



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 AM UTC

PDB ID : 7P9K / pdb_00007p9k
Title : BrxU, GmrSD-family Type IV restriction enzyme
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Deposited on : 2021-07-27
Resolution : 2.12 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

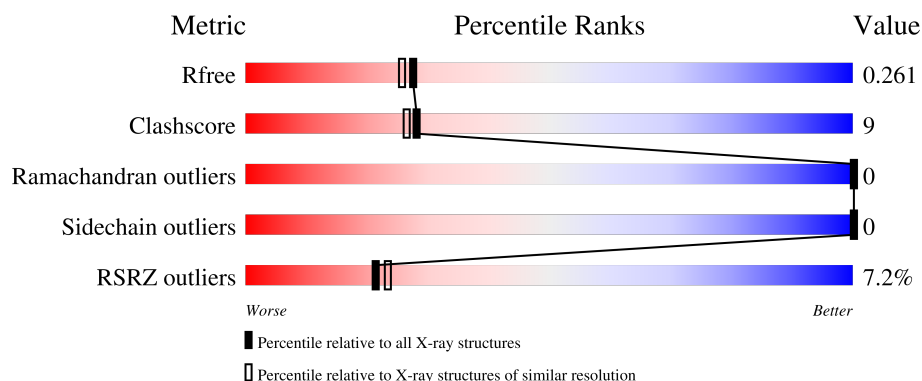
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	587	9% 78% 21% .
1	B	587	6% 82% 17% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	604	-	-	X	-
4	GOL	B	604	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9864 atoms, of which 16 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.

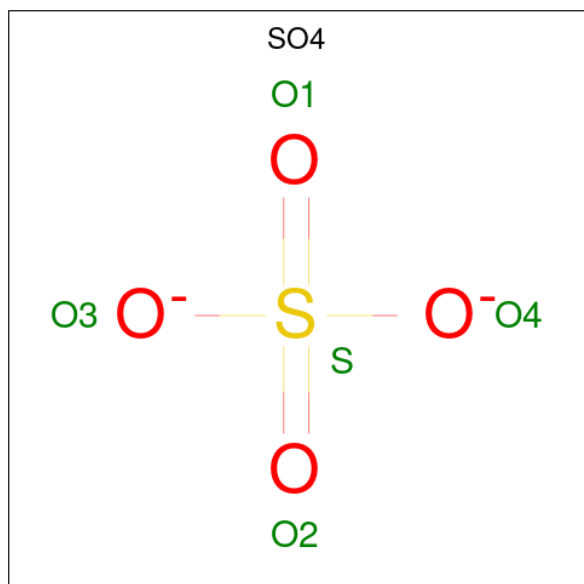
- Molecule 1 is a protein called DUF262 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4732	3011	824	881	16			
1	B	580	Total	C	N	O	S	0	0	0
			4732	3011	824	881	16			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0
4	B	1	Total C H O 14 3 8 3	0	0

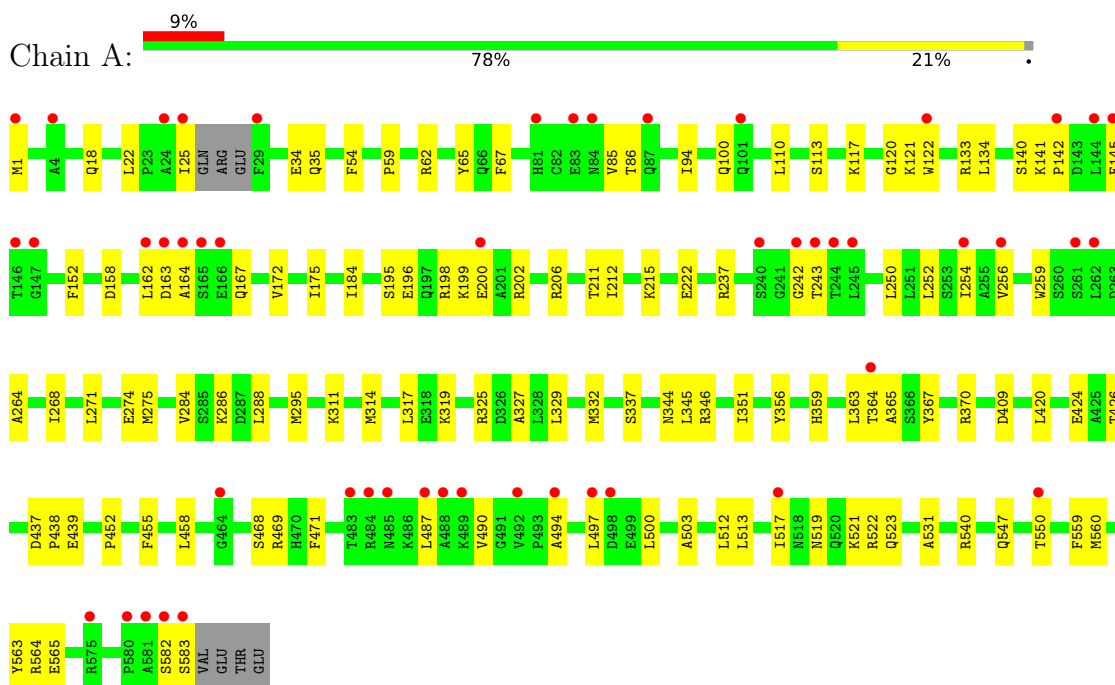
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	162	Total O 162 162	0	0
5	B	188	Total O 188 188	0	0

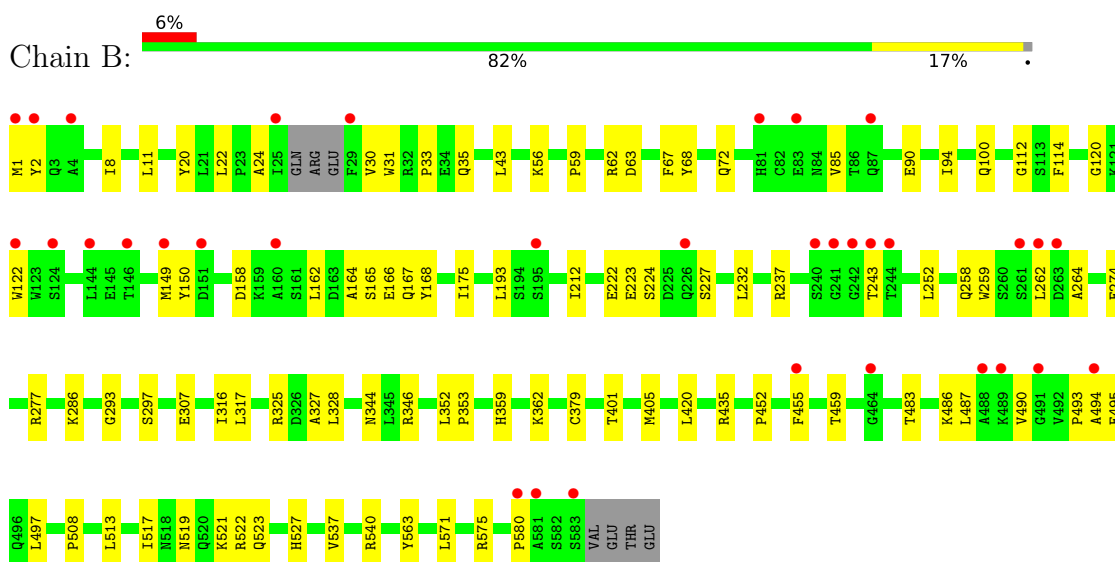
3 Residue-property plots

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: DUF262 domain-containing protein



• Molecule 1: DUF262 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 67.26Å 126.55Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	72.89 – 2.12 72.89 – 2.12	Depositor ED
% Data completeness (in resolution range)	97.4 (72.89-2.12) 99.1 (72.89-2.12)	Depositor ED
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.12Å)	Xtriage
Refinement program	REFMAC CCP4 Program Suite v7.1.015, PHENIX 1.14_3260	Depositor
R, R_{free}	0.204 , 0.252 0.217 , 0.261	Depositor DC
R_{free} test set	5018 reflections (5.04%)	wwPDB
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	ED
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	ED
Total number of atoms	9864	wwPDB
Average B, all atoms (Å ²)	55.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: CL, SO4, 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	0.39	0/4838	0.55	0/6542
1	B	0.37	0/4838	0.52	0/6542
All	All	0.38	0/9676	0.54	0/13084

There are no bond length outliers.

There are no bond angle outliers.

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	4732	0	4655	101	0
1	B	4732	0	4655	72	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	6	8	8	5	0
4	B	6	8	8	4	0
5	A	162	0	0	5	0
5	B	188	0	0	5	0
All	All	9848	16	9326	168	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 9.

All (168) 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:252:LEU:HD22	1:A:286:LYS:HD2	1.49	0.94
1:A:314:MET:HE1	1:A:317:LEU:HD22	1.55	0.89
1:A:494:ALA:HA	1:A:497:LEU:HD12	1.55	0.87
1:A:503:ALA:HB3	1:A:560:MET:HE1	1.57	0.87
1:A:141:LYS:HE3	1:A:200:GLU:OE2	1.77	0.85
1:A:500:LEU:HA	1:A:560:MET:HE3	1.61	0.81
1:A:494:ALA:HA	1:A:497:LEU:CD1	2.10	0.81
1:A:252:LEU:O	1:A:256:VAL:HG23	1.80	0.80
1:B:120:GLY:H	4:B:604:GOL:H31	1.47	0.80
2:B:601:CL:CL	5:B:854:HOH:O	2.37	0.79
1:A:164:ALA:HB3	1:A:167:GLN:HB2	1.64	0.79
1:A:346:ARG:HE	4:A:604:GOL:H2	1.48	0.78
4:B:604:GOL:O1	4:B:604:GOL:O3	1.90	0.76
1:A:503:ALA:HB1	1:A:563:TYR:CE2	2.21	0.75
1:A:237:ARG:HH11	1:B:35:GLN:HG3	1.49	0.74
1:A:140:SER:O	1:A:141:LYS:HE2	1.88	0.74
1:A:469:ARG:HH11	1:A:469:ARG:HB3	1.53	0.73
1:B:59:PRO:O	1:B:62:ARG:HG3	1.89	0.73
1:B:120:GLY:H	4:B:604:GOL:C3	2.03	0.71
1:A:469:ARG:HB3	1:A:469:ARG:NH1	2.08	0.68
1:A:582:SER:O	1:A:583:SER:HB2	1.94	0.68
1:A:314:MET:CE	1:A:317:LEU:HD22	2.24	0.67
1:A:500:LEU:HG	1:A:560:MET:CE	2.24	0.67
1:A:500:LEU:HA	1:A:560:MET:CE	2.24	0.66
1:B:149:MET:HE2	1:B:150:TYR:CE2	2.30	0.66
1:A:59:PRO:O	1:A:62:ARG:HG2	1.97	0.64
1:B:168:TYR:CD1	1:B:193:LEU:HD21	2.33	0.64
1:A:420:LEU:O	1:A:424:GLU:HG3	1.99	0.63
1:A:455:PHE:HE1	1:A:471:PHE:CZ	2.16	0.63
1:A:141:LYS:CE	1:A:200:GLU:OE2	2.47	0.63
1:A:250:LEU:O	1:A:254:ILE:HG12	1.99	0.62
1:A:494:ALA:CA	1:A:497:LEU:HD12	2.30	0.62
1:A:120:GLY:H	4:A:604:GOL:H11	1.63	0.62
1:A:110:LEU:HD23	1:A:172:VAL:HG12	1.81	0.61
1:B:164:ALA:HB1	1:B:167:GLN:HB2	1.81	0.61
1:A:1:MET:HE2	1:A:222:GLU:O	2.01	0.60
1:A:311:LYS:HE3	1:B:63:ASP:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLU:OE1	1:B:227:SER:HB2	2.00	0.60
1:A:500:LEU:HG	1:A:560:MET:HE3	1.83	0.60
1:A:141:LYS:HD3	1:A:142:PRO:HD2	1.83	0.59
1:A:184:ILE:HD11	1:A:206:ARG:HG3	1.84	0.59
1:A:259:TRP:CE3	1:A:264:ALA:HB2	2.36	0.59
1:B:22:LEU:CD2	1:B:100:GLN:HG2	2.32	0.59
1:A:264:ALA:O	1:A:268:ILE:HG12	2.04	0.58
1:B:435:ARG:HG2	1:B:580:PRO:HG3	1.84	0.58
1:B:8:ILE:CD1	1:B:43:LEU:HD21	2.33	0.57
1:B:344:ASN:HB2	1:B:455:PHE:CE1	2.39	0.57
1:A:34:GLU:H	1:A:34:GLU:CD	2.13	0.57
1:B:575:ARG:NE	5:B:708:HOH:O	2.37	0.56
1:A:455:PHE:HE1	1:A:471:PHE:HZ	1.53	0.56
1:A:564:ARG:NH1	5:A:706:HOH:O	2.35	0.56
1:A:314:MET:HA	1:A:314:MET:HE2	1.87	0.56
1:A:256:VAL:HG13	1:A:264:ALA:HB3	1.86	0.56
1:A:274:GLU:CD	1:A:325:ARG:HH22	2.14	0.56
1:B:537:VAL:HG23	1:B:540:ARG:NH2	2.22	0.55
1:B:493:PRO:HB2	1:B:495:GLU:CD	2.32	0.55
1:B:513:LEU:HD11	1:B:521:LYS:HE3	1.88	0.55
1:B:259:TRP:HZ2	1:B:317:LEU:HD22	1.72	0.55
1:B:571:LEU:HB3	1:B:575:ARG:NH2	2.22	0.55
1:B:344:ASN:HB2	1:B:455:PHE:HE1	1.73	0.54
1:A:22:LEU:CD2	1:A:100:GLN:HG2	2.37	0.54
1:B:379:CYS:SG	1:B:420:LEU:HD22	2.48	0.54
1:A:145:GLU:HA	1:A:145:GLU:OE1	2.08	0.54
1:A:513:LEU:HD11	1:A:521:LYS:HE3	1.90	0.54
1:A:22:LEU:HD22	1:A:100:GLN:HG2	1.90	0.54
1:A:122:TRP:N	5:A:701:HOH:O	2.21	0.54
1:A:175:ILE:HD11	1:A:212:ILE:HG13	1.89	0.54
1:A:163:ASP:O	1:A:163:ASP:OD1	2.26	0.54
1:B:1:MET:HG2	1:B:2:TYR:N	2.23	0.54
1:B:352:LEU:HB2	1:B:353:PRO:HD3	1.90	0.54
1:B:274:GLU:OE1	1:B:325:ARG:NH1	2.40	0.53
1:B:455:PHE:O	1:B:459:THR:HG23	2.09	0.53
1:A:503:ALA:HB1	1:A:563:TYR:CD2	2.43	0.53
1:A:437:ASP:OD1	1:A:439:GLU:HG2	2.08	0.53
1:B:232:LEU:HD23	1:B:232:LEU:C	2.34	0.52
1:B:346:ARG:HH21	4:B:604:GOL:H2	1.74	0.52
1:A:519:ASN:O	1:A:523:GLN:HG2	2.09	0.51
1:A:550:THR:HG21	1:A:565:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:O	1:A:199:LYS:HG2	2.11	0.51
1:B:175:ILE:HD11	1:B:212:ILE:HG13	1.93	0.51
1:B:293:GLY:HA3	1:B:317:LEU:HD11	1.92	0.51
1:A:500:LEU:HG	1:A:560:MET:HE2	1.92	0.50
1:A:455:PHE:CE1	1:A:471:PHE:CZ	3.00	0.50
1:B:33:PRO:HG3	1:B:114:PHE:CE1	2.46	0.50
1:A:117:LYS:HE3	1:A:121:LYS:O	2.11	0.50
1:B:494:ALA:HA	1:B:497:LEU:CD1	2.42	0.50
1:B:519:ASN:O	1:B:523:GLN:HG2	2.11	0.50
1:A:559:PHE:CD2	1:A:560:MET:HE2	2.46	0.50
1:A:25:ILE:HG23	5:A:703:HOH:O	2.11	0.49
1:A:120:GLY:H	4:A:604:GOL:C1	2.25	0.49
1:A:284:VAL:HG13	1:A:288:LEU:HD23	1.95	0.49
1:A:455:PHE:CE1	1:A:471:PHE:HZ	2.31	0.49
1:B:158:ASP:O	1:B:162:LEU:HG	2.11	0.49
1:B:94:ILE:HD11	1:B:222:GLU:OE2	2.12	0.49
1:A:337:SER:HA	1:A:468:SER:HB3	1.95	0.49
1:B:344:ASN:HA	1:B:452:PRO:HB3	1.94	0.49
1:A:503:ALA:CB	1:A:560:MET:HE1	2.38	0.49
1:A:54:PHE:HB3	1:A:94:ILE:HG23	1.95	0.48
1:B:67:PHE:O	1:B:85:VAL:HG23	2.13	0.48
1:A:158:ASP:O	1:A:162:LEU:HD13	2.14	0.48
1:A:18:GLN:OE1	1:A:86:THR:O	2.32	0.48
1:A:120:GLY:N	4:A:604:GOL:H11	2.29	0.48
1:A:547:GLN:NE2	5:A:711:HOH:O	2.47	0.48
1:A:211:THR:HA	1:A:215:LYS:HD2	1.94	0.48
1:B:259:TRP:CE3	1:B:264:ALA:HB2	2.49	0.48
1:B:24:ALA:HB2	1:B:68:TYR:HE1	1.77	0.47
1:A:237:ARG:NH1	1:B:35:GLN:HG3	2.23	0.47
1:B:149:MET:HE2	1:B:150:TYR:HE2	1.75	0.47
1:A:65:TYR:HA	1:B:258:GLN:HE22	1.78	0.47
1:B:487:LEU:O	1:B:490:VAL:HG22	2.13	0.47
1:A:559:PHE:HD2	1:A:560:MET:HE2	1.80	0.47
1:B:259:TRP:HZ2	1:B:317:LEU:CD2	2.27	0.47
1:B:122:TRP:HA	1:B:122:TRP:CE3	2.50	0.47
1:B:517:ILE:HD13	1:B:522:ARG:NH2	2.30	0.47
1:B:493:PRO:HB2	1:B:495:GLU:OE2	2.15	0.47
1:B:223:GLU:OE1	1:B:227:SER:CB	2.63	0.46
1:A:67:PHE:O	1:A:85:VAL:HG23	2.15	0.46
1:A:35:GLN:HE21	1:B:237:ARG:NE	2.14	0.46
1:B:72:GLN:O	1:B:112:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:HIS:HD2	5:B:717:HOH:O	1.97	0.46
1:A:437:ASP:HB2	1:A:438:PRO:HD2	1.98	0.46
1:A:370:ARG:NH2	5:A:714:HOH:O	2.48	0.46
1:A:271:LEU:O	1:A:275:MET:HG3	2.16	0.46
1:A:243:THR:HG23	1:B:243:THR:HB	1.98	0.45
1:A:458:LEU:HB3	1:A:512:LEU:HG	1.98	0.45
1:A:327:ALA:CB	1:A:359:HIS:HB2	2.47	0.45
1:B:164:ALA:CB	1:B:167:GLN:HB2	2.47	0.45
1:B:508:PRO:HG2	1:B:563:TYR:CZ	2.52	0.44
1:B:223:GLU:HG3	1:B:224:SER:N	2.31	0.44
1:A:141:LYS:HD3	1:A:141:LYS:HA	1.82	0.44
1:A:363:LEU:HD13	1:A:367:TYR:CD1	2.53	0.44
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.79	0.44
1:A:274:GLU:CD	1:A:329:LEU:HD11	2.43	0.43
1:B:327:ALA:CB	1:B:359:HIS:HB2	2.48	0.43
1:A:295:MET:HE2	1:A:356:TYR:HB2	2.00	0.43
1:A:196:GLU:H	1:A:196:GLU:CD	2.26	0.43
1:A:517:ILE:HD13	1:A:522:ARG:NH1	2.33	0.43
1:B:165:SER:O	1:B:166:GLU:HB2	2.18	0.43
1:A:332:MET:SD	1:A:351:ILE:HD13	2.59	0.43
1:B:362:LYS:HD3	1:B:362:LYS:HA	1.88	0.43
1:A:344:ASN:HA	1:A:452:PRO:HB3	2.01	0.42
1:B:90:GLU:H	1:B:90:GLU:HG2	1.73	0.42
1:A:65:TYR:OH	1:B:307:GLU:HA	2.20	0.42
1:B:252:LEU:HD22	1:B:286:LYS:CD	2.50	0.42
1:B:262:LEU:HD13	1:B:262:LEU:O	2.20	0.42
1:A:487:LEU:O	1:A:490:VAL:HG12	2.20	0.42
1:B:56:LYS:HG3	1:B:222:GLU:HG2	2.02	0.42
1:B:483:THR:OG1	1:B:486:LYS:HG3	2.20	0.41
1:A:242:GLY:O	1:A:243:THR:C	2.63	0.41
1:B:401:THR:O	1:B:405:MET:HG3	2.20	0.41
1:A:409:ASP:OD2	1:A:426:THR:OG1	2.33	0.41
1:B:30:VAL:HG12	1:B:31:TRP:N	2.35	0.41
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.82	0.41
1:B:8:ILE:HD11	1:B:43:LEU:HD21	2.01	0.41
1:A:113:SER:HB3	1:A:133:ARG:HG2	2.01	0.41
1:B:11:LEU:HD12	1:B:20:TYR:CE2	2.54	0.41
1:B:297:SER:HB3	1:B:316:ILE:HG22	2.02	0.41
1:B:277:ARG:NH2	5:B:702:HOH:O	2.51	0.41
1:A:134:LEU:HD11	1:A:152:PHE:HB3	2.02	0.41
1:A:364:THR:OG1	1:A:365:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:MET:HB3	1:A:564:ARG:NH2	2.36	0.41
1:A:259:TRP:CD2	1:A:264:ALA:HB2	2.56	0.40
1:B:158:ASP:N	1:B:158:ASP:OD1	2.54	0.40
1:A:198:ARG:O	1:A:202:ARG:HG3	2.21	0.40
1:B:527:HIS:CD2	5:B:717:HOH:O	2.74	0.40
1:A:120:GLY:CA	4:A:604:GOL:H11	2.52	0.40
1:A:319:LYS:HA	1:A:319:LYS:HD2	1.82	0.40
1:A:531:ALA:HA	1:A:540:ARG:CZ	2.52	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	576/587 (98%)	556 (96%)	20 (4%)	0	100	100
1	B	576/587 (98%)	555 (96%)	21 (4%)	0	100	100
All	All	1152/1174 (98%)	1111 (96%)	41 (4%)	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	509/516 (99%)	509 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	509/516 (99%)	509 (100%)	0	100	100
All	All	1018/1032 (99%)	1018 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	446	GLN
1	A	485	ASN
1	A	527	HIS
1	A	558	GLN
1	B	79	ASN
1	B	258	GLN
1	B	412	GLN
1	B	532	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	604	-	5,5,5	0.80	0	5,5,5	1.27	1 (20%)
4	GOL	A	604	-	5,5,5	0.98	0	5,5,5	1.24	0
3	SO4	B	602	-	4,4,4	0.30	0	6,6,6	0.32	0
3	SO4	B	603	-	4,4,4	0.18	0	6,6,6	0.20	0
3	SO4	A	603	-	4,4,4	0.21	0	6,6,6	0.34	0
3	SO4	A	602	-	4,4,4	0.32	0	6,6,6	0.22	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	604	-	-	2/4/4/4	-
4	GOL	A	604	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	GOL	C3-C2-C1	-2.14	103.94	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	GOL	C1-C2-C3-O3
4	B	604	GOL	C1-C2-C3-O3
4	A	604	GOL	O2-C2-C3-O3
4	B	604	GOL	O2-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	GOL	5	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	580/587 (98%)	0.67	50 (8%)	16 17	37, 53, 79, 122	0
1	B	580/587 (98%)	0.62	34 (5%)	28 30	37, 52, 78, 104	0
All	All	1160/1174 (98%)	0.64	84 (7%)	21 23	37, 53, 79, 122	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	PHE	7.1
1	A	262	LEU	6.8
1	B	262	LEU	6.2
1	A	29	PHE	5.4
1	B	144	LEU	5.3
1	A	25	ILE	4.6
1	A	144	LEU	4.1
1	B	261	SER	3.9
1	B	240	SER	3.9
1	A	581	ALA	3.8
1	B	122	TRP	3.8
1	B	581	ALA	3.7
1	A	464	GLY	3.6
1	A	4	ALA	3.5
1	A	244	THR	3.5
1	B	25	ILE	3.5
1	A	146	THR	3.4
1	A	240	SER	3.4
1	B	242	GLY	3.4
1	B	489	LYS	3.4
1	B	464	GLY	3.4
1	A	243	THR	3.3
1	B	87	GLN	3.3
1	B	243	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	583	SER	3.1
1	A	497	LEU	3.1
1	B	488	ALA	3.0
1	A	1	MET	3.0
1	A	488	ALA	3.0
1	B	83	GLU	3.0
1	A	87	GLN	2.9
1	A	487	LEU	2.9
1	A	492	VAL	2.9
1	A	81	HIS	2.9
1	A	483	THR	2.9
1	A	245	LEU	2.8
1	B	244	THR	2.8
1	A	582	SER	2.8
1	A	163	ASP	2.8
1	A	261	SER	2.8
1	B	1	MET	2.8
1	A	24	ALA	2.7
1	B	580	PRO	2.6
1	A	583	SER	2.6
1	B	81	HIS	2.6
1	B	146	THR	2.6
1	A	142	PRO	2.6
1	B	263	ASP	2.6
1	A	83	GLU	2.6
1	A	575	ARG	2.6
1	A	101	GLN	2.5
1	A	147	GLY	2.5
1	A	164	ALA	2.5
1	A	485	ASN	2.5
1	A	166	GLU	2.5
1	B	124	SER	2.5
1	B	241	GLY	2.4
1	A	254	ILE	2.4
1	A	489	LYS	2.4
1	B	491	GLY	2.4
1	A	256	VAL	2.4
1	A	242	GLY	2.3
1	B	455	PHE	2.3
1	A	550	THR	2.3
1	B	160	ALA	2.3
1	B	226	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	364	THR	2.3
1	A	494	ALA	2.3
1	B	151	ASP	2.3
1	A	517	ILE	2.2
1	B	149	MET	2.2
1	B	2	TYR	2.2
1	A	84	ASN	2.2
1	A	122	TRP	2.2
1	A	580	PRO	2.1
1	A	484	ARG	2.1
1	A	498	ASP	2.1
1	B	494	ALA	2.1
1	A	165	SER	2.1
1	A	200	GLU	2.1
1	A	145	GLU	2.0
1	B	4	ALA	2.1
1	B	195	SER	2.0
1	A	162	LEU	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
3	SO4	A	602	5/5	0.87	0.09	72,76,84,86	0
4	GOL	A	604	6/6	0.88	0.11	56,67,74,78	0
3	SO4	B	602	5/5	0.92	0.08	64,73,73,78	0
4	GOL	B	604	6/6	0.92	0.10	49,68,80,83	0
2	CL	A	601	1/1	0.94	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	601	1/1	0.95	0.10	69,69,69,69	0
3	SO4	A	603	5/5	0.98	0.08	48,52,53,58	0
3	SO4	B	603	5/5	0.98	0.06	48,48,52,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.