



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:29 PM BST

PDB ID : 2PBI
Title : The multifunctional nature of Gbeta5/RGS9 revealed from its crystal structure
Authors : Cheever, M.L.; Snyder, J.T.; Gershburg, S.; Siderovski, D.P.; Harden, T.K.; Sondek, J.
Deposited on : 2007-03-28
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

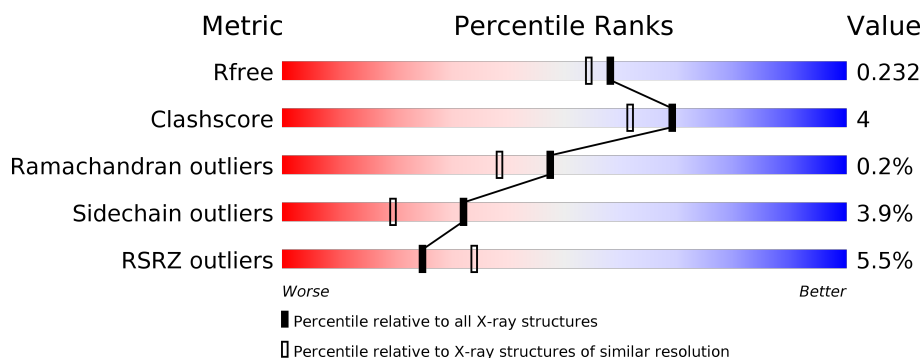
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 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	424	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </div> </div>
1	C	424	<div> <div>11%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>
2	B	354	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>••</div> </div> </div>
2	D	354	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>•</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13309 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 Regulator of G-protein signaling 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	7	0
			3484	2238	598	631	17			
1	C	415	Total	C	N	O	S	0	8	0
			3488	2242	595	632	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP A1L352
A	0	ALA	-	EXPRESSION TAG	UNP A1L352
C	-1	GLY	-	EXPRESSION TAG	UNP A1L352
C	0	ALA	-	EXPRESSION TAG	UNP A1L352

- Molecule 2 is a protein called Guanine nucleotide-binding protein subunit beta 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	345	Total	C	N	O	S	0	3	0
			2664	1657	464	519	24			
2	D	354	Total	C	N	O	S	0	4	0
			2729	1695	474	535	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	EXPRESSION TAG	UNP P62881
D	0	GLY	-	EXPRESSION TAG	UNP P62881

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	276	Total	O	0	0
			276	276		
4	B	214	Total	O	0	0
			214	214		
4	C	199	Total	O	0	0
			199	199		

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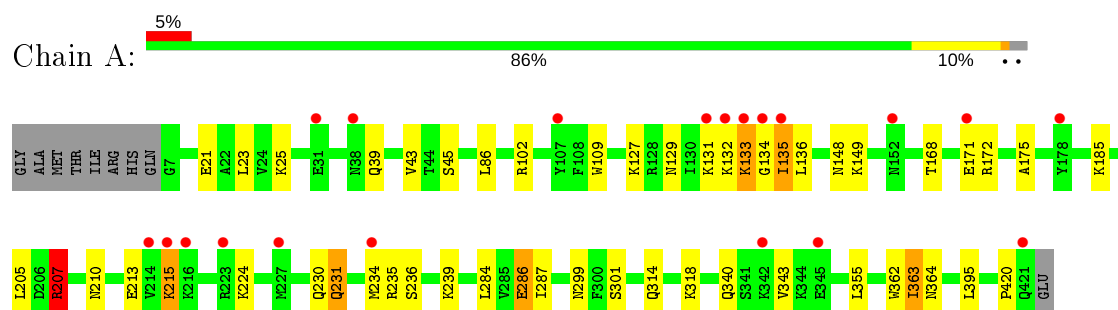
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	201	Total	O	0	0
			201	201		

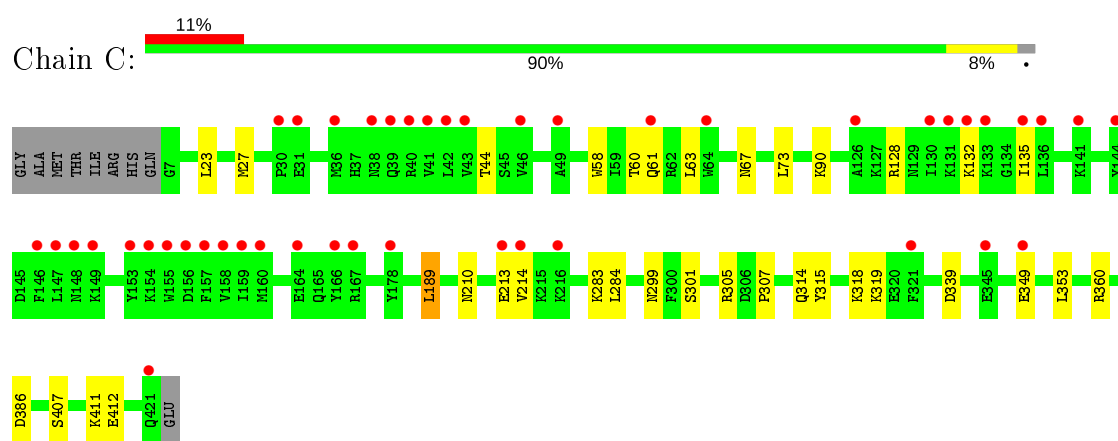
3 Residue-property plots [i](#)

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.

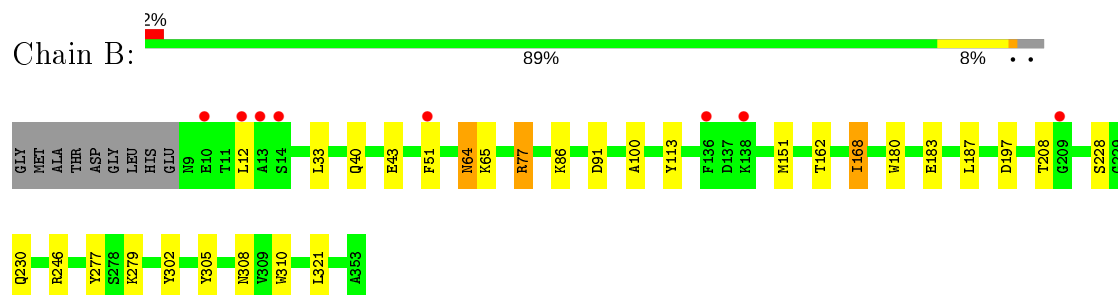
• Molecule 1: Regulator of G-protein signaling 9



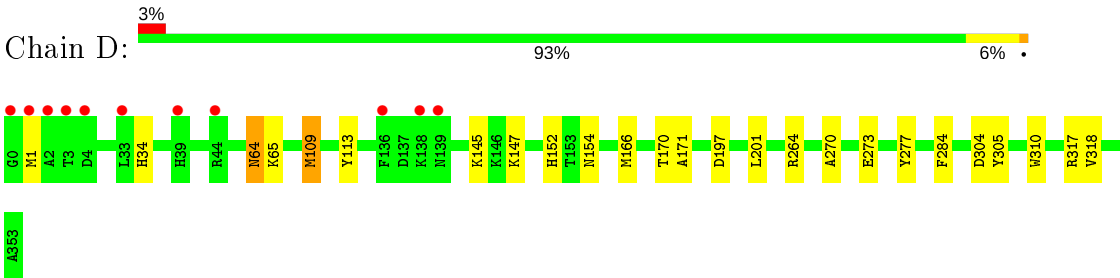
• Molecule 1: Regulator of G-protein signaling 9



• Molecule 2: Guanine nucleotide-binding protein subunit beta 5



• Molecule 2: Guanine nucleotide-binding protein subunit beta 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.17Å 119.03Å 131.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 44.19 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.95) 99.7 (44.19-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.95Å)	Xtriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.183 , 0.225 0.208 , 0.232	Depositor DCC
R_{free} test set	6310 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13309	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.75% 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: 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	0.51	0/3593	0.57	2/4852 (0.0%)
1	C	0.44	0/3599	0.53	0/4859
2	B	0.46	0/2727	0.63	0/3685
2	D	0.52	0/2795	0.62	0/3776
All	All	0.48	0/12714	0.58	2/17172 (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	207	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	207	ARG	NE-CZ-NH2	-6.68	116.96	120.30

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	3484	0	3478	50	0
1	C	3488	0	3482	15	0
2	B	2664	0	2573	17	0
2	D	2729	0	2637	12	0
3	A	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	1	0
3	C	6	0	8	0	0
3	D	18	0	24	0	0
4	A	276	0	0	1	0
4	B	214	0	0	3	0
4	C	199	0	0	0	0
4	D	201	0	0	2	0
All	All	13309	0	12242	92	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HB2	1:A:135:ILE:CG2	1.82	1.10
1:A:132:LYS:CB	1:A:135:ILE:HG22	1.82	1.09
1:A:314:GLN:HE21	1:A:318:LYS:HE3	1.17	1.06
2:B:64:ASN:HD22	2:B:65:LYS:H	1.10	0.98
1:A:132:LYS:HB3	1:A:135:ILE:HG22	1.49	0.93
2:D:64:ASN:HD22	2:D:65:LYS:H	1.09	0.93
1:A:132:LYS:HB2	1:A:135:ILE:HG22	1.45	0.89
1:A:132:LYS:HD3	1:A:135:ILE:HB	1.55	0.89
1:C:214:VAL:O	1:C:214:VAL:HG13	1.73	0.87
1:A:132:LYS:CB	1:A:135:ILE:CG2	2.51	0.82
1:A:314:GLN:NE2	1:A:318:LYS:HE3	1.93	0.82
1:C:214:VAL:O	1:C:214:VAL:CG1	2.30	0.80
1:A:135:ILE:HG12	1:A:135:ILE:O	1.85	0.76
1:C:283:LYS:HG2	1:C:307:PRO:HG2	1.71	0.73
1:A:340:GLN:OE1	1:A:343:VAL:HG11	1.89	0.72
2:D:64:ASN:HD22	2:D:65:LYS:N	1.87	0.71
1:A:215:LYS:H	1:A:215:LYS:HD3	1.57	0.70
2:B:64:ASN:HD22	2:B:65:LYS:N	1.89	0.69
1:A:129:ASN:ND2	1:A:133:LYS:O	2.25	0.68
1:A:132:LYS:CD	1:A:135:ILE:HB	2.24	0.67
1:A:132:LYS:HB2	1:A:135:ILE:HG21	1.76	0.66
1:A:132:LYS:HG3	1:A:133:LYS:H	1.61	0.65
2:B:86:LYS:HE2	2:B:100:ALA:HB1	1.78	0.65
1:A:207:ARG:HD2	4:B:973:HOH:O	1.97	0.64
1:C:210:ASN:HB3	1:C:213:GLU:HB3	1.80	0.62
2:D:64:ASN:ND2	2:D:65:LYS:H	1.90	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:PHE:HE2	2:B:321:LEU:HD21	1.65	0.61
1:C:90:LYS:HD3	1:C:189:LEU:HD21	1.86	0.58
1:A:132:LYS:CG	1:A:135:ILE:HB	2.34	0.57
1:A:134:GLY:C	1:A:136:LEU:H	2.08	0.57
1:A:132:LYS:HB2	1:A:135:ILE:CB	2.36	0.56
2:D:109:MET:HB2	4:D:1048:HOH:O	2.06	0.56
2:B:64:ASN:ND2	2:B:65:LYS:H	1.92	0.56
2:B:77:ARG:HD3	2:B:91:ASP:HA	1.88	0.55
1:C:210:ASN:O	1:C:213:GLU:HG2	2.07	0.54
1:A:231:GLN:OE1	1:A:235:ARG:NE	2.41	0.54
1:A:39:GLN:HE22	1:A:43:VAL:HB	1.72	0.54
1:A:21:GLU:HG2	1:A:109:TRP:CZ3	2.43	0.54
2:D:152:HIS:HE1	2:D:170:THR:OG1	1.90	0.54
1:A:132:LYS:HG2	1:A:135:ILE:N	2.22	0.54
2:B:86:LYS:CE	2:B:100:ALA:HB1	2.38	0.53
1:A:135:ILE:CG1	1:A:135:ILE:O	2.56	0.53
1:C:315:TYR:HA	1:C:318:LYS:HE3	1.91	0.52
2:D:318:VAL:HG13	4:D:980:HOH:O	2.10	0.52
1:A:355:LEU:HD23	1:A:363:ILE:HD11	1.92	0.52
1:C:407:SER:O	1:C:411:LYS:HG2	2.10	0.52
1:A:132:LYS:HB3	1:A:135:ILE:H	1.75	0.51
2:B:168:ILE:HG22	2:B:180:TRP:HB2	1.92	0.51
1:A:210:ASN:ND2	1:A:213:GLU:HG3	2.26	0.51
1:A:239:LYS:HA	2:B:33:LEU:HB3	1.91	0.50
1:A:230:GLN:O	1:A:234:MET:HG2	2.12	0.49
2:D:34:HIS:HE1	2:D:270:ALA:O	1.96	0.49
1:A:355:LEU:HD23	1:A:363:ILE:CD1	2.44	0.47
1:A:132:LYS:CG	1:A:133:LYS:H	2.28	0.47
1:A:340:GLN:OE1	1:A:343:VAL:CG1	2.61	0.47
1:C:301:SER:O	1:C:305:ARG:HG3	2.15	0.47
1:A:127:LYS:HG2	1:A:131:LYS:HE3	1.97	0.47
1:A:355:LEU:CD2	1:A:363:ILE:HD11	2.44	0.47
1:C:339:ASP:OD2	2:D:166:MET:HG2	2.15	0.47
1:C:132:LYS:HB3	1:C:135:ILE:HB	1.97	0.47
1:A:132:LYS:HG2	1:A:135:ILE:H	1.80	0.46
1:A:134:GLY:C	1:A:136:LEU:N	2.69	0.46
1:A:132:LYS:HG3	1:A:133:LYS:N	2.29	0.46
1:C:23:LEU:O	1:C:27:MET:HG3	2.16	0.46
2:B:51:PHE:CE2	2:B:321:LEU:HD21	2.48	0.45
1:A:132:LYS:CG	1:A:133:LYS:N	2.80	0.45
1:A:286:GLU:HG2	1:A:287:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:CB	1:A:135:ILE:CB	2.94	0.44
2:B:279:LYS:HE3	2:B:279:LYS:HB3	1.83	0.44
2:B:40:GLN:HA	2:B:43:GLU:HG3	1.99	0.44
2:B:277:TYR:HB3	2:B:310:TRP:CD2	2.53	0.43
2:D:264:ARG:HD3	2:D:273:GLU:OE2	2.18	0.43
2:D:171:ALA:HB2	2:D:201:LEU:HD23	2.00	0.43
1:A:168:THR:O	1:A:171:GLU:HG2	2.17	0.43
1:A:340:GLN:O	1:A:343:VAL:HG22	2.19	0.43
1:C:27:MET:HG2	1:C:58:TRP:CZ3	2.53	0.43
1:A:86:LEU:HD21	1:A:102:ARG:HG3	2.01	0.43
2:B:86:LYS:HE3	4:B:998:HOH:O	2.19	0.42
1:C:60:THR:HG21	1:C:67:ASN:ND2	2.34	0.42
1:A:45:SER:HB3	1:A:172:ARG:NH2	2.35	0.42
1:A:318:LYS:HD2	4:A:1099:HOH:O	2.19	0.42
2:D:277:TYR:HB3	2:D:310:TRP:CD2	2.54	0.42
2:B:228:SER:OG	2:B:230:GLN:HG2	2.21	0.41
2:D:284:PHE:CD2	2:D:304:ASP:HB3	2.56	0.41
2:B:302:TYR:CE1	2:B:308:ASN:HB2	2.55	0.41
1:A:132:LYS:CB	1:A:135:ILE:H	2.33	0.41
2:B:246:ARG:NH2	4:B:993:HOH:O	2.47	0.41
1:A:301:SER:OG	3:B:909:GOL:H32	2.21	0.40
1:A:43:VAL:HG22	1:A:175:ALA:HB1	2.03	0.40
1:A:132:LYS:HB2	1:A:135:ILE:HB	2.04	0.40
1:A:362:TRP:CH2	1:A:364:ASN:HB2	2.56	0.40
1:C:314:GLN:HG3	1:C:318:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	420/424 (99%)	406 (97%)	12 (3%)	2 (0%)	29 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	420/424 (99%)	410 (98%)	10 (2%)	0	100	100
2	B	346/354 (98%)	331 (96%)	14 (4%)	1 (0%)	41	30
2	D	356/354 (101%)	340 (96%)	16 (4%)	0	100	100
All	All	1542/1556 (99%)	1487 (96%)	52 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	PRO
1	A	135	ILE
2	B	162	THR

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	377/377 (100%)	360 (96%)	17 (4%)	27	15
1	C	378/377 (100%)	364 (96%)	14 (4%)	34	22
2	B	292/295 (99%)	281 (96%)	11 (4%)	33	21
2	D	299/295 (101%)	289 (97%)	10 (3%)	38	26
All	All	1346/1344 (100%)	1294 (96%)	52 (4%)	32	19

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	LYS
1	A	133	LYS
1	A	148	ASN
1	A	149	LYS
1	A	185	LYS
1	A	205	LEU
1	A	207	ARG

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Mol	Chain	Res	Type
1	A	215	LYS
1	A	224	LYS
1	A	231	GLN
1	A	236	SER
1	A	284	LEU
1	A	286	GLU
1	A	299	ASN
1	A	363	ILE
1	A	395	LEU
2	B	12	LEU
2	B	64	ASN
2	B	77	ARG
2	B	113	TYR
2	B	151	MET
2	B	168	ILE
2	B	183	GLU
2	B	187	LEU
2	B	197	ASP
2	B	208	THR
2	B	305	TYR
1	C	44	THR
1	C	61	GLN
1	C	63	LEU
1	C	73	LEU
1	C	128	ARG
1	C	189	LEU
1	C	284	LEU
1	C	299	ASN
1	C	319	LYS
1	C	349	GLU
1	C	353	LEU
1	C	360	ARG
1	C	386	ASP
1	C	412	GLU
2	D	1	MET
2	D	64	ASN
2	D	109	MET
2	D	113	TYR
2	D	145	LYS
2	D	147	LYS
2	D	154	ASN
2	D	197	ASP

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Mol	Chain	Res	Type
2	D	305	TYR
2	D	317	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	39	GLN
1	A	129	ASN
1	A	299	ASN
1	A	314	GLN
2	B	64	ASN
1	C	61	GLN
1	C	67	ASN
1	C	161	GLN
1	C	299	ASN
2	D	34	HIS
2	D	39	HIS
2	D	64	ASN
2	D	152	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	GOL	A	904	-	5,5,5	0.39	0	5,5,5	0.51	0
3	GOL	D	903	-	5,5,5	0.34	0	5,5,5	0.50	0
3	GOL	B	909	-	5,5,5	0.37	0	5,5,5	0.19	0
3	GOL	A	905	-	5,5,5	0.32	0	5,5,5	0.31	0
3	GOL	A	906	-	5,5,5	0.43	0	5,5,5	0.45	0
3	GOL	B	902	-	5,5,5	0.38	0	5,5,5	0.40	0
3	GOL	D	908	-	5,5,5	0.34	0	5,5,5	0.23	0
3	GOL	D	901	-	5,5,5	0.39	0	5,5,5	0.35	0
3	GOL	C	907	-	5,5,5	0.38	0	5,5,5	0.23	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
3	GOL	A	904	-	-	2/4/4/4	-
3	GOL	D	903	-	-	2/4/4/4	-
3	GOL	B	909	-	-	3/4/4/4	-
3	GOL	A	905	-	-	0/4/4/4	-
3	GOL	A	906	-	-	4/4/4/4	-
3	GOL	B	902	-	-	0/4/4/4	-
3	GOL	D	908	-	-	1/4/4/4	-
3	GOL	D	901	-	-	0/4/4/4	-
3	GOL	C	907	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	904	GOL	O1-C1-C2-C3
3	A	906	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	907	GOL	O1-C1-C2-O2
3	C	907	GOL	O1-C1-C2-C3
3	D	903	GOL	O2-C2-C3-O3
3	D	903	GOL	C1-C2-C3-O3
3	B	909	GOL	C1-C2-C3-O3
3	A	906	GOL	O1-C1-C2-C3
3	A	904	GOL	O1-C1-C2-O2
3	A	906	GOL	O1-C1-C2-O2
3	A	906	GOL	O2-C2-C3-O3
3	B	909	GOL	O1-C1-C2-C3
3	D	908	GOL	C1-C2-C3-O3
3	B	909	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	909	GOL	1	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	415/424 (97%)	0.33	20 (4%) 30 40	3, 30, 71, 128	0
1	C	415/424 (97%)	0.73	45 (10%) 5 9	11, 40, 132, 191	0
2	B	345/354 (97%)	0.02	8 (2%) 60 69	-1, 17, 69, 104	0
2	D	354/354 (100%)	0.03	11 (3%) 49 58	1, 19, 58, 155	0
All	All	1529/1556 (98%)	0.30	84 (5%) 25 34	-1, 27, 91, 191	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	8.4
1	C	214	VAL	8.2
1	C	42	LEU	7.0
2	D	0	GLY	6.9
1	C	135	ILE	6.3
1	A	216	LYS	5.9
1	A	214	VAL	5.8
1	C	132	LYS	5.5
1	C	155	TRP	5.3
1	C	133	LYS	5.2
1	A	132	LYS	4.7
2	B	209	GLY	4.6
2	D	2	ALA	4.4
1	A	133	LYS	4.4
1	A	178	TYR	4.2
1	C	144	TYR	3.9
2	D	1	MET	3.9
2	B	138	LYS	3.9
1	C	156	ASP	3.8
1	A	421	GLN	3.8
1	C	421[A]	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	149	LYS	3.8
1	C	40	ARG	3.6
1	C	157	PHE	3.5
1	C	166	TYR	3.4
1	C	158	VAL	3.3
2	D	3	THR	3.3
1	A	107	TYR	3.3
1	C	159	ILE	3.3
1	C	131	LYS	3.2
1	C	146	PHE	3.2
1	C	41	VAL	3.2
1	C	130	ILE	3.2
2	D	136	PHE	3.1
1	A	131	LYS	3.0
2	D	39	HIS	3.0
2	B	14	SER	3.0
1	A	345	GLU	3.0
1	A	134	GLY	3.0
1	C	213	GLU	2.9
1	C	178	TYR	2.9
1	C	136	LEU	2.8
2	D	44	ARG	2.8
1	A	215	LYS	2.7
2	D	138	LYS	2.7
1	A	152[A]	ASN	2.7
1	C	153	TYR	2.7
1	C	147	LEU	2.7
1	C	64	TRP	2.6
1	C	39	GLN	2.6
1	C	43	VAL	2.6
1	C	141	LYS	2.5
1	C	154	LYS	2.5
1	C	216	LYS	2.5
1	A	342	LYS	2.5
1	C	164	GLU	2.4
2	B	10	GLU	2.4
2	B	51	PHE	2.4
1	A	227	MET	2.4
1	A	223	ARG	2.4
1	C	31	GLU	2.4
2	B	13	ALA	2.4
1	C	148	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	234	MET	2.3
1	C	345	GLU	2.3
2	D	139	ASN	2.3
1	C	61	GLN	2.3
1	C	38	ASN	2.3
1	C	160	MET	2.3
2	D	33	LEU	2.3
1	C	321	PHE	2.2
1	A	31	GLU	2.2
2	B	136	PHE	2.2
1	C	126	ALA	2.2
1	C	30	PRO	2.1
1	C	167	ARG	2.1
1	C	46	VAL	2.1
2	D	4	ASP	2.1
2	B	12	LEU	2.1
1	C	36	MET	2.1
1	C	349	GLU	2.0
1	A	38	ASN	2.0
1	C	49	ALA	2.0
1	A	171	GLU	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 monosaccharides 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(\AA^2)	Q<0.9
3	GOL	C	907	6/6	0.63	0.32	69,69,70,71	0
3	GOL	A	905	6/6	0.70	0.28	49,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	904	6/6	0.75	0.28	51,52,53,53	0
3	GOL	B	909	6/6	0.76	0.29	76,77,77,77	0
3	GOL	D	908	6/6	0.86	0.14	52,53,53,53	0
3	GOL	A	906	6/6	0.86	0.45	42,45,46,46	0
3	GOL	D	903	6/6	0.87	0.16	47,50,50,51	0
3	GOL	D	901	6/6	0.92	0.22	27,28,28,29	0
3	GOL	B	902	6/6	0.96	0.31	22,25,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.