.76	0.58	15.06	84,90,96,97	0
7	C8E	B	1340	21/21	0.49	0.64	13.68	103,114,119,119	0
7	C8E	B	1346	10/21	0.78	0.51	12.07	56,69,81,81	0
7	C8E	B	1347	18/21	0.70	0.52	11.13	66,85,94,95	0
3	PLM	A	1334	17/18	0.88	0.53	10.55	79,83,88,89	0
3	PLM	A	1333	17/18	0.92	0.47	8.67	52,56,76,78	0
7	C8E	A	1347	21/21	0.69	0.40	8.32	92,96,103,104	0
7	C8E	A	1346	18/21	0.73	0.32	6.17	60,80,92,92	0
3	PLM	B	1334	17/18	0.83	0.35	5.23	73,78,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	C8E	A	1343	17/21	0.88	0.29	5.19	64,68,73,73	0
7	C8E	B	1345	14/21	0.90	0.28	5.15	45,59,69,71	0
5	PEF	A	1341	20/47	0.91	0.32	4.92	38,52,73,74	0
7	C8E	A	1345	10/21	0.89	0.33	4.54	51,63,75,75	0
5	PEF	B	1342	24/47	0.88	0.29	4.31	42,59,67,68	0
7	C8E	B	1344	14/21	0.88	0.26	4.24	69,75,78,79	0
6	LDA	B	1343	16/16	0.92	0.26	3.72	23,26,31,33	16
6	LDA	B	1348	16/16	0.90	0.23	1.85	26,30,34,35	16
2	RET	B	1332	20/21	0.97	0.18	1.85	28,36,43,43	0
6	LDA	A	1342	16/16	0.90	0.19	1.59	37,52,66,67	0
2	RET	A	1332	20/21	0.96	0.19	1.22	30,38,43,45	0
7	C8E	A	1344	15/21	0.91	0.19	1.08	55,61,70,71	0
8	ZN	B	1349	1/1	0.95	0.16	0.21	75,75,75,75	1
8	ZN	A	1349	1/1	0.97	0.12	-0.61	76,76,76,76	1

6.5 Other polymers [i](#)

There are no such residues in this entry.