



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2017 – 10:33 PM EDT

PDB ID : 2X72
Title : CRYSTAL STRUCTURE OF THE CONSTITUTIVELY ACTIVE E113Q,D2C,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 : unknown
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

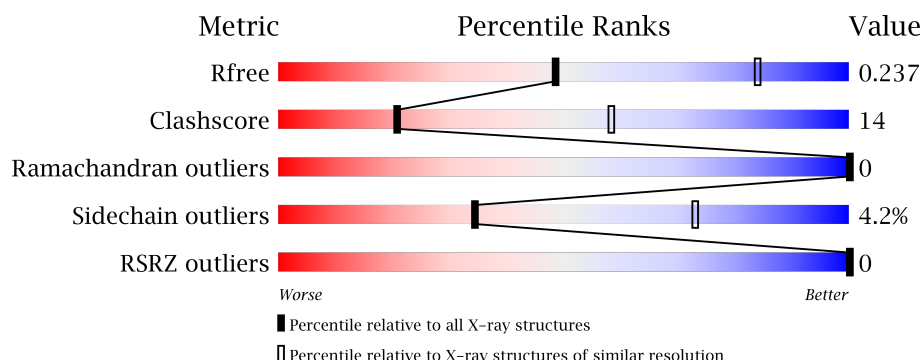
1 Overall quality at a glance

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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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
10	LPP	A	411	-	-	-	X
11	ACT	A	412	-	-	-	X
3	PEF	A	401	-	-	-	X
4	BOG	A	402	-	-	-	X
5	PLM	A	404	-	-	-	X
9	RET	A	410	-	-	X	X

2 Entry composition

There are 12 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).



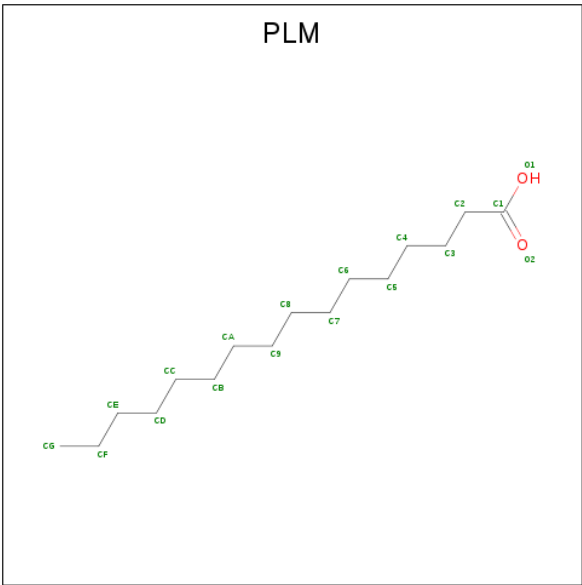
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 47	C 37	N 1	O 8	P 1	0	0

- Molecule 4 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



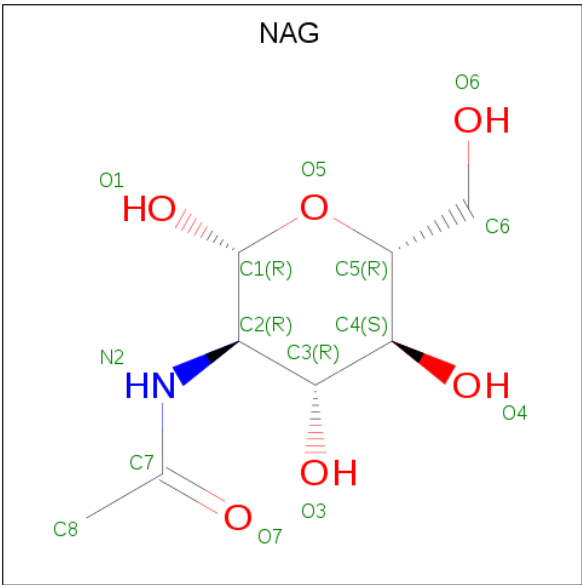
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



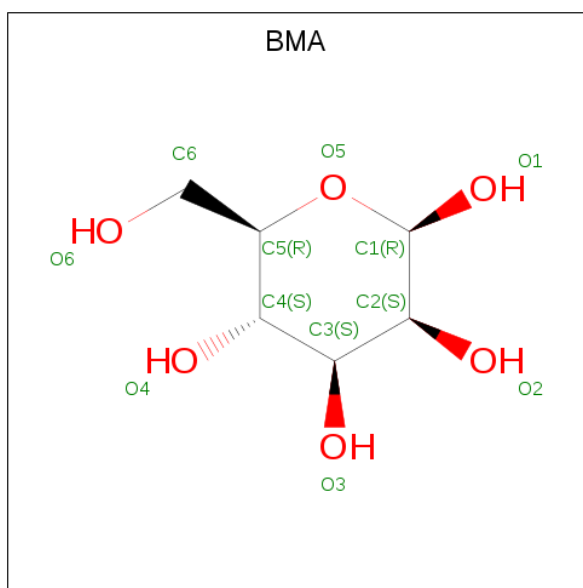
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	16	1		
5	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



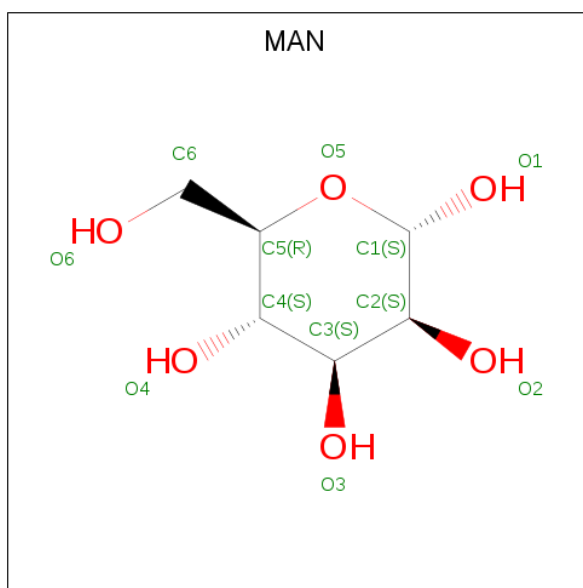
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



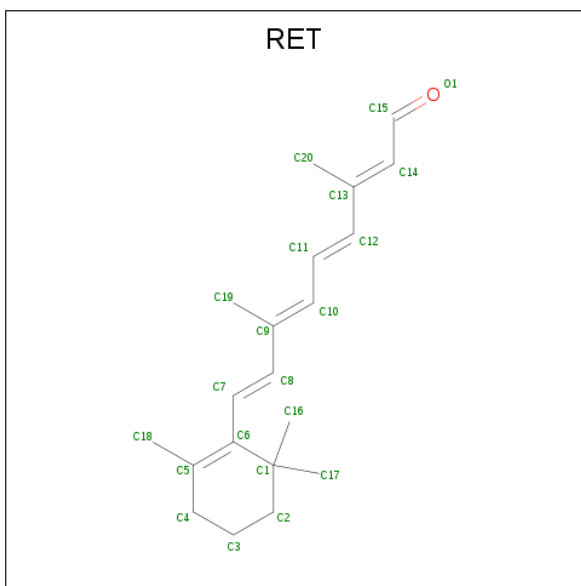
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



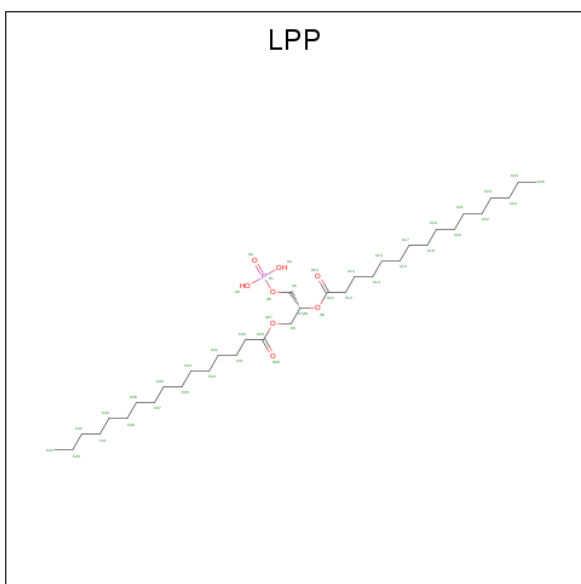
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



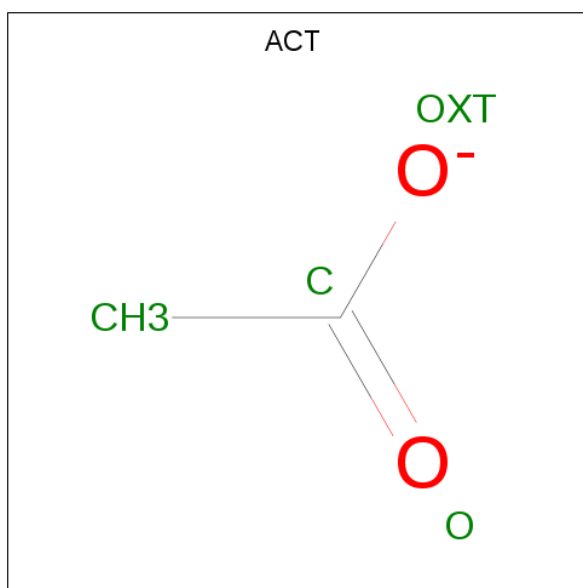
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			21	20	1		

- Molecule 10 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



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

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

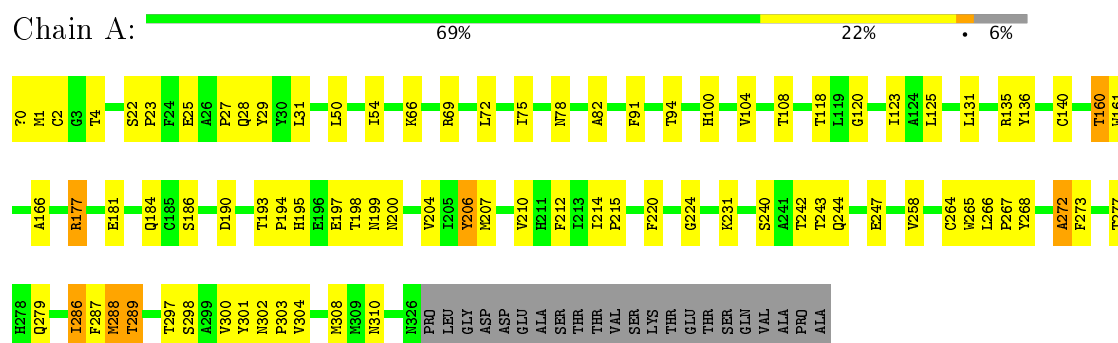
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	16	Total	O	0	0
			16	16		
12	B	2	Total	O	0	0
			2	2		

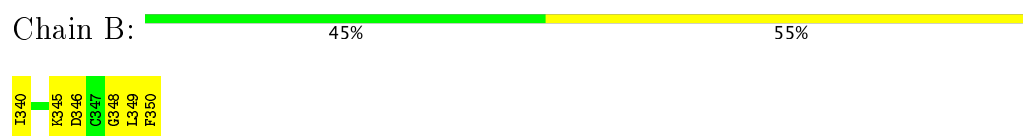
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 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	243.99Å 243.99Å 109.16Å 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 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.244 0.205 , 0.237	Depositor DCC
R_{free} test set	809 reflections (5.17%)	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
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	28	0	24	2	0
7	A	11	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	22	0	20	1	0
9	A	21	0	28	9	0
10	A	37	0	50	8	0
11	A	4	0	3	0	0
12	A	16	0	0	1	0
12	B	2	0	0	0	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.

The worst 5 of 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:401:PEF:H111	2.19	0.77
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.73	0.70

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%)	37	75
2	B	10/10 (100%)	9 (90%)	1 (10%)	9	33
All	All	289/306 (94%)	277 (96%)	12 (4%)	34	73

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	THR
1	A	258	VAL
1	A	288	MET
1	A	206	TYR
1	A	286	ILE

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	401	-	46,46,46	0.91	3 (6%)	48,51,51	1.12	5 (10%)
4	BOG	A	402	-	20,20,20	0.81	1 (5%)	25,25,25	1.20	1 (4%)
5	PLM	A	403	1	16,16,17	1.06	1 (6%)	15,15,17	1.22	2 (13%)
5	PLM	A	404	1	16,16,17	0.92	1 (6%)	15,15,17	1.33	2 (13%)
6	NAG	A	405	1,6	14,14,15	0.55	0	15,19,21	2.39	6 (40%)
6	NAG	A	406	7,6	14,14,15	0.61	0	15,19,21	1.03	0
7	BMA	A	407	8,6	11,11,12	0.87	0	13,15,17	1.94	3 (23%)
8	MAN	A	408	7	11,11,12	0.52	0	13,15,17	1.19	2 (15%)
8	MAN	A	409	7	11,11,12	0.93	1 (9%)	13,15,17	1.70	2 (15%)
9	RET	A	410	-	21,21,21	0.90	1 (4%)	27,28,28	1.84	8 (29%)
10	LPP	A	411	-	36,36,43	1.15	2 (5%)	40,41,48	1.25	4 (10%)
11	ACT	A	412	-	1,3,3	2.41	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	401	-	-	0/50/50/50	0/0/0/0
4	BOG	A	402	-	-	0/11/31/31	0/1/1/1
5	PLM	A	403	1	-	0/13/14/15	0/0/0/0
5	PLM	A	404	1	-	0/13/14/15	0/0/0/0
6	NAG	A	405	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	406	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	407	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	408	7	-	0/2/19/22	0/1/1/1
8	MAN	A	409	7	-	0/2/19/22	0/1/1/1
9	RET	A	410	-	-	0/13/31/31	0/1/1/1
10	LPP	A	411	-	-	1/38/38/45	0/0/0/0
11	ACT	A	412	-	-	0/0/0/0	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	410	RET	C1-C6	-3.15	1.49	1.53
3	A	401	PEF	C31-C30	2.01	1.56	1.50
3	A	401	PEF	P-O4P	2.06	1.68	1.59
3	A	401	PEF	P-O2P	2.10	1.65	1.55
4	A	402	BOG	O1-C1	2.18	1.44	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	410	RET	C11-C10-C9	-4.16	121.38	127.31
7	A	407	BMA	O5-C1-C2	-3.86	104.75	110.79
9	A	410	RET	C3-C4-C5	-3.33	108.05	113.78
9	A	410	RET	C16-C1-C6	-3.24	105.06	110.31
6	A	405	NAG	O7-C7-C8	-3.12	116.38	122.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	411	LPP	C7-O9-C11-C12

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	PEF	6	0
4	A	402	BOG	2	0
5	A	403	PLM	1	0
6	A	405	NAG	2	0
7	A	407	BMA	1	0
8	A	409	MAN	1	0
9	A	410	RET	9	0
10	A	411	LPP	8	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 [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](#)

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
9	RET	A	410	21/21	0.80	0.38	9.05	73,84,87,90	21
10	LPP	A	411	37/44	0.90	0.32	7.76	79,117,175,186	0
3	PEF	A	401	47/47	0.87	0.36	6.78	63,105,124,147	0
11	ACT	A	412	4/4	0.96	0.41	4.16	83,88,96,98	0
5	PLM	A	404	17/18	0.92	0.26	3.66	84,100,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BOG	A	402	20/20	0.93	0.30	3.56	78,116,134,137	0
5	PLM	A	403	17/18	0.95	0.20	1.92	79,88,112,116	0
6	NAG	A	405	14/15	0.98	0.10	-1.44	55,59,66,70	0
6	NAG	A	406	14/15	0.98	0.12	-	51,59,73,77	0
7	BMA	A	407	11/12	0.95	0.14	-	78,92,103,111	0
8	MAN	A	408	11/12	0.94	0.25	-	81,89,94,100	0
8	MAN	A	409	11/12	0.91	0.25	-	104,112,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.