



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 11:14 AM UTC

PDB ID : 5JYK / pdb_00005jyk
Title : Deg9 crystal under 289K
Authors : Ouyang, M.; Zhang, L.X.
Deposited on : 2016-05-14
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

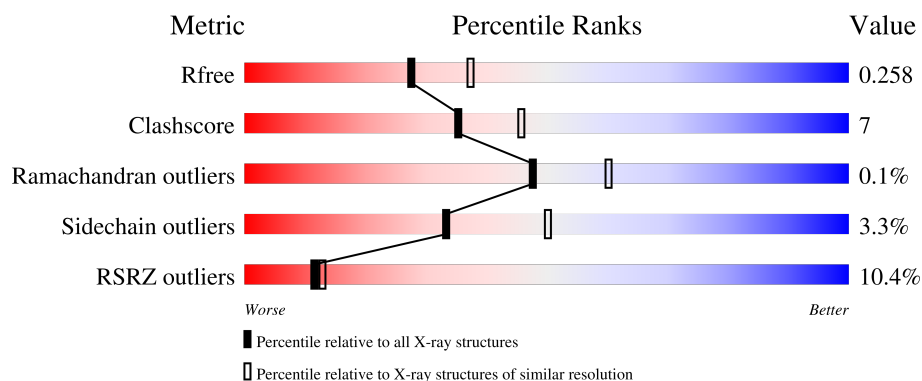
1 Overall quality at a glance

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)
Sidechain outliers	187428	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	566	% 72% 9% • 18%
1	B	566	15% 58% 13% • 27%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7294 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 Protease Do-like 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	6	0
			3611	2311	602	682	16			
1	B	412	Total	C	N	O	S	0	7	0
			3176	2031	535	598	12			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9FL12
A	28	GLY	-	expression tag	UNP Q9FL12
A	29	SER	-	expression tag	UNP Q9FL12
A	30	SER	-	expression tag	UNP Q9FL12
A	31	HIS	-	expression tag	UNP Q9FL12
A	32	HIS	-	expression tag	UNP Q9FL12
A	33	HIS	-	expression tag	UNP Q9FL12
A	34	HIS	-	expression tag	UNP Q9FL12
A	35	HIS	-	expression tag	UNP Q9FL12
A	36	HIS	-	expression tag	UNP Q9FL12
A	37	SER	-	expression tag	UNP Q9FL12
A	38	SER	-	expression tag	UNP Q9FL12
A	39	GLY	-	expression tag	UNP Q9FL12
A	40	LEU	-	expression tag	UNP Q9FL12
A	41	VAL	-	expression tag	UNP Q9FL12
A	42	PRO	-	expression tag	UNP Q9FL12
A	43	ARG	-	expression tag	UNP Q9FL12
A	44	GLY	-	expression tag	UNP Q9FL12
A	45	SER	-	expression tag	UNP Q9FL12
A	46	HIS	-	expression tag	UNP Q9FL12
A	47	MET	-	expression tag	UNP Q9FL12
A	48	ALA	-	expression tag	UNP Q9FL12
A	49	SER	-	expression tag	UNP Q9FL12
A	50	MET	-	expression tag	UNP Q9FL12
A	51	THR	-	expression tag	UNP Q9FL12

Continued on next page...

Continued from previous page...

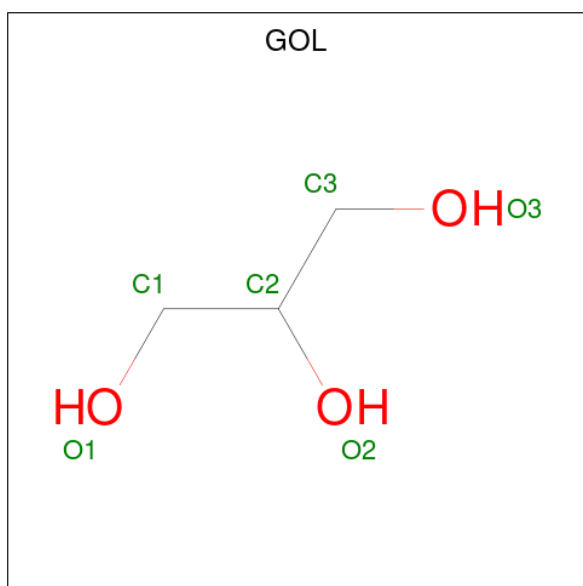
Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	expression tag	UNP Q9FL12
A	53	GLY	-	expression tag	UNP Q9FL12
A	54	GLN	-	expression tag	UNP Q9FL12
A	55	GLN	-	expression tag	UNP Q9FL12
A	56	MET	-	expression tag	UNP Q9FL12
A	57	GLY	-	expression tag	UNP Q9FL12
A	58	ARG	-	expression tag	UNP Q9FL12
A	59	GLY	-	expression tag	UNP Q9FL12
A	60	SER	-	expression tag	UNP Q9FL12
A	61	GLU	-	expression tag	UNP Q9FL12
A	62	PHE	-	expression tag	UNP Q9FL12
A	63	GLU	-	expression tag	UNP Q9FL12
A	64	LEU	-	expression tag	UNP Q9FL12
B	27	MET	-	expression tag	UNP Q9FL12
B	28	GLY	-	expression tag	UNP Q9FL12
B	29	SER	-	expression tag	UNP Q9FL12
B	30	SER	-	expression tag	UNP Q9FL12
B	31	HIS	-	expression tag	UNP Q9FL12
B	32	HIS	-	expression tag	UNP Q9FL12
B	33	HIS	-	expression tag	UNP Q9FL12
B	34	HIS	-	expression tag	UNP Q9FL12
B	35	HIS	-	expression tag	UNP Q9FL12
B	36	HIS	-	expression tag	UNP Q9FL12
B	37	SER	-	expression tag	UNP Q9FL12
B	38	SER	-	expression tag	UNP Q9FL12
B	39	GLY	-	expression tag	UNP Q9FL12
B	40	LEU	-	expression tag	UNP Q9FL12
B	41	VAL	-	expression tag	UNP Q9FL12
B	42	PRO	-	expression tag	UNP Q9FL12
B	43	ARG	-	expression tag	UNP Q9FL12
B	44	GLY	-	expression tag	UNP Q9FL12
B	45	SER	-	expression tag	UNP Q9FL12
B	46	HIS	-	expression tag	UNP Q9FL12
B	47	MET	-	expression tag	UNP Q9FL12
B	48	ALA	-	expression tag	UNP Q9FL12
B	49	SER	-	expression tag	UNP Q9FL12
B	50	MET	-	expression tag	UNP Q9FL12
B	51	THR	-	expression tag	UNP Q9FL12
B	52	GLY	-	expression tag	UNP Q9FL12
B	53	GLY	-	expression tag	UNP Q9FL12
B	54	GLN	-	expression tag	UNP Q9FL12
B	55	GLN	-	expression tag	UNP Q9FL12

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	56	MET	-	expression tag	UNP Q9FL12
B	57	GLY	-	expression tag	UNP Q9FL12
B	58	ARG	-	expression tag	UNP Q9FL12
B	59	GLY	-	expression tag	UNP Q9FL12
B	60	SER	-	expression tag	UNP Q9FL12
B	61	GLU	-	expression tag	UNP Q9FL12
B	62	PHE	-	expression tag	UNP Q9FL12
B	63	GLU	-	expression tag	UNP Q9FL12
B	64	LEU	-	expression tag	UNP Q9FL12

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

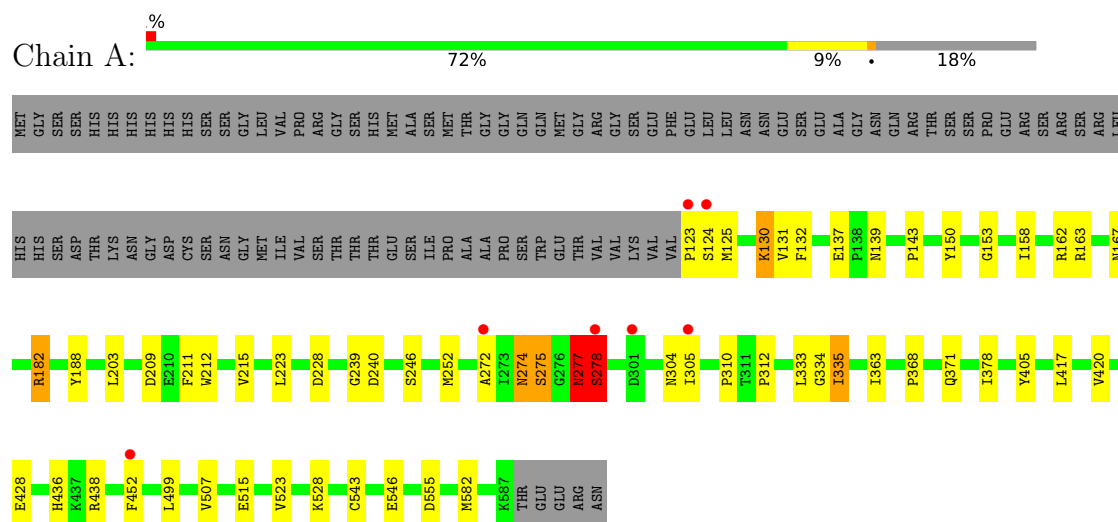
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	277	Total	O	0	0
			277	277		
3	B	224	Total	O	0	0
			224	224		

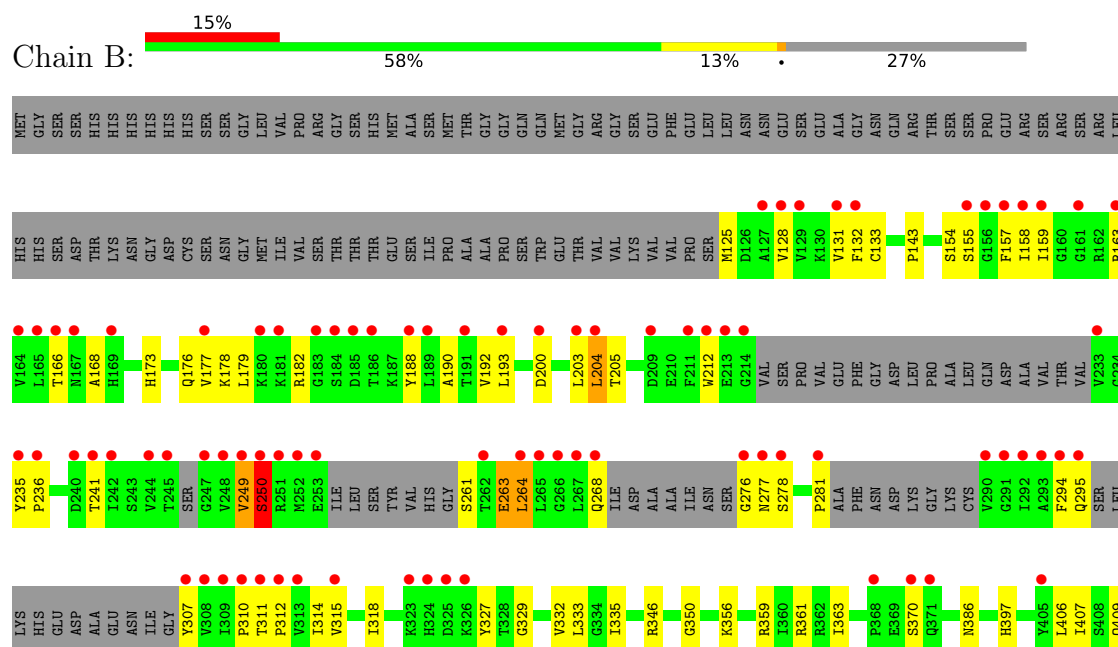
3 Residue-property plots [i](#)

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: Protease Do-like 9



• Molecule 1: Protease Do-like 9





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	132.16Å 132.16Å 154.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.66 – 2.30 35.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	84.5 (35.66-2.30) 84.5 (35.66-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.76 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.198 , 0.256 0.201 , 0.258	Depositor DCC
R_{free} test set	2549 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.017 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7294	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	0.41	2/3696 (0.1%)	0.55	2/5018 (0.0%)
1	B	0.35	0/3244	0.58	0/4396
All	All	0.38	2/6940 (0.0%)	0.57	2/9414 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	SER	C-N	-8.29	1.20	1.33
1	A	274	ASN	CA-C	-5.53	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ASN	CB-CA-C	-5.48	98.44	110.67
1	A	277	ASN	N-CA-C	5.22	119.36	112.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	249	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	263	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3611	0	3567	44	0
1	B	3176	0	3058	57	0
2	A	6	0	8	3	0
3	A	277	0	0	8	0
3	B	224	0	0	23	0
All	All	7294	0	6633	100	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 7.

All (100) 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:274:ASN:ND2	1:A:275:SER:O	1.88	1.06
1:B:178:LYS:O	3:B:601:HOH:O	1.88	0.91
1:A:272:ALA:HB2	1:A:304:ASN:HA	1.53	0.90
1:B:178:LYS:O	3:B:602:HOH:O	1.96	0.81
1:B:192:VAL:HG22	1:B:204:LEU:HD12	1.65	0.78
1:B:386[B]:ASN:OD1	3:B:603:HOH:O	2.02	0.76
1:B:176:GLN:O	3:B:604:HOH:O	2.04	0.74
1:A:167:ASN:OD1	1:A:278:SER:OG	2.05	0.73
1:B:132:PHE:O	3:B:602:HOH:O	2.05	0.72
1:B:177:VAL:HG13	1:B:190:ALA:HB3	1.73	0.71
1:B:264:LEU:HD11	1:B:310:PRO:HG2	1.73	0.71
1:A:130:LYS:NZ	1:A:239:GLY:O	2.24	0.70
1:A:163[A]:ARG:NH2	3:A:708:HOH:O	2.24	0.69
1:A:274:ASN:H	1:A:277:ASN:HD21	1.40	0.69
1:B:261:SER:N	3:B:612:HOH:O	2.26	0.68
1:B:350:GLY:HA3	1:B:424:LYS:HG3	1.76	0.67
1:A:123:PRO:HA	1:A:125:MET:H	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:OE1	3:A:701:HOH:O	2.15	0.64
1:B:549:LYS:NZ	3:B:613:HOH:O	2.29	0.64
1:B:157:PHE:O	3:B:605:HOH:O	2.16	0.62
1:B:333:LEU:HB2	1:B:407:ILE:HD13	1.81	0.62
1:B:158:ILE:HG23	1:B:212:TRP:HZ3	1.64	0.62
1:B:179:LEU:N	1:B:188:TYR:O	2.29	0.61
1:A:228:ASP:OD2	3:A:702:HOH:O	2.15	0.60
1:A:130:LYS:HD3	1:A:132:PHE:CZ	2.37	0.58
1:B:397:HIS:O	3:B:606:HOH:O	2.17	0.58
1:B:310:PRO:O	1:B:314:ILE:HG13	2.05	0.57
1:B:327:TYR:CZ	1:B:329:GLY:HA2	2.39	0.57
1:B:332:VAL:HG21	1:B:436:HIS:HB2	1.87	0.56
1:B:249:VAL:O	1:B:250:SER:HB2	2.05	0.56
1:B:182[B]:ARG:NH1	3:B:621:HOH:O	2.38	0.56
1:A:274:ASN:O	1:A:277:ASN:ND2	2.39	0.56
1:B:363:ILE:HG21	1:B:370:SER:HA	1.88	0.55
1:A:277:ASN:HD22	1:A:277:ASN:H	1.55	0.55
1:A:368:PRO:HA	1:A:371:GLN:HG2	1.89	0.54
1:A:310:PRO:HB2	1:A:312:PRO:HD2	1.89	0.54
1:B:235:TYR:O	1:B:277:ASN:HB2	2.06	0.54
1:A:162:ARG:HG3	1:A:212:TRP:CE2	2.43	0.54
1:A:333:LEU:H	2:A:601:GOL:H11	1.73	0.53
1:A:507:VAL:HG22	1:A:515:GLU:HG2	1.90	0.53
1:B:268:GLN:O	3:B:607:HOH:O	2.19	0.52
1:B:132:PHE:O	3:B:604:HOH:O	2.19	0.52
1:A:123:PRO:HA	1:A:125:MET:N	2.24	0.52
1:A:277:ASN:HD22	1:A:277:ASN:N	2.07	0.51
1:A:158:ILE:HG23	1:A:212:TRP:HZ3	1.75	0.51
1:B:278:SER:OG	1:B:294:PHE:HA	2.11	0.51
1:A:335:ILE:H	2:A:601:GOL:H12	1.77	0.50
1:B:143:PRO:HB3	1:B:449:PRO:HB2	1.93	0.50
1:B:536:LEU:HA	1:B:539:MET:HE3	1.94	0.50
1:A:543:CYS:O	3:A:703:HOH:O	2.19	0.50
1:B:278:SER:HB2	1:B:295:GLN:H	1.77	0.49
1:B:236:PRO:HD2	1:B:241:THR:O	2.11	0.49
1:B:335:ILE:HG22	1:B:363:ILE:HG12	1.95	0.49
1:A:378:ILE:O	1:A:420:VAL:HA	2.13	0.49
1:B:159:ILE:HG12	3:B:605:HOH:O	2.13	0.49
1:B:166:THR:OG1	3:B:608:HOH:O	2.19	0.49
1:B:311:THR:O	1:B:315:VAL:HG22	2.13	0.48
1:A:555:ASP:O	1:B:361:ARG:HG2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155[A]:SER:OG	1:B:277:ASN:HB3	2.14	0.48
1:B:346[B]:ARG:NH2	3:B:627:HOH:O	2.45	0.48
1:A:223:LEU:HD11	1:A:252[A]:MET:HE1	1.96	0.48
1:B:193:LEU:HD11	1:B:205:THR:HB	1.97	0.47
1:B:311:THR:N	1:B:312:PRO:HD2	2.29	0.47
1:B:356[B]:LYS:NZ	3:B:629:HOH:O	2.48	0.47
1:A:182:ARG:H	1:A:182:ARG:HG3	1.48	0.47
1:A:209:ASP:OD1	3:A:704:HOH:O	2.20	0.47
1:B:276:GLY:HA2	1:B:277:ASN:HA	1.64	0.46
1:B:173:HIS:ND1	3:B:611:HOH:O	2.24	0.46
1:B:168:ALA:HB3	1:B:200:ASP:HA	1.98	0.46
1:A:240:ASP:HB2	3:A:721:HOH:O	2.15	0.46
1:A:436:HIS:CE1	1:A:438:ARG:HG3	2.51	0.45
1:B:159:ILE:HG13	1:B:163:ARG:HB2	1.98	0.45
1:B:193:LEU:N	1:B:203:LEU:O	2.43	0.45
1:A:131:VAL:O	1:A:153:GLY:HA2	2.17	0.45
1:A:334:GLY:H	2:A:601:GOL:C1	2.29	0.45
1:A:163[A]:ARG:HG2	1:A:203:LEU:HD11	1.99	0.45
1:B:131:VAL:HB	1:B:154:SER:HG	1.81	0.45
1:B:133:CYS:HA	3:B:604:HOH:O	2.17	0.45
1:A:274:ASN:O	1:A:275:SER:C	2.60	0.44
1:A:335:ILE:HG22	1:A:363:ILE:HG12	1.99	0.44
1:B:157:PHE:CG	1:B:281:PRO:HG3	2.53	0.44
1:B:131:VAL:HB	1:B:154:SER:OG	2.18	0.43
1:A:452:PHE:HD1	1:A:582:MET:HE2	1.82	0.43
1:A:212:TRP:O	1:A:215:VAL:HG22	2.19	0.43
1:B:278:SER:HB3	3:B:771:HOH:O	2.18	0.43
1:A:528:LYS:NZ	3:A:720:HOH:O	2.38	0.42
1:A:137:GLU:OE2	1:A:150:TYR:OH	2.26	0.42
1:B:498:GLN:OE1	1:B:532:ASN:HB2	2.19	0.41
1:B:132:PHE:HD1	3:B:601:HOH:O	2.02	0.41
1:A:274:ASN:ND2	1:A:274:ASN:C	2.78	0.41
1:A:277:ASN:ND2	1:A:277:ASN:H	2.18	0.41
1:B:314:ILE:O	1:B:318:ILE:HG12	2.21	0.41
1:A:124:SER:HB2	3:A:884:HOH:O	2.20	0.41
1:B:356[A]:LYS:O	3:B:603:HOH:O	2.18	0.41
1:A:417:LEU:HD22	1:A:428:GLU:HG2	2.03	0.40
1:B:359:ARG:NH2	3:B:625:HOH:O	2.43	0.40
1:B:128:VAL:HG22	1:B:281:PRO:HG2	2.03	0.40
1:A:139:ASN:O	1:A:143:PRO:HA	2.22	0.40
1:A:188:TYR:CD2	1:A:211:PHE:HB2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:HD3	3:B:675:HOH:O	2.20	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	469/566 (83%)	460 (98%)	9 (2%)	0	100	100
1	B	405/566 (72%)	384 (95%)	20 (5%)	1 (0%)	43	55
All	All	874/1132 (77%)	844 (97%)	29 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	250	SER

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	391/490 (80%)	380 (97%)	11 (3%)	38	56
1	B	329/490 (67%)	317 (96%)	12 (4%)	31	47
All	All	720/980 (74%)	697 (97%)	23 (3%)	33	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LYS
1	A	182	ARG
1	A	246	SER
1	A	275	SER
1	A	277	ASN
1	A	278	SER
1	A	305	ILE
1	A	335	ILE
1	A	405	TYR
1	A	499	LEU
1	A	523	VAL
1	B	125	MET
1	B	204	LEU
1	B	250	SER
1	B	263	GLU
1	B	264	LEU
1	B	307	TYR
1	B	406	LEU
1	B	409	GLN
1	B	435	ILE
1	B	494	SER
1	B	512	ILE
1	B	516	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	304	ASN
1	A	409	GLN
1	B	493	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

1 ligand is 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	$\# Z > 2$
2	GOL	A	601	-	5,5,5	0.49	0	5,5,5	0.24	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
2	GOL	A	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	3	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	465/566 (82%)	-0.11	7 (1%) 72 73	8, 27, 47, 72	6 (1%)
1	B	412/566 (72%)	0.64	84 (20%) 3 3	9, 32, 71, 86	10 (2%)
All	All	877/1132 (77%)	0.24	91 (10%) 11 13	8, 29, 65, 86	16 (1%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	GLY	6.5
1	B	310	PRO	6.5
1	B	295	GLN	6.4
1	B	128	VAL	6.2
1	B	129	VAL	6.0
1	B	308	VAL	5.9
1	B	236	PRO	5.7
1	B	278	SER	5.4
1	B	158	ILE	5.0
1	B	155[A]	SER	4.9
1	B	244	VAL	4.8
1	B	164	VAL	4.8
1	B	281	PRO	4.4
1	B	127	ALA	4.3
1	B	264	LEU	4.3
1	B	309	ILE	4.1
1	A	123	PRO	4.1
1	B	167	ASN	4.0
1	B	204	LEU	3.9
1	B	132	PHE	3.9
1	B	166	THR	3.9
1	B	249	VAL	3.8
1	B	188	TYR	3.8
1	B	266	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	268	GLN	3.7
1	B	262	THR	3.7
1	B	165	LEU	3.6
1	B	235	TYR	3.5
1	A	301	ASP	3.5
1	B	245	THR	3.5
1	B	267	LEU	3.5
1	B	241	THR	3.5
1	B	277	ASN	3.4
1	B	233	VAL	3.4
1	B	253	GLU	3.3
1	B	324	HIS	3.3
1	B	307	TYR	3.2
1	B	157	PHE	3.1
1	B	156	GLY	3.1
1	B	185	ASP	3.1
1	B	312	PRO	3.1
1	A	278	SER	3.1
1	B	290	VAL	3.1
1	B	252	MET	3.1
1	B	250	SER	3.0
1	B	265	LEU	3.0
1	B	248	VAL	2.9
1	B	323	LYS	2.8
1	B	211	PHE	2.8
1	B	313	VAL	2.7
1	B	247	GLY	2.7
1	B	131	VAL	2.7
1	B	292	ILE	2.7
1	A	124	SER	2.6
1	B	368	PRO	2.6
1	A	272	ALA	2.5
1	B	184	SER	2.5
1	B	181	LYS	2.5
1	B	177	VAL	2.5
1	B	213	GLU	2.5
1	B	588	THR	2.4
1	B	214	GLY	2.4
1	B	159	ILE	2.4
1	B	293	ALA	2.4
1	B	240	ASP	2.4
1	B	193	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	163	ARG	2.4
1	B	251	ARG	2.3
1	B	180	LYS	2.3
1	B	326	LYS	2.3
1	B	242	ILE	2.3
1	B	186	THR	2.3
1	B	169	HIS	2.3
1	B	212	TRP	2.2
1	B	294	PHE	2.2
1	B	371	GLN	2.2
1	B	311	THR	2.2
1	B	203	LEU	2.2
1	B	291	GLY	2.2
1	B	370	SER	2.1
1	B	405	TYR	2.1
1	B	200	ASP	2.1
1	B	161	GLY	2.1
1	B	191	THR	2.1
1	B	209	ASP	2.1
1	B	315	VAL	2.1
1	B	325	ASP	2.1
1	B	183	GLY	2.1
1	A	452	PHE	2.0
1	B	189	LEU	2.0
1	A	305	ILE	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	GOL	A	601	6/6	0.88	0.13	23,34,39,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.