Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 06:25 PM EDT

PDB ID	:	3STG
Title	:	Crystal structure of A58P, DEL(N59), and loop 7 truncated mutant 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	:	2011-07-09
Resolution	:	2.20 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:

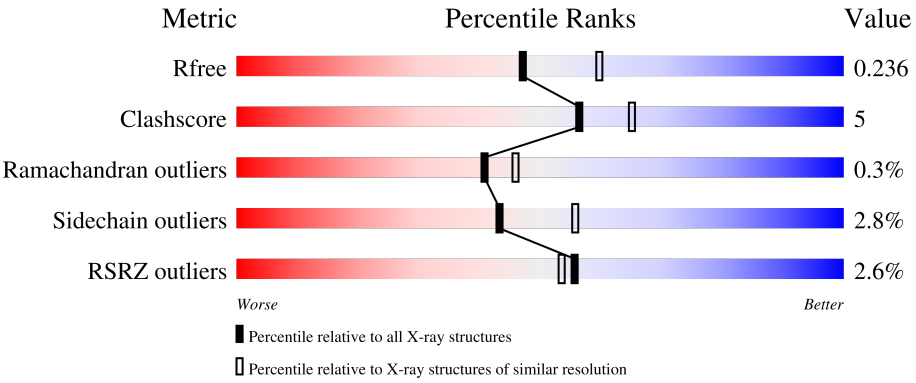
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	268	88% 7%
1	B	268	4% 88% 11%
1	C	268	3% 82% 14%
1	D	268	87% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8729 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	260	Total	C	N	O	S	0	2	0
			2020	1298	340	371	11			
1	B	268	Total	C	N	O	S	0	4	0
			2080	1337	349	382	12			
1	C	260	Total	C	N	O	S	0	4	0
			2030	1307	342	369	12			
1	D	258	Total	C	N	O	S	0	3	0
			2013	1296	339	366	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	PRO	ALA	ENGINEERED MUTATION	UNP Q9JZ55
A	?	-	ASN	DELETION	UNP Q9JZ55
A	?	-	GLN	DELETION	UNP Q9JZ55
A	?	-	THR	DELETION	UNP Q9JZ55
A	?	-	ARG	DELETION	UNP Q9JZ55
A	?	-	ASP	DELETION	UNP Q9JZ55
A	?	-	ALA	DELETION	UNP Q9JZ55
A	?	-	GLY	DELETION	UNP Q9JZ55
A	?	-	SER	DELETION	UNP Q9JZ55
A	?	-	ALA	DELETION	UNP Q9JZ55
A	?	-	ALA	DELETION	UNP Q9JZ55
A	?	-	SER	DELETION	UNP Q9JZ55
A	?	-	GLY	DELETION	UNP Q9JZ55
B	58	PRO	ALA	ENGINEERED MUTATION	UNP Q9JZ55
B	?	-	ASN	DELETION	UNP Q9JZ55
B	?	-	GLN	DELETION	UNP Q9JZ55
B	?	-	THR	DELETION	UNP Q9JZ55
B	?	-	ARG	DELETION	UNP Q9JZ55
B	?	-	ASP	DELETION	UNP Q9JZ55
B	?	-	ALA	DELETION	UNP Q9JZ55
B	?	-	GLY	DELETION	UNP Q9JZ55

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	DELETION	UNP Q9JZ55
B	?	-	ALA	DELETION	UNP Q9JZ55
B	?	-	ALA	DELETION	UNP Q9JZ55
B	?	-	SER	DELETION	UNP Q9JZ55
B	?	-	GLY	DELETION	UNP Q9JZ55
C	58	PRO	ALA	ENGINEERED MUTATION	UNP Q9JZ55
C	?	-	ASN	DELETION	UNP Q9JZ55
C	?	-	GLN	DELETION	UNP Q9JZ55
C	?	-	THR	DELETION	UNP Q9JZ55
C	?	-	ARG	DELETION	UNP Q9JZ55
C	?	-	ASP	DELETION	UNP Q9JZ55
C	?	-	ALA	DELETION	UNP Q9JZ55
C	?	-	GLY	DELETION	UNP Q9JZ55
C	?	-	SER	DELETION	UNP Q9JZ55
C	?	-	ALA	DELETION	UNP Q9JZ55
C	?	-	ALA	DELETION	UNP Q9JZ55
C	?	-	SER	DELETION	UNP Q9JZ55
C	?	-	GLY	DELETION	UNP Q9JZ55
D	58	PRO	ALA	ENGINEERED MUTATION	UNP Q9JZ55
D	?	-	ASN	DELETION	UNP Q9JZ55
D	?	-	GLN	DELETION	UNP Q9JZ55
D	?	-	THR	DELETION	UNP Q9JZ55
D	?	-	ARG	DELETION	UNP Q9JZ55
D	?	-	ASP	DELETION	UNP Q9JZ55
D	?	-	ALA	DELETION	UNP Q9JZ55
D	?	-	GLY	DELETION	UNP Q9JZ55
D	?	-	SER	DELETION	UNP Q9JZ55
D	?	-	ALA	DELETION	UNP Q9JZ55
D	?	-	ALA	DELETION	UNP Q9JZ55
D	?	-	SER	DELETION	UNP Q9JZ55
D	?	-	GLY	DELETION	UNP Q9JZ55

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	4	Total Cl 4 4	0	0
2	C	2	Total Cl 2 2	0	0
2	D	3	Total Cl 3 3	0	0

- Molecule 3 is water.

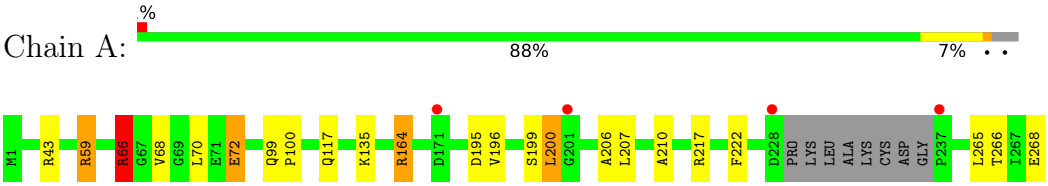
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	150	Total O 150 150	0	0
3	B	138	Total O 138 138	0	0
3	C	135	Total O 135 135	0	0
3	D	151	Total O 151 151	0	0

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.

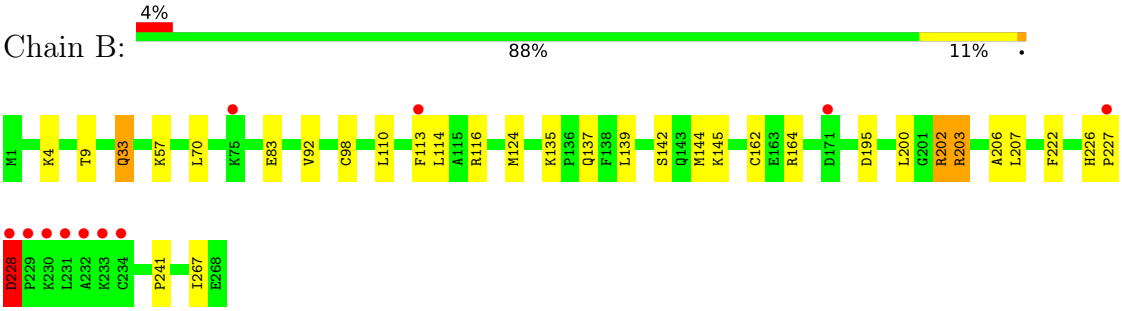
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain A:



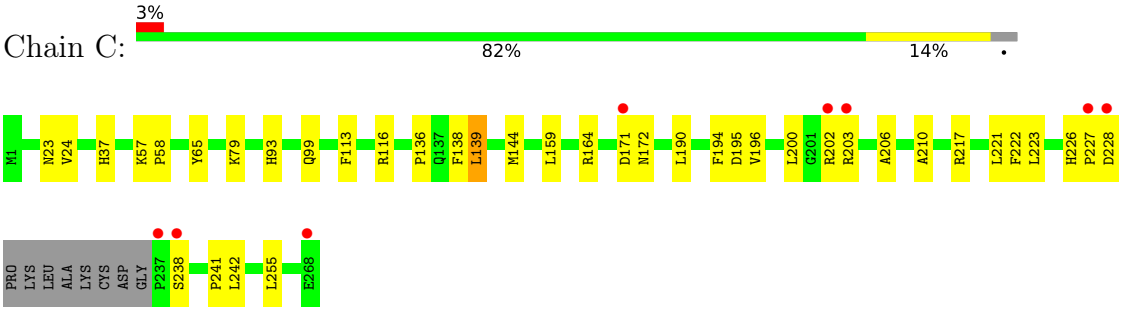
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain B:



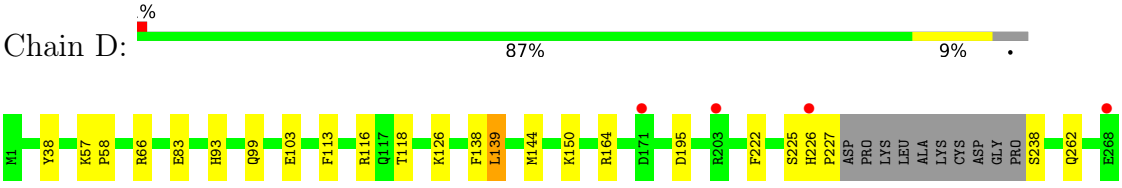
• Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.69Å 104.05Å 149.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.99 – 2.20 36.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.99-2.20) 100.0 (36.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.77 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.238 0.199 , 0.236	Depositor DCC
R_{free} test set	3250 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8729	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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

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	1/2061 (0.0%)	0.60	3/2789 (0.1%)
1	B	0.66	1/2127 (0.0%)	0.66	2/2884 (0.1%)
1	C	0.61	1/2071 (0.0%)	0.59	0/2802
1	D	0.51	0/2053	0.59	0/2777
All	All	0.59	3/8312 (0.0%)	0.61	5/11252 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	CYS	CB-SG	-5.65	1.72	1.81
1	C	65	TYR	CD2-CE2	-5.26	1.31	1.39
1	A	199	SER	CB-OG	-5.05	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	59	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	200	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	228[A]	ASP	N-CA-C	-5.25	96.82	111.00
1	B	228[B]	ASP	N-CA-C	-5.25	96.82	111.00

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	2020	0	2073	15	0
1	B	2080	0	2120	32	0
1	C	2030	0	2087	25	0
1	D	2013	0	2076	16	0
2	A	3	0	0	1	0
2	B	4	0	0	2	0
2	C	2	0	0	0	0
2	D	3	0	0	1	0
3	A	150	0	0	1	0
3	B	138	0	0	6	0
3	C	135	0	0	2	0
3	D	151	0	0	3	0
All	All	8729	0	8356	82	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 5.

All (82) 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:228[A]:ASP:CB	3:B:300:HOH:O	2.20	0.88
1:A:68:VAL:HB	1:A:72:GLU:HG2	1.62	0.81
1:B:228[A]:ASP:HB2	3:B:300:HOH:O	1.80	0.77
1:B:228[A]:ASP:HB3	3:B:300:HOH:O	1.89	0.70
1:D:150:LYS:NZ	3:D:613:HOH:O	2.22	0.68
1:C:202:ARG:NH2	3:C:547:HOH:O	2.27	0.66
1:B:70:LEU:C	1:B:70:LEU:HD13	2.20	0.62
1:D:38:TYR:OH	1:D:225:SER:HB2	2.00	0.61
1:B:33:GLN:NE2	1:B:228[B]:ASP:OD2	2.33	0.61
1:B:110:LEU:CD1	1:B:124:MET:HE3	2.31	0.61
1:C:194:PHE:CE2	1:C:196[B]:VAL:HG12	2.34	0.61
1:B:4:LYS:HE2	1:B:9:THR:OG1	2.01	0.61
1:C:226:HIS:CB	1:C:227:PRO:HD2	2.31	0.60
1:B:110:LEU:HD13	1:B:124:MET:HE3	1.85	0.58
1:B:92[A]:VAL:HG23	1:B:124:MET:CE	2.33	0.58
1:A:196[B]:VAL:HG11	1:A:210:ALA:HB2	1.87	0.56
1:C:255[B]:LEU:C	1:C:255[B]:LEU:HD23	2.25	0.56
1:B:92[B]:VAL:HG11	1:B:98:CYS:SG	2.47	0.55
1:A:195:ASP:HA	1:A:222:PHE:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:PRO:HG2	1:C:139:LEU:HD22	1.88	0.54
1:B:57:LYS:NZ	3:B:348:HOH:O	2.40	0.53
1:B:92[A]:VAL:HG23	1:B:124:MET:HE2	1.89	0.53
1:C:138:PHE:CD2	1:C:139:LEU:HD13	2.46	0.51
1:A:117:GLN:NE2	1:C:113:PHE:CD1	2.79	0.51
1:B:135:LYS:HG3	1:B:144:MET:HE3	1.93	0.50
1:A:59:ARG:HB2	2:A:271:CL:CL	2.49	0.50
1:C:138:PHE:CE2	1:C:139:LEU:HD13	2.47	0.49
1:A:207:LEU:HB2	1:B:267:ILE:HD11	1.94	0.49
1:C:23:ASN:OD1	1:C:57:LYS:NZ	2.37	0.49
1:B:116:ARG:HG3	1:D:113:PHE:CE2	2.48	0.48
1:B:113[B]:PHE:CD1	1:B:114:LEU:HG	2.48	0.48
1:B:113[A]:PHE:HZ	1:D:116:ARG:HH11	1.60	0.48
1:C:79:LYS:HA	1:C:79:LYS:HD2	1.64	0.47
1:D:139:LEU:HD23	1:D:144[B]:MET:HE2	1.95	0.47
1:C:139:LEU:HD23	1:C:144[B]:MET:CE	2.45	0.46
1:B:57:LYS:HG3	2:B:271:CL:CL	2.53	0.46
1:A:70:LEU:C	1:A:70:LEU:HD23	2.36	0.46
1:D:118:THR:OG1	1:D:150:LYS:HE2	2.16	0.46
1:D:116:ARG:HA	3:D:377:HOH:O	2.15	0.46
1:C:203:ARG:HD3	1:C:241:PRO:HD3	1.97	0.45
1:C:58:PRO:HG3	1:C:93:HIS:CD2	2.51	0.45
1:C:37[B]:HIS:HD2	1:C:242:LEU:HG	1.81	0.45
1:B:195:ASP:HA	1:B:222:PHE:HB3	1.97	0.45
1:D:226:HIS:CD2	3:D:274:HOH:O	2.70	0.45
1:C:200:LEU:HD11	1:C:206:ALA:HA	1.99	0.45
3:A:329:HOH:O	1:C:171:ASP:CB	2.64	0.44
1:B:139:LEU:HD23	1:B:144:MET:HE2	1.98	0.44
1:D:195:ASP:HA	1:D:222:PHE:HB3	1.98	0.44
1:A:68:VAL:HB	1:A:72:GLU:CG	2.42	0.44
1:A:265:LEU:HD23	1:B:207:LEU:HD22	2.00	0.44
1:B:92[A]:VAL:HG23	1:B:124:MET:HE1	2.00	0.44
1:C:195:ASP:HA	1:C:222:PHE:HB3	2.00	0.44
1:D:139:LEU:HD23	1:D:144[B]:MET:CE	2.48	0.43
1:A:200:LEU:HD11	1:A:206:ALA:HA	1.99	0.43
1:A:99:GLN:N	1:A:100:PRO:HD2	2.34	0.43
1:D:138:PHE:CE2	1:D:139:LEU:HD13	2.54	0.43
1:B:137:GLN:HG2	2:B:272:CL:CL	2.55	0.43
1:B:226:HIS:HD2	1:B:241:PRO:HA	1.82	0.43
1:C:226:HIS:CB	1:C:227:PRO:CD	2.97	0.43
1:B:70:LEU:HD13	1:B:70:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HD12	1:B:124:MET:HE3	1.99	0.42
1:D:57:LYS:HE3	2:D:271:CL:CL	2.56	0.42
1:D:58:PRO:HA	1:D:66:ARG:HH21	1.85	0.42
1:B:203:ARG:H	1:B:203:ARG:HG3	1.59	0.42
1:B:142:SER:O	1:B:145:LYS:HG2	2.20	0.42
1:C:159:LEU:HB2	1:C:190:LEU:HD13	2.00	0.42
1:A:66:ARG:HH21	1:A:66:ARG:HD3	1.59	0.42
1:A:135:LYS:O	1:A:164:ARG:HD2	2.20	0.41
1:D:99:GLN:O	1:D:103:GLU:HG2	2.20	0.41
1:A:66:ARG:HE	1:A:66:ARG:HB3	1.74	0.41
1:A:59:ARG:HG2	1:C:116:ARG:HB2	2.02	0.41
1:D:226:HIS:HA	1:D:227:PRO:HD3	1.93	0.41
1:C:202:ARG:NH2	3:C:548:HOH:O	2.54	0.41
1:B:92[A]:VAL:CG2	1:B:124:MET:CE	2.99	0.41
1:B:200:LEU:HD11	1:B:206:ALA:HA	2.03	0.41
1:C:24:VAL:HG21	1:C:57:LYS:HG3	2.03	0.41
1:B:57:LYS:HE2	3:B:600:HOH:O	2.20	0.40
1:B:202:ARG:O	3:B:601:HOH:O	2.22	0.40
1:C:37[B]:HIS:CD2	1:C:242:LEU:HG	2.57	0.40
1:C:196[B]:VAL:HG11	1:C:210:ALA:HA	2.03	0.40
1:D:58:PRO:HG2	1:D:93:HIS:CD2	2.57	0.40
1:C:196[B]:VAL:CG1	1:C:221:LEU:HD11	2.52	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	258/268 (96%)	253 (98%)	4 (2%)	1 (0%)	34	37
1	B	270/268 (101%)	265 (98%)	4 (2%)	1 (0%)	34	37
1	C	260/268 (97%)	254 (98%)	5 (2%)	1 (0%)	34	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	257/268 (96%)	253 (98%)	4 (2%)	0	100 100
All	All	1045/1072 (98%)	1025 (98%)	17 (2%)	3 (0%)	41 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	PRO
1	A	217	ARG
1	C	217	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	226/230 (98%)	220 (97%)	6 (3%)	44 57
1	B	231/230 (100%)	224 (97%)	7 (3%)	41 53
1	C	226/230 (98%)	219 (97%)	7 (3%)	40 51
1	D	225/230 (98%)	219 (97%)	6 (3%)	44 57
All	All	908/920 (99%)	882 (97%)	26 (3%)	43 54

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	66	ARG
1	A	72	GLU
1	A	164	ARG
1	A	266	THR
1	A	268	GLU
1	B	33	GLN
1	B	83	GLU
1	B	164	ARG
1	B	202	ARG
1	B	203	ARG

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Mol	Chain	Res	Type
1	B	228[A]	ASP
1	B	228[B]	ASP
1	C	99	GLN
1	C	139	LEU
1	C	164	ARG
1	C	172	ASN
1	C	223	LEU
1	C	228	ASP
1	C	238	SER
1	D	83	GLU
1	D	126	LYS
1	D	139	LEU
1	D	164	ARG
1	D	238	SER
1	D	262	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	262	GLN
1	B	33	GLN
1	B	243	HIS
1	C	93	HIS
1	C	152	HIS
1	D	152	HIS
1	D	226	HIS

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 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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	260/268 (97%)	-0.26	4 (1%) 73 72	11, 21, 38, 60	0
1	B	268/268 (100%)	-0.02	11 (4%) 37 35	11, 24, 45, 57	0
1	C	260/268 (97%)	-0.23	8 (3%) 49 47	14, 24, 45, 84	0
1	D	258/268 (96%)	-0.31	4 (1%) 72 70	12, 20, 37, 76	0
All	All	1046/1072 (97%)	-0.20	27 (2%) 56 53	11, 22, 43, 84	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	ALA	12.5
1	B	229	PRO	7.0
1	B	233	LYS	6.8
1	C	237	PRO	5.8
1	B	113[A]	PHE	4.2
1	B	171	ASP	4.0
1	A	237	PRO	3.8
1	C	171	ASP	3.7
1	C	227	PRO	3.6
1	D	268	GLU	3.5
1	B	231	LEU	3.5
1	B	227	PRO	3.5
1	A	171	ASP	3.4
1	D	226	HIS	3.3
1	B	234	CYS	3.1
1	B	228[A]	ASP	3.0
1	C	268	GLU	2.9
1	C	228	ASP	2.7
1	C	202	ARG	2.5
1	A	228	ASP	2.5
1	B	75	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	203	ARG	2.2
1	D	171	ASP	2.2
1	A	201	GLY	2.1
1	C	238	SER	2.1
1	D	203	ARG	2.1
1	B	230	LYS	2.1

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
2	CL	A	269	1/1	0.97	0.05	22,22,22,22	0
2	CL	A	270	1/1	0.97	0.11	27,27,27,27	0
2	CL	A	271	1/1	0.97	0.05	33,33,33,33	0
2	CL	B	271	1/1	0.97	0.08	31,31,31,31	0
2	CL	C	270	1/1	0.97	0.13	35,35,35,35	0
2	CL	B	269	1/1	0.98	0.12	28,28,28,28	0
2	CL	B	272	1/1	0.98	0.15	30,30,30,30	0
2	CL	B	270	1/1	0.98	0.10	22,22,22,22	0
2	CL	D	271	1/1	0.98	0.05	35,35,35,35	0
2	CL	D	269	1/1	0.99	0.06	24,24,24,24	0
2	CL	D	270	1/1	0.99	0.06	26,26,26,26	0
2	CL	C	269	1/1	0.99	0.06	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.