



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:33 PM GMT

PDB ID : 1C9U
Title : CRYSTAL STRUCTURE OF THE SOLUBLE QUINOPROTEIN GLUCOSE
DEHYDROGENASE IN COMPLEX WITH PQQ
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Deposited on : 1999-08-03
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

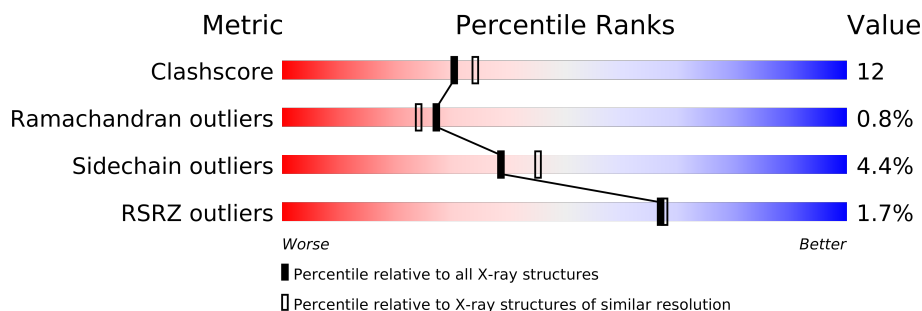
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	454	
1	B	454	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	1005	-	X
4	GOL	A	1007	-	X
4	GOL	B	1005	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7634 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

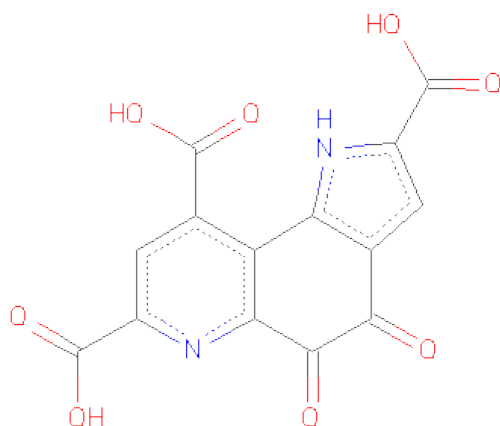
- Molecule 1 is a protein called SOLUBLE QUINOPROTEIN GLUCOSE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3470	2206	590	669	5			
1	B	452	Total	C	N	O	S	0	0	0
			3538	2249	600	684	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is PYRROLOQUINOLINE QUINONE (three-letter code: PQQ) (formula: C₁₄H₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	14	2	8		
3	B	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	255	Total	O	0	0
			255	255		
5	B	293	Total	O	0	0
			293	293		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.59Å 158.72Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 39.85 – 2.13	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-2.20) 80.4 (39.85-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.12Å)	Xtriage
Refinement program	REFMAC, X-PLOR 3.843	Depositor
R, R_{free}	0.223 , 0.286 0.227 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 48621 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7634	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, PQQ

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	0.30	0/3558	0.71	1/4847 (0.0%)
1	B	0.30	0/3628	0.71	1/4943 (0.0%)
All	All	0.30	0/7186	0.71	2/9790 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	B	109	GLU	N-CA-CB	7.34	123.81	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3470	0	3408	84	0
1	B	3538	0	3476	81	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	24	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	3	1	0
4	A	18	0	24	1	0
4	B	6	0	8	0	0
5	A	255	0	0	7	0
5	B	293	0	0	2	0
All	All	7634	0	6922	167	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (167) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:GLU:C	1:B:111:PRO:HD3	1.81	1.01
1:A:405:ASN:HD21	1:A:442:ASN:H	1.11	0.95
1:B:405:ASN:HD21	1:B:442:ASN:H	1.22	0.85
1:B:110:LEU:N	1:B:111:PRO:HD3	1.99	0.75
1:B:110:LEU:N	1:B:111:PRO:CD	2.52	0.72
1:A:431:LYS:HD2	1:A:437:THR:HB	1.72	0.72
1:A:23:LEU:HD11	1:A:60:VAL:HG21	1.71	0.71
1:B:22:ILE:HD11	1:B:448:LYS:HB3	1.72	0.71
1:A:268:VAL:HG22	1:A:309:GLU:HB3	1.72	0.70
3:A:1004:PQQ:N1	3:A:1004:PQQ:O9B	2.26	0.68
1:A:405:ASN:HD21	1:A:442:ASN:N	1.89	0.67
1:A:160:THR:HG23	1:A:233:LEU:HD22	1.75	0.67
1:A:66:VAL:HB	1:A:69:ILE:HD13	1.77	0.67
1:B:171:TYR:HB3	1:B:174:LEU:HD12	1.76	0.66
3:B:1004:PQQ:O9B	3:B:1004:PQQ:N1	2.27	0.65
1:B:227:HIS:HB3	1:B:230:PRO:HG3	1.79	0.64
1:A:447:ILE:HD11	1:A:449:PHE:CZ	2.33	0.64
1:A:420:TYR:HB3	1:A:446:LEU:HD21	1.79	0.63
1:B:109:GLU:CA	1:B:111:PRO:HD3	2.29	0.63
1:A:19:LYS:HG3	1:A:447:ILE:HD12	1.82	0.62
1:B:181:THR:HG21	1:B:216:ASN:HD22	1.63	0.62
1:A:140:SER:HA	1:A:145:GLN:HE22	1.64	0.61
1:B:250:SER:HA	1:B:348:THR:HG23	1.82	0.61
1:A:89:LYS:HD2	1:A:89:LYS:H	1.66	0.61
1:A:40:ILE:HG13	1:A:55:PRO:HG3	1.83	0.60
1:A:248:PRO:HB2	1:A:296:ASN:HD21	1.66	0.60
1:A:32:LEU:HD22	1:A:422:LEU:HD13	1.83	0.60
1:A:295:GLN:HE21	1:A:299:LYS:HE2	1.67	0.60
1:B:431:LYS:HD3	1:B:437:THR:HG21	1.84	0.59
1:A:418:VAL:HG12	1:A:450:THR:HG23	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:370:THR:HG21	1:B:383:ARG:HD3	1.85	0.58
1:B:265:TRP:CD2	1:B:266:PRO:HA	2.38	0.58
1:A:52:ARG:NH2	1:A:61:LYS:HD3	2.17	0.58
1:B:39:GLN:NE2	1:B:55:PRO:HD2	2.19	0.57
1:B:89:LYS:HD2	1:B:89:LYS:H	1.68	0.57
1:A:405:ASN:ND2	1:A:442:ASN:H	1.92	0.56
1:B:179:GLN:HA	1:B:225:LEU:HD13	1.87	0.56
1:A:246:GLN:NE2	1:A:350:ALA:HA	2.19	0.56
1:B:32:LEU:HB3	1:B:422:LEU:HD11	1.86	0.56
1:B:332:ASN:HD22	1:B:334:ASN:H	1.53	0.56
1:B:109:GLU:OE1	1:B:110:LEU:N	2.37	0.56
1:A:53:VAL:HG22	1:A:60:VAL:HG22	1.87	0.56
1:B:344:ILE:HD13	1:B:436:VAL:HG11	1.87	0.56
1:A:42:LEU:HD11	1:A:51:LEU:HD12	1.87	0.55
1:A:410:VAL:HG23	1:A:421:VAL:HG12	1.89	0.55
1:A:265:TRP:CD2	1:A:266:PRO:HA	2.41	0.55
1:A:5:THR:HB	1:A:6:PRO:HD2	1.90	0.54
1:B:417:ASN:HD22	1:B:417:ASN:H	1.55	0.54
1:B:246:GLN:NE2	1:B:350:ALA:HA	2.23	0.54
1:B:109:GLU:C	1:B:111:PRO:CD	2.65	0.54
1:B:410:VAL:HG23	1:B:421:VAL:HG12	1.90	0.53
1:B:8:GLN:HA	1:B:11:LYS:HE2	1.90	0.53
1:A:406:ARG:HB2	1:A:424:ASP:HB2	1.90	0.53
1:A:183:THR:H	1:A:186:GLU:HG3	1.73	0.53
1:B:383:ARG:NH1	1:B:383:ARG:HB3	2.24	0.53
1:A:160:THR:HG22	1:A:199:VAL:HG22	1.90	0.53
1:A:425:THR:HA	1:A:444:GLY:H	1.74	0.52
1:A:186:GLU:HB3	1:A:191:ASP:HB3	1.92	0.52
1:B:352:SER:HB3	1:B:376:LEU:HG	1.92	0.52
1:A:346:TRP:C	5:A:1102:HOH:O	2.48	0.52
1:A:301:ALA:O	1:A:304:VAL:HG12	2.09	0.51
1:A:28:LYS:HD2	1:A:46:ALA:HB2	1.93	0.51
1:A:121:TYR:HE2	1:A:123:LYS:HG2	1.74	0.51
1:A:341:MET:HB3	1:A:344:ILE:CD1	2.40	0.51
1:A:23:LEU:HD21	1:A:60:VAL:HG21	1.93	0.51
1:B:352:SER:OG	1:B:374:PRO:HB2	2.11	0.51
1:A:114:THR:HB	1:A:138:LEU:HB2	1.93	0.51
1:A:352:SER:HB3	1:A:376:LEU:HG	1.93	0.51
1:A:425:THR:HA	1:A:444:GLY:N	2.26	0.51
1:B:418:VAL:HG22	1:B:450:THR:HG23	1.94	0.50
1:B:202:LEU:HB3	1:B:221:HIS:HD2	1.76	0.50
1:B:287:ASN:HB2	5:B:1170:HOH:O	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:249:ASN:H	1:B:296:ASN:ND2	2.10	0.50
1:B:405:ASN:ND2	1:B:442:ASN:H	2.00	0.50
1:B:248:PRO:HB2	1:B:296:ASN:HD21	1.77	0.50
1:A:157:ILE:HB	1:A:202:LEU:HG	1.93	0.50
1:B:344:ILE:HA	1:B:377:LYS:HD2	1.93	0.50
1:B:381:ILE:HD11	1:B:421:VAL:HG11	1.95	0.49
1:A:249:ASN:H	1:A:296:ASN:ND2	2.10	0.49
1:A:97:SER:HA	1:A:115:ILE:O	2.13	0.48
1:B:143:ASP:HB2	1:B:165:GLY:HA3	1.95	0.48
1:B:236:THR:OG1	1:B:238:ASN:ND2	2.47	0.48
1:B:344:ILE:HD13	1:B:436:VAL:CG1	2.43	0.48
1:B:270:GLY:HA2	1:B:320:PRO:HG3	1.95	0.47
1:A:6:PRO:HG3	5:A:1122:HOH:O	2.14	0.47
1:A:169:LEU:HD11	4:A:1005:GOL:H2	1.97	0.47
1:A:5:THR:C	5:A:1250:HOH:O	2.53	0.47
1:B:40:ILE:HG13	1:B:55:PRO:HG3	1.96	0.47
1:A:341:MET:HB3	1:A:344:ILE:HD13	1.97	0.47
1:B:312:TRP:CE2	1:B:314:GLY:HA3	2.50	0.47
1:B:147:GLY:HA2	1:B:159:TYR:CZ	2.50	0.47
1:B:114:THR:HB	1:B:138:LEU:HB2	1.98	0.46
1:B:374:PRO:HG3	1:B:410:VAL:HG12	1.97	0.46
1:B:144:HIS:ND1	1:B:165:GLY:HA2	2.31	0.46
1:A:248:PRO:HB2	1:A:296:ASN:ND2	2.29	0.46
1:B:338:CYS:HB3	1:B:341:MET:O	2.15	0.46
1:A:181:THR:HG23	1:A:182:PRO:HD2	1.98	0.46
1:A:362:LYS:HD2	1:A:415:ASP:HB3	1.96	0.46
1:B:53:VAL:O	1:B:55:PRO:HD3	2.16	0.45
1:B:52:ARG:NH2	1:B:61:LYS:HD3	2.31	0.45
1:B:406:ARG:HB2	1:B:424:ASP:HB2	1.98	0.45
1:A:238:ASN:HD22	1:A:238:ASN:H	1.65	0.45
1:B:32:LEU:HD11	1:B:411:ILE:HG12	1.99	0.45
1:A:181:THR:C	1:A:194:THR:HG21	2.36	0.45
1:B:37:ASP:O	1:B:39:GLN:HG2	2.16	0.45
1:A:324:LEU:HD12	1:A:349:VAL:HG21	1.99	0.45
1:B:431:LYS:HD3	1:B:437:THR:CG2	2.47	0.45
1:B:381:ILE:CD1	1:B:421:VAL:HG11	2.47	0.45
1:B:248:PRO:HB2	1:B:296:ASN:ND2	2.32	0.45
1:A:76:GLN:NE2	1:A:144:HIS:H	2.15	0.45
1:B:405:ASN:HD21	1:B:442:ASN:N	2.03	0.45
1:A:347:PRO:N	5:A:1102:HOH:O	2.50	0.45
1:A:121:TYR:CE2	1:A:123:LYS:HG2	2.51	0.45
1:A:413:SER:HB2	1:A:414:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:181:THR:HG21	1:B:216:ASN:ND2	2.29	0.44
1:A:357:TYR:OH	1:A:364:ILE:HD12	2.18	0.44
1:B:23:LEU:HD13	1:B:26:LEU:HD21	1.98	0.44
1:B:97:SER:HA	1:B:115:ILE:O	2.18	0.44
1:A:166:ARG:NH1	5:A:1139:HOH:O	2.51	0.44
1:B:107:ASP:HB3	1:B:110:LEU:HB2	2.01	0.43
1:B:331:TYR:CE2	1:B:347:PRO:HD3	2.53	0.43
1:B:77:ASN:HB2	1:B:99:THR:OG1	2.18	0.43
1:B:108:LYS:C	1:B:109:GLU:O	2.53	0.43
1:B:362:LYS:HB3	1:B:417:ASN:HB3	2.01	0.43
1:A:83:ALA:HB2	1:A:149:LEU:O	2.19	0.43
1:A:300:VAL:HG21	1:A:306:VAL:HG21	2.01	0.43
1:A:168:GLN:N	1:A:172:LEU:HA	2.33	0.42
1:A:312:TRP:CZ2	1:A:314:GLY:HA3	2.54	0.42
1:B:218:VAL:HB	5:B:1225:HOH:O	2.20	0.42
1:A:262:ASN:O	1:A:317:PHE:HA	2.18	0.42
1:A:304:VAL:HA	1:A:305:PRO:HD3	1.89	0.42
1:B:267:ASN:O	1:B:309:GLU:HG2	2.20	0.42
1:A:331:TYR:CE2	1:A:347:PRO:HD3	2.55	0.42
1:B:238:ASN:HD22	1:B:238:ASN:H	1.67	0.42
1:B:246:GLN:HE21	1:B:246:GLN:HB3	1.67	0.42
1:A:381:ILE:CD1	1:A:421:VAL:HG11	2.50	0.42
1:B:119:TYR:CE2	1:B:131:PRO:HB3	2.55	0.42
1:A:440:LEU:HD13	5:A:1046:HOH:O	2.20	0.42
1:A:85:HIS:HD2	1:A:87:ASP:H	1.68	0.41
1:A:160:THR:HB	1:A:230:PRO:HG2	2.00	0.41
1:A:69:ILE:HD12	1:A:100:PHE:CE2	2.55	0.41
1:A:387:ASP:HB2	1:A:388:PRO:HD2	2.01	0.41
1:A:225:LEU:HD23	1:A:262:ASN:HA	2.02	0.41
1:A:74:ASP:OD1	1:A:142:LYS:HD3	2.20	0.41
1:B:352:SER:HG	1:B:374:PRO:HB2	1.86	0.41
1:A:215:PHE:CE2	1:A:225:LEU:HD22	2.55	0.41
1:A:146:SER:OG	1:A:230:PRO:HD2	2.19	0.41
1:B:140:SER:HA	1:B:145:GLN:HE22	1.85	0.41
1:A:443:PRO:O	1:A:444:GLY:C	2.57	0.41
1:B:379:GLY:HA2	1:B:405:ASN:O	2.21	0.41
1:A:232:GLY:O	1:A:243:GLN:HG2	2.20	0.41
1:A:177:GLN:HA	1:A:180:HIS:CD2	2.55	0.41
1:A:33:LEU:HD11	1:A:82:PHE:O	2.21	0.41
1:B:108:LYS:NZ	1:B:108:LYS:HB3	2.36	0.41
1:B:334:ASN:O	1:B:336:PRO:HD3	2.21	0.41
1:A:344:ILE:HD13	1:A:436:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:GLY:O	1:A:402:LYS:HA	2.21	0.41
1:A:287:ASN:ND2	1:A:289:SER:OG	2.53	0.41
1:B:224:THR:HG21	1:B:257:ILE:HG23	2.02	0.40
1:B:341:MET:HB2	1:B:436:VAL:HG21	2.03	0.40
1:B:232:GLY:O	1:B:243:GLN:HG2	2.21	0.40
1:B:202:LEU:HA	1:B:209:PRO:HD3	2.03	0.40
1:A:252:ASP:OD2	1:A:348:THR:HB	2.22	0.40
1:B:335:ASP:HA	1:B:336:PRO:HD3	1.82	0.40
1:B:379:GLY:O	1:B:402:LYS:HA	2.21	0.40
1:B:213:PRO:HD3	1:B:259:LYS:HE3	2.04	0.40
1:A:286:ALA:HB1	5:A:1204:HOH:O	2.22	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	440/454 (97%)	400 (91%)	35 (8%)	5 (1%)	21	16
1	B	450/454 (99%)	418 (93%)	30 (7%)	2 (0%)	43	45
All	All	890/908 (98%)	818 (92%)	65 (7%)	7 (1%)	27	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	PRO
1	B	248	PRO
1	A	286	ALA
1	B	110	LEU
1	A	146	SER
1	A	170	ALA
1	A	339	GLY

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	382/391 (98%)	363 (95%)	19 (5%)	34	39
1	B	390/391 (100%)	375 (96%)	15 (4%)	44	53
All	All	772/782 (99%)	738 (96%)	34 (4%)	39	45

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	15	GLU
1	A	39	GLN
1	A	68	GLU
1	A	101	LYS
1	A	156	LYS
1	A	181	THR
1	A	186	GLU
1	A	202	LEU
1	A	238	ASN
1	A	243	GLN
1	A	246	GLN
1	A	296	ASN
1	A	315	LYS
1	A	377	LYS
1	A	417	ASN
1	A	433	ASP
1	A	446	LEU
1	A	447	ILE
1	B	107	ASP
1	B	108	LYS
1	B	109	GLU
1	B	202	LEU
1	B	238	ASN
1	B	243	GLN
1	B	246	GLN
1	B	296	ASN
1	B	332	ASN
1	B	335	ASP

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Mol	Chain	Res	Type
1	B	348	THR
1	B	383	ARG
1	B	396	ASP
1	B	417	ASN
1	B	436	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	85	HIS
1	A	145	GLN
1	A	216	ASN
1	A	238	ASN
1	A	246	GLN
1	A	287	ASN
1	A	295	GLN
1	A	296	ASN
1	A	332	ASN
1	A	404	ASN
1	A	405	ASN
1	A	417	ASN
1	A	428	ASN
1	B	71	ASN
1	B	91	ASN
1	B	145	GLN
1	B	180	HIS
1	B	184	GLN
1	B	193	HIS
1	B	216	ASN
1	B	238	ASN
1	B	246	GLN
1	B	296	ASN
1	B	332	ASN
1	B	334	ASN
1	B	404	ASN
1	B	405	ASN
1	B	417	ASN
1	B	428	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 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	$\# Z > 2$
3	PQQ	A	1004	2	26,26,26	3.91	12 (46%)	39,40,40	2.16	14 (35%)
4	GOL	A	1005	-	5,5,5	0.65	0	5,5,5	0.34	0
4	GOL	A	1006	-	5,5,5	0.65	0	5,5,5	0.41	0
4	GOL	A	1007	-	5,5,5	0.64	0	5,5,5	0.51	0
3	PQQ	B	1004	2	26,26,26	3.92	12 (46%)	39,40,40	2.10	14 (35%)
4	GOL	B	1005	-	5,5,5	0.63	0	5,5,5	0.32	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	PQQ	A	1004	2	-	0/10/28/28	0/0/3/3
4	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1007	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PQQ	B	1004	2	-	0/10/28/28	0/0/3/3
4	GOL	B	1005	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	PQQ	C2-C2X	-11.25	1.38	1.51
3	A	1004	PQQ	C2-C2X	-11.23	1.38	1.51
3	B	1004	PQQ	O4-C4	7.15	1.39	1.23
3	A	1004	PQQ	C7-C7X	-7.06	1.41	1.50
3	A	1004	PQQ	O4-C4	7.04	1.38	1.23
3	B	1004	PQQ	C7-C7X	-7.03	1.41	1.50
3	B	1004	PQQ	O5-C5	6.03	1.36	1.23
3	A	1004	PQQ	O5-C5	6.00	1.36	1.23
3	A	1004	PQQ	C6A-C5	-5.73	1.42	1.49
3	B	1004	PQQ	C6A-C5	-5.65	1.42	1.49
3	A	1004	PQQ	C5-C4	-5.26	1.37	1.53
3	B	1004	PQQ	C5-C4	-5.24	1.37	1.53
3	A	1004	PQQ	C3A-C4	-4.22	1.39	1.48
3	B	1004	PQQ	C3A-C4	-4.21	1.39	1.48
3	A	1004	PQQ	C9A-C1A	-4.13	1.41	1.49
3	B	1004	PQQ	C9A-C1A	-4.09	1.41	1.49
3	B	1004	PQQ	C9-C9X	-3.16	1.42	1.49
3	A	1004	PQQ	C9-C9X	-3.15	1.42	1.49
3	A	1004	PQQ	O2B-C2X	-2.65	1.22	1.30
3	B	1004	PQQ	O2B-C2X	-2.61	1.22	1.30
3	B	1004	PQQ	O9B-C9X	-2.62	1.22	1.30
3	A	1004	PQQ	O9B-C9X	-2.57	1.22	1.30
3	B	1004	PQQ	C3-C3A	-2.06	1.35	1.39
3	A	1004	PQQ	C3-C3A	-2.01	1.36	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	PQQ	C9-C9A-C1A	5.94	127.91	122.52
3	A	1004	PQQ	C9-C9A-C1A	5.85	127.83	122.52
3	A	1004	PQQ	O9B-C9X-O9A	-3.81	114.71	123.35
3	B	1004	PQQ	O9B-C9X-O9A	-3.56	115.28	123.35
3	A	1004	PQQ	C9A-C6A-N6	3.49	128.58	123.37
3	B	1004	PQQ	C9A-C6A-N6	3.42	128.48	123.37
3	A	1004	PQQ	C8-C7-C7X	3.37	125.75	119.55
3	A	1004	PQQ	C5-C6A-N6	-3.34	110.94	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	PQQ	C7X-C7-N6	-3.14	111.93	116.51
3	B	1004	PQQ	O2B-C2X-C2	3.12	121.12	113.39
3	A	1004	PQQ	O9B-C9X-C9	3.09	124.69	115.47
3	B	1004	PQQ	C8-C7-C7X	3.07	125.20	119.55
3	B	1004	PQQ	C5-C6A-N6	-3.03	111.43	116.23
3	A	1004	PQQ	O2B-C2X-C2	2.88	120.53	113.39
3	B	1004	PQQ	C2X-C2-N1	2.86	119.06	116.85
3	A	1004	PQQ	C2X-C2-N1	2.81	119.02	116.85
3	A	1004	PQQ	O7B-C7X-C7	2.71	120.88	114.68
3	B	1004	PQQ	O9B-C9X-C9	2.70	123.54	115.47
3	B	1004	PQQ	C3A-C1A-C9A	-2.70	120.29	121.70
3	A	1004	PQQ	C3A-C1A-C9A	-2.70	120.29	121.70
3	B	1004	PQQ	O7B-C7X-C7	2.61	120.66	114.68
3	B	1004	PQQ	C7X-C7-N6	-2.54	112.80	116.51
3	B	1004	PQQ	C9-C9A-C6A	-2.53	113.96	118.53
3	A	1004	PQQ	C9-C9A-C6A	-2.38	114.22	118.53
3	B	1004	PQQ	O7B-C7X-O7A	-2.35	118.01	123.35
3	A	1004	PQQ	C6A-N6-C7	-2.22	114.49	117.97
3	A	1004	PQQ	C1A-C9A-C6A	-2.04	117.94	119.78
3	B	1004	PQQ	C6A-N6-C7	-2.02	114.81	117.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	444/454 (97%)	-0.15	6 (1%) 72 72	11, 30, 52, 66	0
1	B	452/454 (99%)	-0.17	9 (1%) 62 62	12, 25, 52, 69	0
All	All	896/908 (98%)	-0.16	15 (1%) 67 68	11, 27, 52, 69	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	ASN	6.4
1	B	340	GLU	3.8
1	B	338	CYS	3.8
1	B	106	THR	3.1
1	B	339	GLY	3.0
1	B	335	ASP	2.9
1	A	103	PRO	2.4
1	A	289	SER	2.4
1	B	124	SER	2.4
1	A	363	ALA	2.2
1	B	361	LYS	2.2
1	B	90	ASN	2.2
1	B	452	LYS	2.1
1	A	15	GLU	2.1
1	A	185	GLN	2.1

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	A	1007	6/6	0.25	5.27	42,47,52,52	0
4	GOL	B	1005	6/6	0.16	3.66	43,50,51,51	0
4	GOL	A	1005	6/6	0.18	2.84	41,43,45,46	0
2	CA	A	1001	1/1	0.15	1.62	23,23,23,23	0
4	GOL	A	1006	6/6	0.18	1.39	48,52,54,55	0
2	CA	B	1002	1/1	0.15	0.95	21,21,21,21	0
3	PQQ	A	1004	24/24	0.12	0.76	29,35,44,47	0
3	PQQ	B	1004	24/24	0.12	0.25	22,32,36,37	0
2	CA	A	1002	1/1	0.10	-0.86	15,15,15,15	0
2	CA	B	1003	1/1	0.06	-3.50	23,23,23,23	0
2	CA	B	1001	1/1	0.05	-3.80	12,12,12,12	0
2	CA	A	1003	1/1	0.03	-4.27	19,19,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.