



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 01:37 PM EDT

PDB ID : 3FYO
Title : Crystal structure of the triple mutant (N23C/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 : 1.90 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 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	:	2.23.2
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)	:	2.23.2

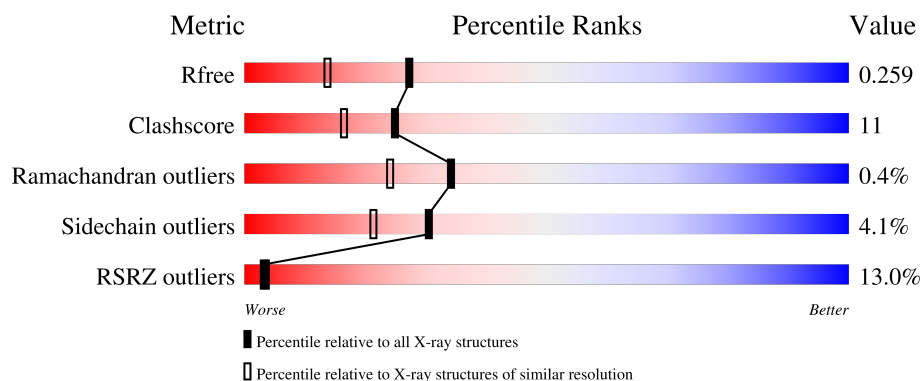
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	<div> <div>19%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	280	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	280	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	280	<div> <div>14%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8610 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	255	Total	C	N	O	S	0	10	0
			1995	1287	335	361	12			
1	B	262	Total	C	N	O	S	0	11	0
			2082	1337	352	381	12			
1	C	256	Total	C	N	O	S	0	5	0
			2002	1290	336	364	12			
1	D	261	Total	C	N	O	S	0	12	0
			2064	1327	348	374	15			

There are 12 discrepancies between the modelled and reference sequences:

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

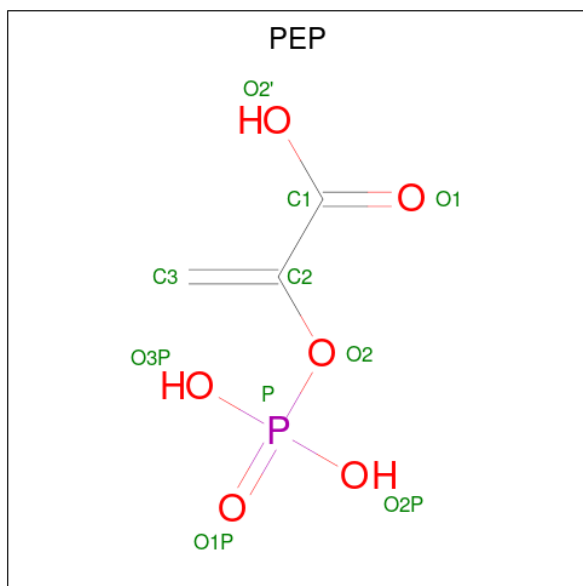
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: C₃H₅O₆P).



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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

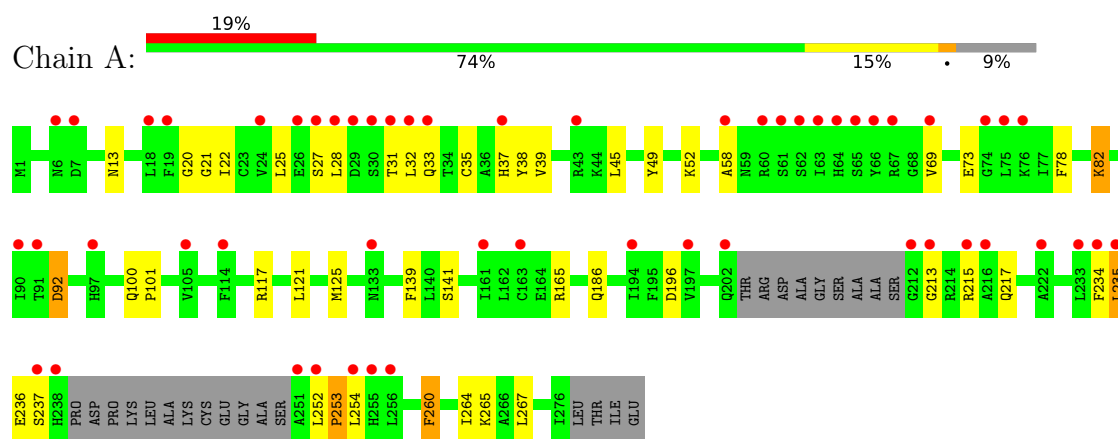
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	86	Total	O	0	0
			86	86		
6	B	122	Total	O	0	0
			122	122		
6	C	123	Total	O	0	0
			123	123		
6	D	122	Total	O	0	0
			122	122		

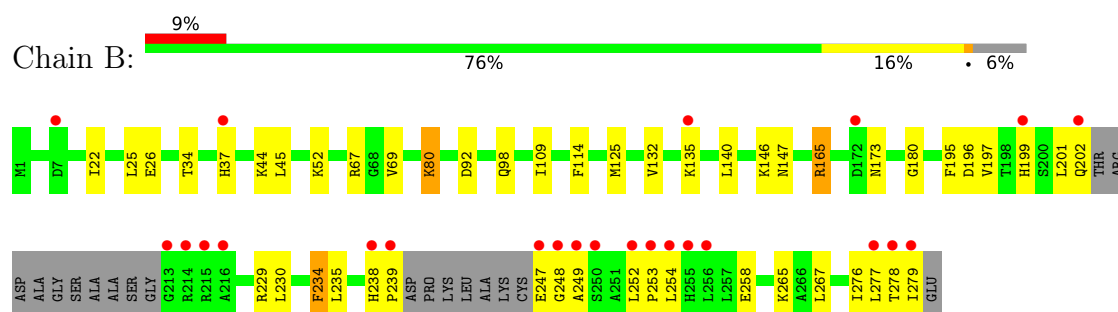
3 Residue-property plots

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.

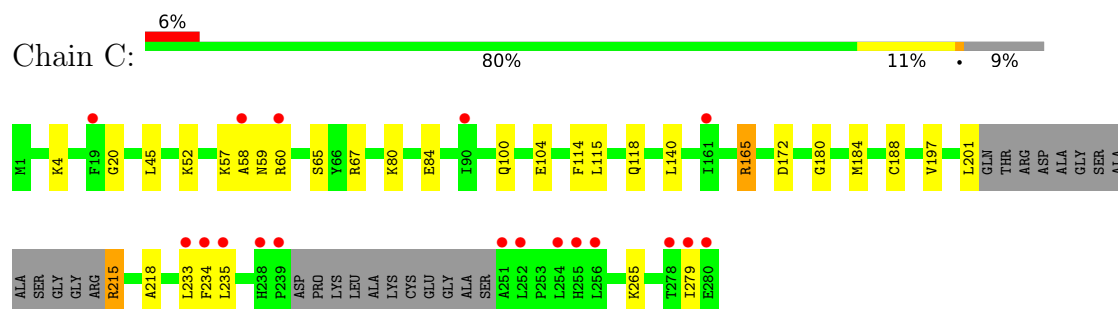
- Molecule 1: 3-deoxy-D-manno-octulosonic acid 8-phosphate synthetase



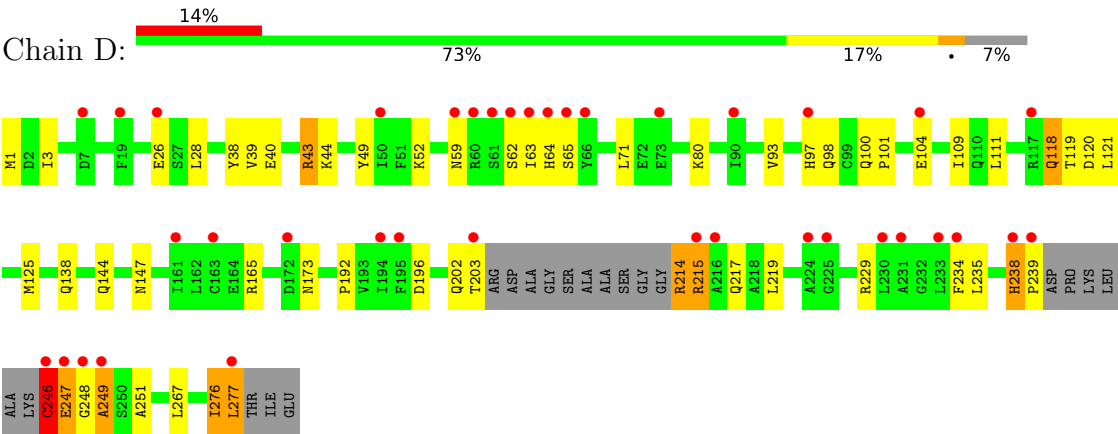
- Molecule 1: 3-deoxy-D-manno-octulosonic acid 8-phosphate synthetase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.74Å 86.20Å 163.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.94 – 1.90 33.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.94-1.90) 99.4 (33.95-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.257 0.217 , 0.259	Depositor DCC
R_{free} test set	4644 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8610	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEP, NA, MN, 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	0.45	0/2042	0.54	0/2763
1	B	0.50	0/2134	0.56	0/2884
1	C	0.49	0/2043	0.56	0/2760
1	D	0.48	0/2137	0.56	2/2889 (0.1%)
All	All	0.48	0/8356	0.55	2/11296 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1[A]	MET	N-CA-C	6.53	128.64	111.00
1	D	1[B]	MET	N-CA-C	6.53	128.64	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	215	ARG	Peptide
1	D	246	CYS	Peptide

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	1995	0	2023	51	0
1	B	2082	0	2129	70	0
1	C	2002	0	2056	24	0
1	D	2064	0	2126	45	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	C	1	0	0	0	0
4	D	10	0	2	0	0
5	D	1	0	0	0	0
6	A	86	0	0	8	0
6	B	122	0	0	13	0
6	C	123	0	0	4	0
6	D	122	0	0	1	0
All	All	8610	0	8336	179	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 11.

All (179) 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:B:37[B]:HIS:CD2	1:B:254:LEU:HD11	1.54	1.39
1:B:135:LYS:HE2	1:B:165[B]:ARG:NH1	1.42	1.30
1:D:118:GLN:NE2	1:D:120:ASP:OD2	1.70	1.25
1:B:165[B]:ARG:NH2	6:B:548:HOH:O	1.57	1.24
1:A:141[A]:SER:OG	6:A:305:HOH:O	1.62	1.16
1:A:235:LEU:HD12	1:A:235:LEU:C	1.66	1.15
1:C:165[B]:ARG:HG3	1:C:165[B]:ARG:HH11	0.96	1.12
1:A:254[B]:LEU:O	6:A:281:HOH:O	1.71	1.09
1:A:139:PHE:O	6:A:306:HOH:O	1.70	1.08
1:A:254[A]:LEU:O	6:A:281:HOH:O	1.71	1.08
1:B:37[B]:HIS:CD2	1:B:254:LEU:CD1	2.38	1.07
1:B:52:LYS:HD3	1:B:234:PHE:HZ	1.20	1.04
1:C:165[B]:ARG:HG3	1:C:165[B]:ARG:NH1	1.65	0.99
1:B:37[B]:HIS:HD2	1:B:254:LEU:CD1	1.73	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37[B]:HIS:CD2	1:B:254:LEU:HD21	1.99	0.98
1:C:165[B]:ARG:HH11	1:C:165[B]:ARG:CG	1.76	0.97
1:A:235:LEU:CD1	1:A:236:GLU:N	2.30	0.95
1:D:246:CYS:O	1:D:247:GLU:CG	2.15	0.95
1:A:260[B]:PHE:CE2	1:A:264[B]:ILE:HD11	2.02	0.94
1:A:235:LEU:C	1:A:235:LEU:CD1	2.35	0.94
1:B:52:LYS:HD3	1:B:234:PHE:CZ	2.00	0.94
1:B:109:ILE:HG22	1:B:125:MET:HE3	1.47	0.94
1:B:199[B]:HIS:CG	6:B:548:HOH:O	2.23	0.91
1:B:135:LYS:HE2	1:B:165[B]:ARG:HH12	1.09	0.89
1:B:37[B]:HIS:HD2	1:B:254:LEU:HD11	0.91	0.89
1:D:246:CYS:O	1:D:247:GLU:HG3	1.76	0.86
1:A:260[B]:PHE:CE2	1:A:264[B]:ILE:CD1	2.59	0.85
1:B:235:LEU:C	1:B:235:LEU:HD13	1.97	0.84
1:A:235:LEU:HD13	1:A:236:GLU:N	1.91	0.84
1:B:98:GLN:OE1	6:B:409:HOH:O	1.96	0.83
1:A:58:ALA:HB1	1:C:118:GLN:HE22	1.45	0.82
1:B:199[A]:HIS:ND1	6:B:548:HOH:O	2.11	0.81
1:B:109:ILE:CG2	1:B:125:MET:HE3	2.10	0.81
1:B:235:LEU:HD13	1:B:235:LEU:O	1.80	0.80
1:B:109:ILE:HG22	1:B:125:MET:CE	2.10	0.79
1:B:52:LYS:CD	1:B:234:PHE:CZ	2.59	0.76
1:C:172:ASP:OD1	6:C:671:HOH:O	2.03	0.76
1:B:37[B]:HIS:CD2	1:B:254:LEU:CD2	2.69	0.74
1:B:135:LYS:HE2	1:B:165[B]:ARG:HH11	1.49	0.74
1:A:237:SER:HB3	1:A:252:LEU:O	1.88	0.74
1:B:135:LYS:CE	1:B:165[B]:ARG:NH1	2.38	0.72
1:B:92[B]:ASP:OD1	6:B:284:HOH:O	2.07	0.72
1:A:267:LEU:HD13	1:B:267[A]:LEU:CD1	2.22	0.70
1:D:238[B]:HIS:ND1	1:D:239:PRO:HD2	2.07	0.69
1:A:235:LEU:HD12	1:A:236:GLU:N	1.97	0.69
1:B:199[A]:HIS:O	1:B:202:GLN:N	2.23	0.69
1:B:235:LEU:O	1:B:235:LEU:CD1	2.39	0.69
1:A:37[A]:HIS:CD2	6:A:282:HOH:O	2.46	0.69
1:B:165[A]:ARG:NH2	1:B:199[A]:HIS:CE1	2.61	0.69
1:A:22:ILE:HD11	1:A:25:LEU:HD23	1.74	0.68
1:B:252:LEU:HD22	1:B:253:PRO:HD2	1.75	0.68
1:B:37[B]:HIS:NE2	1:B:254:LEU:HD21	2.09	0.67
1:B:247:GLU:HA	6:B:577:HOH:O	1.95	0.67
1:A:27:SER:O	1:A:31:THR:HG23	1.95	0.66
1:B:247:GLU:OE1	1:B:249:ALA:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLU:HB3	1:D:249:ALA:H	1.61	0.65
1:A:260[B]:PHE:CD2	1:A:264[B]:ILE:HD12	2.31	0.65
1:B:92[A]:ASP:OD1	6:B:549:HOH:O	2.15	0.65
1:B:199[A]:HIS:CG	6:B:548:HOH:O	2.49	0.64
1:C:58:ALA:O	1:C:59:ASN:CB	2.43	0.64
1:D:246:CYS:O	1:D:247:GLU:CB	2.45	0.64
1:C:215:ARG:N	6:C:611:HOH:O	2.30	0.64
1:A:58:ALA:HB1	1:C:118:GLN:NE2	2.12	0.64
1:A:260[B]:PHE:CD2	1:A:264[B]:ILE:CD1	2.82	0.63
1:A:78:PHE:O	1:A:82:LYS:HG3	1.98	0.63
1:A:235:LEU:HD12	1:A:235:LEU:O	1.98	0.63
1:B:26:GLU:O	1:B:69:VAL:HG11	1.98	0.63
1:D:235:LEU:C	1:D:235:LEU:HD12	2.19	0.62
1:B:125:MET:HE2	1:B:132:VAL:HG13	1.82	0.62
1:A:13[B]:ASN:HB2	6:A:441:HOH:O	1.98	0.62
1:B:26:GLU:O	1:B:69:VAL:CG1	2.47	0.62
1:B:52:LYS:CD	1:B:234:PHE:HZ	1.96	0.62
1:D:121:LEU:O	1:D:125[A]:MET:HG3	1.99	0.62
1:A:196:ASP:HA	1:A:234:PHE:HB3	1.81	0.61
1:B:67:ARG:NH2	1:D:119:THR:HG22	2.15	0.60
1:A:100:GLN:N	1:A:101:PRO:HD2	2.16	0.60
1:B:80:LYS:N	1:B:80:LYS:HD3	2.16	0.60
1:A:52[B]:LYS:NZ	1:A:236:GLU:OE2	2.30	0.60
1:B:235:LEU:C	1:B:235:LEU:CD1	2.69	0.59
1:B:196:ASP:HA	1:B:234:PHE:HB3	1.83	0.59
1:C:100:GLN:O	1:C:104:GLU:HG3	2.03	0.58
1:B:247:GLU:CD	1:B:248:GLY:H	2.06	0.58
1:B:92[B]:ASP:CG	6:B:284:HOH:O	2.42	0.58
1:B:37[B]:HIS:CD2	1:B:254:LEU:CG	2.87	0.57
1:A:267:LEU:CD1	1:B:267[A]:LEU:HD13	2.35	0.56
1:D:173[A]:ASN:OD1	1:D:203:THR:CG2	2.53	0.56
1:B:37[B]:HIS:CG	1:B:254:LEU:HD21	2.39	0.56
1:C:279:ILE:HD11	1:D:219:LEU:HB2	1.87	0.55
1:B:196:ASP:OD2	1:B:199[B]:HIS:HD2	1.90	0.55
1:A:254[A]:LEU:O	1:A:254[A]:LEU:HD23	2.06	0.55
1:D:109:ILE:HD12	1:D:125[B]:MET:HG2	1.89	0.55
1:C:52:LYS:C	1:C:52:LYS:HD3	2.28	0.54
1:D:100:GLN:HB3	1:D:101:PRO:HD3	1.90	0.54
1:D:93:VAL:CG2	1:D:125[B]:MET:HE2	2.38	0.54
1:A:237:SER:CB	1:A:252:LEU:O	2.56	0.54
1:B:22:ILE:CG2	1:B:34:THR:HG21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146[B]:LYS:HE2	1:B:147:ASN:HD21	1.72	0.54
1:A:25:LEU:HD22	1:A:31:THR:HG21	1.90	0.53
1:D:111:LEU:HA	1:D:125[B]:MET:HE3	1.91	0.53
1:A:28:LEU:O	1:A:32:LEU:HG	2.10	0.52
1:D:100:GLN:O	1:D:104:GLU:HG2	2.09	0.52
1:A:254[B]:LEU:O	1:A:254[B]:LEU:HD23	2.09	0.52
1:B:37[B]:HIS:NE2	1:B:254:LEU:HD11	2.15	0.52
1:D:97:HIS:HD2	6:D:572:HOH:O	1.93	0.52
1:A:235:LEU:HD13	1:A:236:GLU:H	1.73	0.52
1:A:267:LEU:CD1	1:B:267[A]:LEU:CD1	2.88	0.51
1:C:197:VAL:HG21	1:C:233:LEU:HD11	1.92	0.51
1:D:202:GLN:O	1:D:203:THR:HG23	2.11	0.51
1:B:135:LYS:CE	1:B:165[B]:ARG:HH12	2.00	0.51
1:C:197:VAL:CG2	1:C:233:LEU:HD11	2.40	0.51
1:A:69:VAL:HG22	1:A:73:GLU:CB	2.41	0.50
1:B:199[B]:HIS:HB3	6:B:548:HOH:O	2.10	0.50
1:D:39:VAL:O	1:D:43:ARG:HG2	2.12	0.50
1:B:238:HIS:HB2	1:B:239:PRO:HD2	1.94	0.49
1:D:248:GLY:O	1:D:249:ALA:HB3	2.13	0.49
1:B:67:ARG:NH2	1:D:119:THR:CG2	2.76	0.49
1:D:63:ILE:HG13	1:D:64:HIS:CD2	2.48	0.48
1:A:117:ARG:O	1:C:59:ASN:HA	2.14	0.48
1:A:215:ARG:O	1:A:260[A]:PHE:HZ	1.96	0.48
1:B:278:THR:O	1:B:279:ILE:C	2.51	0.48
1:A:213:GLY:O	1:A:217:GLN:N	2.39	0.48
1:B:146[B]:LYS:HD2	1:B:147:ASN:ND2	2.29	0.48
1:B:195:PHE:CE2	1:B:197[B]:VAL:HG22	2.48	0.47
1:B:199[A]:HIS:HB2	6:B:548:HOH:O	2.14	0.47
1:C:67:ARG:HG3	6:C:662:HOH:O	2.13	0.47
1:B:25:LEU:O	1:B:69:VAL:HG13	2.14	0.47
1:D:246:CYS:O	1:D:247:GLU:HG2	2.10	0.47
1:D:93:VAL:HG22	1:D:125[B]:MET:HE1	1.95	0.47
1:B:199[B]:HIS:CB	6:B:548:HOH:O	2.53	0.46
1:D:173[B]:ASN:HA	1:D:203:THR:HG22	1.97	0.46
1:D:173[A]:ASN:HA	1:D:203:THR:HG22	1.97	0.45
1:A:20:GLY:HA2	1:A:235:LEU:O	2.16	0.45
1:D:93:VAL:HG22	1:D:125[B]:MET:CE	2.47	0.45
1:D:215:ARG:NH2	1:D:251:ALA:O	2.42	0.45
1:A:141[B]:SER:HB2	6:A:305:HOH:O	2.16	0.45
1:C:201:LEU:HD11	1:C:218:ALA:HA	1.98	0.45
1:A:35:CYS:O	1:A:39:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ILE:O	1:D:277:LEU:CB	2.65	0.44
1:D:52:LYS:HD3	1:D:52:LYS:C	2.38	0.44
1:A:267:LEU:HD13	1:B:267[A]:LEU:HD11	1.98	0.43
1:A:37[A]:HIS:CG	6:A:282:HOH:O	2.70	0.43
1:B:229:ARG:CD	1:B:276:ILE:HD11	2.49	0.43
1:C:114:PHE:CE2	1:C:115:LEU:HD21	2.54	0.43
1:A:236:GLU:O	1:A:237:SER:OG	2.29	0.43
1:B:44:LYS:HE2	1:B:258:GLU:OE2	2.19	0.43
1:A:38:TYR:HB3	1:A:49:TYR:CZ	2.53	0.42
1:A:92:ASP:OD1	1:A:92:ASP:N	2.36	0.42
1:D:267:LEU:C	1:D:267:LEU:HD23	2.40	0.42
1:D:39:VAL:O	1:D:43:ARG:CG	2.66	0.42
1:A:121:LEU:O	1:A:125:MET:HG3	2.19	0.42
1:D:196:ASP:HA	1:D:234:PHE:HB3	2.01	0.42
1:D:38:TYR:HB3	1:D:49:TYR:CZ	2.55	0.42
1:A:252:LEU:O	1:A:253:PRO:O	2.38	0.42
1:D:71:LEU:CD1	1:D:98:GLN:HG2	2.49	0.42
1:D:93:VAL:CG2	1:D:125[B]:MET:CE	2.98	0.42
1:C:180:GLY:HA3	6:C:417:HOH:O	2.19	0.42
1:D:3:ILE:HD12	1:D:192:PRO:HG2	2.01	0.42
1:B:180:GLY:HA3	6:B:406:HOH:O	2.19	0.41
1:C:80:LYS:NZ	1:C:84:GLU:OE1	2.53	0.41
1:B:45:LEU:O	1:B:265:LYS:HE3	2.20	0.41
1:C:184:MET:O	1:C:188:CYS:HB2	2.20	0.41
1:D:28:LEU:HD13	1:D:80:LYS:HD2	2.02	0.41
1:C:165[B]:ARG:NH1	1:C:165[B]:ARG:CG	2.46	0.41
1:D:173[B]:ASN:OD1	1:D:203:THR:HG22	2.20	0.41
1:B:114:PHE:HE1	1:D:118:GLN:HG3	1.85	0.41
1:B:199[A]:HIS:O	1:B:201:LEU:N	2.54	0.41
1:C:45:LEU:O	1:C:265:LYS:HE3	2.21	0.41
1:D:214:ARG:O	1:D:217:GLN:N	2.39	0.41
1:D:144:GLN:OE1	1:D:147:ASN:ND2	2.54	0.40
1:B:37[B]:HIS:CE1	1:B:254:LEU:HD21	2.56	0.40
1:A:45:LEU:O	1:A:265:LYS:HE3	2.21	0.40
1:B:252:LEU:HD22	1:B:253:PRO:CD	2.48	0.40
1:C:20:GLY:HA2	1:C:235:LEU:O	2.22	0.40
1:C:235:LEU:C	1:C:235:LEU:HD12	2.41	0.40
1:D:62:SER:HB3	1:D:65:SER:OG	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	259/280 (92%)	249 (96%)	9 (4%)	1 (0%)	34	24
1	B	267/280 (95%)	258 (97%)	9 (3%)	0	100	100
1	C	255/280 (91%)	250 (98%)	5 (2%)	0	100	100
1	D	266/280 (95%)	257 (97%)	6 (2%)	3 (1%)	14	5
All	All	1047/1120 (94%)	1014 (97%)	29 (3%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO
1	D	249	ALA
1	D	247	GLU
1	D	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	217/235 (92%)	209 (96%)	8 (4%)	34	25
1	B	232/235 (99%)	224 (97%)	8 (3%)	37	28
1	C	221/235 (94%)	213 (96%)	8 (4%)	35	26
1	D	232/235 (99%)	216 (93%)	16 (7%)	15	7
All	All	902/940 (96%)	862 (96%)	40 (4%)	30	19

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	82	LYS
1	A	92	ASP
1	A	165	ARG
1	A	186	GLN
1	A	235	LEU
1	A	260[A]	PHE
1	A	260[B]	PHE
1	B	80	LYS
1	B	140	LEU
1	B	165[A]	ARG
1	B	165[B]	ARG
1	B	173	ASN
1	B	230	LEU
1	B	234	PHE
1	B	277	LEU
1	C	4	LYS
1	C	57	LYS
1	C	60	ARG
1	C	65	SER
1	C	140	LEU
1	C	165[A]	ARG
1	C	165[B]	ARG
1	C	234	PHE
1	D	26	GLU
1	D	40	GLU
1	D	43	ARG
1	D	44	LYS
1	D	59	ASN
1	D	118	GLN
1	D	138[A]	GLN
1	D	138[B]	GLN
1	D	165	ARG
1	D	214	ARG
1	D	215	ARG
1	D	238[A]	HIS
1	D	238[B]	HIS
1	D	246	CYS
1	D	276	ILE
1	D	277	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	118	GLN
1	B	94	HIS
1	B	98	GLN
1	B	147	ASN
1	B	173	ASN
1	B	202	GLN
1	C	100	GLN
1	C	118	GLN
1	D	64	HIS
1	D	255	HIS

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 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	PEP	D	281	-	6,9,9	3.98	1 (16%)	8,13,13	2.02	2 (25%)

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	PEP	D	281	-	-	0/5/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	281	PEP	C3-C2	9.44	1.51	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	281	PEP	O2-C2-C3	-3.61	117.83	124.79
4	D	281	PEP	C1-C2-C3	-3.43	114.66	121.07

There are no chirality outliers.

There are no torsion outliers.

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, 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	255/280 (91%)	1.02	54 (21%) 0 0	17, 27, 58, 63	1 (0%)
1	B	262/280 (93%)	0.60	24 (9%) 9 10	15, 24, 51, 66	6 (2%)
1	C	256/280 (91%)	0.39	18 (7%) 16 18	16, 24, 42, 60	2 (0%)
1	D	261/280 (93%)	0.81	38 (14%) 2 2	16, 25, 47, 58	3 (1%)
All	All	1034/1120 (92%)	0.70	134 (12%) 3 3	15, 25, 50, 66	12 (1%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	GLU	11.1
1	D	248	GLY	11.0
1	B	248	GLY	8.4
1	B	279	ILE	8.1
1	B	249	ALA	7.3
1	A	61	SER	7.1
1	A	66	TYR	6.9
1	C	239	PRO	6.6
1	D	277	LEU	6.5
1	A	212	GLY	6.4
1	D	249	ALA	6.0
1	D	66	TYR	5.9
1	C	255	HIS	5.7
1	A	251	ALA	5.7
1	B	239	PRO	5.6
1	B	256	LEU	5.6
1	A	64	HIS	5.5
1	C	278	THR	5.0
1	B	255	HIS	5.0
1	A	63	ILE	4.9
1	B	254	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	65	SER	4.7
1	A	213	GLY	4.6
1	B	277	LEU	4.6
1	C	280	GLU	4.5
1	C	279	ILE	4.5
1	A	26	GLU	4.3
1	D	64	HIS	4.3
1	D	246	CYS	4.2
1	B	278	THR	4.2
1	B	250	SER	4.2
1	A	29	ASP	4.1
1	D	247	GLU	4.1
1	A	30	SER	4.0
1	B	215	ARG	4.0
1	D	203	THR	4.0
1	B	238	HIS	3.9
1	B	135	LYS	3.9
1	D	233	LEU	3.8
1	D	194	ILE	3.7
1	A	7	ASP	3.7
1	A	235	LEU	3.6
1	B	253	PRO	3.5
1	D	239	PRO	3.5
1	D	7	ASP	3.4
1	A	28	LEU	3.4
1	A	234	PHE	3.4
1	D	61	SER	3.4
1	B	213	GLY	3.4
1	A	67	ARG	3.3
1	A	19	PHE	3.3
1	D	63	ILE	3.2
1	D	104	GLU	3.2
1	D	60	ARG	3.2
1	B	202	GLN	3.2
1	D	59	ASN	3.2
1	A	33	GLN	3.1
1	B	7[A]	ASP	3.1
1	D	161	ILE	3.1
1	A	197	VAL	3.1
1	A	27	SER	3.1
1	B	252	LEU	3.0
1	A	215	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	215	ARG	3.0
1	A	202	GLN	3.0
1	A	237	SER	2.9
1	B	172	ASP	2.9
1	A	37[A]	HIS	2.9
1	C	238	HIS	2.9
1	A	97	HIS	2.9
1	A	216	ALA	2.9
1	A	62	SER	2.8
1	A	60	ARG	2.8
1	A	24	VAL	2.8
1	A	32	LEU	2.8
1	D	224	ALA	2.8
1	D	19	PHE	2.8
1	A	254[A]	LEU	2.8
1	D	65	SER	2.8
1	D	230	LEU	2.7
1	A	31	THR	2.7
1	A	6	ASN	2.7
1	C	19	PHE	2.6
1	A	238	HIS	2.6
1	A	114[A]	PHE	2.6
1	D	195	PHE	2.6
1	D	172	ASP	2.6
1	A	255	HIS	2.5
1	A	69	VAL	2.5
1	A	233	LEU	2.5
1	A	18	LEU	2.5
1	D	225	GLY	2.5
1	C	252	LEU	2.5
1	A	256	LEU	2.5
1	A	161	ILE	2.4
1	A	194	ILE	2.4
1	D	73	GLU	2.4
1	D	163	CYS	2.4
1	A	222	ALA	2.4
1	C	234	PHE	2.4
1	B	216	ALA	2.4
1	D	117[A]	ARG	2.4
1	D	97	HIS	2.4
1	B	199[A]	HIS	2.3
1	B	214	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	163	CYS	2.3
1	D	238[A]	HIS	2.3
1	A	76	LYS	2.2
1	A	43	ARG	2.2
1	A	252	LEU	2.2
1	C	235	LEU	2.2
1	C	58	ALA	2.2
1	A	74	GLY	2.2
1	C	256	LEU	2.2
1	D	90	ILE	2.2
1	A	90	ILE	2.2
1	D	50	ILE	2.2
1	A	75	LEU	2.2
1	C	233	LEU	2.2
1	A	91	THR	2.2
1	A	105	VAL	2.2
1	B	37[A]	HIS	2.1
1	C	60	ARG	2.1
1	C	251	ALA	2.1
1	C	90	ILE	2.1
1	A	133	ASN	2.1
1	A	58	ALA	2.1
1	D	216	ALA	2.1
1	D	62	SER	2.1
1	D	26	GLU	2.0
1	D	231	ALA	2.0
1	D	234	PHE	2.0
1	C	161	ILE	2.0
1	C	254	LEU	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MN	D	282	1/1	0.90	0.33	27,27,27,27	1
4	PEP	D	281	10/10	0.95	0.19	19,21,26,27	10
2	CL	C	281	1/1	0.96	0.34	24,24,24,24	1
2	CL	B	281	1/1	0.97	0.11	15,15,15,15	1
3	NA	C	282	1/1	0.99	0.07	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.