



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:20 AM UTC

PDB ID : 2PBI / pdb_00002pbi
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 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

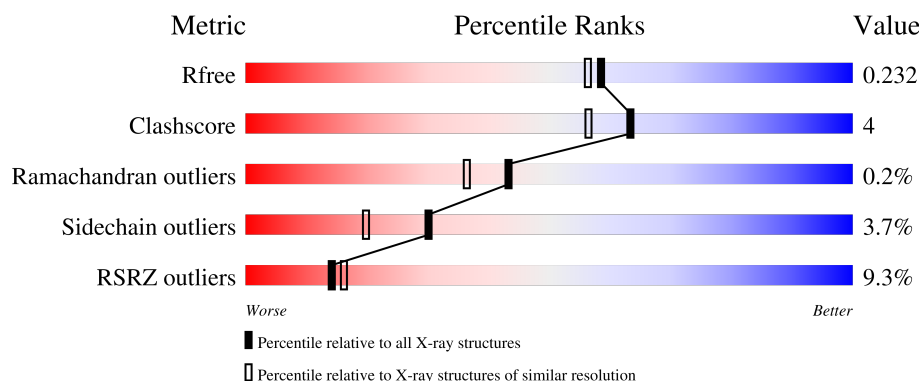
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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	424	5% 86% 11% ..
1	C	424	21% 88% 9% ..
2	B	354	5% 89% 7% ..
2	D	354	3% 93% 6% .

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 (CCD ID: 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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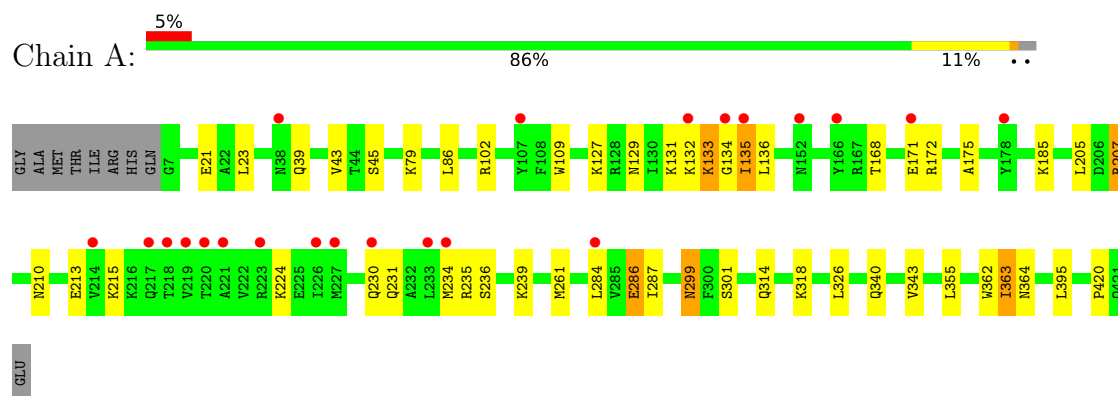
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	201	Total 201	O 201	0	0

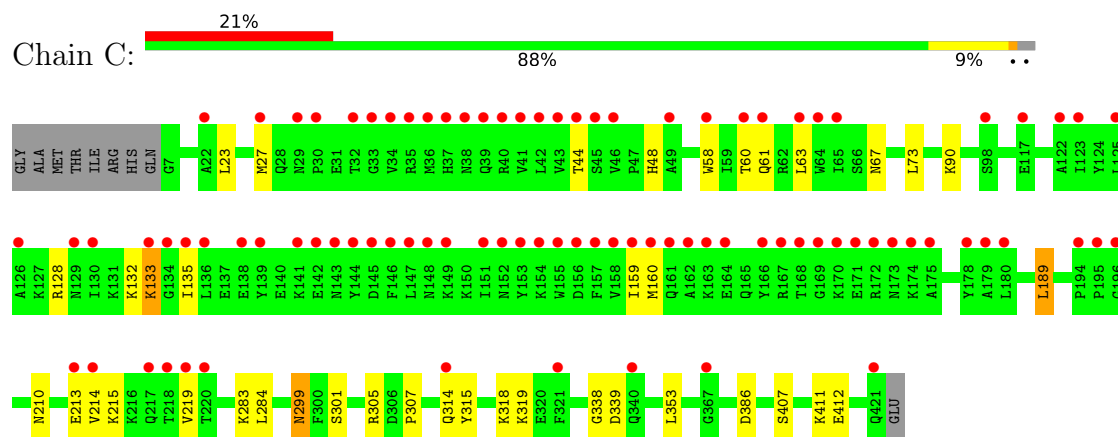
3 Residue-property plots [i](#)

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.

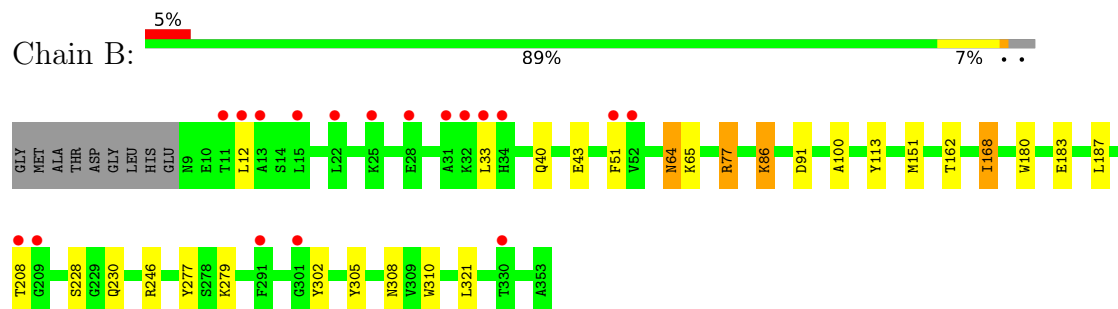
• Molecule 1: Regulator of G-protein signaling 9



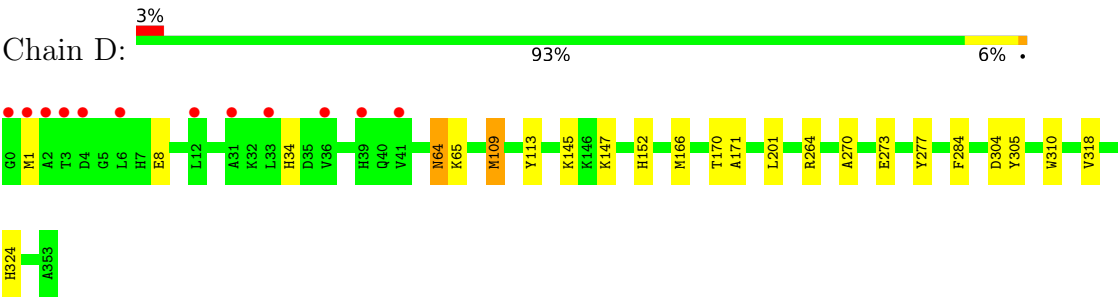
• Molecule 1: Regulator of G-protein signaling 9



• 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 20.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.95) 99.5 (20.00-1.95)	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 0.209 , 0.232	Depositor DCC
R_{free} test set	6310 reflections (3.65%)	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 , 53.9	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	0.62	0/3593	0.82	0/4852
1	C	0.55	0/3599	0.81	2/4859 (0.0%)
2	B	0.54	0/2727	0.76	0/3685
2	D	0.60	1/2795 (0.0%)	0.76	0/3776
All	All	0.58	1/12714 (0.0%)	0.79	2/17172 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	324	HIS	C-O	-5.24	1.17	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	LYS	CB-CA-C	6.71	118.05	109.80
1	C	133	LYS	N-CA-C	-5.98	101.79	110.64

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	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3488	0	3482	18	0
2	B	2664	0	2573	17	0
2	D	2729	0	2637	13	0
3	A	18	0	24	0	0
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	3	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	98	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 (98) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:51:PHE:HE2	2:B:321:LEU:HD21	1.65	0.61
1:A:134:GLY:C	1:A:136:LEU:H	2.08	0.60
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: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:39:GLN:HE22	1:A:43:VAL:HB	1.72	0.54
1:A:231:GLN:OE1	1:A:235:ARG:NE	2.41	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
1:A:261:MET:HE1	4:A:939:HOH:O	2.07	0.54
2:B:86:LYS:CE	2:B:100:ALA:HB1	2.38	0.53
1:A:135:ILE:O	1:A:135:ILE:CG1	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:C:338:GLY:HA2	2:D:166:MET:HE2	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:134:GLY:C	1:A:136:LEU:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HG2	1:A:135:ILE:H	1.80	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
1:A:132:LYS:CB	1:A:135:ILE:CB	2.94	0.44
2:B:279:LYS:HB3	2:B:279:LYS:HE3	1.83	0.44
2:B:40:GLN:HA	2:B:43:GLU:HG3	1.99	0.44
1:C:132:LYS:O	1:C:133:LYS:C	2.61	0.44
1:C:299:ASN:HD22	1:C:299:ASN:C	2.26	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:299:ASN:C	1:A:299:ASN:HD22	2.27	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
1:A:79:LYS:NZ	4:A:1121:HOH:O	2.54	0.41
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%)	24	16
1	C	420/424 (99%)	410 (98%)	10 (2%)	0	100	100
2	B	346/354 (98%)	331 (96%)	14 (4%)	1 (0%)	36	28
2	D	356/354 (101%)	340 (96%)	16 (4%)	0	100	100
All	All	1542/1556 (99%)	1487 (96%)	52 (3%)	3 (0%)	43	36

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%)	364 (97%)	13 (3%)	32	23
1	C	378/377 (100%)	361 (96%)	17 (4%)	24	14
2	B	292/295 (99%)	281 (96%)	11 (4%)	29	19
2	D	299/295 (101%)	291 (97%)	8 (3%)	39	32
All	All	1346/1344 (100%)	1297 (96%)	49 (4%)	30	21

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	133	LYS
1	A	185	LYS
1	A	205	LEU
1	A	207	ARG
1	A	224	LYS
1	A	236	SER
1	A	284	LEU
1	A	286	GLU
1	A	299	ASN
1	A	326	LEU
1	A	363	ILE
1	A	395	LEU
2	B	12	LEU
2	B	64	ASN
2	B	77	ARG
2	B	86	LYS
2	B	113	TYR
2	B	151	MET
2	B	168	ILE
2	B	183	GLU
2	B	187	LEU
2	B	208	THR
2	B	305	TYR
1	C	44	THR
1	C	48	HIS
1	C	61	GLN
1	C	63	LEU
1	C	73	LEU
1	C	128	ARG
1	C	159	ILE
1	C	160	MET
1	C	189	LEU
1	C	215	LYS
1	C	219	VAL
1	C	284	LEU
1	C	299	ASN
1	C	319	LYS
1	C	353	LEU
1	C	386	ASP
1	C	412	GLU
2	D	1	MET
2	D	8	GLU

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Mol	Chain	Res	Type
2	D	64	ASN
2	D	109	MET
2	D	113	TYR
2	D	145	LYS
2	D	147	LYS
2	D	305	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	38	ASN
1	A	39	GLN
1	A	72	ASN
1	A	87	GLN
1	A	129	ASN
1	A	148	ASN
1	A	198	ASN
1	A	299	ASN
1	A	314	GLN
1	A	364	ASN
2	B	9	ASN
2	B	50	GLN
2	B	64	ASN
1	C	61	GLN
1	C	67	ASN
1	C	148	ASN
1	C	212	ASN
1	C	299	ASN
1	C	391	HIS
2	D	34	HIS
2	D	64	ASN
2	D	152	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	906	-	5,5,5	0.44	0	5,5,5	0.50	0
3	GOL	D	903	-	5,5,5	0.34	0	5,5,5	0.54	0
3	GOL	A	905	-	5,5,5	0.33	0	5,5,5	0.34	0
3	GOL	D	901	-	5,5,5	0.41	0	5,5,5	0.38	0
3	GOL	C	907	-	5,5,5	0.38	0	5,5,5	0.25	0
3	GOL	D	908	-	5,5,5	0.35	0	5,5,5	0.26	0
3	GOL	B	909	-	5,5,5	0.37	0	5,5,5	0.21	0
3	GOL	B	902	-	5,5,5	0.39	0	5,5,5	0.45	0
3	GOL	A	904	-	5,5,5	0.39	0	5,5,5	0.54	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	906	-	-	4/4/4/4	-
3	GOL	D	903	-	-	2/4/4/4	-
3	GOL	A	905	-	-	0/4/4/4	-
3	GOL	D	901	-	-	0/4/4/4	-
3	GOL	C	907	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	908	-	-	0/4/4/4	-
3	GOL	B	909	-	-	3/4/4/4	-
3	GOL	B	902	-	-	0/4/4/4	-
3	GOL	A	904	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) 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
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	A	906	GOL	O1-C1-C2-C3
3	B	909	GOL	C1-C2-C3-O3
3	D	903	GOL	C1-C2-C3-O3
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-O2
3	B	909	GOL	O2-C2-C3-O3

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 [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	415/424 (97%)	0.33	22 (5%) 32 37	3, 30, 71, 128	7 (1%)
1	C	415/424 (97%)	0.95	90 (21%) 2 2	11, 40, 132, 191	8 (1%)
2	B	340/354 (96%)	0.02	18 (5%) 32 37	-1, 18, 70, 104	3 (0%)
2	D	354/354 (100%)	-0.06	12 (3%) 48 54	1, 19, 58, 155	4 (1%)
All	All	1524/1556 (97%)	0.34	142 (9%) 14 16	-1, 27, 91, 191	22 (1%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	301	GLY	7.4
1	C	155	TRP	6.5
1	C	159	ILE	6.4
1	C	136	LEU	5.5
1	C	157	PHE	5.2
1	C	158	VAL	4.9
1	C	167	ARG	4.8
2	D	3	THR	4.8
1	A	219	VAL	4.7
2	B	209	GLY	4.5
1	C	141	LYS	4.4
1	C	218	THR	4.4
1	C	151	ILE	4.3
1	C	42	LEU	4.3
1	C	163	LYS	4.2
1	C	144	TYR	4.2
2	D	0	GLY	4.1
1	C	40	ARG	4.0
2	D	2	ALA	4.0
1	C	166	TYR	3.9
1	C	46	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	30	PRO	3.8
2	D	1	MET	3.8
1	C	130	ILE	3.7
1	C	123	ILE	3.7
1	C	153	TYR	3.6
2	B	12	LEU	3.6
1	C	196	GLY	3.6
1	C	135	ILE	3.6
1	A	178	TYR	3.5
1	C	34	VAL	3.5
1	C	170	LYS	3.5
1	C	217	GLN	3.4
1	C	49	ALA	3.4
1	C	179	ALA	3.4
1	A	135	ILE	3.4
2	B	291	PHE	3.3
2	D	4	ASP	3.3
1	C	38	ASN	3.2
1	C	43	VAL	3.2
1	C	214	VAL	3.2
1	A	152[A]	ASN	3.1
1	C	32	THR	3.1
2	B	13	ALA	3.1
1	C	41	VAL	3.1
1	C	147	LEU	3.1
1	C	174	LYS	3.0
1	C	213	GLU	3.0
1	C	126	ALA	3.0
1	C	162	ALA	3.0
1	C	160	MET	3.0
1	C	146	PHE	3.0
1	C	156	ASP	3.0
2	B	11	THR	3.0
1	C	152	ASN	3.0
1	A	226	ILE	2.9
1	A	223	ARG	2.9
1	A	134	GLY	2.9
1	C	37	HIS	2.9
1	C	149	LYS	2.9
1	C	138	GLU	2.9
1	A	38	ASN	2.9
1	C	122	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	218	THR	2.8
1	A	214	VAL	2.8
1	C	421[A]	GLN	2.8
1	A	220	THR	2.8
1	C	220	THR	2.8
1	C	33	GLY	2.8
1	C	168	THR	2.8
1	C	173	ASN	2.7
1	A	132	LYS	2.7
1	C	169	GLY	2.7
2	D	12	LEU	2.7
1	C	219	VAL	2.7
1	C	58	TRP	2.7
1	C	64	TRP	2.7
1	C	142	GLU	2.7
1	C	36	MET	2.7
2	B	33	LEU	2.7
1	C	125	LEU	2.6
2	B	32	LYS	2.6
1	C	195	PRO	2.5
1	C	44	THR	2.5
1	C	61	GLN	2.5
1	C	154	LYS	2.5
1	A	107	TYR	2.5
1	C	98	SER	2.5
1	A	166	TYR	2.4
1	C	148	ASN	2.4
1	A	233	LEU	2.4
2	B	15	LEU	2.4
1	A	217	GLN	2.4
1	C	45	SER	2.4
2	B	31	ALA	2.4
2	B	52	VAL	2.4
2	D	6	LEU	2.4
2	D	41	VAL	2.4
1	A	227	MET	2.4
1	C	194	PRO	2.4
1	A	234	MET	2.4
1	C	133	LYS	2.4
1	C	145	ASP	2.3
1	C	139	TYR	2.3
2	B	208	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	143	ASN	2.3
2	D	39	HIS	2.3
1	C	172	ARG	2.3
1	C	171	GLU	2.3
2	B	22	LEU	2.3
1	C	129	ASN	2.3
2	B	34[A]	HIS	2.3
1	C	178	TYR	2.3
2	B	51	PHE	2.3
2	D	31	ALA	2.3
2	D	36	VAL	2.3
1	C	180	LEU	2.3
1	C	164	GLU	2.2
1	C	65	ILE	2.2
1	C	117	GLU	2.2
1	C	340[A]	GLN	2.2
1	C	367	GLY	2.2
1	C	29	ASN	2.2
2	B	28	GLU	2.2
1	C	314	GLN	2.2
2	D	33	LEU	2.2
1	C	175	ALA	2.2
1	C	321	PHE	2.2
1	A	221	ALA	2.2
1	C	22	ALA	2.2
1	A	171	GLU	2.1
1	C	60	THR	2.1
1	A	284	LEU	2.1
1	C	35	ARG	2.1
2	B	330	THR	2.1
1	A	230	GLN	2.1
2	B	25	LYS	2.0
1	C	134	GLY	2.0
1	C	63	LEU	2.0
1	C	27	MET	2.0
1	C	39	GLN	2.0
1	C	161	GLN	2.0

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

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
3	GOL	C	907	6/6	0.67	0.23	69,69,70,71	0
3	GOL	A	905	6/6	0.75	0.13	49,51,51,51	0
3	GOL	A	906	6/6	0.84	0.20	42,45,46,46	0
3	GOL	B	909	6/6	0.85	0.19	76,77,77,77	0
3	GOL	A	904	6/6	0.85	0.13	51,52,53,53	0
3	GOL	D	908	6/6	0.86	0.10	52,53,53,53	0
3	GOL	D	903	6/6	0.91	0.08	47,50,50,51	0
3	GOL	D	901	6/6	0.91	0.10	27,28,28,29	0
3	GOL	B	902	6/6	0.93	0.09	22,25,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.