



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:10 AM UTC

PDB ID : 4QAM / pdb_00004qam
Title : Crystal Structure of the RPGR RCC1-like domain in complex with the RPGR-interacting domain of RPGRIP1
Authors : Remans, K.; Buerger, M.; Vetter, I.R.; Wittinghofer, A.
Deposited on : 2014-05-05
Resolution : 1.83 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

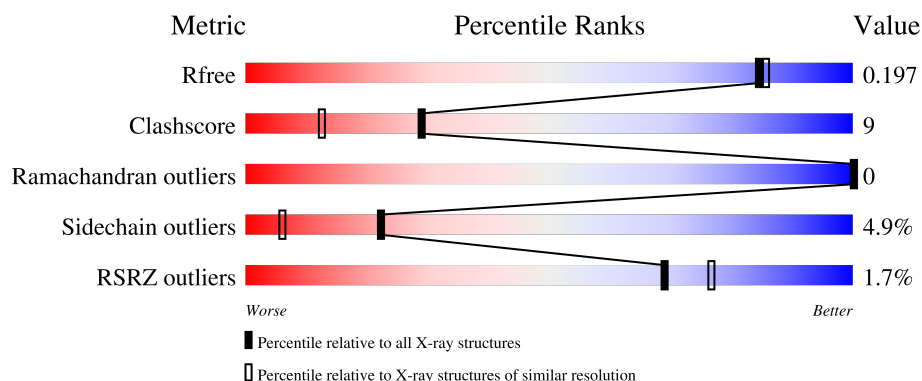
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

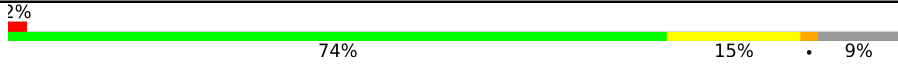
The reported resolution of this entry is 1.83 Å.

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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	400	
2	B	201	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4654 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 X-linked retinitis pigmentosa GTPase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	11	0
			2824	1793	482	531	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	VAL	ILE	engineered mutation	UNP Q92834
A	393	TRP	-	expression tag	UNP Q92834
A	394	SER	-	expression tag	UNP Q92834
A	395	HIS	-	expression tag	UNP Q92834
A	396	PRO	-	expression tag	UNP Q92834
A	397	GLN	-	expression tag	UNP Q92834
A	398	PHE	-	expression tag	UNP Q92834
A	399	GLU	-	expression tag	UNP Q92834
A	400	LYS	-	expression tag	UNP Q92834

- Molecule 2 is a protein called X-linked retinitis pigmentosa GTPase regulator-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S Se	0	2	0
			1464	930	233	294	2 5			

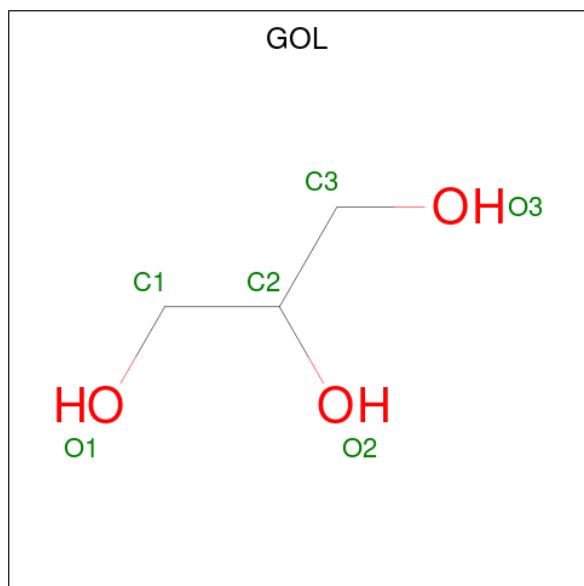
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1086	GLY	-	expression tag	UNP Q96KN7
B	1087	ALA	-	expression tag	UNP Q96KN7
B	1088	MSE	-	expression tag	UNP Q96KN7
B	1089	GLY	-	expression tag	UNP Q96KN7
B	1090	SER	-	expression tag	UNP Q96KN7

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total	O	0	0
			239	239		

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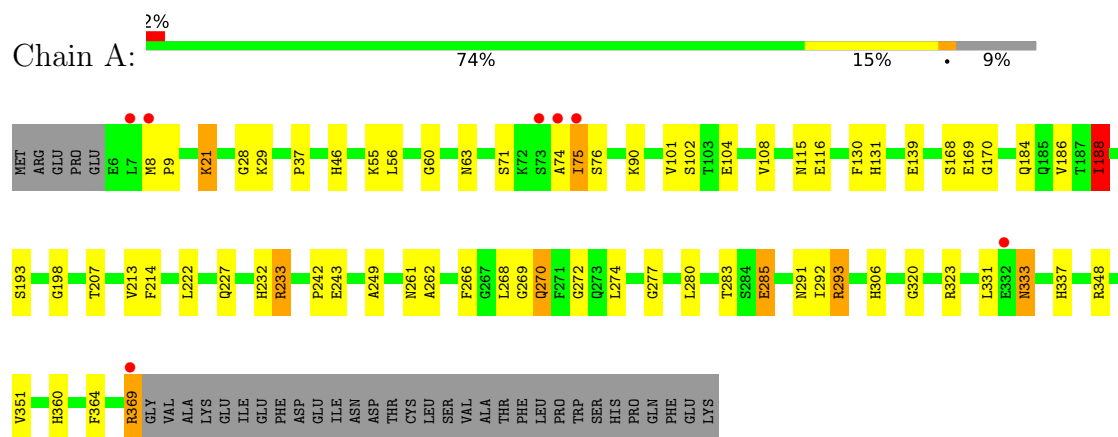
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	83	Total	O	0	0
			83	83		

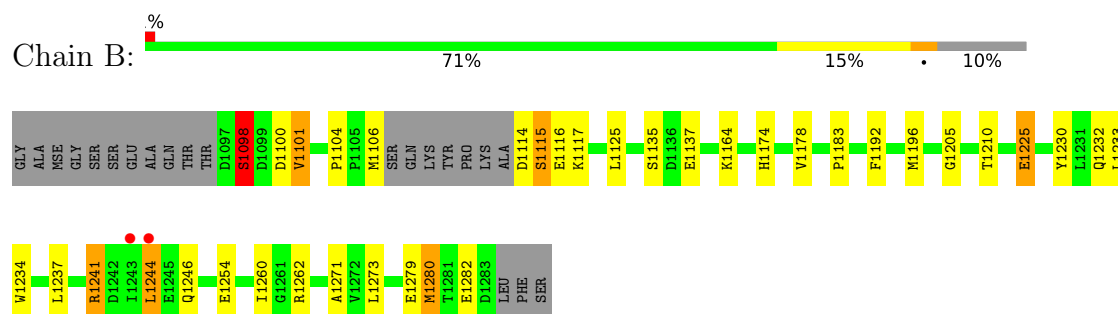
3 Residue-property plots [i](#)

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

- Molecule 1: X-linked retinitis pigmentosa GTPase regulator



- Molecule 2: X-linked retinitis pigmentosa GTPase regulator-interacting protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.12Å 63.80Å 161.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.23 – 1.83 43.23 – 1.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.23-1.83) 100.0 (43.23-1.83)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.197 0.163 , 0.197	Depositor DCC
R_{free} test set	2917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4654	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL

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	1.55	19/2918 (0.7%)	1.25	8/3952 (0.2%)
2	B	1.32	6/1493 (0.4%)	1.26	5/2010 (0.2%)
All	All	1.47	25/4411 (0.6%)	1.25	13/5962 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLY	N-CA	9.16	1.53	1.44
1	A	333	ASN	N-CA	7.64	1.55	1.46
1	A	75	ILE	C-O	7.37	1.31	1.24
1	A	306	HIS	CE1-NE2	7.32	1.39	1.32
2	B	1164	LYS	CA-C	6.85	1.60	1.53
1	A	337	HIS	ND1-CE1	6.62	1.39	1.32
1	A	232	HIS	ND1-CE1	6.45	1.39	1.32
1	A	320	GLY	C-O	6.37	1.28	1.24
1	A	323	ARG	N-CA	6.07	1.53	1.46
1	A	102	SER	CA-C	6.07	1.60	1.52
1	A	272	GLY	N-CA	6.07	1.53	1.45
1	A	351	VAL	C-O	5.94	1.30	1.24
1	A	277	GLY	N-CA	5.92	1.52	1.45
2	B	1135	SER	N-CA	5.55	1.53	1.46
2	B	1230	TYR	C-O	5.50	1.30	1.24
2	B	1254	GLU	N-CA	5.48	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	VAL	CA-C	5.43	1.59	1.52
1	A	249	ALA	C-O	5.31	1.30	1.23
1	A	360	HIS	CG-CD2	5.29	1.41	1.35
1	A	46	HIS	N-CA	5.22	1.52	1.45
2	B	1174	HIS	CG-CD2	5.17	1.41	1.35
1	A	198	GLY	N-CA	5.11	1.51	1.45
1	A	131	HIS	ND1-CE1	5.10	1.37	1.32
2	B	1104	PRO	CA-C	5.04	1.56	1.52
1	A	169	GLU	CA-C	5.01	1.59	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ILE	N-CA-C	-7.97	104.59	112.17
1	A	186	VAL	N-CA-C	-6.69	97.47	107.37
2	B	1115	SER	N-CA-C	-6.63	105.50	112.93
1	A	261	ASN	N-CA-C	5.85	118.89	111.69
1	A	233	ARG	CG-CD-NE	-5.68	99.50	112.00
1	A	75	ILE	N-CA-C	-5.59	100.08	108.12
2	B	1262	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	B	1260	ILE	N-CA-C	-5.26	108.16	113.47
2	B	1225	GLU	CA-CB-CG	-5.24	103.63	114.10
1	A	71	SER	N-CA-C	-5.18	101.39	108.38
1	A	333	ASN	N-CA-C	5.13	117.10	108.73
2	B	1101	VAL	CB-CA-C	5.04	119.19	111.68
1	A	55	LYS	CD-CE-NZ	-5.03	95.81	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1098	SER	Peptide

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	2824	0	2785	46	0
2	B	1464	0	1426	25	0
3	A	2	0	0	0	0
4	A	30	0	40	4	0
4	B	12	0	16	4	0
5	A	239	0	0	14	1
5	B	83	0	0	3	0
All	All	4654	0	4267	75	1

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 9.

All (75) 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:293:ARG:HH11	1:A:293:ARG:HG3	1.15	1.09
4:A:505:GOL:H31	5:A:838:HOH:O	1.57	1.01
1:A:291[B]:ASN:ND2	5:A:834:HOH:O	1.93	0.99
1:A:333:ASN:ND2	5:A:756:HOH:O	1.95	0.96
1:A:115:ASN:HB2	5:A:722:HOH:O	1.69	0.93
1:A:270[B]:GLN:NE2	5:A:776:HOH:O	2.07	0.86
1:A:293:ARG:HG3	1:A:293:ARG:NH1	1.87	0.86
1:A:8[B]:MET:HE2	1:A:29:LYS:NZ	1.90	0.85
1:A:8[B]:MET:HE2	1:A:29:LYS:HZ2	1.41	0.85
2:B:1232:GLN:HE21	2:B:1234:TRP:HB3	1.40	0.84
1:A:369:ARG:HB2	1:A:369:ARG:NH1	1.95	0.81
1:A:188:ILE:CD1	5:A:782:HOH:O	2.28	0.80
1:A:188:ILE:HD12	5:A:782:HOH:O	1.81	0.79
1:A:369:ARG:HB2	1:A:369:ARG:HH11	1.48	0.79
1:A:213[A]:VAL:HG21	1:A:222:LEU:O	1.86	0.75
2:B:1244:LEU:HD12	2:B:1244:LEU:H	1.50	0.75
1:A:242:PRO:HD2	1:A:243:GLU:OE1	1.90	0.71
1:A:90:LYS:HE3	1:A:104:GLU:OE2	1.91	0.70
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.01	0.69
2:B:1098:SER:C	2:B:1100:ASP:H	2.00	0.69
2:B:1241:ARG:CZ	2:B:1241:ARG:HB2	2.23	0.69
2:B:1116:GLU:HG2	2:B:1183:PRO:HD3	1.74	0.68
1:A:262:ALA:HB2	1:A:293:ARG:HE	1.60	0.67
1:A:8[B]:MET:CE	1:A:29:LYS:NZ	2.58	0.67
2:B:1114:ASP:HB2	2:B:1117[A]:LYS:HG2	1.77	0.65
2:B:1232:GLN:NE2	2:B:1234:TRP:HB3	2.11	0.65
2:B:1225:GLU:H	4:B:1302:GOL:H11	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8[B]:MET:CE	1:A:29:LYS:HZ2	2.12	0.63
2:B:1137:GLU:HG2	5:B:1432:HOH:O	2.00	0.62
4:A:506:GOL:H31	5:A:839:HOH:O	2.01	0.60
2:B:1114:ASP:HB3	2:B:1116:GLU:H	1.68	0.57
1:A:293:ARG:HD3	5:A:668:HOH:O	2.04	0.56
1:A:9:PRO:HG3	5:A:835:HOH:O	2.05	0.56
1:A:227:GLN:H	1:A:227:GLN:CD	2.14	0.54
2:B:1241:ARG:HB2	2:B:1241:ARG:NH1	2.23	0.54
2:B:1210:THR:HG21	2:B:1225:GLU:HG2	1.90	0.53
1:A:168:SER:O	1:A:233:ARG:NH2	2.42	0.53
1:A:101[A]:VAL:HG23	1:A:130:PHE:CE1	2.44	0.52
1:A:74:ALA:HB2	5:A:667:HOH:O	2.09	0.52
2:B:1244:LEU:H	2:B:1244:LEU:CD1	2.22	0.52
2:B:1098:SER:C	2:B:1100:ASP:N	2.67	0.52
1:A:56:LEU:HD22	1:A:101[B]:VAL:HG11	1.92	0.51
2:B:1225:GLU:H	4:B:1302:GOL:C1	2.24	0.51
1:A:8[A]:MET:HE2	1:A:29:LYS:HD2	1.94	0.50
2:B:1196:MSE:O	2:B:1205:GLY:HA2	2.12	0.49
2:B:1115:SER:HB3	2:B:1271:ALA:HB1	1.94	0.49
1:A:116:GLU:OE1	4:A:505:GOL:H2	2.13	0.49
1:A:8[B]:MET:CE	1:A:29:LYS:HZ1	2.26	0.49
1:A:21:LYS:HB2	1:A:60:GLY:HA2	1.96	0.48
1:A:227:GLN:H	1:A:227:GLN:NE2	2.12	0.48
2:B:1192:PHE:CZ	2:B:1196:MSE:HE1	2.49	0.47
2:B:1192:PHE:CE2	2:B:1196:MSE:HE1	2.51	0.45
2:B:1098:SER:CA	2:B:1100:ASP:H	2.29	0.45
2:B:1116:GLU:CG	2:B:1183:PRO:HD3	2.46	0.44
1:A:348[B]:ARG:NH2	5:A:699:HOH:O	2.51	0.43
1:A:63:ASN:OD1	4:A:504:GOL:O1	2.36	0.43
1:A:193:SER:HB3	1:A:207:THR:HG22	1.99	0.43
2:B:1279:GLU:OE1	2:B:1280:MSE:HE3	2.18	0.43
1:A:37:PRO:HG2	1:A:364:PHE:CD1	2.53	0.43
1:A:269:GLY:HA3	1:A:274:LEU:HG	2.01	0.43
4:B:1301:GOL:C2	5:B:1483:HOH:O	2.67	0.43
1:A:170:GLY:HA3	1:A:233:ARG:HA	2.00	0.42
1:A:266:PHE:HA	1:A:283:THR:HG23	2.01	0.42
2:B:1117[A]:LYS:HD2	2:B:1178:VAL:HG11	2.01	0.42
1:A:21:LYS:O	1:A:76:SER:HA	2.19	0.42
1:A:90:LYS:CE	1:A:104:GLU:OE2	2.64	0.42
1:A:184:GLN:HB2	5:A:781:HOH:O	2.20	0.42
1:A:262:ALA:CB	1:A:293:ARG:HE	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HA	1:A:280:LEU:HD12	1.89	0.41
2:B:1196:MSE:HE2	2:B:1196:MSE:HB2	1.51	0.41
1:A:285[B]:GLU:OE2	5:A:779:HOH:O	2.22	0.41
1:A:8[B]:MET:HE2	1:A:29:LYS:HZ1	1.78	0.40
2:B:1125:LEU:C	2:B:1125:LEU:HD12	2.46	0.40
4:B:1301:GOL:H11	5:B:1483:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:689:HOH:O	5:A:829:HOH:O[4_445]	2.10	0.10

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	373/400 (93%)	365 (98%)	8 (2%)	0	100	100
2	B	178/201 (89%)	170 (96%)	8 (4%)	0	100	100
All	All	551/601 (92%)	535 (97%)	16 (3%)	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	312/334 (93%)	298 (96%)	14 (4%)	24	7
2	B	166/174 (95%)	155 (93%)	11 (7%)	15	3
All	All	478/508 (94%)	453 (95%)	25 (5%)	22	5

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	75	ILE
1	A	139	GLU
1	A	188	ILE
1	A	214	PHE
1	A	268	LEU
1	A	270[A]	GLN
1	A	270[B]	GLN
1	A	285[A]	GLU
1	A	285[B]	GLU
1	A	292	ILE
1	A	293	ARG
1	A	331	LEU
1	A	369	ARG
2	B	1098	SER
2	B	1101	VAL
2	B	1106	MSE
2	B	1233	LEU
2	B	1237	LEU
2	B	1241	ARG
2	B	1244	LEU
2	B	1246	GLN
2	B	1273	LEU
2	B	1280	MSE
2	B	1282	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
1	A	333	ASN
1	A	368	HIS
2	B	1200	GLN
2	B	1232	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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$
4	GOL	B	1302	-	5,5,5	0.49	0	5,5,5	1.63	1 (20%)
4	GOL	B	1301	-	5,5,5	0.24	0	5,5,5	1.48	2 (40%)
4	GOL	A	503	-	5,5,5	1.48	1 (20%)	5,5,5	1.57	0
4	GOL	A	504	-	5,5,5	1.36	1 (20%)	5,5,5	1.01	0
4	GOL	A	506	-	5,5,5	0.44	0	5,5,5	0.79	0
4	GOL	A	505	-	5,5,5	0.64	0	5,5,5	1.65	2 (40%)
4	GOL	A	502	-	5,5,5	0.34	0	5,5,5	1.25	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	GOL	B	1302	-	-	3/4/4/4	-
4	GOL	B	1301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	503	-	-	3/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	A	506	-	-	4/4/4/4	-
4	GOL	A	505	-	-	1/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	GOL	O3-C3	2.48	1.52	1.42
4	A	503	GOL	O2-C2	2.48	1.50	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1302	GOL	O2-C2-C3	-3.30	95.52	109.18
4	B	1301	GOL	O3-C3-C2	-2.35	99.78	110.38
4	B	1301	GOL	O1-C1-C2	-2.29	100.06	110.38
4	A	505	GOL	O3-C3-C2	-2.24	100.31	110.38
4	A	505	GOL	O1-C1-C2	-2.23	100.32	110.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	GOL	O1-C1-C2-C3
4	A	503	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
4	B	1301	GOL	C1-C2-C3-O3
4	B	1302	GOL	O1-C1-C2-C3
4	B	1302	GOL	C1-C2-C3-O3
4	A	506	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-O2
4	B	1301	GOL	O2-C2-C3-O3
4	B	1302	GOL	O2-C2-C3-O3
4	A	502	GOL	O1-C1-C2-O2
4	A	503	GOL	O1-C1-C2-O2
4	A	503	GOL	O2-C2-C3-O3
4	A	506	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	GOL	2	0
4	B	1301	GOL	2	0
4	A	504	GOL	1	0
4	A	506	GOL	1	0
4	A	505	GOL	2	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	364/400 (91%)	-0.50	7 (1%) 66 73	12, 25, 50, 83	11 (3%)
2	B	175/201 (87%)	-0.13	2 (1%) 78 84	15, 32, 76, 107	2 (1%)
All	All	539/601 (89%)	-0.38	9 (1%) 69 77	12, 27, 63, 107	13 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1244	LEU	4.2
1	A	7	LEU	2.9
1	A	74	ALA	2.5
1	A	8[A]	MET	2.4
1	A	369	ARG	2.3
1	A	75	ILE	2.2
1	A	73	SER	2.1
1	A	332	GLU	2.0
2	B	1243	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	1302	6/6	0.73	0.16	42,45,53,60	0
4	GOL	B	1301	6/6	0.77	0.18	46,67,69,70	0
4	GOL	A	505	6/6	0.77	0.16	47,52,56,59	0
4	GOL	A	506	6/6	0.86	0.11	45,56,59,64	0
4	GOL	A	504	6/6	0.90	0.12	22,37,38,41	0
4	GOL	A	502	6/6	0.94	0.12	20,24,26,31	0
4	GOL	A	503	6/6	0.95	0.10	16,22,26,30	0
3	MG	A	501	1/1	0.95	0.05	49,49,49,49	0
3	MG	A	507	1/1	0.99	0.14	28,28,28,28	1

6.5 Other polymers [i](#)

There are no such residues in this entry.