Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 10:13 AM EDT

PDB ID	:	2QKF
Title	:	Crystal structure of 3-deoxy-d-manno-octulosonate 8-phosphate synthase (KDO8PS) from Neisseria meningitidis
Authors	:	Cochrane, F.C.; Patchett, M.L.; Jameson, G.B.; Parker, E.J.
Deposited on	:	2007-07-11
Resolution	:	1.75 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:

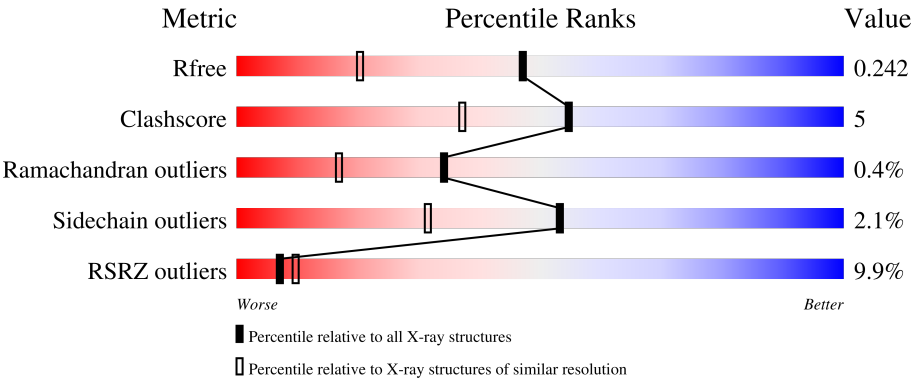
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 <=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	280	13% 82% 5% • 10%
1	B	280	6% 77% 11% • 10%
1	C	280	4% 81% 10% 9%
1	D	280	13% 81% 9% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	D	282	-	-	X	-
4	GOL	C	286	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8466 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 3-deoxy-D-manno-octulosonic acid 8- phosphate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	2	0
			1927	1240	324	352	11			
1	B	251	Total	C	N	O	S	0	12	0
			1991	1287	331	361	12			
1	C	256	Total	C	N	O	S	0	8	0
			2014	1298	339	366	11			
1	D	253	Total	C	N	O	S	0	7	0
			1976	1273	330	362	11			

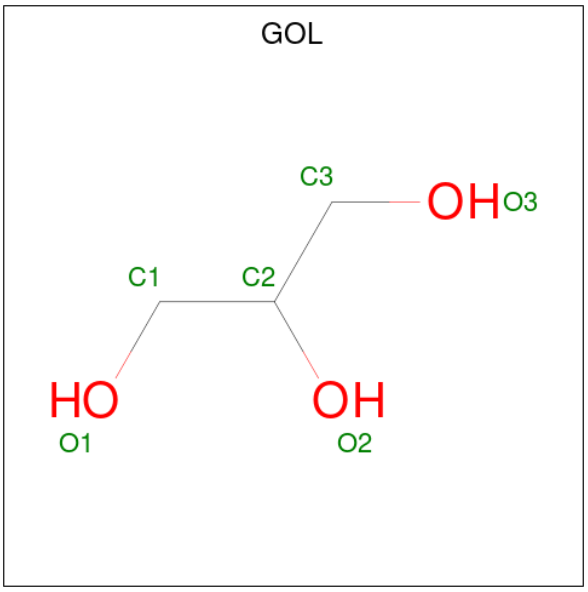
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Na	0	0
			1	1		

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



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

- Molecule 5 is water.

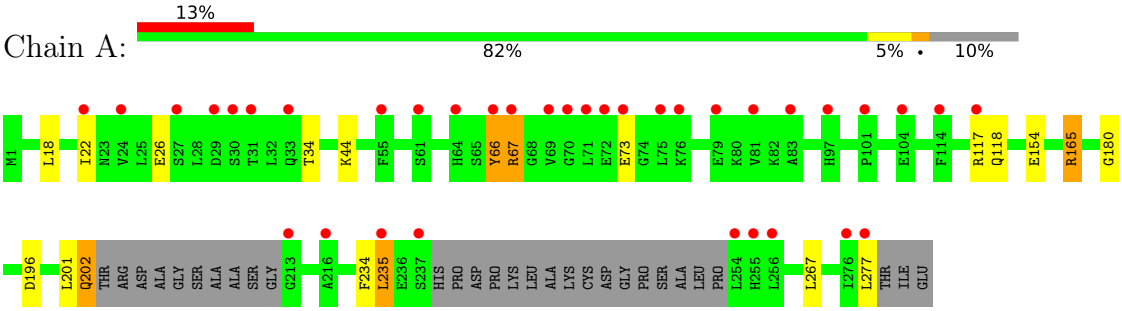
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	100	Total O 100 100	0	0
5	B	146	Total O 146 146	0	3
5	C	148	Total O 148 148	0	0
5	D	134	Total O 134 134	0	1

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.

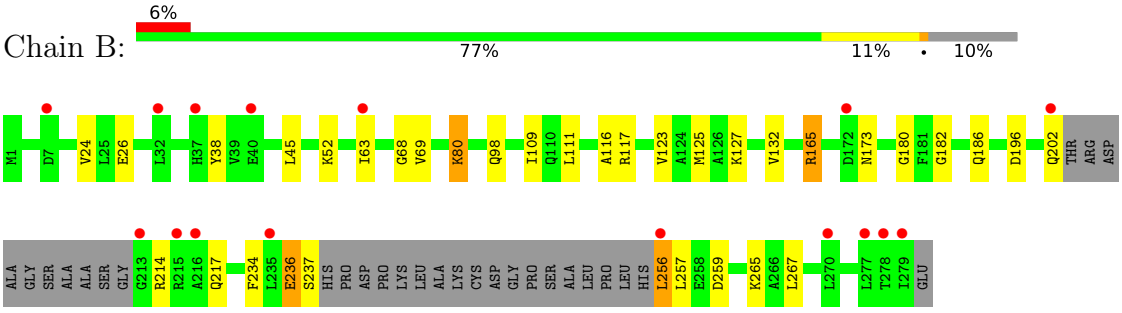
• Molecule 1: 3-deoxy-D-manno-octulosonic acid 8- phosphate synthetase

Chain A:



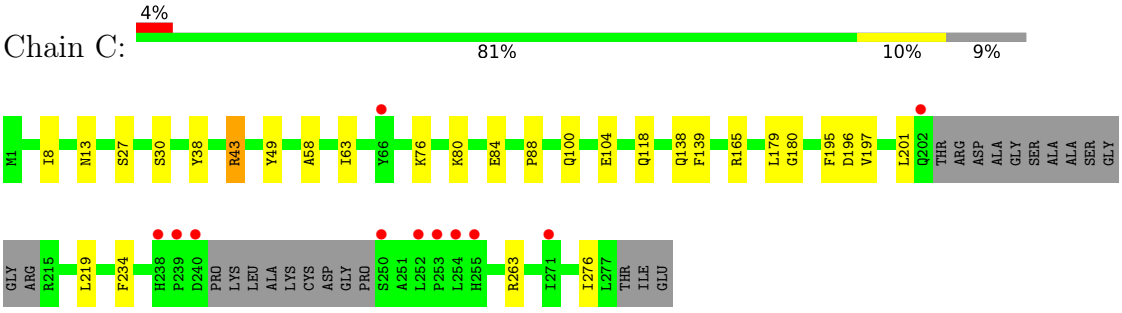
• Molecule 1: 3-deoxy-D-manno-octulosonic acid 8- phosphate synthetase

Chain B:



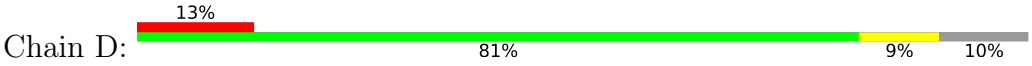
• Molecule 1: 3-deoxy-D-manno-octulosonic acid 8- phosphate synthetase

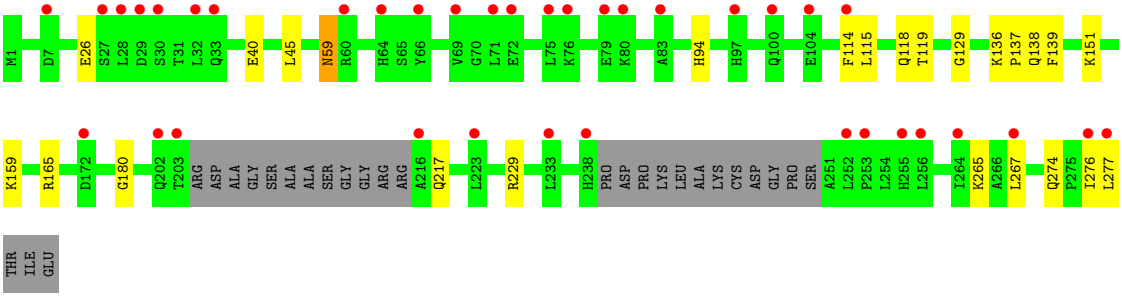
Chain C:



• Molecule 1: 3-deoxy-D-manno-octulosonic acid 8- phosphate synthetase

Chain D:




M1
D7
E26
S27
L28
D29
S30
T31
L32
Q33
E40
L45
N59
R60
H64
S65
Y66
V69
G70
L71
E72
L75
K76
E79
K80
A83
H94
H97
Q100
E104
F114
L115
Q118
T119
G129
K136
P137
Q138
F139
K151
K159
R165
D172
G180
Q202
T203
ARG
ASP
ALA
GLY
SER
ALA
ALA
SER
GLY
GLY
ARG
ARG
A216
Q217
L223
R229
L233
H238
PRO
ASP
PRO
LYS
LEU
ALA
LYS
CYS
ASP
GLY
PRO
SER
A251
L252
P253
L254
H255
L256
I264
K265
A266
L267
Q274
P275
I276
L277
THR
ILE
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.52Å 85.30Å 162.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 39.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.00-1.75) 97.0 (39.90-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.235 0.203 , 0.242	Depositor DCC
R_{free} test set	5588 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8466	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 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, GOL, 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	0/1965	0.65	1/2656 (0.0%)
1	B	0.58	0/2052	0.67	0/2770
1	C	0.60	0/2068	0.67	1/2795 (0.0%)
1	D	0.58	0/2027	0.65	0/2743
All	All	0.58	0/8112	0.66	2/10964 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	43	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	165	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1927	0	1967	23	0
1	B	1991	0	2079	32	0
1	C	2014	0	2079	18	1
1	D	1976	0	2014	24	1
2	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	1	0
2	D	2	0	0	2	0
3	C	1	0	0	0	0
4	C	18	0	24	0	0
4	D	6	0	8	0	0
5	A	100	0	0	4	0
5	B	146	0	0	3	0
5	C	148	0	0	2	0
5	D	134	0	0	3	0
All	All	8466	0	8171	84	1

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 5.

All (84) 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:D:94[B]:HIS:HE1	1:D:114[B]:PHE:CZ	1.48	1.30
1:D:94[B]:HIS:CE1	1:D:114[B]:PHE:CZ	2.36	1.12
1:D:94[B]:HIS:CE1	1:D:114[B]:PHE:HZ	1.69	1.09
1:D:114[B]:PHE:CD2	5:D:366:HOH:O	2.21	0.91
1:D:94[B]:HIS:CE1	1:D:114[B]:PHE:CE1	2.60	0.89
1:D:94[B]:HIS:HE1	1:D:114[B]:PHE:HZ	0.84	0.81
1:B:98:GLN:OE1	5:B:368:HOH:O	1.96	0.81
1:B:38:TYR:OH	1:B:237:SER:C	2.28	0.71
1:C:13:ASN:HD21	1:C:276:ILE:HD11	1.55	0.70
1:D:114[B]:PHE:CD1	1:D:115:LEU:HG	2.29	0.67
1:A:154:GLU:HG3	1:C:63:ILE:HD11	1.77	0.67
5:A:310:HOH:O	1:C:139:PHE:HB3	1.96	0.64
1:B:24[B]:VAL:HG13	1:B:68:GLY:HA2	1.81	0.63
1:B:196:ASP:HA	1:B:234:PHE:HB3	1.81	0.62
1:A:267:LEU:CD1	1:B:267[B]:LEU:HD13	2.30	0.61
1:D:114[B]:PHE:CE2	5:D:366:HOH:O	2.46	0.60
1:A:267:LEU:HD13	1:B:267[B]:LEU:CD1	2.32	0.60
1:A:66:TYR:O	1:A:67:ARG:CB	2.51	0.58
1:A:118:GLN:HA	1:A:118:GLN:HE21	1.69	0.57
1:B:109:ILE:HG22	1:B:125[A]:MET:HE3	1.85	0.57
1:B:182:GLY:O	1:B:186:GLN:HG2	2.05	0.57
1:B:52:LYS:HE2	1:B:234:PHE:CZ	2.39	0.57
1:D:94[B]:HIS:CE1	1:D:114[B]:PHE:HE1	2.21	0.56
1:A:196:ASP:HA	1:A:234:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:HA	1:A:118:GLN:NE2	2.21	0.56
1:A:66:TYR:O	1:A:67:ARG:HB2	2.08	0.54
1:B:256:LEU:HD12	1:B:257:LEU:H	1.73	0.54
1:B:125[A]:MET:HE2	1:B:132:VAL:HG13	1.91	0.53
1:B:180:GLY:HA3	5:B:335:HOH:O	2.08	0.53
1:A:26:GLU:HA	1:A:66:TYR:OH	2.09	0.52
1:B:165[B]:ARG:NH2	2:B:281:CL:CL	2.78	0.52
1:A:18:LEU:HD11	1:A:235:LEU:HG	1.92	0.51
1:B:165[A]:ARG:HH11	1:B:165[A]:ARG:CG	2.24	0.51
1:D:59:ASN:ND2	1:D:114[B]:PHE:CZ	2.75	0.51
1:B:186:GLN:NE2	5:B:376:HOH:O	2.44	0.50
1:A:118:GLN:HE22	1:C:58:ALA:HB3	1.78	0.49
1:A:118:GLN:HE22	1:C:58:ALA:CB	2.25	0.49
1:D:129:GLY:O	1:D:159:LYS:CE	2.60	0.49
1:D:114[B]:PHE:HD1	1:D:115:LEU:HG	1.78	0.49
1:B:63:ILE:HD13	1:D:119:THR:CG2	2.43	0.48
1:A:267:LEU:HD13	1:B:267[B]:LEU:HD13	1.94	0.47
1:D:138:GLN:NE2	2:D:282:CL:CL	2.80	0.47
1:A:180:GLY:HA3	5:A:295:HOH:O	2.14	0.47
1:B:80:LYS:HA	1:B:80:LYS:HE2	1.95	0.47
1:C:80:LYS:NZ	1:C:84:GLU:OE1	2.47	0.47
1:C:195:PHE:CE2	1:C:197[B]:VAL:HG12	2.48	0.47
1:A:117[B]:ARG:HG2	5:A:353:HOH:O	2.14	0.47
1:A:235:LEU:HD12	1:A:235:LEU:C	2.35	0.47
1:D:276:ILE:O	1:D:277:LEU:CB	2.63	0.46
1:B:52:LYS:NZ	1:B:236:GLU:OE1	2.48	0.46
1:D:267:LEU:C	1:D:267:LEU:HD23	2.37	0.45
1:A:22:ILE:HG23	1:A:34:THR:HG21	1.97	0.45
1:A:277:LEU:HD22	1:B:259[B]:ASP:OD2	2.16	0.45
1:A:44:LYS:HB2	5:A:346:HOH:O	2.15	0.45
1:C:196:ASP:HA	1:C:234:PHE:HB3	1.98	0.45
1:B:123:VAL:O	1:B:127[B]:LYS:HG2	2.17	0.45
1:C:8:ILE:HD12	1:C:88:PRO:HG2	2.00	0.44
1:C:43:ARG:HD3	5:C:379:HOH:O	2.17	0.44
1:B:165[A]:ARG:HH11	1:B:165[A]:ARG:HG3	1.82	0.44
1:B:24[B]:VAL:HG13	1:B:68:GLY:CA	2.48	0.44
1:B:214:ARG:HA	1:B:217:GLN:HE21	1.81	0.44
1:B:52:LYS:HE2	1:B:234:PHE:CE2	2.53	0.43
1:D:180:GLY:HA3	5:D:310:HOH:O	2.18	0.43
1:C:179:LEU:HD22	1:D:217:GLN:HB3	2.01	0.43
1:D:45:LEU:O	1:D:265:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:CG2	1:A:34:THR:HG21	2.48	0.43
1:B:45:LEU:O	1:B:265:LYS:HE3	2.18	0.43
1:C:138:GLN:HG2	2:C:281:CL:CL	2.56	0.42
1:D:114[B]:PHE:CE1	1:D:115:LEU:HG	2.54	0.42
1:B:26:GLU:O	1:B:69:VAL:CG1	2.67	0.42
1:C:27:SER:OG	1:C:30:SER:HB3	2.19	0.42
1:C:100:GLN:O	1:C:104:GLU:HG3	2.19	0.42
1:C:38:TYR:HB3	1:C:49:TYR:CZ	2.54	0.42
1:A:201:LEU:O	1:A:202:GLN:C	2.57	0.42
1:B:111:LEU:HD21	1:B:116:ALA:HA	2.01	0.42
1:A:267:LEU:CD1	1:B:267[B]:LEU:CD1	2.93	0.41
1:D:138:GLN:HG2	2:D:282:CL:CL	2.56	0.41
1:C:180:GLY:HA3	5:C:341:HOH:O	2.20	0.41
1:C:263:ARG:HA	1:D:274:GLN:HE22	1.86	0.41
1:C:219:LEU:HD21	1:C:263:ARG:HD3	2.03	0.40
1:B:63:ILE:HD11	1:D:151:LYS:HB3	2.02	0.40
1:D:137:PRO:HB3	1:D:139:PHE:CE2	2.56	0.40
1:A:267:LEU:HD11	1:B:267[B]:LEU:HD13	2.01	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:LYS:NZ	1:D:40:GLU:OE2[3_655]	2.19	0.01

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	247/280 (88%)	238 (96%)	7 (3%)	2 (1%)	19 6
1	B	257/280 (92%)	250 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	258/280 (92%)	252 (98%)	5 (2%)	1 (0%)	34 17
1	D	254/280 (91%)	250 (98%)	3 (1%)	1 (0%)	34 17
All	All	1016/1120 (91%)	990 (97%)	22 (2%)	4 (0%)	34 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	C	201	LEU
1	A	66	TYR
1	D	229	ARG

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	211/236 (89%)	207 (98%)	4 (2%)	57 37
1	B	224/236 (95%)	216 (96%)	8 (4%)	35 13
1	C	226/236 (96%)	224 (99%)	2 (1%)	78 67
1	D	220/236 (93%)	215 (98%)	5 (2%)	50 28
All	All	881/944 (93%)	862 (98%)	19 (2%)	53 29

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

Mol	Chain	Res	Type
1	A	73	GLU
1	A	165	ARG
1	A	202	GLN
1	A	235	LEU
1	B	80	LYS
1	B	117	ARG
1	B	165[A]	ARG
1	B	165[B]	ARG

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Mol	Chain	Res	Type
1	B	173	ASN
1	B	202	GLN
1	B	236	GLU
1	B	256	LEU
1	C	118	GLN
1	C	165	ARG
1	D	26	GLU
1	D	59	ASN
1	D	118	GLN
1	D	136	LYS
1	D	165	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	23	ASN
1	A	118	GLN
1	A	138	GLN
1	B	118	GLN
1	B	173	ASN
1	B	217	GLN
1	C	13	ASN
1	C	37	HIS
1	C	97	HIS
1	C	100	GLN
1	C	217	GLN
1	C	238	HIS
1	D	23	ASN
1	D	59	ASN
1	D	186	GLN
1	D	274	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	C	285	-	5,5,5	0.48	0	5,5,5	0.84	0
4	GOL	C	286	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	C	284	-	5,5,5	0.48	0	5,5,5	0.48	0
4	GOL	D	283	-	5,5,5	0.43	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
4	GOL	C	285	-	-	2/4/4/4	-
4	GOL	C	286	-	-	0/4/4/4	-
4	GOL	C	284	-	-	0/4/4/4	-
4	GOL	D	283	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	285	GOL	O1-C1-C2-C3
4	D	283	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	285	GOL	O1-C1-C2-O2
4	D	283	GOL	O1-C1-C2-O2
4	D	283	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	251/280 (89%)	0.75	36 (14%) 2 3	22, 35, 56, 65	1 (0%)
1	B	251/280 (89%)	0.36	16 (6%) 19 25	21, 28, 45, 66	0
1	C	256/280 (91%)	0.28	11 (4%) 35 41	22, 29, 46, 77	0
1	D	253/280 (90%)	0.72	37 (14%) 2 3	21, 32, 49, 64	0
All	All	1011/1120 (90%)	0.53	100 (9%) 7 10	21, 31, 50, 77	1 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	TYR	8.7
1	A	277	LEU	7.1
1	D	277	LEU	6.2
1	C	250	SER	5.9
1	A	69	VAL	5.8
1	A	254	LEU	5.7
1	C	239	PRO	5.5
1	D	66	TYR	5.1
1	D	114[A]	PHE	4.9
1	A	30	SER	4.9
1	C	255	HIS	4.8
1	B	279	ILE	4.5
1	C	240	ASP	4.5
1	A	72	GLU	4.4
1	A	71	LEU	4.1
1	A	61	SER	4.0
1	D	72	GLU	4.0
1	C	238	HIS	3.9
1	A	97	HIS	3.9
1	A	76	LYS	3.8
1	B	256	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	104	GLU	3.6
1	A	67	ARG	3.6
1	D	30[A]	SER	3.5
1	B	278	THR	3.5
1	A	256	LEU	3.5
1	A	22	ILE	3.5
1	A	117[A]	ARG	3.5
1	D	203	THR	3.4
1	A	276	ILE	3.4
1	A	73	GLU	3.4
1	A	75	LEU	3.3
1	B	37	HIS	3.2
1	A	213	GLY	3.2
1	D	69	VAL	3.2
1	D	267	LEU	3.2
1	A	29	ASP	3.2
1	B	216	ALA	3.2
1	A	237	SER	3.2
1	D	276	ILE	3.1
1	C	202	GLN	3.1
1	D	33	GLN	3.1
1	D	255	HIS	3.0
1	D	80	LYS	3.0
1	A	114	PHE	3.0
1	D	27	SER	3.0
1	A	33	GLN	3.0
1	D	238	HIS	2.9
1	B	277	LEU	2.9
1	A	255	HIS	2.9
1	D	253	PRO	2.9
1	C	252	LEU	2.9
1	D	233	LEU	2.9
1	B	202	GLN	2.9
1	D	252	LEU	2.8
1	B	172	ASP	2.8
1	A	235	LEU	2.8
1	A	216	ALA	2.8
1	D	216	ALA	2.8
1	A	64	HIS	2.7
1	B	215	ARG	2.7
1	A	31	THR	2.6
1	D	32	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	100	GLN	2.6
1	A	104	GLU	2.6
1	D	29	ASP	2.6
1	D	264	ILE	2.5
1	D	28	LEU	2.5
1	A	27	SER	2.5
1	A	101	PRO	2.5
1	B	40	GLU	2.5
1	C	254	LEU	2.4
1	D	71	LEU	2.4
1	B	32	LEU	2.4
1	A	79	GLU	2.3
1	D	7	ASP	2.3
1	C	253	PRO	2.2
1	A	83	ALA	2.2
1	D	76	LYS	2.2
1	C	271	ILE	2.2
1	D	79	GLU	2.2
1	D	75	LEU	2.2
1	B	213	GLY	2.2
1	A	55	PHE	2.1
1	C	66	TYR	2.1
1	D	60	ARG	2.1
1	D	64	HIS	2.1
1	B	7	ASP	2.1
1	B	63	ILE	2.1
1	D	172	ASP	2.1
1	A	70	GLY	2.1
1	D	97	HIS	2.1
1	D	256	LEU	2.1
1	D	202	GLN	2.1
1	A	24	VAL	2.1
1	A	81	VAL	2.1
1	D	83	ALA	2.1
1	B	235	LEU	2.0
1	B	270	LEU	2.0
1	D	223	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	C	286	6/6	0.66	0.44	42,42,43,43	6
4	GOL	C	285	6/6	0.73	0.23	47,47,48,49	0
4	GOL	D	283	6/6	0.83	0.17	40,40,41,41	6
4	GOL	C	284	6/6	0.93	0.14	33,35,36,36	0
2	CL	C	281	1/1	0.97	0.06	41,41,41,41	0
2	CL	C	282	1/1	0.97	0.06	36,36,36,36	0
2	CL	B	281	1/1	0.97	0.11	41,41,41,41	0
2	CL	D	281	1/1	0.98	0.09	35,35,35,35	0
2	CL	D	282	1/1	0.98	0.06	48,48,48,48	0
3	NA	C	283	1/1	0.99	0.05	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.