



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 3RIP / pdb_00003rip
Title : Crystal Structure of human gamma-tubulin complex protein 4 (GCP4)
Authors : Gregory-Pauron, L.; Guillet, V.; Mourey, L.
Deposited on : 2011-04-14
Resolution : 2.30 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

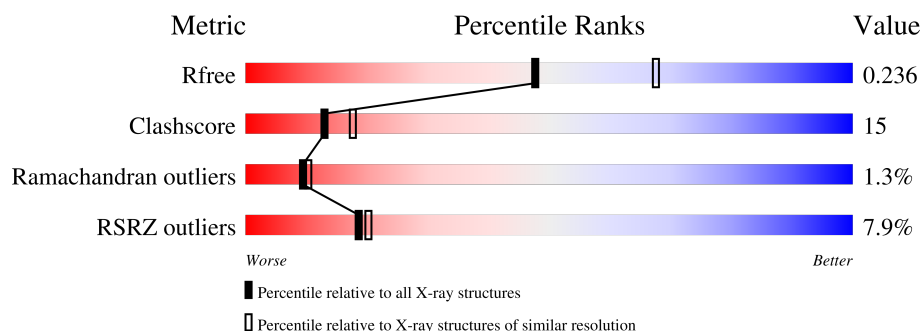
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	677	7% 61% 22% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4843 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 Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	4	0
			4572	2963	774	816	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	667	CYS	-	expression tag	UNP Q9UGJ1
A	668	GLY	-	expression tag	UNP Q9UGJ1
A	669	ARG	-	expression tag	UNP Q9UGJ1
A	670	LEU	-	expression tag	UNP Q9UGJ1
A	671	GLU	-	expression tag	UNP Q9UGJ1
A	672	HIS	-	expression tag	UNP Q9UGJ1
A	673	HIS	-	expression tag	UNP Q9UGJ1
A	674	HIS	-	expression tag	UNP Q9UGJ1
A	675	HIS	-	expression tag	UNP Q9UGJ1
A	676	HIS	-	expression tag	UNP Q9UGJ1
A	677	HIS	-	expression tag	UNP Q9UGJ1

- Molecule 2 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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		

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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	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

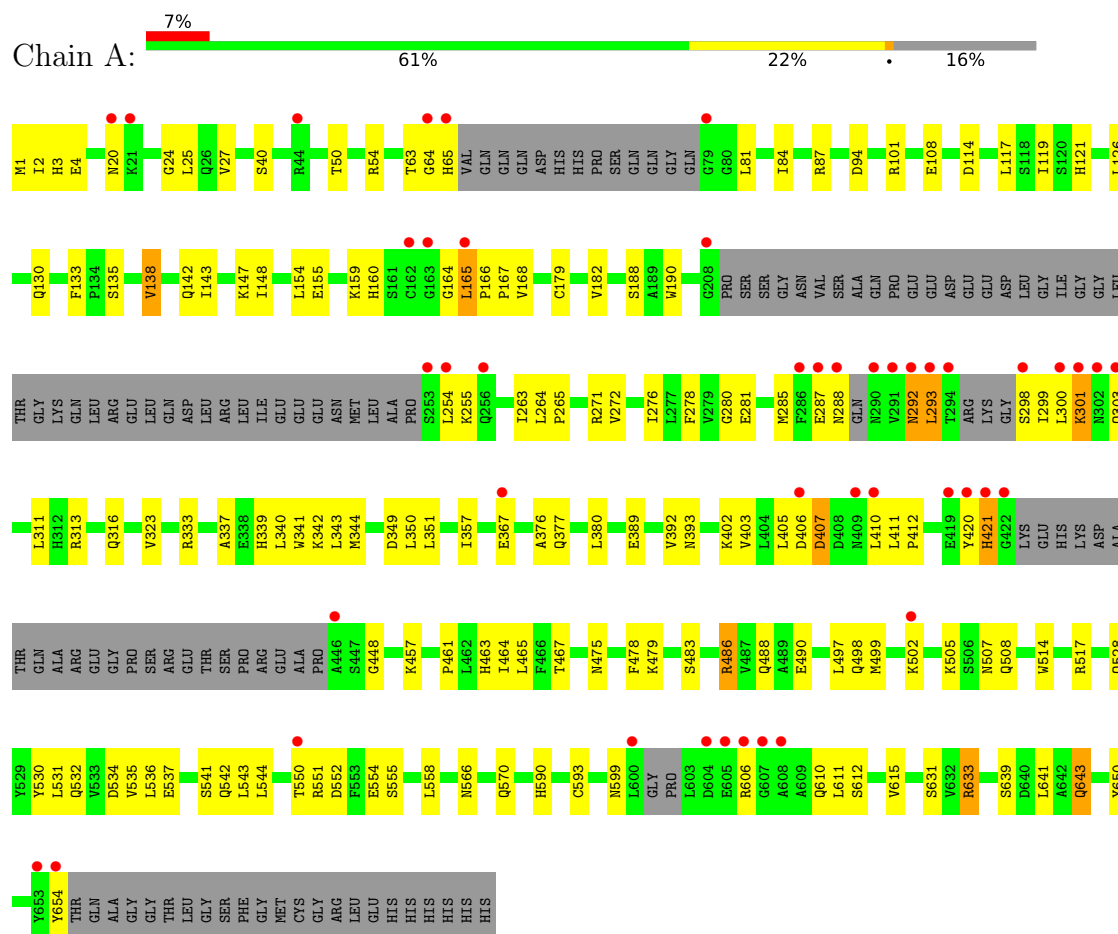
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	2
			215	215		

3 Residue-property plots

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: Gamma-tubulin complex component 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	214.95Å 214.95Å 128.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.30) 99.3 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.227 , 0.260 (Not available) , 0.236	Depositor DCC
R_{free} test set	4414 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4843	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: GOL, MRD

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	1.28	10/4676 (0.2%)	1.26	26/6334 (0.4%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	PHE	N-CA	-6.54	1.38	1.46
1	A	641	LEU	CA-C	5.55	1.59	1.52
1	A	631	SER	CA-C	-5.51	1.45	1.52
1	A	558	LEU	N-CA	-5.40	1.40	1.46
1	A	367[A]	GLU	CD-OE2	5.21	1.35	1.25
1	A	367[B]	GLU	CD-OE2	5.21	1.35	1.25
1	A	119	ILE	N-CA	-5.14	1.40	1.46
1	A	486	ARG	N-CA	-5.07	1.40	1.46
1	A	323	VAL	CA-CB	5.04	1.59	1.54
1	A	40	SER	N-CA	-5.00	1.40	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	PHE	CA-C-N	-13.39	106.12	119.64
1	A	133	PHE	C-N-CA	-13.39	106.12	119.64
1	A	367[A]	GLU	CG-CD-OE1	9.33	139.85	118.40
1	A	367[B]	GLU	CG-CD-OE1	9.33	139.85	118.40
1	A	27	VAL	CB-CA-C	-8.55	97.66	110.82
1	A	633	ARG	NE-CZ-NH2	-7.82	112.16	119.20
1	A	465	LEU	N-CA-C	-7.31	103.20	112.93
1	A	323	VAL	N-CA-CB	6.97	118.25	110.51
1	A	276	ILE	N-CA-C	-6.07	104.59	110.72
1	A	467	THR	CA-C-N	-5.95	113.56	119.56
1	A	467	THR	C-N-CA	-5.95	113.56	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	SER	CB-CA-C	-5.87	101.04	110.79
1	A	138	VAL	N-CA-CB	5.68	117.19	110.55
1	A	403	VAL	CB-CA-C	5.65	119.03	111.85
1	A	303	GLN	N-CA-C	-5.64	106.24	113.01
1	A	643	GLN	CB-CA-C	-5.57	99.99	110.67
1	A	631	SER	N-CA-C	-5.49	105.20	111.07
1	A	114	ASP	CA-C-N	-5.45	114.07	120.12
1	A	114	ASP	C-N-CA	-5.45	114.07	120.12
1	A	87	ARG	N-CA-C	-5.22	105.58	111.28
1	A	367[A]	GLU	CG-CD-OE2	-5.20	106.45	118.40
1	A	367[B]	GLU	CG-CD-OE2	-5.20	106.45	118.40
1	A	357	ILE	N-CA-C	-5.19	105.35	111.00
1	A	536	LEU	N-CA-C	5.07	116.50	110.97
1	A	633	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	54	ARG	CB-CG-CD	5.03	122.87	111.30

There are no chirality outliers.

There are no planarity outliers.

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	4572	0	4505	136	0
2	A	8	0	14	4	0
3	A	48	0	64	4	0
4	A	215	0	0	11	0
All	All	4843	0	4583	138	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 15.

All (138) 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:612:SER:HB3	4:A:888:HOH:O	1.44	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASN:HD22	1:A:288:ASN:H	1.11	0.99
1:A:410:LEU:HD23	1:A:411:LEU:N	1.80	0.96
1:A:550:THR:HG22	1:A:552:ASP:H	1.35	0.91
1:A:639:SER:O	1:A:643:GLN:HG2	1.73	0.89
1:A:497:LEU:C	1:A:497:LEU:HD23	1.98	0.87
1:A:164:GLY:O	1:A:165:LEU:HG	1.80	0.82
1:A:316:GLN:HA	1:A:316:GLN:OE1	1.81	0.81
1:A:117:LEU:HD11	1:A:121:HIS:HD2	1.48	0.79
1:A:288:ASN:H	1:A:288:ASN:ND2	1.79	0.79
1:A:1[B]:MET:HE2	1:A:3:HIS:H	1.47	0.78
1:A:606:ARG:O	1:A:610:GLN:HG2	1.85	0.77
1:A:534:ASP:OD2	1:A:633:ARG:CD	2.34	0.75
1:A:285:MET:C	1:A:285:MET:SD	2.70	0.74
1:A:502[A]:LYS:HG2	4:A:901:HOH:O	1.86	0.74
1:A:188:SER:HB2	1:A:311:LEU:HD12	1.70	0.74
1:A:165:LEU:HB2	1:A:168:VAL:HG13	1.72	0.71
1:A:316:GLN:OE1	1:A:316:GLN:CA	2.39	0.70
1:A:505:LYS:NZ	1:A:599:ASN:OD1	2.22	0.70
1:A:508:GLN:NE2	1:A:508:GLN:HA	2.06	0.70
1:A:534:ASP:OD2	1:A:633:ARG:HD2	1.93	0.69
2:A:678:MRD:O2	2:A:678:MRD:H5C2	1.92	0.69
1:A:117:LEU:HD11	1:A:121:HIS:CD2	2.29	0.68
1:A:499:MET:HE2	1:A:517:ARG:CD	2.25	0.67
1:A:135:SER:O	1:A:138:VAL:HG22	1.95	0.67
1:A:497:LEU:HD23	1:A:497:LEU:O	1.96	0.65
1:A:534:ASP:OD2	1:A:633:ARG:HD3	1.97	0.65
1:A:84:ILE:HD12	1:A:182:VAL:HG13	1.80	0.64
1:A:142:GLN:OE1	1:A:160:HIS:NE2	2.28	0.64
1:A:554:GLU:OE1	3:A:685:GOL:O3	2.15	0.64
1:A:20:ASN:O	1:A:24:GLY:N	2.27	0.64
1:A:1[B]:MET:CE	1:A:3:HIS:H	2.11	0.63
1:A:650:TYR:CE1	1:A:654:TYR:HB2	2.34	0.63
1:A:81:LEU:HD21	1:A:147:LYS:HA	1.80	0.62
1:A:63:THR:O	1:A:65:HIS:N	2.26	0.61
1:A:410:LEU:HD23	1:A:410:LEU:C	2.25	0.61
1:A:497:LEU:C	1:A:497:LEU:CD2	2.70	0.61
1:A:499:MET:HE2	1:A:517:ARG:HD3	1.82	0.60
1:A:285:MET:SD	1:A:285:MET:O	2.60	0.59
1:A:566:ASN:O	1:A:570:GLN:HG2	2.03	0.59
1:A:190:TRP:CE2	1:A:280:GLY:HA3	2.37	0.59
1:A:1[B]:MET:HE3	1:A:2:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:MET:HE2	1:A:461:PRO:HG2	1.84	0.58
1:A:287:GLU:O	1:A:287:GLU:HG3	2.04	0.58
1:A:410:LEU:HD23	1:A:411:LEU:H	1.66	0.57
1:A:550:THR:HG21	1:A:555:SER:CB	2.34	0.57
1:A:550:THR:HG21	1:A:555:SER:HB2	1.86	0.57
1:A:508:GLN:NE2	1:A:508:GLN:CA	2.68	0.56
1:A:288:ASN:ND2	1:A:288:ASN:N	2.51	0.55
1:A:531:LEU:O	1:A:535:VAL:HB	2.06	0.54
1:A:499:MET:HE2	1:A:517:ARG:HD2	1.88	0.54
1:A:411:LEU:N	1:A:412:PRO:HD2	2.23	0.54
1:A:287:GLU:O	1:A:287:GLU:CG	2.56	0.53
1:A:281:GLU:OE2	4:A:834:HOH:O	2.18	0.53
2:A:678:MRD:O2	2:A:678:MRD:C5	2.56	0.53
1:A:508:GLN:CA	1:A:508:GLN:HE21	2.21	0.53
1:A:499:MET:HE3	1:A:514:TRP:HE3	1.73	0.53
1:A:143:ILE:HA	1:A:148:ILE:HG13	1.91	0.53
1:A:488:GLN:OE1	1:A:528:GLN:NE2	2.36	0.53
1:A:271:ARG:HG2	1:A:272:VAL:N	2.23	0.52
1:A:155:GLU:OE2	1:A:159:LYS:HE2	2.09	0.52
1:A:166:PRO:HB2	1:A:167:PRO:HD3	1.90	0.52
1:A:505:LYS:HE2	4:A:692:HOH:O	2.09	0.51
1:A:188:SER:HB2	1:A:311:LEU:CD1	2.41	0.50
1:A:108:GLU:HG3	4:A:792:HOH:O	2.10	0.50
1:A:498:GLN:CD	1:A:593:CYS:HB2	2.37	0.50
1:A:341:TRP:NE1	1:A:550:THR:O	2.45	0.50
1:A:550:THR:HG22	1:A:551:ARG:N	2.27	0.49
1:A:420:TYR:O	1:A:421:HIS:HB2	2.12	0.49
1:A:84:ILE:HD12	1:A:182:VAL:CG1	2.41	0.49
1:A:537:GLU:O	1:A:541:SER:HB2	2.12	0.49
1:A:593:CYS:SG	2:A:678:MRD:H5C1	2.53	0.49
1:A:486:ARG:O	1:A:490:GLU:HG3	2.12	0.49
1:A:1[B]:MET:HE2	1:A:3:HIS:HB3	1.95	0.49
1:A:406:ASP:O	1:A:407:ASP:C	2.55	0.49
1:A:502[B]:LYS:HE3	4:A:811:HOH:O	2.13	0.48
1:A:507:ASN:OD1	1:A:507:ASN:C	2.56	0.48
1:A:405:LEU:HD12	1:A:406:ASP:N	2.28	0.48
1:A:313:ARG:O	1:A:316:GLN:HB2	2.13	0.48
1:A:532:GLN:O	1:A:537:GLU:HG2	2.13	0.48
1:A:502[A]:LYS:HE3	4:A:727:HOH:O	2.13	0.48
1:A:126:LEU:O	1:A:130:GLN:HG3	2.14	0.48
1:A:254:LEU:O	1:A:255:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.69	0.48
1:A:463:HIS:N	1:A:463:HIS:ND1	2.62	0.47
1:A:499:MET:HE3	1:A:514:TRP:CE3	2.49	0.47
1:A:643:GLN:HG2	1:A:643:GLN:H	1.58	0.47
1:A:292:ASN:O	1:A:293:LEU:CB	2.62	0.47
1:A:389:GLU:O	1:A:393:ASN:ND2	2.41	0.47
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.60	0.46
1:A:333:ARG:HD2	3:A:685:GOL:H11	1.97	0.46
1:A:342:LYS:O	1:A:343:LEU:C	2.55	0.46
1:A:479:LYS:NZ	4:A:830:HOH:O	2.49	0.46
1:A:1[B]:MET:HG2	1:A:4:GLU:HG2	1.98	0.45
1:A:285:MET:O	1:A:285:MET:CG	2.65	0.45
1:A:117:LEU:CD1	1:A:121:HIS:CD2	2.99	0.45
1:A:263:ILE:O	1:A:263:ILE:HG23	2.17	0.45
1:A:299:ILE:O	1:A:339:HIS:ND1	2.49	0.45
1:A:457:LYS:N	1:A:457:LYS:CD	2.80	0.45
1:A:341:TRP:HE3	1:A:342:LYS:N	2.14	0.45
1:A:337:ALA:HB1	1:A:552:ASP:OD1	2.17	0.45
1:A:376:ALA:O	1:A:377:GLN:C	2.58	0.45
1:A:281:GLU:OE1	3:A:686:GOL:O2	2.28	0.45
1:A:351:LEU:HD22	1:A:544:LEU:HD22	1.98	0.45
1:A:410:LEU:CD2	1:A:411:LEU:N	2.66	0.45
1:A:154:LEU:HD23	1:A:179:CYS:HB3	1.98	0.45
1:A:566:ASN:O	1:A:570:GLN:CG	2.64	0.45
1:A:570:GLN:HG2	1:A:570:GLN:H	1.59	0.44
1:A:278:PHE:HB2	3:A:686:GOL:H2	1.98	0.44
1:A:94:ASP:OD1	1:A:101:ARG:NH2	2.51	0.44
1:A:341:TRP:CZ2	1:A:551:ARG:NH1	2.85	0.44
1:A:25:LEU:HB2	1:A:50:THR:OG1	2.18	0.44
1:A:155:GLU:O	1:A:159:LYS:HG2	2.18	0.44
1:A:344:MET:CE	1:A:461:PRO:HG2	2.48	0.44
1:A:499:MET:CE	1:A:517:ARG:HD3	2.48	0.44
1:A:349:ASP:HA	4:A:720:HOH:O	2.18	0.43
1:A:461:PRO:O	1:A:464:ILE:HG23	2.19	0.43
1:A:411:LEU:O	1:A:412:PRO:C	2.62	0.43
1:A:264:LEU:O	1:A:265:PRO:C	2.61	0.42
1:A:271:ARG:CG	1:A:272:VAL:N	2.75	0.42
1:A:590:HIS:ND1	2:A:678:MRD:H5C3	2.35	0.42
1:A:448:GLY:HA3	4:A:900:HOH:O	2.20	0.41
1:A:164:GLY:O	1:A:165:LEU:CG	2.60	0.41
1:A:350:LEU:N	4:A:720:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLN:O	1:A:543:LEU:C	2.61	0.41
1:A:402:LYS:O	1:A:402:LYS:HG2	2.20	0.41
1:A:611:LEU:O	1:A:615:VAL:HG23	2.20	0.41
1:A:380:LEU:HD21	1:A:392:VAL:HG21	2.03	0.41
1:A:63:THR:C	1:A:65:HIS:H	2.22	0.41
1:A:164:GLY:O	1:A:165:LEU:CB	2.69	0.41
1:A:298:SER:C	1:A:300:LEU:H	2.29	0.40
1:A:300:LEU:O	1:A:301:LYS:CB	2.69	0.40
1:A:530:TYR:CD1	1:A:633:ARG:HD3	2.56	0.40
1:A:475:ASN:O	1:A:479:LYS:HG3	2.22	0.40
1:A:499:MET:HE1	1:A:514:TRP:HA	2.03	0.40
1:A:405:LEU:HD12	1:A:405:LEU:C	2.47	0.40
1:A:457:LYS:N	1:A:457:LYS:HD2	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	557/677 (82%)	525 (94%)	25 (4%)	7 (1%)	9 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	LEU
1	A	292	ASN
1	A	293	LEU
1	A	301	LYS
1	A	407	ASP
1	A	64	GLY
1	A	421	HIS

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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	684	-	5,5,5	1.29	0	5,5,5	1.46	1 (20%)
3	GOL	A	683	-	5,5,5	0.79	0	5,5,5	0.70	0
3	GOL	A	685	-	5,5,5	0.62	0	5,5,5	0.67	0
3	GOL	A	686	-	5,5,5	0.48	0	5,5,5	0.68	0
3	GOL	A	681	-	5,5,5	0.68	0	5,5,5	1.65	1 (20%)
3	GOL	A	679	-	5,5,5	0.71	0	5,5,5	1.42	1 (20%)
3	GOL	A	680	-	5,5,5	0.84	0	5,5,5	1.12	0
3	GOL	A	682	-	5,5,5	0.57	0	5,5,5	0.76	0
2	MRD	A	678	-	7,7,7	1.13	0	9,10,10	0.38	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	684	-	-	4/4/4/4	-
3	GOL	A	683	-	-	2/4/4/4	-
3	GOL	A	685	-	-	0/4/4/4	-
3	GOL	A	686	-	-	2/4/4/4	-
3	GOL	A	681	-	-	4/4/4/4	-
3	GOL	A	679	-	-	4/4/4/4	-
3	GOL	A	680	-	-	2/4/4/4	-
3	GOL	A	682	-	-	2/4/4/4	-
2	MRD	A	678	-	-	3/5/5/5	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	684	GOL	C3-C2-C1	-2.92	101.07	111.80
3	A	679	GOL	O1-C1-C2	-2.19	100.51	110.38
3	A	681	GOL	O3-C3-C2	-2.19	100.53	110.38

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	679	GOL	C1-C2-C3-O3
3	A	680	GOL	O1-C1-C2-C3
3	A	681	GOL	O1-C1-C2-O2
3	A	681	GOL	O1-C1-C2-C3
3	A	682	GOL	C1-C2-C3-O3
3	A	684	GOL	O1-C1-C2-C3
3	A	684	GOL	C1-C2-C3-O3
3	A	686	GOL	O1-C1-C2-O2
3	A	686	GOL	O1-C1-C2-C3
3	A	679	GOL	O2-C2-C3-O3
3	A	682	GOL	O2-C2-C3-O3
3	A	679	GOL	O1-C1-C2-C3
3	A	681	GOL	C1-C2-C3-O3
3	A	683	GOL	C1-C2-C3-O3
3	A	684	GOL	O1-C1-C2-O2
3	A	684	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	679	GOL	O1-C1-C2-O2
3	A	680	GOL	O1-C1-C2-O2
2	A	678	MRD	C1-C2-C3-C4
2	A	678	MRD	C2-C3-C4-C5
3	A	683	GOL	O2-C2-C3-O3
3	A	681	GOL	O2-C2-C3-O3
2	A	678	MRD	CM-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	685	GOL	2	0
3	A	686	GOL	2	0
2	A	678	MRD	4	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	568/677 (83%)	0.41	45 (7%) 18 20	15, 51, 82, 119	5 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	LEU	7.0
1	A	291	VAL	6.9
1	A	301	LYS	5.8
1	A	654	TYR	5.8
1	A	208	GLY	5.1
1	A	294	THR	5.0
1	A	163	GLY	4.5
1	A	253	SER	4.4
1	A	64	GLY	4.3
1	A	254	LEU	4.2
1	A	422	GLY	4.1
1	A	79	GLY	4.0
1	A	292	ASN	4.0
1	A	302	ASN	3.9
1	A	298	SER	3.9
1	A	287	GLU	3.9
1	A	419	GLU	3.8
1	A	409	ASN	3.6
1	A	290	ASN	3.6
1	A	286	PHE	3.6
1	A	162	CYS	3.5
1	A	65	HIS	3.5
1	A	406	ASP	3.5
1	A	288	ASN	3.4
1	A	21	LYS	3.3
1	A	421	HIS	3.3
1	A	653	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	605	GLU	3.1
1	A	256	GLN	3.0
1	A	303	GLN	2.8
1	A	410	LEU	2.8
1	A	20	ASN	2.6
1	A	293	LEU	2.6
1	A	300	LEU	2.6
1	A	165	LEU	2.6
1	A	608	ALA	2.6
1	A	604	ASP	2.6
1	A	502[A]	LYS	2.5
1	A	606	ARG	2.4
1	A	420	TYR	2.3
1	A	367[A]	GLU	2.3
1	A	550	THR	2.3
1	A	44	ARG	2.3
1	A	446	ALA	2.0
1	A	607	GLY	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(Å ²)	Q<0.9
2	MRD	A	678	8/8	0.60	0.25	56,68,77,83	0
3	GOL	A	685	6/6	0.70	0.30	63,72,76,79	0
3	GOL	A	683	6/6	0.73	0.19	39,41,45,46	6
3	GOL	A	679	6/6	0.81	0.17	43,45,49,49	0
3	GOL	A	686	6/6	0.82	0.31	63,69,71,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	680	6/6	0.86	0.14	34,36,39,40	6
3	GOL	A	682	6/6	0.90	0.13	39,43,46,46	0
3	GOL	A	681	6/6	0.92	0.10	46,48,48,49	0
3	GOL	A	684	6/6	0.97	0.06	33,35,43,46	6

6.5 Other polymers [i](#)

There are no such residues in this entry.