Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 03:28 PM EDT

PDB ID	:	3QPY
Title	:	Crystal structure of a mutant (K57A) of 3-deoxy-D-manno-octulosonate 8-phosphate synthase (KDO8PS) from Neisseria meningitidis
Authors	:	Allison, T.M.; Jameson, G.B.; Parker, E.J.
Deposited on	:	2011-02-14
Resolution	:	1.95 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:

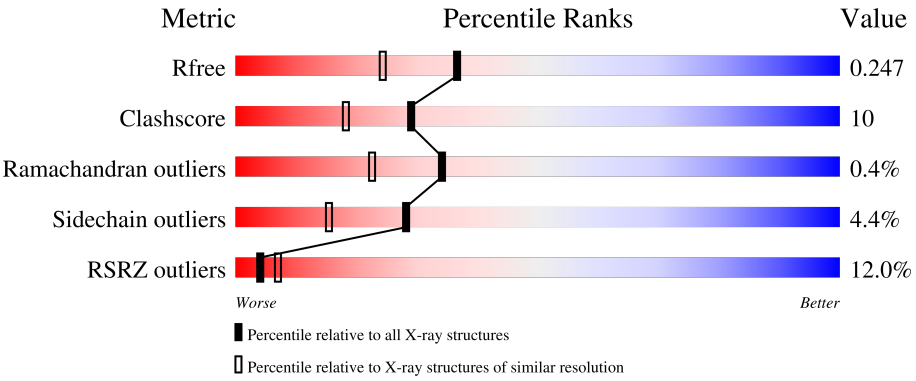
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	11% 73% 15% • 11%
1	B	280	8% 74% 14% • 11%
1	C	280	7% 74% 14% • 10%
1	D	280	16% 71% 16% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8574 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 2-dehydro-3-deoxyphosphooctonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	3	0
			1939	1242	331	355	11			
1	B	250	Total	C	N	O	S	0	6	0
			1956	1261	327	357	11			
1	C	251	Total	C	N	O	S	0	7	0
			1982	1277	335	359	11			
1	D	249	Total	C	N	O	S	0	7	0
			1950	1252	325	362	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55
B	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55
C	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55
D	57	ALA	LYS	ENGINEERED MUTATION	UNP Q9JZ55

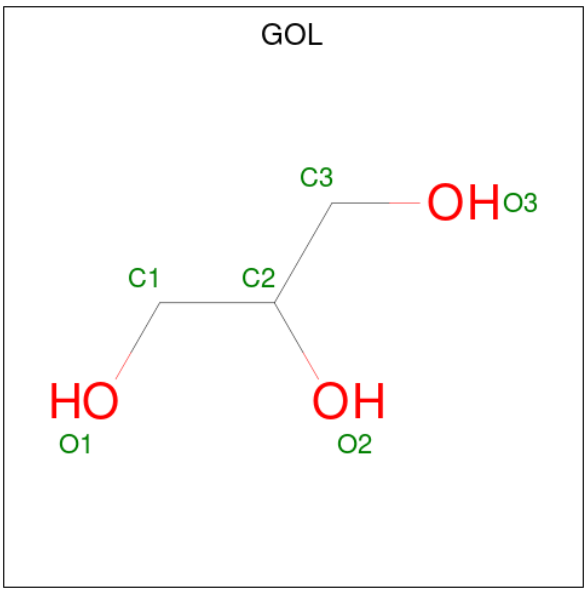
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	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

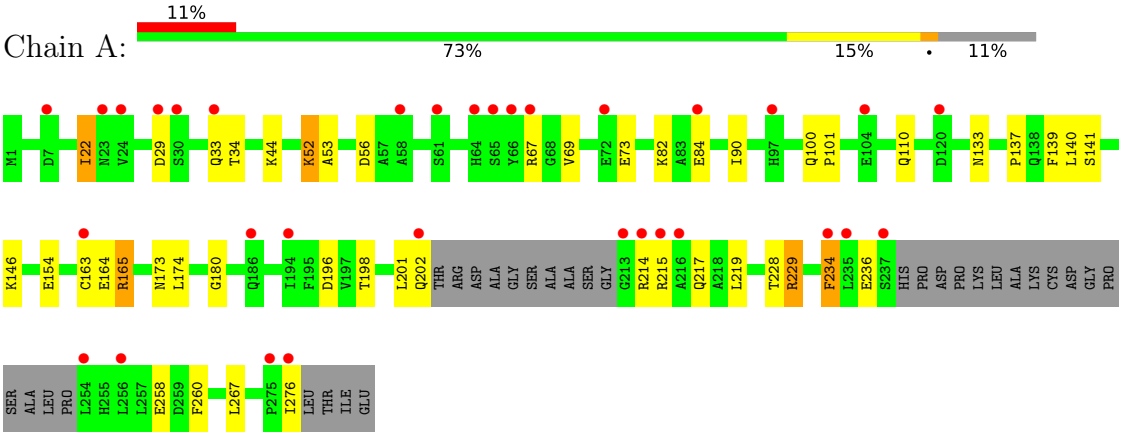
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	163	Total O 163 163	0	0
5	B	243	Total O 243 243	0	0
5	C	188	Total O 188 188	0	0
5	D	143	Total O 143 143	0	0

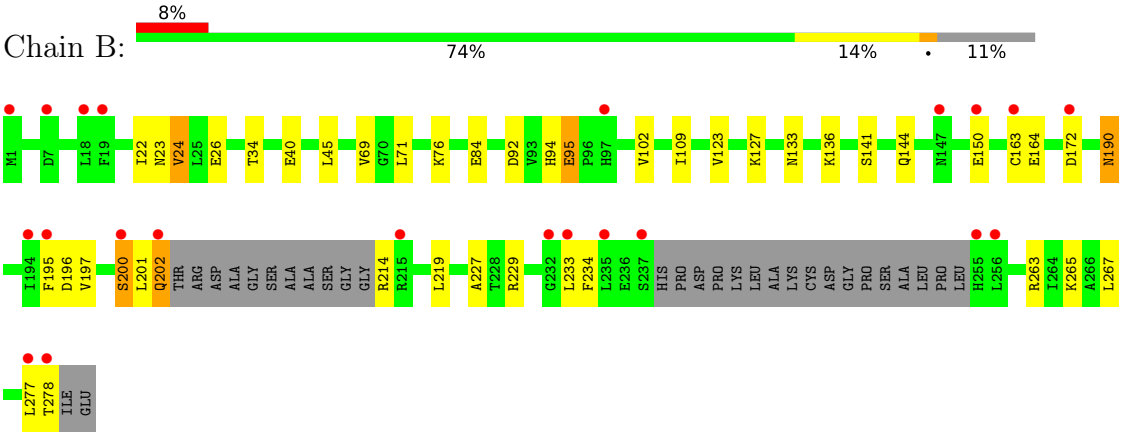
3 Residue-property plots (i)

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.

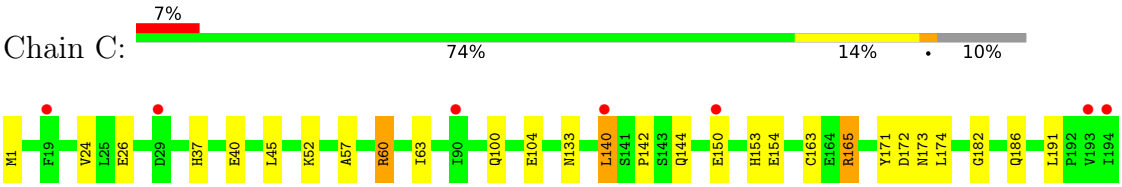
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

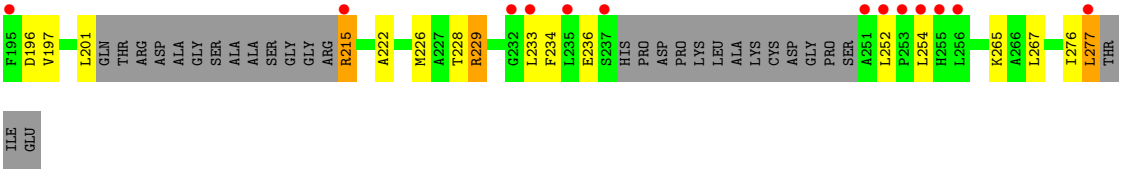


• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

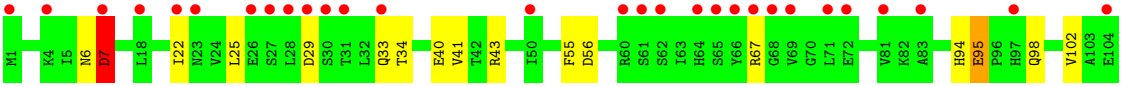


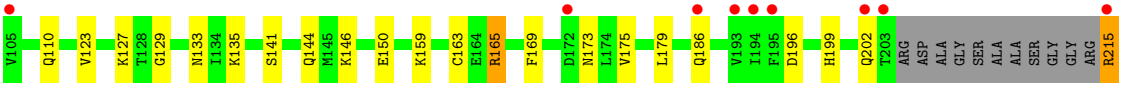
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

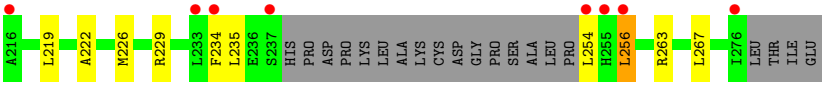




• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.43Å 86.18Å 163.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.84 – 1.95 31.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (33.84-1.95) 97.9 (31.26-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.252 0.200 , 0.247	Depositor DCC
R_{free} test set	4210 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8574	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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.*

[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: CL, NA, 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	0.55	1/1974 (0.1%)	0.57	0/2665
1	B	0.53	0/2003	0.58	1/2707 (0.0%)
1	C	0.51	0/2023	0.58	0/2733
1	D	0.49	0/1993	0.59	2/2695 (0.1%)
All	All	0.52	1/7993 (0.0%)	0.58	3/10800 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	GLU	CD-OE2	-5.04	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	7[A]	ASP	CB-CG-OD1	6.00	123.69	118.30
1	D	7[B]	ASP	CB-CG-OD1	6.00	123.69	118.30
1	B	172	ASP	CB-CG-OD2	5.61	123.35	118.30

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	1939	0	1980	42	0
1	B	1956	0	2025	38	0
1	C	1982	0	2051	48	0
1	D	1950	0	1991	34	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	1	0	0	0	0
4	C	6	0	8	1	0
5	A	163	0	0	6	0
5	B	243	0	0	6	0
5	C	188	0	0	6	0
5	D	143	0	0	1	0
All	All	8574	0	8055	152	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 10.

All (152) 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:214[B]:ARG:HH11	1:A:214[B]:ARG:HG2	1.10	1.11
1:B:40:GLU:HG3	5:B:382:HOH:O	1.49	1.09
1:A:29:ASP:O	1:A:33:GLN:HG2	1.67	0.95
1:A:196:ASP:HA	1:A:234:PHE:HB2	1.54	0.89
1:D:165:ARG:HG2	5:D:689:HOH:O	1.72	0.88
1:A:267:LEU:HD13	1:B:267[B]:LEU:HD21	1.59	0.84
1:D:6:ASN:HB3	1:D:7[A]:ASP:OD2	1.77	0.84
1:C:215:ARG:HD3	1:C:215:ARG:N	1.92	0.83
1:C:140:LEU:CD2	1:C:144:GLN:HB2	2.09	0.83
1:B:277:LEU:HD23	1:B:278:THR:N	1.95	0.80
1:A:214[B]:ARG:HG2	1:A:214[B]:ARG:NH1	1.88	0.80
1:A:52:LYS:HB2	1:A:90:ILE:HG23	1.65	0.79
1:B:277:LEU:HD23	1:B:278:THR:H	1.47	0.78
1:D:215:ARG:NH1	1:D:215:ARG:HA	1.98	0.77
1:D:141:SER:H	1:D:144:GLN:HE21	1.29	0.76
1:A:154:GLU:HG3	1:C:63:ILE:HD11	1.66	0.76
1:A:202:GLN:HA	5:A:316:HOH:O	1.86	0.74
1:C:45:LEU:O	1:C:265:LYS:HE3	1.87	0.74
1:A:267:LEU:CD1	1:B:267[B]:LEU:HD21	2.17	0.74
1:C:57:ALA:O	1:C:60[B]:ARG:HD2	1.87	0.73
1:B:141:SER:H	1:B:144:GLN:HE21	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:HD21	1:C:144:GLN:HB2	1.71	0.72
1:D:215:ARG:HA	1:D:215:ARG:HH11	1.53	0.72
1:C:140:LEU:HD21	1:C:144:GLN:CB	2.20	0.71
1:D:6:ASN:CB	1:D:7[A]:ASP:OD2	2.38	0.71
1:B:102:VAL:HG12	1:B:109[A]:ILE:HD12	1.74	0.69
1:B:190:ASN:ND2	5:B:824:HOH:O	2.25	0.69
1:C:140:LEU:HD23	1:C:144:GLN:HB2	1.75	0.69
1:A:214[B]:ARG:HH11	1:A:214[B]:ARG:CG	1.93	0.68
1:A:133:ASN:HD21	1:A:163:CYS:HB2	1.60	0.66
1:C:100:GLN:O	1:C:104:GLU:HG3	1.96	0.66
1:A:198:THR:HG21	1:A:236:GLU:HG3	1.78	0.66
1:D:40:GLU:HG3	1:D:41:VAL:N	2.10	0.66
1:D:7[A]:ASP:OD2	1:D:7[A]:ASP:N	2.30	0.65
1:A:215:ARG:O	1:A:260:PHE:HZ	1.81	0.64
1:C:52:LYS:NZ	1:C:236:GLU:HG2	2.13	0.63
1:A:214[B]:ARG:NH1	1:A:214[B]:ARG:CG	2.56	0.62
1:D:133:ASN:HD21	1:D:163:CYS:HB2	1.64	0.62
1:C:267[A]:LEU:HD13	1:D:267[A]:LEU:CD1	2.28	0.62
1:C:52:LYS:HE2	1:C:234:PHE:CE1	2.35	0.61
1:C:165[B]:ARG:NH1	5:C:883:HOH:O	2.33	0.61
1:B:133:ASN:HD21	1:B:163:CYS:HB2	1.64	0.61
1:B:95:GLU:HG3	5:B:828:HOH:O	2.00	0.61
1:D:165:ARG:O	1:D:165:ARG:HD3	2.01	0.60
1:A:236:GLU:HG2	5:A:324:HOH:O	2.00	0.60
1:B:102:VAL:HG12	1:B:109[A]:ILE:CD1	2.31	0.60
1:B:195:PHE:CE2	1:B:197[B]:VAL:HG22	2.38	0.59
1:D:123:VAL:HG12	1:D:127:LYS:HE2	1.83	0.59
1:C:52:LYS:HZ3	1:C:236:GLU:HG2	1.66	0.59
1:A:110:GLN:HE22	1:A:234:PHE:HZ	1.50	0.58
1:B:92:ASP:OD1	1:B:94:HIS:HE1	1.86	0.58
1:C:215:ARG:N	1:C:215:ARG:CD	2.61	0.58
1:C:37:HIS:HE1	1:C:254:LEU:O	1.86	0.58
1:C:196:ASP:HA	1:C:234:PHE:HB3	1.84	0.58
1:B:219:LEU:HD21	1:B:263:ARG:HD3	1.85	0.58
1:C:52:LYS:CD	1:C:234:PHE:CZ	2.87	0.57
1:A:201:LEU:O	1:A:202:GLN:CB	2.53	0.57
1:D:129:GLY:O	1:D:159:LYS:NZ	2.33	0.57
1:A:201:LEU:O	1:A:202:GLN:HB3	2.04	0.56
1:C:133:ASN:HD21	1:C:163:CYS:HB2	1.69	0.56
1:C:276:ILE:HG22	1:C:277:LEU:N	2.21	0.55
1:C:267[A]:LEU:HD13	1:D:267[A]:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HE2	5:A:334:HOH:O	2.06	0.55
1:D:22:ILE:HG23	1:D:34:THR:HG21	1.88	0.54
1:C:52:LYS:HD2	1:C:234:PHE:CZ	2.43	0.54
1:A:215:ARG:O	1:A:260:PHE:CZ	2.60	0.54
1:B:136:LYS:CE	1:B:164:GLU:OE1	2.55	0.53
1:C:52:LYS:HE2	1:C:234:PHE:CZ	2.43	0.53
1:A:214[B]:ARG:HD3	1:A:215:ARG:N	2.24	0.53
1:A:69:VAL:HB	1:A:73:GLU:HG2	1.91	0.53
1:C:1:MET:HE2	1:C:191:LEU:HD23	1.89	0.53
1:A:267:LEU:HD13	1:B:267[B]:LEU:CD2	2.34	0.53
1:B:141:SER:H	1:B:144:GLN:NE2	2.02	0.53
1:A:22:ILE:HG23	1:A:34:THR:HG21	1.91	0.52
1:C:24:VAL:HG22	1:C:57:ALA:HB2	1.91	0.52
1:C:153:HIS:HE1	5:C:454:HOH:O	1.93	0.52
1:C:228:THR:O	1:C:229:ARG:HB3	2.11	0.51
1:C:267[A]:LEU:CD1	1:D:267[A]:LEU:CD1	2.89	0.51
1:C:37:HIS:CE1	1:C:254:LEU:O	2.63	0.50
1:B:123:VAL:O	1:B:127[B]:LYS:HG2	2.11	0.50
1:B:201:LEU:C	1:B:202:GLN:HG2	2.31	0.49
1:B:22:ILE:HG23	1:B:34:THR:HG21	1.94	0.49
1:D:110:GLN:NE2	1:D:135:LYS:HE3	2.28	0.49
1:B:40:GLU:CG	5:B:382:HOH:O	2.31	0.49
1:C:165[B]:ARG:CD	5:C:625:HOH:O	2.61	0.48
1:D:141:SER:H	1:D:144:GLN:NE2	2.03	0.48
1:A:69:VAL:HB	1:A:73:GLU:CG	2.44	0.48
1:A:196:ASP:HA	1:A:234:PHE:CB	2.36	0.48
1:C:182:GLY:O	1:C:186:GLN:HG2	2.14	0.48
1:C:222:ALA:O	1:C:226:MET:HG2	2.13	0.48
1:C:140:LEU:HD21	1:C:144:GLN:HB3	1.93	0.47
1:C:252:LEU:HD22	5:C:338:HOH:O	2.14	0.47
1:A:137:PRO:HG2	1:A:140:LEU:HD12	1.96	0.47
1:C:1:MET:CE	1:C:191:LEU:HD23	2.45	0.47
1:B:136:LYS:HE2	1:B:164:GLU:OE1	2.15	0.46
1:B:71:LEU:HD21	1:B:102:VAL:HG23	1.98	0.46
1:C:24:VAL:CG2	1:C:57:ALA:HB2	2.45	0.46
5:A:665:HOH:O	1:C:142:PRO:HG3	2.15	0.46
1:C:267[A]:LEU:CD1	1:D:267[A]:LEU:HD13	2.45	0.46
1:C:60[B]:ARG:CG	5:C:404:HOH:O	2.64	0.46
1:B:190:ASN:CG	5:B:824:HOH:O	2.54	0.46
1:C:228:THR:O	1:C:229:ARG:CB	2.65	0.45
1:B:22:ILE:CG2	1:B:34:THR:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASP:OD1	1:B:94:HIS:CE1	2.68	0.45
1:D:22:ILE:HD11	1:D:25:LEU:HD23	1.98	0.45
1:A:276:ILE:C	5:A:297:HOH:O	2.54	0.45
1:A:52:LYS:HD2	1:A:53:ALA:N	2.32	0.45
1:A:180:GLY:HA3	5:A:288:HOH:O	2.16	0.45
1:A:219:LEU:HD22	1:B:277:LEU:HD12	2.00	0.44
1:C:277:LEU:HD12	1:C:277:LEU:C	2.38	0.44
1:B:202:GLN:HG3	5:B:373:HOH:O	2.17	0.44
1:B:45:LEU:O	1:B:265:LYS:HE3	2.18	0.44
1:A:146:LYS:HB3	1:A:146:LYS:HE2	1.42	0.43
1:C:201[B]:LEU:C	5:C:370:HOH:O	2.56	0.43
1:C:197[B]:VAL:CG1	1:C:233:LEU:HD11	2.48	0.43
1:A:44:LYS:NZ	1:A:258:GLU:OE2	2.47	0.43
1:D:40:GLU:HG3	1:D:41:VAL:H	1.80	0.43
1:D:169:PHE:CD2	1:D:175[B]:VAL:HG23	2.54	0.42
1:A:267:LEU:HD11	1:B:267[B]:LEU:HD21	2.00	0.42
1:B:197[B]:VAL:CG2	1:B:233:LEU:HD11	2.49	0.42
1:C:171:TYR:O	1:C:172:ASP:HB2	2.19	0.42
1:D:146:LYS:O	1:D:150:GLU:HG3	2.20	0.42
1:A:100:GLN:N	1:A:101:PRO:HD2	2.34	0.42
1:B:197[B]:VAL:HG21	1:B:233:LEU:HD11	2.02	0.42
1:C:150:GLU:OE1	1:C:154:GLU:HG3	2.19	0.42
1:C:24:VAL:O	1:C:26:GLU:HG2	2.20	0.42
1:D:6:ASN:HB2	1:D:7[A]:ASP:OD2	2.18	0.42
1:D:222:ALA:O	1:D:226:MET:HG2	2.19	0.42
1:D:256:LEU:HD12	1:D:256:LEU:HA	1.89	0.42
1:B:196:ASP:HA	1:B:234:PHE:HB3	2.02	0.42
1:B:200[B]:SER:C	1:B:202:GLN:H	2.24	0.42
1:A:165:ARG:HH12	1:A:174:LEU:CD1	2.33	0.41
1:B:267[B]:LEU:HD23	1:B:267[B]:LEU:HA	1.86	0.41
1:B:227:ALA:HA	1:B:267[A]:LEU:HD21	2.02	0.41
1:A:198:THR:CG2	1:A:236:GLU:HG3	2.49	0.41
4:C:281:GOL:H32	1:D:179:LEU:HD12	2.02	0.41
1:A:137:PRO:HB3	1:A:139:PHE:CE1	2.56	0.41
1:D:135:LYS:NZ	1:D:196:ASP:OD2	2.42	0.41
1:C:52:LYS:CE	1:C:234:PHE:CZ	3.04	0.41
1:A:228:THR:O	1:A:229:ARG:CB	2.68	0.41
1:B:26:GLU:O	1:B:69:VAL:CG1	2.69	0.41
1:C:173:ASN:ND2	1:C:174:LEU:H	2.20	0.40
1:D:196:ASP:HA	1:D:234:PHE:HB3	2.02	0.40
1:D:55:PHE:CD1	1:D:56:ASP:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:O	1:A:229:ARG:HB3	2.21	0.40
1:B:23:ASN:ND2	1:B:24[B]:VAL:HG23	2.37	0.40
1:D:98:GLN:O	1:D:102:VAL:HG23	2.21	0.40
1:D:219:LEU:HD21	1:D:263:ARG:HD3	2.02	0.40
1:D:94:HIS:C	1:D:95:GLU:HG2	2.42	0.40
1:D:199:HIS:O	1:D:202:GLN:HG2	2.21	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	247/280 (88%)	242 (98%)	4 (2%)	1 (0%)	34	22
1	B	250/280 (89%)	245 (98%)	4 (2%)	1 (0%)	34	22
1	C	251/280 (90%)	247 (98%)	3 (1%)	1 (0%)	34	22
1	D	249/280 (89%)	246 (99%)	2 (1%)	1 (0%)	34	22
All	All	997/1120 (89%)	980 (98%)	13 (1%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	ARG
1	A	229	ARG
1	D	229	ARG
1	B	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	213/235 (91%)	204 (96%)	9 (4%)	30 17
1	B	219/235 (93%)	208 (95%)	11 (5%)	24 11
1	C	221/235 (94%)	213 (96%)	8 (4%)	35 23
1	D	218/235 (93%)	204 (94%)	14 (6%)	17 6
All	All	871/940 (93%)	829 (95%)	42 (5%)	28 12

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	52	LYS
1	A	56	ASP
1	A	67	ARG
1	A	84	GLU
1	A	141	SER
1	A	165	ARG
1	A	173	ASN
1	A	234	PHE
1	B	24[A]	VAL
1	B	24[B]	VAL
1	B	76	LYS
1	B	84	GLU
1	B	95	GLU
1	B	150	GLU
1	B	190	ASN
1	B	200[A]	SER
1	B	200[B]	SER
1	B	202	GLN
1	B	214	ARG
1	C	40	GLU
1	C	60[A]	ARG
1	C	60[B]	ARG
1	C	140	LEU
1	C	165[A]	ARG
1	C	165[B]	ARG
1	C	215	ARG
1	C	277	LEU

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Mol	Chain	Res	Type
1	D	7[A]	ASP
1	D	7[B]	ASP
1	D	29	ASP
1	D	33	GLN
1	D	43	ARG
1	D	67	ARG
1	D	95	GLU
1	D	165	ARG
1	D	173	ASN
1	D	186	GLN
1	D	215	ARG
1	D	235	LEU
1	D	254	LEU
1	D	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	130	ASN
1	A	133	ASN
1	A	173	ASN
1	B	33	GLN
1	B	94	HIS
1	B	133	ASN
1	B	138	GLN
1	B	144	GLN
1	B	190	ASN
1	B	274	GLN
1	C	37	HIS
1	C	94	HIS
1	C	100	GLN
1	C	110	GLN
1	C	118	GLN
1	C	130	ASN
1	C	133	ASN
1	C	144	GLN
1	C	173	ASN
1	D	23	ASN
1	D	133	ASN
1	D	144	GLN
1	D	147	ASN

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Mol	Chain	Res	Type
1	D	173	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	GOL	C	281	-	5,5,5	0.59	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
4	GOL	C	281	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	281	GOL	O1-C1-C2-C3
4	C	281	GOL	O2-C2-C3-O3
4	C	281	GOL	C1-C2-C3-O3
4	C	281	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	281	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	250/280 (89%)	0.81	32 (12%) 3 6	19, 36, 54, 75	1 (0%)
1	B	250/280 (89%)	0.60	22 (8%) 10 16	20, 30, 46, 67	1 (0%)
1	C	251/280 (89%)	0.61	20 (7%) 12 19	21, 32, 48, 63	0
1	D	249/280 (88%)	0.94	46 (18%) 1 1	21, 40, 63, 72	0
All	All	1000/1120 (89%)	0.74	120 (12%) 4 7	19, 34, 58, 75	2 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	SER	7.9
1	D	66	TYR	6.7
1	A	214[A]	ARG	5.9
1	C	255	HIS	5.5
1	C	252	LEU	5.5
1	A	66	TYR	5.3
1	C	277	LEU	5.2
1	A	213	GLY	5.2
1	D	30[A]	SER	5.1
1	A	67	ARG	5.0
1	B	277	LEU	4.9
1	D	276	ILE	4.9
1	A	215	ARG	4.8
1	B	278	THR	4.7
1	B	255	HIS	4.5
1	A	64	HIS	4.4
1	D	62	SER	4.4
1	C	237	SER	4.4
1	A	30	SER	4.3
1	D	254	LEU	4.3
1	A	202	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	275	PRO	4.1
1	B	233	LEU	4.0
1	C	233	LEU	4.0
1	B	194	ILE	3.9
1	C	253	PRO	3.9
1	C	256	LEU	3.9
1	A	216	ALA	3.8
1	D	72	GLU	3.8
1	D	33	GLN	3.7
1	D	71	LEU	3.7
1	D	202	GLN	3.7
1	A	276	ILE	3.6
1	D	22	ILE	3.6
1	D	97	HIS	3.6
1	A	254	LEU	3.5
1	A	61	SER	3.5
1	D	203	THR	3.5
1	C	251	ALA	3.4
1	C	254	LEU	3.4
1	A	33	GLN	3.3
1	D	61	SER	3.3
1	D	67	ARG	3.3
1	D	27	SER	3.3
1	D	104	GLU	3.2
1	B	256	LEU	3.2
1	D	172	ASP	3.2
1	A	256	LEU	3.1
1	D	28	LEU	3.1
1	D	105	VAL	3.1
1	D	26	GLU	3.1
1	D	83	ALA	3.1
1	D	1	MET	3.1
1	D	233	LEU	3.0
1	D	237[A]	SER	3.0
1	A	7	ASP	3.0
1	D	255	HIS	2.9
1	D	31	THR	2.9
1	D	60	ARG	2.9
1	B	237	SER	2.8
1	D	64	HIS	2.8
1	C	215	ARG	2.8
1	A	97	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	2.8
1	D	29	ASP	2.8
1	A	65	SER	2.8
1	B	235	LEU	2.7
1	A	29	ASP	2.7
1	D	23	ASN	2.7
1	D	215	ARG	2.7
1	B	18	LEU	2.7
1	D	256	LEU	2.7
1	D	7[A]	ASP	2.6
1	D	193	VAL	2.6
1	C	232	GLY	2.6
1	A	234	PHE	2.6
1	D	65	SER	2.6
1	D	68	GLY	2.6
1	D	194	ILE	2.6
1	D	81	VAL	2.5
1	A	58	ALA	2.5
1	D	69	VAL	2.5
1	C	235	LEU	2.5
1	B	200[A]	SER	2.4
1	C	195	PHE	2.4
1	C	19	PHE	2.4
1	B	172	ASP	2.4
1	B	163	CYS	2.4
1	C	140	LEU	2.3
1	B	19	PHE	2.3
1	C	150	GLU	2.3
1	C	194	ILE	2.3
1	B	147	ASN	2.3
1	B	1	MET	2.3
1	D	216	ALA	2.3
1	B	7	ASP	2.3
1	B	232	GLY	2.2
1	D	195	PHE	2.2
1	A	194	ILE	2.2
1	C	90	ILE	2.2
1	A	84	GLU	2.2
1	D	186	GLN	2.2
1	D	18	LEU	2.2
1	C	29	ASP	2.2
1	B	202	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	23	ASN	2.1
1	A	120	ASP	2.1
1	D	50	ILE	2.1
1	A	186	GLN	2.1
1	B	195	PHE	2.1
1	D	234	PHE	2.1
1	B	97	HIS	2.1
1	D	4	LYS	2.1
1	C	193	VAL	2.0
1	A	163	CYS	2.0
1	A	24	VAL	2.0
1	B	215	ARG	2.0
1	B	150	GLU	2.0
1	A	235	LEU	2.0
1	A	72	GLU	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	281	6/6	0.87	0.25	17,25,29,30	0
3	NA	B	281	1/1	0.90	0.22	26,26,26,26	0
2	CL	A	281	1/1	0.91	0.13	29,29,29,29	0
2	CL	D	281	1/1	0.97	0.10	27,27,27,27	0
2	CL	C	282	1/1	0.98	0.19	19,19,19,19	1

6.5 Other polymers (i)

There are no such residues in this entry.