



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:53 PM UTC

PDB ID : 8THP / pdb_00008thp
Title : PorX phosphatase null mutant (T271V)
Authors : Saran, A.; Zeytuni, N.
Deposited on : 2023-07-17
Resolution : 2.60 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

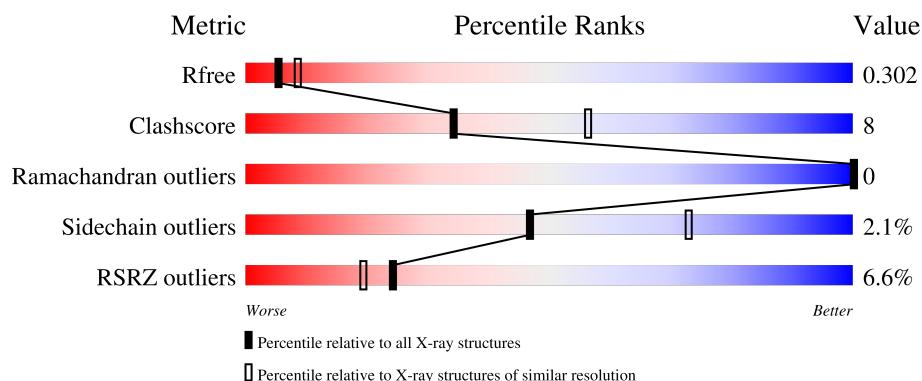
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	520	12% 73% 21% 5%
1	B	520	% 78% 19% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8325 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 Response regulator receiver protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	10	2	0
			4072	2647	642	769	14			
1	B	511	Total	C	N	O	S	0	0	0
			4199	2728	664	792	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A5FFU4
A	-1	SER	-	expression tag	UNP A5FFU4
A	0	HIS	-	expression tag	UNP A5FFU4
A	271	VAL	THR	engineered mutation	UNP A5FFU4
B	-2	GLY	-	expression tag	UNP A5FFU4
B	-1	SER	-	expression tag	UNP A5FFU4
B	0	HIS	-	expression tag	UNP A5FFU4
B	271	VAL	THR	engineered mutation	UNP A5FFU4

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- 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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total	O	0	0
			22	22		
4	B	22	Total	O	0	0
			22	22		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.09Å 96.98Å 130.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 2.60 45.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.95-2.60) 99.7 (45.95-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.250 , 0.305 0.252 , 0.302	Depositor DCC
R_{free} test set	1800 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8325	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CA, 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	0.52	2/4161 (0.0%)	0.90	1/5612 (0.0%)
1	B	0.54	0/4290	0.89	1/5791 (0.0%)
All	All	0.53	2/8451 (0.0%)	0.90	2/11403 (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	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	LYS	CA-CB	-5.32	1.43	1.54
1	A	456	GLU	C-N	-5.27	1.26	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	477	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	242	ASP	CA-CB-CG	5.29	117.89	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	ARG	Sidechain
1	B	196	ARG	Sidechain

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	4072	0	4080	67	0
1	B	4199	0	4222	60	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	8	0	0
4	A	22	0	0	4	0
4	B	22	0	0	6	0
All	All	8325	0	8310	125	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 8.

All (125) 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:276:ASN:HB3	1:A:287:MET:HE1	1.45	0.99
1:B:129:THR:HB	1:B:170:ILE:HD11	1.63	0.79
1:B:283:MET:HE3	1:B:284:PRO:HD2	1.66	0.78
1:A:360:ASP:O	4:A:701:HOH:O	2.04	0.75
1:A:229:LYS:HE3	1:A:516:PRO:HD2	1.69	0.72
1:A:452:TYR:HB3	1:A:473:PHE:HB2	1.74	0.69
1:B:379:ASP:O	1:B:383:ARG:HG3	1.95	0.67
1:A:283:MET:HE3	1:A:284:PRO:HD2	1.78	0.65
1:B:272:GLN:HG3	1:B:304:LYS:HB3	1.79	0.63
1:B:380:LYS:HA	1:B:383:ARG:HE	1.63	0.62
1:A:364:HIS:HB2	4:A:701:HOH:O	2.00	0.61
1:A:333:TYR:N	4:A:703:HOH:O	2.33	0.61
1:B:10:ASP:OD2	1:B:104:LYS:NZ	2.32	0.61
1:A:129:THR:HG22	1:A:167:LEU:HD23	1.82	0.60
1:B:13:ILE:HD12	1:B:16:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD13	1:A:99:ALA:HB3	1.85	0.58
1:A:167:LEU:HD22	1:A:170:ILE:HD13	1.85	0.58
1:B:284:PRO:HA	1:B:287:MET:HE3	1.85	0.57
1:A:167:LEU:O	1:A:170:ILE:HG12	2.05	0.57
1:A:12:GLU:HB3	1:A:15:LEU:HD13	1.87	0.56
1:A:17:LYS:N	1:A:18:PRO:HD2	2.19	0.56
1:B:22:PHE:O	1:B:25:LYS:HG2	2.06	0.56
1:B:217:LYS:HG3	1:B:319:LEU:HD21	1.88	0.56
1:B:20:ILE:O	1:B:24:GLU:HG2	2.04	0.56
1:A:436:LEU:HD23	1:A:479:PHE:HB2	1.87	0.55
1:A:170:ILE:HB	4:A:708:HOH:O	2.06	0.55
1:B:69:MET:SD	1:B:78:MET:HE1	2.47	0.55
1:A:343:PHE:HB3	1:A:401:GLN:HG2	1.89	0.55
1:A:456:GLU:O	1:A:459:THR:HG22	2.06	0.55
1:B:236:ILE:HD11	1:B:411:LEU:HD11	1.89	0.54
1:B:248:GLU:O	1:B:251:ILE:HG22	2.07	0.54
1:B:22:PHE:CD2	1:B:108:PRO:HB2	2.42	0.54
1:B:165:LEU:O	1:B:168:GLU:HG2	2.08	0.54
1:A:167:LEU:HD12	1:A:179:LEU:HD22	1.90	0.53
1:A:460:ILE:HG13	1:A:462:LEU:HG	1.90	0.52
1:A:490:VAL:O	1:A:494:LYS:HB2	2.09	0.52
1:A:11:ASP:HB3	1:A:58:PRO:HD2	1.92	0.52
1:A:83:LYS:HG2	1:A:104:LYS:HB2	1.91	0.52
1:A:211:GLN:HA	1:A:264:PHE:O	2.09	0.52
1:A:279:PHE:HD1	1:A:312:LEU:HD13	1.74	0.52
1:B:216:PHE:CE2	1:B:312:LEU:HD11	2.45	0.52
1:B:211:GLN:HA	1:B:264:PHE:O	2.10	0.52
1:B:86:GLU:O	1:B:89:ILE:HG22	2.10	0.51
1:A:144:LEU:O	1:A:147:VAL:HG22	2.10	0.51
1:A:69:MET:HB3	1:A:78:MET:HE1	1.93	0.51
1:A:420:VAL:HG22	1:A:496:THR:O	2.11	0.50
1:B:454:VAL:HG21	1:B:460:ILE:HD13	1.93	0.50
1:A:220:VAL:HG12	1:A:224:ILE:HD11	1.94	0.50
1:B:147:VAL:HG11	1:B:153:TRP:CD2	2.47	0.49
1:A:60:MET:HE1	1:A:68:GLU:HG3	1.94	0.49
1:A:84:SER:HB3	1:A:89:ILE:HD12	1.95	0.48
1:B:17:LYS:N	1:B:18:PRO:HD2	2.28	0.48
1:B:362:LEU:HD11	1:B:385:LEU:HD21	1.95	0.48
1:A:248:GLU:O	1:A:251:ILE:HG22	2.13	0.48
1:A:402:ALA:HB1	1:A:407:PHE:HB2	1.96	0.48
1:B:151:GLU:O	1:B:155:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LYS:HG3	1:A:348:GLY:N	2.29	0.47
1:B:273:TYR:OH	1:B:298:ASP:OD1	2.31	0.47
1:B:490:VAL:O	1:B:494:LYS:HB2	2.15	0.47
1:A:294:TYR:CE2	1:A:310:GLU:HB3	2.49	0.47
1:A:285:LEU:HG	1:A:289:LYS:HE2	1.96	0.47
1:A:479:PHE:HE2	1:A:490:VAL:HA	1.80	0.46
1:B:65:THR:HG22	1:B:69:MET:HE3	1.96	0.46
1:A:267:LEU:HD21	1:A:502:ILE:HG12	1.97	0.46
1:B:144:LEU:HD11	1:B:186:ALA:HA	1.96	0.46
1:B:359:VAL:N	4:B:701:HOH:O	2.21	0.46
1:B:417:THR:HG21	4:B:715:HOH:O	2.16	0.46
1:A:195:GLU:HG3	1:A:452:TYR:CD1	2.51	0.46
1:A:220:VAL:O	1:A:224:ILE:HG13	2.16	0.46
1:B:11:ASP:HB3	1:B:58:PRO:HD2	1.98	0.46
1:B:35:ASN:HD21	1:B:59:GLY:HA3	1.81	0.46
1:B:255:TYR:HB3	1:B:514:PHE:HB3	1.97	0.46
1:B:221:VAL:HG21	1:B:319:LEU:HD22	1.98	0.45
1:B:12:GLU:HB3	1:B:15:LEU:HD13	1.97	0.45
1:A:240:ARG:HB2	1:A:243:GLN:HG3	1.98	0.45
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.75	0.45
1:A:267:LEU:HB3	1:A:473:PHE:CE1	2.52	0.45
1:A:225:LYS:HE2	1:A:321:LEU:HD11	1.99	0.45
1:B:305:ASN:N	4:B:702:HOH:O	2.23	0.44
1:B:438:TYR:HA	1:B:472:ILE:O	2.18	0.44
1:A:142:MET:O	1:A:146:MET:HG2	2.18	0.44
1:A:43:PHE:CE2	1:A:73:LYS:HB2	2.53	0.44
1:A:367:THR:HG23	1:A:496:THR:HG21	1.98	0.44
1:B:195:GLU:HG3	1:B:452:TYR:CD1	2.53	0.44
1:A:240:ARG:H	1:A:243:GLN:HE21	1.65	0.43
1:B:499:HIS:HA	1:B:506:GLU:OE2	2.18	0.43
1:B:79:ILE:HD13	1:B:114:SER:HB3	2.00	0.43
1:B:324:LYS:HG3	1:B:349:ASN:OD1	2.18	0.43
1:A:279:PHE:O	1:A:312:LEU:HA	2.18	0.43
1:B:425:LYS:HG2	1:B:486:TYR:CE1	2.54	0.43
1:B:460:ILE:HD11	1:B:462:LEU:HD12	2.01	0.43
1:A:242:ASP:HB2	1:A:383:ARG:HD3	2.01	0.43
1:B:17:LYS:N	1:B:18:PRO:CD	2.81	0.42
1:A:65:THR:HG22	1:A:69:MET:HE3	2.01	0.42
1:B:164:GLU:HG2	4:B:706:HOH:O	2.18	0.42
1:A:371:VAL:HA	1:B:358:PHE:HE1	1.84	0.42
1:A:212:SER:H	1:A:266:ILE:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:HE2	1:A:408:LYS:HB2	2.02	0.42
1:A:435:ASN:OD1	1:A:436:LEU:N	2.53	0.42
1:A:7:LEU:HB3	1:A:51:VAL:HG22	2.02	0.42
1:A:90:MET:HE1	1:B:109:ASN:HB3	2.00	0.42
1:B:221:VAL:N	1:B:222:PRO:CD	2.83	0.42
1:A:136:GLU:OE2	1:A:139:LYS:HD2	2.18	0.42
1:A:144:LEU:HD13	1:A:156:LEU:CD2	2.50	0.41
1:A:257:LEU:HD21	1:A:260:GLU:HB2	2.02	0.41
1:A:425:LYS:HG2	1:A:486:TYR:CE1	2.55	0.41
1:B:242:ASP:C	4:B:707:HOH:O	2.63	0.41
1:B:53:LEU:HD11	1:B:78:MET:HE3	2.02	0.41
1:A:104:LYS:HA	1:A:106:VAL:HG23	2.01	0.41
1:B:167:LEU:HD12	1:B:179:LEU:HD22	2.02	0.41
1:A:25:LYS:HA	1:A:25:LYS:HD3	1.99	0.41
1:B:267:LEU:HD23	1:B:269:THR:HG23	2.03	0.41
1:B:383:ARG:HD3	4:B:707:HOH:O	2.20	0.41
1:B:440:THR:HB	1:B:471:PHE:CE1	2.55	0.41
1:A:317:LYS:HG2	1:A:318:ARG:N	2.35	0.40
1:A:479:PHE:CE2	1:A:490:VAL:HA	2.56	0.40
1:B:78:MET:HE3	1:B:78:MET:HB3	1.91	0.40
1:B:219:LEU:C	1:B:222:PRO:HD2	2.45	0.40
1:B:246:SER:O	1:B:387:LEU:HD13	2.20	0.40
1:A:265:SER:HB2	1:A:509:ILE:HD13	2.03	0.40
1:A:315:GLN:HG3	1:A:319:LEU:HD23	2.03	0.40
1:A:341:GLU:O	1:A:344:LYS:HE2	2.21	0.40
1:B:22:PHE:HA	1:B:25:LYS:NZ	2.37	0.40
1:B:172:ASP:O	1:B:176:ILE:HG12	2.22	0.40
1:B:221:VAL:HG21	1:B:319:LEU:CD2	2.51	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	484/520 (93%)	474 (98%)	10 (2%)	0	100	100
1	B	507/520 (98%)	498 (98%)	9 (2%)	0	100	100
All	All	991/1040 (95%)	972 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	453/475 (95%)	447 (99%)	6 (1%)	61	82
1	B	467/475 (98%)	454 (97%)	13 (3%)	38	66
All	All	920/950 (97%)	901 (98%)	19 (2%)	47	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	TYR
1	A	271	VAL
1	A	286	ASP
1	A	321	LEU
1	A	342	ASN
1	A	369	MET
1	B	14	ASP
1	B	27	ASN
1	B	78	MET
1	B	148	ASN
1	B	241	TYR
1	B	282	LEU
1	B	368	GLU
1	B	383	ARG
1	B	417	THR
1	B	435	ASN
1	B	436	LEU
1	B	438	TYR

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Mol	Chain	Res	Type
1	B	467	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	243	GLN
1	A	315	GLN
1	A	364	HIS
1	B	35	ASN
1	B	118	ASN
1	B	197	ASN
1	B	211	GLN
1	B	238	ASN
1	B	315	GLN
1	B	435	ASN

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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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
3	GOL	A	603	-	5,5,5	0.28	0	5,5,5	0.72	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	603	-	-	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
3	A	603	GOL	C1-C2-C3-O3
3	A	603	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	492/520 (94%)	0.85	60 (12%) 8 6	21, 53, 94, 112	4 (0%)
1	B	511/520 (98%)	0.36	6 (1%) 76 73	21, 44, 77, 92	0
All	All	1003/1040 (96%)	0.60	66 (6%) 24 19	21, 48, 88, 112	4 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	4.1
1	A	351	LEU	3.9
1	A	321	LEU	3.9
1	A	454	VAL	3.8
1	A	453	VAL	3.6
1	A	426	VAL	3.5
1	A	460	ILE	3.4
1	A	472	ILE	3.4
1	B	285	LEU	3.3
1	A	231	ILE	3.3
1	B	435	ASN	3.3
1	A	144	LEU	3.2
1	A	273	TYR	3.2
1	A	323	ILE	3.0
1	A	268	PRO	3.0
1	A	265	SER	3.0
1	A	348	GLY	2.9
1	A	304	LYS	2.9
1	A	251	ILE	2.8
1	A	202	PHE	2.8
1	A	285	LEU	2.7
1	B	299	VAL	2.7
1	A	458	LYS	2.7
1	A	311	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	407	PHE	2.7
1	A	266	ILE	2.7
1	A	203	ALA	2.7
1	A	406	GLY	2.6
1	A	439	LYS	2.6
1	A	267	LEU	2.6
1	A	215	LEU	2.6
1	B	434	LEU	2.6
1	A	299	VAL	2.6
1	A	471	PHE	2.6
1	A	500	GLY	2.5
1	A	342	ASN	2.5
1	A	443	SER	2.5
1	A	307	TYR	2.5
1	A	483	VAL	2.5
1	A	502	ILE	2.5
1	A	451	VAL	2.4
1	A	350	ASP	2.4
1	A	196	ARG	2.4
1	A	475	LYS	2.3
1	A	201	TRP	2.3
1	A	473	PHE	2.3
1	A	217	LYS	2.3
1	A	403	GLN	2.3
1	A	232	LEU	2.2
1	A	353	THR	2.2
1	A	269	THR	2.2
1	A	457	PRO	2.2
1	A	369	MET	2.2
1	A	319	LEU	2.2
1	B	44	GLU	2.1
1	A	349	ASN	2.1
1	A	507	MET	2.1
1	A	404	LEU	2.1
1	A	221	VAL	2.1
1	A	200	ASP	2.1
1	A	352	VAL	2.1
1	B	468	SER	2.0
1	A	324	LYS	2.0
1	A	455	LYS	2.0
1	A	263	TYR	2.0
1	A	452	TYR	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($\text{\AA}^2$)	Q<0.9
3	GOL	A	603	6/6	0.86	0.10	34,38,42,43	0
2	CA	A	602	1/1	0.94	0.07	52,52,52,52	0
2	CA	A	601	1/1	0.96	0.04	44,44,44,44	0
2	CA	B	601	1/1	0.98	0.03	48,48,48,48	0
2	CA	B	602	1/1	0.99	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.