



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X72
Title : CRYSTAL STRUCTURE OF THE CONSTITUTIVELY ACTIVE E113Q,N2C, D282C RHODOPSIN MUTANT WITH BOUND GALPHACT PEPTIDE.
Authors : Standfuss, J.; Edwards, P.C.; Dantona, A.; Fransen, M.; Xie, G.; Oprian, D.D.; Schertler, G.F.X.
Deposited on : 2010-02-22
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (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

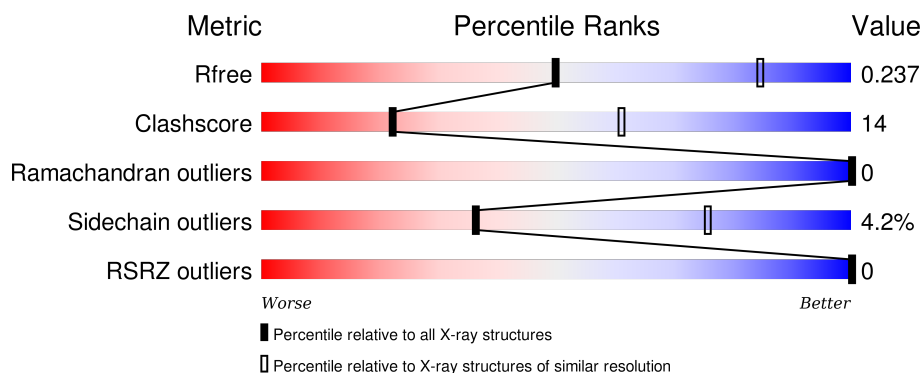
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	349	
2	B	11	

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	PEF	A	1329	-	-	-	X
4	BOG	A	1330	-	-	-	X
5	PLM	A	1332	-	-	-	X
7	RET	A	1338	-	-	X	X
8	LPP	A	1340	-	-	-	X
9	ACT	A	1351	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 2932 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	327	Total	C	N	O	S	0	1	0
			2602	1735	401	438	28			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	CYS	ASN	ENGINEERED MUTATION	UNP P02699
A	113	GLN	GLU	ENGINEERED MUTATION	UNP P02699
A	282	CYS	ASP	ENGINEERED MUTATION	UNP P02699

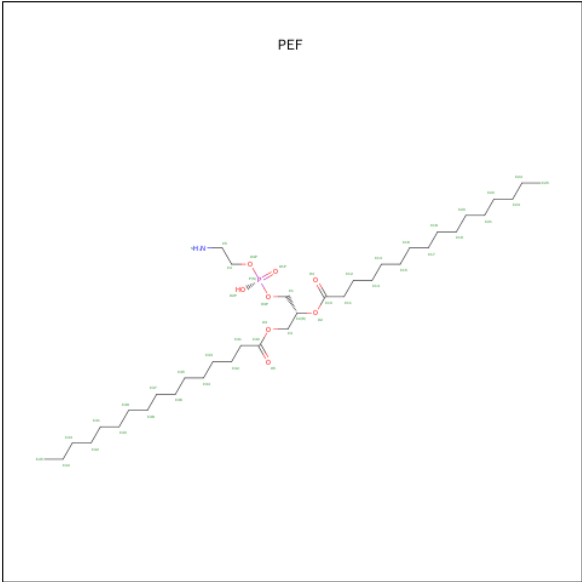
- Molecule 2 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN G(T) SUB-UNIT ALPHA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	S	0	0	0
			88	57	13	17	1			

There is a discrepancy between the modelled and reference sequences:

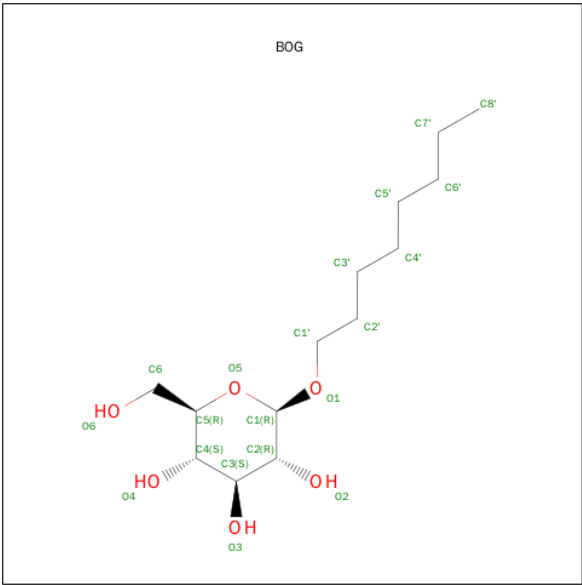
Chain	Residue	Modelled	Actual	Comment	Reference
B	341	LEU	LYS	ENGINEERED MUTATION	UNP P04695

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



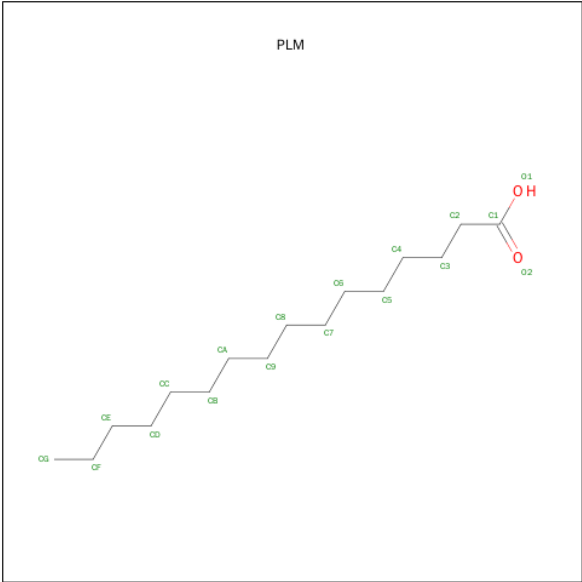
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).

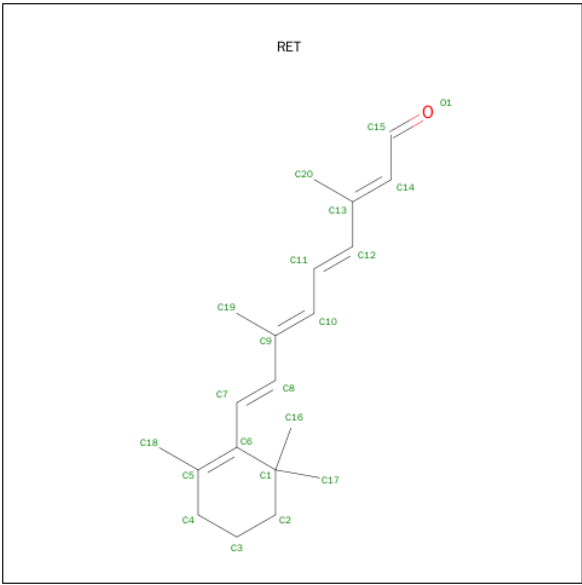


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	16	1		
5	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

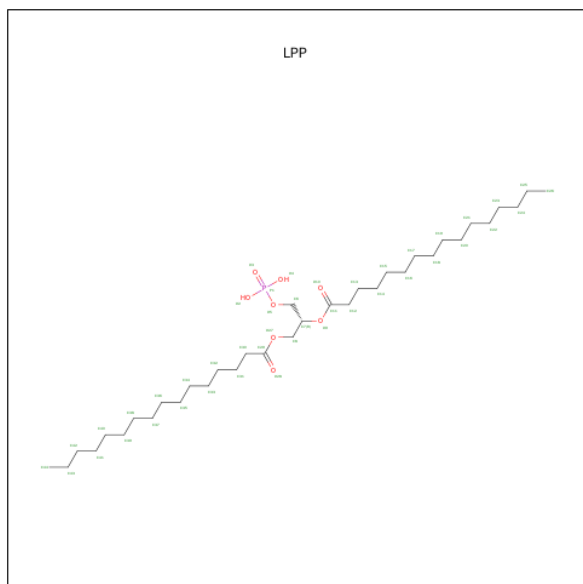
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



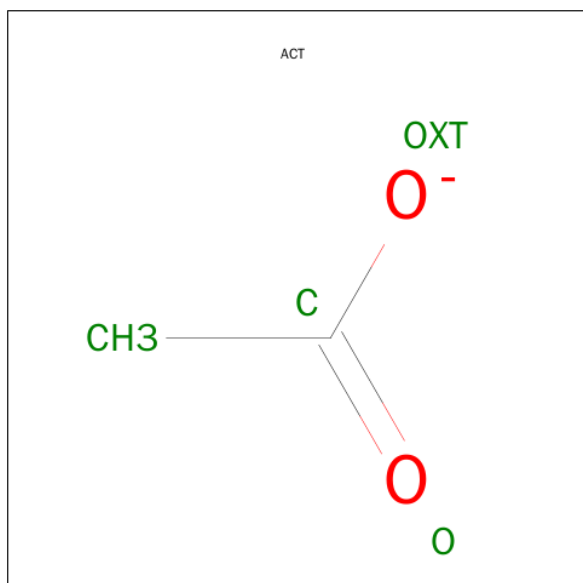
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			21	20	1		

- Molecule 8 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			37	28	8	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		

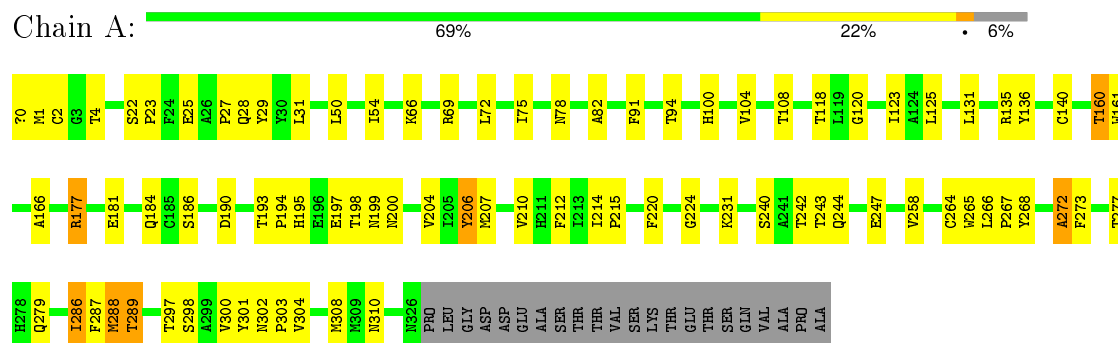
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	18	Total	O	0	0
			18	18		

3 Residue-property plots

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 2: GUANINE NUCLEOTIDE-BINDING PROTEIN G(T) SUBUNIT ALPHA-1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	243.99 Å 243.99 Å 109.16 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.94 – 3.00 39.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (39.94-3.00) 62.7 (39.94-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.244 0.215 , 0.237	Depositor DCC
R_{free} test set	810 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 15641 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2932	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ACE, RET, LPP, ACT, PEF, BOG, PLM, MAN

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	0.51	0/2687	0.65	2/3662 (0.1%)
2	B	0.72	0/88	0.61	0/115
All	All	0.52	0/2775	0.65	2/3777 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	ACE	C-N-CA	8.50	142.95	121.70
1	A	272	ALA	CB-CA-C	-7.25	99.23	110.10

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	2602	0	2579	64	0
2	B	88	0	89	4	0
3	A	47	0	73	6	0
4	A	20	0	28	2	0
5	A	34	0	62	1	0
6	A	61	0	52	3	0
7	A	21	0	28	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	37	0	50	8	0
9	A	4	0	3	0	0
10	A	18	0	0	1	0
All	All	2932	0	2964	81	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 14.

All (81) 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:78:ASN:HD21	1:A:160:THR:HG21	1.17	1.08
1:A:200:ASN:O	1:A:204:VAL:HG23	1.67	0.94
1:A:78:ASN:ND2	1:A:160:THR:HG21	1.87	0.87
1:A:100:HIS:CE1	3:A:1329:PEF:H111	2.19	0.77
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.73	0.70
1:A:28:GLN:HB3	1:A:31:LEU:HD12	1.74	0.69
1:A:27:PRO:HB3	1:A:29:TYR:CE2	2.27	0.69
3:A:1329:PEF:O4	3:A:1329:PEF:H12	1.92	0.68
3:A:1329:PEF:H391	3:A:1329:PEF:H351	1.75	0.67
1:A:100:HIS:O	3:A:1329:PEF:H52	1.98	0.64
1:A:75:ILE:HG21	1:A:131:LEU:HD13	1.80	0.62
1:A:75:ILE:CG2	1:A:131:LEU:HD13	2.30	0.62
1:A:224:GLY:N	4:A:1330:BOG:H8'2	2.15	0.61
1:A:78:ASN:HD21	1:A:160:THR:CG2	2.05	0.61
1:A:181:GLU:HB3	10:A:2010:HOH:O	2.01	0.61
1:A:4:THR:HG21	6:A:1333:NAG:H82	1.83	0.61
7:A:1338:RET:H181	7:A:1338:RET:H8	1.82	0.60
1:A:123:ILE:HG23	1:A:160:THR:CG2	2.31	0.60
8:A:1340:LPP:C8	8:A:1340:LPP:H122	2.32	0.58
5:A:1331:PLM:H22	8:A:1340:LPP:H161	1.85	0.58
1:A:100:HIS:CD2	1:A:104:VAL:HG11	2.39	0.58
1:A:220:PHE:HA	4:A:1330:BOG:H8'1	1.85	0.57
1:A:288:MET:CE	1:A:288:MET:HA	2.35	0.57
1:A:23:PRO:HB3	1:A:184:GLN:HB3	1.86	0.56
1:A:72:LEU:HD12	2:B:346:ASP:HB3	1.88	0.56
1:A:298:SER:O	1:A:302:ASN:HB2	2.06	0.56
1:A:264:CYS:HB2	1:A:301:TYR:OH	2.06	0.55
8:A:1340:LPP:H122	8:A:1340:LPP:HC81	1.89	0.54
1:A:118:THR:OG1	7:A:1338:RET:H203	2.08	0.54
1:A:287:PHE:HD1	1:A:288:MET:HE3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1340:LPP:C8	8:A:1340:LPP:C12	2.86	0.53
1:A:272:ALA:HB2	7:A:1338:RET:C16	2.39	0.53
1:A:300:VAL:O	1:A:303:PRO:HD2	2.08	0.53
1:A:66:LYS:HA	1:A:69:ARG:NH2	2.24	0.53
1:A:100:HIS:CG	1:A:104:VAL:HG11	2.46	0.51
3:A:1329:PEF:C39	3:A:1329:PEF:H351	2.42	0.50
1:A:286:ILE:HA	1:A:289:THR:HB	1.92	0.50
1:A:22:SER:HB3	1:A:25:GLU:HB2	1.94	0.50
1:A:304:VAL:HA	1:A:308:MET:HG3	1.93	0.50
7:A:1338:RET:C8	7:A:1338:RET:H181	2.42	0.50
1:A:210:VAL:O	1:A:215:PRO:HD3	2.13	0.49
1:A:135:ARG:HD3	2:B:349:LEU:HD11	1.94	0.48
1:A:272:ALA:HB2	7:A:1338:RET:H162	1.95	0.48
1:A:4:THR:CG2	6:A:1333:NAG:H82	2.43	0.48
1:A:198:THR:O	1:A:199:ASN:HB2	2.14	0.48
1:A:304:VAL:HA	1:A:308:MET:CG	2.44	0.47
1:A:297:THR:HG22	1:A:297:THR:O	2.14	0.47
1:A:288:MET:HA	1:A:288:MET:HE3	1.97	0.47
1:A:166:ALA:O	1:A:206:TYR:OH	2.26	0.46
8:A:1340:LPP:C12	8:A:1340:LPP:HC81	2.44	0.46
1:A:207:MET:HB2	7:A:1338:RET:H173	1.98	0.46
1:A:123:ILE:HG23	1:A:160:THR:HG23	1.98	0.46
1:A:240:SER:O	1:A:244:GLN:HG2	2.15	0.45
1:A:197:GLU:OE1	1:A:197:GLU:N	2.50	0.45
1:A:94:THR:OG1	1:A:186:SER:HB3	2.17	0.45
1:A:207:MET:CB	7:A:1338:RET:H173	2.46	0.44
1:A:28:GLN:CB	1:A:31:LEU:HD12	2.44	0.44
1:A:50:LEU:O	1:A:54:ILE:HG13	2.17	0.44
7:A:1338:RET:H11	7:A:1338:RET:H191	1.80	0.44
1:A:266:LEU:HB3	1:A:267:PRO:HD3	1.99	0.44
1:A:193:THR:HG22	1:A:195:HIS:HB2	2.00	0.43
1:A:136:TYR:O	1:A:140:CYS:HB2	2.18	0.43
1:A:1:MET:O	1:A:1:MET:HG3	2.18	0.43
8:A:1340:LPP:H332	8:A:1340:LPP:O28	2.19	0.43
2:B:345:LYS:HA	2:B:350:PHE:OXT	2.18	0.43
1:A:91:PHE:N	1:A:91:PHE:CD1	2.86	0.42
1:A:273:PHE:O	1:A:277:THR:HG23	2.19	0.42
7:A:1338:RET:H7	7:A:1338:RET:H161	1.84	0.42
1:A:194:PRO:HG3	1:A:279:GLN:OE1	2.18	0.42
1:A:177:ARG:NH1	1:A:190:ASP:OD2	2.49	0.42
6:A:1335:BMA:H62	6:A:1337:MAN:H2	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:NZ	1:A:247:GLU:OE2	2.53	0.41
1:A:240:SER:HB3	1:A:243:THR:HB	2.02	0.41
1:A:160:THR:HG22	1:A:161[A]:TRP:CD1	2.56	0.41
1:A:100:HIS:HA	3:A:1329:PEF:H52	2.02	0.41
1:A:212:PHE:C	1:A:215:PRO:HD2	2.41	0.41
1:A:310:ASN:ND2	2:B:348:GLY:HA3	2.35	0.41
8:A:1340:LPP:H122	8:A:1340:LPP:HC82	2.02	0.40
8:A:1340:LPP:H132	8:A:1340:LPP:H161	1.80	0.40
1:A:82:ALA:HB1	1:A:120:GLY:O	2.21	0.40
1:A:125:LEU:HD13	1:A:265:TRP:NE1	2.36	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%)	294 (90%)	32 (10%)	0	100	100
2	B	9/11 (82%)	9 (100%)	0	0	100	100
All	All	335/360 (93%)	303 (90%)	32 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/296 (94%)	268 (96%)	11 (4%)	39	77
2	B	10/10 (100%)	9 (90%)	1 (10%)	9	34
All	All	289/306 (94%)	277 (96%)	12 (4%)	36	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	CYS
1	A	108	THR
1	A	160	THR
1	A	177	ARG
1	A	206	TYR
1	A	242	THR
1	A	258	VAL
1	A	268	TYR
1	A	286	ILE
1	A	288	MET
1	A	289	THR
2	B	340	ILE

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

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 ⓘ

5 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	$\# Z > 2$
6	NAG	A	1333	1,6	14,14,15	0.54	0	15,19,21	2.31	4 (26%)
6	NAG	A	1334	6	14,14,15	0.59	0	15,19,21	1.21	1 (6%)
6	BMA	A	1335	6	11,11,12	0.84	0	14,15,17	1.94	4 (28%)
6	MAN	A	1336	6	11,11,12	0.51	0	14,15,17	1.19	2 (14%)
6	MAN	A	1337	6	11,11,12	0.92	1 (9%)	14,15,17	1.90	3 (21%)

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
6	NAG	A	1333	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1334	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1335	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1336	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1337	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1337	MAN	C2-C3	2.23	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1335	BMA	O5-C1-C2	-3.77	104.75	110.86
6	A	1333	NAG	O7-C7-C8	-3.10	116.38	122.06
6	A	1337	MAN	C3-C4-C5	-2.33	106.14	110.20
6	A	1336	MAN	O5-C1-C2	-2.15	107.36	110.86
6	A	1335	BMA	C1-C2-C3	2.16	112.09	109.54
6	A	1333	NAG	O7-C7-N2	2.65	127.27	121.86
6	A	1335	BMA	C2-C3-C4	2.76	115.74	111.04
6	A	1334	NAG	O5-C5-C6	2.78	113.37	107.35
6	A	1337	MAN	O5-C5-C6	2.95	113.74	107.35
6	A	1336	MAN	C1-O5-C5	3.55	116.75	112.25
6	A	1335	BMA	C3-C4-C5	3.89	116.98	110.20
6	A	1333	NAG	C2-N2-C7	4.49	128.81	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1337	MAN	C1-C2-C3	5.22	115.72	109.54
6	A	1333	NAG	C1-O5-C5	5.69	119.47	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1333	NAG	2	0
6	A	1335	BMA	1	0
6	A	1337	MAN	1	0

5.6 Ligand geometry [i](#)

7 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
3	PEF	A	1329	-	45,46,46	0.91	1 (2%)	46,51,51	1.09	4 (8%)
4	BOG	A	1330	-	20,20,20	0.78	1 (5%)	25,25,25	1.22	2 (8%)
5	PLM	A	1331	1	16,16,17	1.06	1 (6%)	14,15,17	1.15	2 (14%)
5	PLM	A	1332	1	16,16,17	0.91	1 (6%)	14,15,17	1.33	2 (14%)
7	RET	A	1338	-	21,21,21	0.89	1 (4%)	27,28,28	1.86	8 (29%)
8	LPP	A	1340	-	36,36,43	1.12	2 (5%)	39,41,48	1.23	3 (7%)
9	ACT	A	1351	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-

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	PEF	A	1329	-	-	0/50/50/50	0/0/0/0
4	BOG	A	1330	-	-	0/11/31/31	0/1/1/1
5	PLM	A	1331	1	-	0/13/14/15	0/0/0/0
5	PLM	A	1332	1	-	0/13/14/15	0/0/0/0
7	RET	A	1338	-	-	0/14/31/31	0/1/1/1
8	LPP	A	1340	-	-	1/38/38/45	0/0/0/0
9	ACT	A	1351	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1338	RET	C1-C6	-3.04	1.49	1.53
4	A	1330	BOG	O1-C1	2.13	1.44	1.40
9	A	1351	ACT	CH3-C	2.19	1.51	1.48
3	A	1329	PEF	P-O2P	2.52	1.65	1.54
5	A	1332	PLM	C2-C1	2.79	1.57	1.49
5	A	1331	PLM	C2-C1	3.44	1.59	1.49
8	A	1340	LPP	O27-C29	4.14	1.45	1.33
8	A	1340	LPP	O9-C11	4.40	1.47	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1338	RET	C11-C10-C9	-4.03	121.38	127.20
7	A	1338	RET	C3-C4-C5	-3.67	108.05	113.87
7	A	1338	RET	C16-C1-C6	-3.34	105.06	110.30
5	A	1332	PLM	CB-CA-C9	-2.76	100.30	114.53
3	A	1329	PEF	C22-C21-C20	-2.73	100.45	114.53
7	A	1338	RET	C1-C6-C7	-2.58	108.60	115.82
8	A	1340	LPP	O9-C11-O10	-2.57	116.76	123.67
7	A	1338	RET	C7-C8-C9	-2.45	122.48	126.22
5	A	1331	PLM	C3-C2-C1	-2.39	106.50	113.36
5	A	1332	PLM	C3-C2-C1	-2.28	106.81	113.36
7	A	1338	RET	C11-C12-C13	-2.19	119.87	126.32
3	A	1329	PEF	O2-C2-C3	-2.17	100.72	108.36
8	A	1340	LPP	O27-C29-O28	-2.16	117.93	123.49
3	A	1329	PEF	C13-C12-C11	-2.07	105.71	113.29
3	A	1329	PEF	C32-C31-C30	2.18	122.17	113.59
5	A	1331	PLM	C4-C3-C2	2.26	122.67	113.86
7	A	1338	RET	C12-C13-C14	2.36	122.79	118.98
4	A	1330	BOG	O1-C1-C2	2.44	111.12	108.04
7	A	1338	RET	C7-C6-C5	3.01	128.27	121.37
4	A	1330	BOG	C1'-O1-C1	3.43	119.94	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1340	LPP	O9-C11-C12	4.85	122.08	111.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1340	LPP	C7-O9-C11-C12

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1329	PEF	6	0
4	A	1330	BOG	2	0
5	A	1331	PLM	1	0
7	A	1338	RET	9	0
8	A	1340	LPP	8	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	326/349 (93%)	-0.87	0	100 100	59, 74, 98, 135	0
2	B	11/11 (100%)	-0.89	0	100 100	83, 90, 97, 100	0
All	All	337/360 (93%)	-0.87	0	100 100	59, 75, 99, 135	0

There are no RSRZ outliers to report.

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](#)

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
6	NAG	A	1333	14/15	0.98	0.10	-1.44	55,59,66,70	0
6	NAG	A	1334	14/15	0.98	0.12	-	51,59,73,77	0
6	BMA	A	1335	11/12	0.95	0.14	-	78,92,103,111	0
6	MAN	A	1336	11/12	0.94	0.25	-	81,89,94,100	0
6	MAN	A	1337	11/12	0.91	0.25	-	104,112,118,118	0

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
7	RET	A	1338	21/21	0.80	0.38	9.03	73,84,87,90	21
8	LPP	A	1340	37/44	0.90	0.32	7.76	79,117,175,186	0
3	PEF	A	1329	47/47	0.87	0.36	6.78	63,105,124,147	0
9	ACT	A	1351	4/4	0.96	0.41	4.16	83,88,96,98	0
5	PLM	A	1332	17/18	0.92	0.26	3.64	84,100,114,117	0
4	BOG	A	1330	20/20	0.93	0.31	3.58	78,116,134,137	0
5	PLM	A	1331	17/18	0.95	0.20	1.91	79,88,112,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.