



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:51 AM GMT

PDB ID : 3FYP
Title : Crystal structure of the quadruple mutant (N23C/C246S/D247E/P249A) of 3-deoxy-D-manno-octulosonate 8-phosphate synthase (KDO8PS) from *Neisseria meningitidis*
Authors : Jameson, G.B.; Parker, E.J.; Cochrane, F.P.; Patchett, M.L.
Deposited on : 2009-01-22
Resolution : 1.85 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>

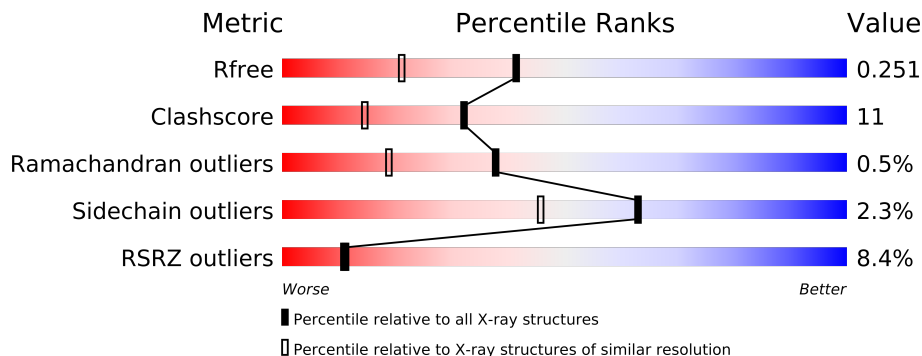
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.85 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}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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	280	
1	B	280	
1	C	280	
1	D	280	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	2647	-	X
3	GOL	B	281	-	X
4	NA	D	283	-	X
6	MN	D	284	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8586 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 3-deoxy-D-manno-octulosonicacid 8-phosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	8	0
			2004	1288	339	365	12			
1	B	253	Total	C	N	O	S	0	12	0
			1990	1290	325	363	12			
1	C	256	Total	C	N	O	S	0	7	0
			1994	1287	333	362	12			
1	D	255	Total	C	N	O	S	0	6	0
			1981	1276	330	362	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	CYS	ASN	ENGINEERED	UNP Q9JZ55
A	246	SER	CYS	ENGINEERED	UNP Q9JZ55
A	247	GLU	ASP	ENGINEERED	UNP Q9JZ55
A	249	ALA	PRO	ENGINEERED	UNP Q9JZ55
B	23	CYS	ASN	ENGINEERED	UNP Q9JZ55
B	246	SER	CYS	ENGINEERED	UNP Q9JZ55
B	247	GLU	ASP	ENGINEERED	UNP Q9JZ55
B	249	ALA	PRO	ENGINEERED	UNP Q9JZ55
C	23	CYS	ASN	ENGINEERED	UNP Q9JZ55
C	246	SER	CYS	ENGINEERED	UNP Q9JZ55
C	247	GLU	ASP	ENGINEERED	UNP Q9JZ55
C	249	ALA	PRO	ENGINEERED	UNP Q9JZ55
D	23	CYS	ASN	ENGINEERED	UNP Q9JZ55
D	246	SER	CYS	ENGINEERED	UNP Q9JZ55
D	247	GLU	ASP	ENGINEERED	UNP Q9JZ55
D	249	ALA	PRO	ENGINEERED	UNP Q9JZ55

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

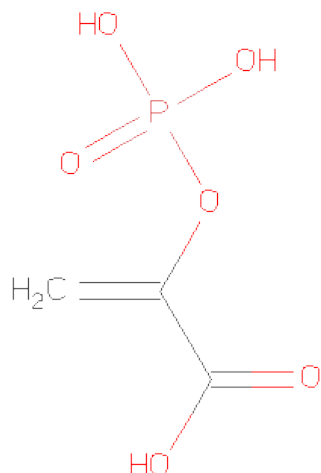


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



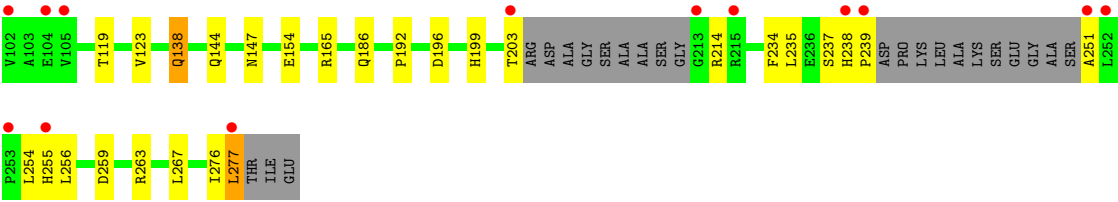
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	131	Total	O	0	0
			131	131		
7	B	163	Total	O	0	0
			163	163		
7	C	162	Total	O	0	0
			162	162		
7	D	134	Total	O	0	0
			134	134		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.78Å 85.68Å 163.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.96 – 1.85 37.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.96-1.85) 99.6 (37.96-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.205 , 0.247 0.214 , 0.251	Depositor DCC
R_{free} test set	4964 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.2	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 98470 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8586	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, MN, PEP, NA, CL

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	0.56	0/2056	0.65	0/2779
1	B	0.62	0/2055	0.66	0/2776
1	C	0.62	0/2046	0.70	0/2763
1	D	0.58	0/2026	0.70	0/2740
All	All	0.60	0/8183	0.68	0/11058

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	3
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	GLU	Peptide
1	B	200	SER	Mainchain
1	B	201	LEU	Peptide
1	B	255	HIS	Peptide

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	2004	0	2050	54	0
1	B	1990	0	2069	55	1
1	C	1994	0	2063	40	0
1	D	1981	0	2029	52	1
2	A	1	0	0	0	0
2	D	1	0	0	1	0
3	B	12	0	16	8	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	D	10	0	2	0	0
6	D	1	0	0	0	0
7	A	131	0	0	8	0
7	B	163	0	0	6	1
7	C	162	0	0	6	3
7	D	134	0	0	8	0
All	All	8586	0	8229	185	3

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 11.

All (185) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:63[A]:ILE:HD13	1:D:119[A]:THR:CG2	1.56	1.35
1:A:277:LEU:O	1:A:278:THR:HG22	1.37	1.24
1:C:190:ASN:HB2	7:C:682:HOH:O	1.53	1.07
1:B:63[A]:ILE:HD13	1:D:119[A]:THR:HG23	1.03	1.02
1:B:63[A]:ILE:CD1	1:D:119[A]:THR:HG23	1.89	1.01
1:A:236:GLU:HB2	7:A:462:HOH:O	1.64	0.96
1:B:63[A]:ILE:CD1	1:D:119[A]:THR:CG2	2.42	0.94
1:C:238:HIS:ND1	1:C:251:ALA:HB3	1.83	0.94
1:A:135:LYS:NZ	1:A:165[B]:ARG:HH21	1.70	0.89
1:B:150[A]:GLU:HG3	7:B:304:HOH:O	1.73	0.87
1:A:118[B]:GLN:OE1	1:C:58:ALA:HB1	1.76	0.84
1:D:24:VAL:HA	7:D:800:HOH:O	1.77	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:237:SER:HB3	7:D:721:HOH:O	1.77	0.83
1:C:201:LEU:O	1:C:202:GLN:HG2	1.79	0.81
1:A:277:LEU:O	1:A:278:THR:CG2	2.25	0.80
1:B:63[A]:ILE:HA	1:D:119[A]:THR:HG21	1.64	0.78
1:A:135:LYS:HZ2	1:A:165[B]:ARG:HH21	1.34	0.76
1:B:63[A]:ILE:HD13	1:D:119[A]:THR:HG22	1.68	0.75
1:D:76:LYS:NZ	7:D:553:HOH:O	2.09	0.75
1:C:100:GLN:O	1:C:104:GLU:HG3	1.87	0.75
1:C:140:LEU:HD12	1:C:144:GLN:HB2	1.69	0.74
1:A:135:LYS:HZ2	1:A:165[B]:ARG:NH2	1.86	0.74
1:A:138:GLN:OE1	7:A:796:HOH:O	2.04	0.74
1:D:61:SER:O	1:D:62:SER:CB	2.35	0.74
1:A:32:LEU:HD22	1:A:84:GLU:OE1	1.89	0.73
1:A:135:LYS:NZ	1:A:165[B]:ARG:HD2	2.04	0.72
1:A:115:LEU:HD22	1:A:118[A]:GLN:OE1	1.91	0.71
1:C:267:LEU:C	1:C:267:LEU:HD23	2.12	0.69
1:A:22:ILE:HD11	1:A:25:LEU:HD23	1.73	0.69
1:C:238:HIS:ND1	1:C:251:ALA:CB	2.56	0.69
1:A:73:GLU:HA	1:A:76:LYS:HG3	1.76	0.68
1:D:154[A]:GLU:OE2	7:D:524:HOH:O	0.69	0.68
1:C:251:ALA:HB2	7:C:549:HOH:O	1.95	0.67
1:D:94:HIS:ND1	7:D:550:HOH:O	2.27	0.67
1:C:139:PHE:CE1	1:C:140:LEU:HD23	2.30	0.67
1:B:63[A]:ILE:HA	1:D:119[A]:THR:CG2	2.25	0.67
1:A:23:CYS:HA	1:A:236:GLU:OE2	1.95	0.66
1:B:28:LEU:HD11	1:B:80:LYS:HG2	1.78	0.66
1:D:73:GLU:O	1:D:76:LYS:HB2	1.95	0.66
1:B:62[B]:SER:OG	7:B:464:HOH:O	2.13	0.65
1:B:212:GLY:CA	1:B:216:ALA:HB2	2.27	0.65
1:B:63[A]:ILE:HD12	1:D:123:VAL:CG2	2.26	0.65
1:B:63[A]:ILE:CD1	1:D:119[A]:THR:HG22	2.25	0.64
1:A:165[B]:ARG:HG3	1:A:196:ASP:HB3	1.79	0.64
1:A:146:LYS:NZ	1:A:147:ASN:OD1	2.31	0.63
1:D:186:GLN:NE2	7:D:778:HOH:O	2.31	0.63
1:A:135:LYS:NZ	1:A:165[B]:ARG:NH2	2.43	0.62
1:D:71:LEU:CD1	1:D:98:GLN:HG2	2.30	0.62
1:D:267:LEU:C	1:D:267:LEU:HD23	2.20	0.62
1:D:100:GLN:O	1:D:100:GLN:NE2	2.33	0.62
1:B:123:VAL:O	1:B:127[B]:LYS:HG2	2.00	0.62
1:A:199[B]:HIS:HB2	7:A:334:HOH:O	1.99	0.62
1:C:201:LEU:O	1:C:202:GLN:CG	2.47	0.62
1:D:62:SER:O	1:D:63:ILE:C	2.39	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:238:HIS:CE1	1:C:251:ALA:HB3	2.34	0.61
1:B:109[A]:ILE:HG22	1:B:125:MET:HE3	1.83	0.61
1:A:173:ASN:CG	7:A:823:HOH:O	2.40	0.60
1:A:135:LYS:HZ3	1:A:165[B]:ARG:HD2	1.66	0.60
1:A:135:LYS:HD2	1:A:165[B]:ARG:HD3	1.82	0.59
1:B:71[A]:LEU:HD11	1:B:75:LEU:HD11	1.84	0.59
1:A:154:GLU:HG2	1:C:63:ILE:HD11	1.85	0.59
1:D:61:SER:O	1:D:62:SER:HB2	2.03	0.58
1:D:54:SER:N	7:D:800:HOH:O	2.19	0.58
1:B:236:GLU:HA	3:B:281:GOL:H2	1.85	0.58
1:B:237:SER:HA	7:B:311:HOH:O	2.02	0.57
1:C:80:LYS:NZ	1:C:84:GLU:OE1	2.37	0.57
1:A:72:GLU:O	1:A:76:LYS:HG2	2.03	0.57
1:B:212:GLY:HA3	1:B:216:ALA:HB2	1.86	0.57
1:D:276:ILE:O	1:D:277:LEU:HB2	2.04	0.57
1:B:22:ILE:HG23	1:B:34:THR:HG21	1.85	0.57
1:B:23:CYS:CA	3:B:281:GOL:H11	2.35	0.56
1:A:22:ILE:HG23	1:A:34:THR:HG21	1.87	0.55
1:C:140:LEU:HD12	1:C:144:GLN:CB	2.35	0.55
1:B:52:LYS:HE2	1:B:234:PHE:CZ	2.42	0.55
1:B:23:CYS:HA	3:B:281:GOL:H11	1.88	0.55
1:B:45:LEU:O	1:B:265:LYS:HE3	2.07	0.54
1:D:251:ALA:N	7:D:607:HOH:O	2.40	0.54
1:A:110:GLN:NE2	1:A:135:LYS:HE3	2.23	0.54
1:D:73:GLU:HA	1:D:76:LYS:HD3	1.89	0.54
1:D:138:GLN:NE2	1:D:138:GLN:H	2.05	0.54
1:B:195:PHE:CE2	1:B:197[B]:VAL:HG22	2.43	0.53
1:D:24:VAL:HB	1:D:57:LYS:HD3	1.90	0.53
1:D:119[A]:THR:O	1:D:123:VAL:HG23	2.08	0.53
1:B:63[A]:ILE:HD12	1:D:123:VAL:HG23	1.90	0.52
1:B:23:CYS:SG	3:B:281:GOL:H31	2.49	0.52
1:B:25:LEU:O	1:B:69:VAL:HG13	2.10	0.52
1:B:237:SER:N	3:B:281:GOL:H12	2.24	0.52
1:A:100:GLN:N	1:A:101:PRO:HD2	2.24	0.52
1:C:27:SER:OG	1:C:30:SER:HB3	2.09	0.52
1:A:135:LYS:HD2	1:A:165[A]:ARG:HD2	1.92	0.52
1:D:276:ILE:O	1:D:277:LEU:CB	2.58	0.51
1:B:199:HIS:HB2	1:B:236:GLU:OE2	2.10	0.51
1:B:95:GLU:HB2	1:B:98:GLN:HG3	1.92	0.51
1:D:61:SER:O	1:D:62:SER:HB3	2.10	0.51
1:C:165:ARG:NH1	1:C:165:ARG:HG3	2.24	0.51
1:B:199:HIS:C	1:B:201:LEU:H	2.15	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:186:GLN:NE2	7:B:751:HOH:O	2.43	0.51
1:B:22:ILE:CG2	1:B:34:THR:HG21	2.41	0.51
1:C:276:ILE:HD12	7:C:507:HOH:O	2.10	0.51
1:B:237:SER:H	3:B:281:GOL:H12	1.75	0.50
1:B:13[A]:ASN:OD1	1:B:229:ARG:NH2	2.37	0.50
1:C:197[A]:VAL:CG1	1:C:198:THR:N	2.74	0.50
1:A:119:THR:HG21	1:C:63:ILE:HA	1.92	0.50
1:C:165:ARG:HG3	1:C:165:ARG:HH11	1.75	0.50
1:A:140:LEU:HD11	1:A:144:GLN:HB2	1.94	0.50
1:C:197[A]:VAL:HG13	1:C:198:THR:N	2.26	0.50
1:D:138:GLN:HE21	1:D:138:GLN:H	1.60	0.49
1:A:159:LYS:HD2	7:A:696:HOH:O	2.10	0.49
1:A:173:ASN:CB	7:A:823:HOH:O	2.59	0.49
1:C:140:LEU:CD1	1:C:144:GLN:CB	2.91	0.49
1:A:173:ASN:HB2	7:A:823:HOH:O	2.13	0.49
1:A:140:LEU:HD11	1:A:144:GLN:CB	2.43	0.49
1:B:141:SER:OG	1:B:144:GLN:HG2	2.13	0.49
1:B:196:ASP:HA	1:B:234:PHE:HB3	1.94	0.48
1:D:71:LEU:HD23	1:D:75:LEU:HD22	1.96	0.48
1:A:258:GLU:O	1:A:262:ILE:HG13	2.13	0.48
1:D:144:GLN:OE1	1:D:147:ASN:ND2	2.47	0.48
1:A:28:LEU:HD11	1:A:32:LEU:HD11	1.95	0.48
1:D:196:ASP:HA	1:D:234:PHE:HB3	1.95	0.47
1:A:198:THR:HG21	1:A:236:GLU:HB3	1.97	0.47
1:D:71:LEU:HD11	1:D:98:GLN:HG2	1.94	0.47
1:A:196:ASP:HA	1:A:234:PHE:HB3	1.95	0.47
1:C:140:LEU:CD1	1:C:144:GLN:HB2	2.42	0.47
1:D:196:ASP:OD2	1:D:199:HIS:ND1	2.30	0.47
1:A:26:GLU:HG3	1:A:66:TYR:HE2	1.79	0.46
1:A:121:LEU:O	1:A:125:MET:HG3	2.16	0.46
1:A:212:GLY:HA3	1:A:216:ALA:HB2	1.97	0.46
1:A:259:ASP:O	1:A:263[B]:ARG:HD2	2.15	0.46
1:B:140:LEU:HG	1:B:144:GLN:HB2	1.97	0.46
1:D:38:TYR:HB3	1:D:49:TYR:CZ	2.51	0.46
1:D:235:LEU:C	1:D:235:LEU:HD12	2.36	0.46
1:B:143:SER:O	1:B:146:LYS:HE2	2.16	0.46
1:B:212:GLY:HA2	1:B:216:ALA:HB2	1.96	0.46
1:C:267:LEU:O	1:C:267:LEU:HD23	2.15	0.45
1:B:236:GLU:HB3	3:B:281:GOL:H2	1.98	0.45
1:B:212:GLY:HA3	1:B:216:ALA:CB	2.47	0.45
1:B:236:GLU:CA	3:B:281:GOL:H2	2.45	0.45
1:C:267:LEU:CD2	1:C:267:LEU:C	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:26:GLU:O	1:B:69:VAL:CG1	2.64	0.45
1:C:139:PHE:CD1	1:C:140:LEU:HD23	2.51	0.45
1:A:214:ARG:O	1:A:214:ARG:HG3	2.14	0.45
1:A:18:LEU:HD11	1:A:235:LEU:HD22	1.99	0.45
1:C:37:HIS:HE1	1:C:254:LEU:O	2.00	0.44
1:B:199:HIS:C	1:B:201:LEU:N	2.69	0.44
1:C:275:PRO:O	1:D:263:ARG:NH2	2.44	0.44
1:C:238:HIS:CE1	1:C:251:ALA:CB	3.01	0.44
1:A:26:GLU:HA	1:A:66:TYR:OH	2.17	0.44
1:D:255:HIS:CE1	1:D:256:LEU:CD2	3.00	0.44
1:A:119:THR:CG2	1:C:63:ILE:HA	2.47	0.44
1:C:45:LEU:O	1:C:265:LYS:HE3	2.18	0.43
1:D:238:HIS:HB2	1:D:239:PRO:HD2	2.00	0.43
1:D:255:HIS:CE1	1:D:256:LEU:HD21	2.54	0.43
1:C:27:SER:HB2	7:C:472:HOH:O	2.19	0.43
1:C:277:LEU:HB2	1:D:263:ARG:CZ	2.49	0.43
1:B:72:GLU:HG2	7:B:505:HOH:O	2.18	0.43
1:D:119[B]:THR:O	1:D:123:VAL:HG23	2.18	0.43
1:B:199:HIS:O	1:B:201:LEU:N	2.52	0.43
1:B:182:GLY:O	1:B:186:GLN:HG2	2.18	0.43
1:C:252:LEU:HD12	7:C:669:HOH:O	2.18	0.42
1:D:63:ILE:HD12	1:D:63:ILE:HA	1.90	0.42
1:C:110:GLN:NE2	1:C:135:LYS:HD2	2.35	0.42
1:D:76:LYS:HB2	1:D:76:LYS:HZ3	1.84	0.42
1:A:100:GLN:N	1:A:101:PRO:CD	2.83	0.42
1:C:24:VAL:HG22	1:C:57:LYS:HB2	2.01	0.42
1:A:135:LYS:HZ2	1:A:165[B]:ARG:HD2	1.82	0.42
1:A:100:GLN:O	1:A:104:GLU:HG2	2.19	0.42
1:A:165[A]:ARG:NH1	7:A:333:HOH:O	2.52	0.42
1:A:214:ARG:HB2	1:A:214:ARG:HE	1.64	0.42
1:B:52:LYS:CD	1:B:234:PHE:CZ	3.02	0.42
1:D:52:LYS:HE3	2:D:282:CL:CL	2.57	0.41
1:B:4:LYS:HD2	1:B:4:LYS:HA	1.85	0.41
1:C:52[A]:LYS:HG2	1:C:90:ILE:HG23	2.02	0.41
1:D:37:HIS:HD2	1:D:254:LEU:HD11	1.84	0.41
1:B:52:LYS:CE	1:B:234:PHE:CZ	3.04	0.41
1:B:95:GLU:OE1	7:B:662:HOH:O	2.21	0.41
1:A:26:GLU:HG3	1:A:66:TYR:CE2	2.55	0.41
1:A:103:ALA:HB1	1:A:130:ASN:OD1	2.20	0.41
1:D:57:LYS:HB3	1:D:60:ARG:HG2	2.03	0.40
1:A:199[B]:HIS:C	1:A:201:LEU:H	2.24	0.40
1:D:3:ILE:HD12	1:D:192:PRO:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:LEU:HB3	1:A:256:LEU:CD2	2.51	0.40
1:C:94:HIS:CD2	7:C:713:HOH:O	2.74	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:689:HOH:O	7:C:544:HOH:O[2_555]	1.94	0.26
1:B:104:GLU:OE1	7:C:544:HOH:O[2_555]	1.95	0.25
1:D:259:ASP:CG	7:C:795:HOH:O[3_645]	2.16	0.04

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	259/280 (92%)	248 (96%)	10 (4%)	1 (0%)	43	24
1	B	259/280 (92%)	252 (97%)	7 (3%)	0	100	100
1	C	257/280 (92%)	250 (97%)	5 (2%)	2 (1%)	27	10
1	D	252/280 (90%)	245 (97%)	5 (2%)	2 (1%)	27	10
All	All	1027/1120 (92%)	995 (97%)	27 (3%)	5 (0%)	38	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	GLY
1	D	60	ARG
1	D	62	SER
1	A	237	SER
1	C	229	ARG

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	221/235 (94%)	218 (99%)	3 (1%)	78	68
1	B	223/235 (95%)	221 (99%)	2 (1%)	87	83
1	C	222/235 (94%)	217 (98%)	5 (2%)	63	46
1	D	219/235 (93%)	209 (95%)	10 (5%)	37	16
All	All	885/940 (94%)	865 (98%)	20 (2%)	63	46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LYS
1	A	214	ARG
1	A	235	LEU
1	B	4	LYS
1	B	146	LYS
1	C	57	LYS
1	C	118	GLN
1	C	136	LYS
1	C	140	LEU
1	C	165	ARG
1	D	40	GLU
1	D	54	SER
1	D	61	SER
1	D	66	TYR
1	D	75	LEU
1	D	138	GLN
1	D	165	ARG
1	D	203	THR
1	D	214	ARG
1	D	277	LEU

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

Mol	Chain	Res	Type
1	A	6	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	217	GLN
1	B	118	GLN
1	B	186	GLN
1	C	37	HIS
1	C	100	GLN
1	C	118	GLN
1	D	59	ASN
1	D	138	GLN

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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	B	2647	-	5,5,5	0.35	0	5,5,5	0.27	0
3	GOL	B	281	-	5,5,5	0.46	0	5,5,5	0.55	0
5	PEP	D	281	-	9,9,9	1.01	0	13,13,13	1.48	2 (15%)

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	B	2647	-	-	0/4/4/4	0/0/0/0
3	GOL	B	281	-	-	0/4/4/4	0/0/0/0
5	PEP	D	281	-	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	281	PEP	O2'-C1-C2	3.39	119.83	113.90
5	D	281	PEP	O1-C1-C2	-3.14	116.96	121.81

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	257/280 (91%)	0.45	32 (12%) 5 4	12, 25, 60, 74	1 (0%)
1	B	253/280 (90%)	-0.02	5 (1%) 62 61	13, 20, 37, 65	1 (0%)
1	C	256/280 (91%)	-0.03	10 (3%) 37 34	11, 19, 40, 70	1 (0%)
1	D	255/280 (91%)	0.66	36 (14%) 3 3	13, 24, 55, 82	0
All	All	1021/1120 (91%)	0.27	83 (8%) 11 11	11, 22, 50, 82	3 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	63	ILE	7.8
1	A	278	THR	6.3
1	B	279	ILE	6.2
1	A	253	PRO	6.1
1	A	211	SER	5.8
1	A	66	TYR	5.7
1	D	66	TYR	5.7
1	C	255	HIS	5.4
1	A	237	SER	5.3
1	C	212	GLY	5.0
1	A	277	LEU	4.7
1	C	252	LEU	4.6
1	D	97	HIS	4.4
1	B	212	GLY	4.3
1	D	203	THR	4.3
1	D	105	VAL	4.1
1	C	253	PRO	4.0
1	C	277	LEU	3.7
1	D	78	PHE	3.7
1	D	27	SER	3.7
1	A	32	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	29	ASP	3.5
1	D	75	LEU	3.5
1	D	101	PRO	3.5
1	D	213	GLY	3.4
1	A	33	GLN	3.4
1	D	253	PRO	3.4
1	D	68	GLY	3.4
1	D	239	PRO	3.3
1	D	76	LYS	3.2
1	D	77	ILE	3.1
1	B	237	SER	3.1
1	A	61	SER	3.1
1	D	81	VAL	3.1
1	A	30	SER	3.1
1	C	254	LEU	3.0
1	A	105	VAL	2.9
1	D	80	LYS	2.9
1	D	277	LEU	2.9
1	D	29	ASP	2.8
1	A	28	LEU	2.8
1	A	71	LEU	2.8
1	A	254	LEU	2.8
1	A	31	THR	2.7
1	A	63	ILE	2.7
1	A	203	THR	2.7
1	A	69	VAL	2.7
1	A	72	GLU	2.7
1	D	255	HIS	2.7
1	D	74	GLY	2.7
1	D	251	ALA	2.7
1	B	255	HIS	2.6
1	B	278	THR	2.6
1	D	252	LEU	2.6
1	D	31	THR	2.5
1	A	97	HIS	2.5
1	D	62	SER	2.5
1	D	83	ALA	2.5
1	C	213	GLY	2.5
1	D	61	SER	2.5
1	D	60	ARG	2.4
1	A	76	LYS	2.4
1	D	102	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	69	VAL	2.4
1	A	78	PHE	2.3
1	A	73	GLU	2.3
1	D	67	ARG	2.3
1	A	26	GLU	2.3
1	A	67	ARG	2.3
1	D	215	ARG	2.3
1	C	251	ALA	2.3
1	A	79	GLU	2.3
1	A	68	GLY	2.2
1	D	33	GLN	2.2
1	C	238	HIS	2.2
1	D	104	GLU	2.2
1	C	202	GLN	2.1
1	D	26	GLU	2.1
1	A	74	GLY	2.1
1	A	81	VAL	2.1
1	A	75	LEU	2.1
1	D	238	HIS	2.0
1	A	64	HIS	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 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	NA	D	283	1/1	0.38	20.93	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	2647	6/6	0.17	8.78	40,43,45,46	0
3	GOL	B	281	6/6	0.47	5.06	26,30,30,32	6
6	MN	D	284	1/1	0.29	3.64	31,31,31,31	1
5	PEP	D	281	10/10	0.15	0.90	17,22,24,25	10
2	CL	A	281	1/1	0.06	-1.61	33,33,33,33	0
2	CL	D	282	1/1	0.08	-2.66	37,37,37,37	1
4	NA	C	281	1/1	0.05	-2.96	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.