Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:53 PM GMT

PDB ID	:	4JTJ
Title	:	Crystal structure of R117K mutant of 3-deoxy-D-manno-octulosonate 8-phosphate synthase (KDO8PS) from Neisseria meningitidis
Authors	:	Allison, T.M.; Cochrane, F.C.; Jameson, G.B.; Parker, E.J.
Deposited on	:	2013-03-23
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

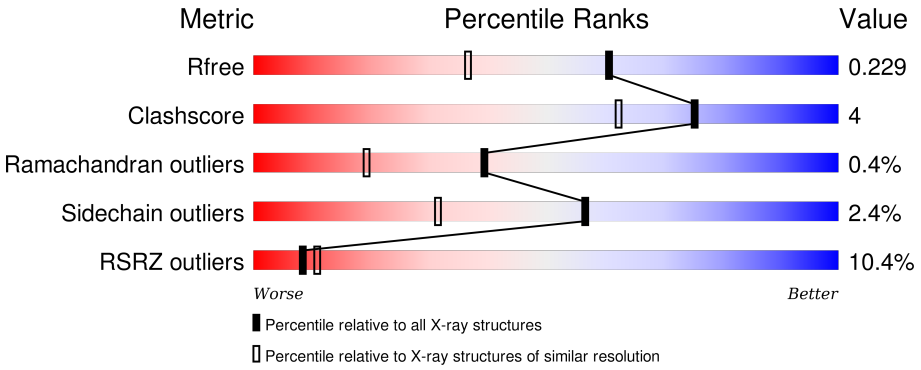
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 81% 9% 10%
1	B	280	4% 79% 10% • 10%
1	C	280	6% 84% 7% 8%
1	D	280	15% 84% 7% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8274 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	253	Total	C	N	O	S	0	2	0
			1963	1260	332	360	11			
1	B	253	Total	C	N	O	S	0	5	0
			1981	1274	333	362	12			
1	C	257	Total	C	N	O	S	0	3	0
			1991	1282	334	364	11			
1	D	259	Total	C	N	O	S	0	1	0
			1997	1280	338	368	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	LYS	ARG	ENGINEERED MUTATION	UNP Q9JZ55
B	117	LYS	ARG	ENGINEERED MUTATION	UNP Q9JZ55
C	117	LYS	ARG	ENGINEERED MUTATION	UNP Q9JZ55
D	117	LYS	ARG	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	D	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		

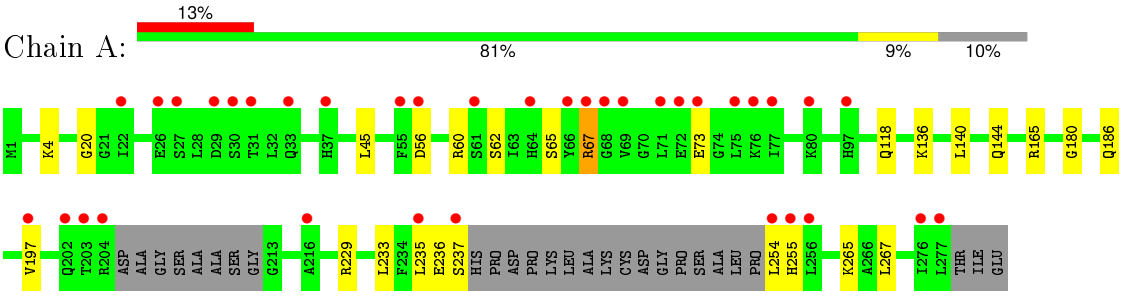
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	77	Total O 77 77	0	0
4	B	96	Total O 96 96	0	0
4	C	92	Total O 92 92	0	0
4	D	73	Total O 73 73	0	0

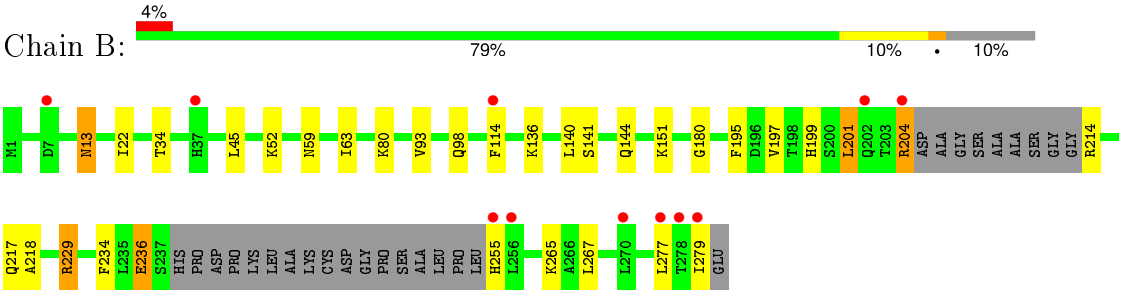
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

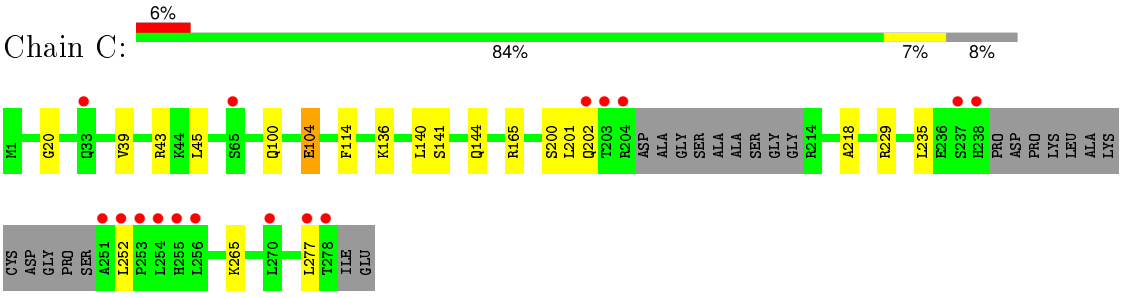
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



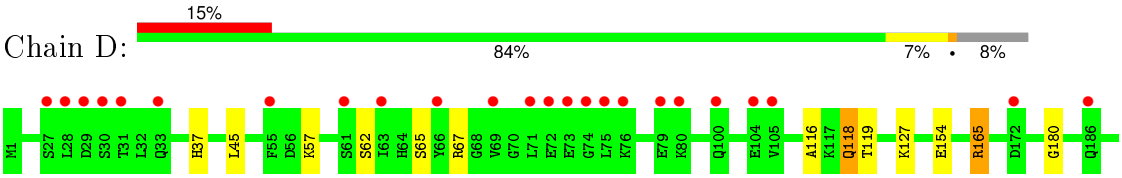
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

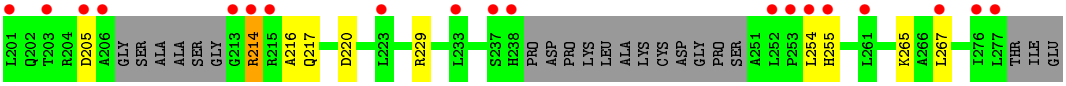


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



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




L201
Q202
T203
R204
D205
A206
GLY
SER
ALA
ALA
SER
GLY
G213
R214
R215
A216
Q217
D220
L223
R229
L233
S237
H238
PRO
ASP
PRO
LYS
LEU
ALA
LYS
CYS
ASP
GLY
PRO
SER
A251
L252
P253
L254
H255
L261
K265
A266
L267
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	81.47Å 85.37Å 163.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.55 – 1.75 39.52 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.55-1.75) 98.6 (39.52-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.197 , 0.226 0.203 , 0.229	Depositor DCC
R_{free} test set	5686 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.2	EDS
Estimated twinning fraction	0.004 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 113637 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8274	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.80	0/1998	0.85	2/2698 (0.1%)
1	B	0.88	1/2025 (0.0%)	0.90	2/2735 (0.1%)
1	C	0.93	2/2034 (0.1%)	0.87	1/2749 (0.0%)
1	D	0.84	0/2034	0.89	3/2748 (0.1%)
All	All	0.86	3/8091 (0.0%)	0.88	8/10930 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	200	SER	CB-OG	-5.88	1.34	1.42
1	C	104	GLU	CB-CG	-5.80	1.41	1.52
1	B	236	GLU	CD-OE2	-5.58	1.19	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	LYS	CD-CE-NZ	5.86	125.18	111.70
1	C	136	LYS	CD-CE-NZ	5.77	124.97	111.70
1	D	67	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	165	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	136	LYS	CD-CE-NZ	5.41	124.14	111.70
1	D	220	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	201	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	60	ARG	NE-CZ-NH2	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1963	0	2017	21	0
1	B	1981	0	2047	28	0
1	C	1991	0	2053	9	0
1	D	1997	0	2039	13	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	1	0	0	0	0
4	A	77	0	0	1	0
4	B	96	0	0	2	0
4	C	92	0	0	0	0
4	D	73	0	0	3	0
All	All	8274	0	8156	62	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 4.

All (62) 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:204:ARG:HG2	1:B:204:ARG:HH21	1.37	0.89
1:B:13:ASN:HD21	1:B:229:ARG:HH21	1.26	0.80
1:A:118:GLN:NE2	1:C:114:PHE:HE2	1.84	0.74
1:D:37:HIS:CD2	1:D:254:LEU:HG	2.25	0.71
1:A:118:GLN:NE2	1:C:114:PHE:CE2	2.61	0.69
1:B:214:ARG:HB3	1:B:217:GLN:HE21	1.60	0.67
1:B:204:ARG:HH21	1:B:204:ARG:CG	2.08	0.66
1:D:116:ALA:HB2	4:D:466:HOH:O	1.95	0.64
1:A:236:GLU:O	1:A:237:SER:CB	2.47	0.63
1:B:13:ASN:ND2	1:B:229:ARG:HH21	1.97	0.62
1:A:197[B]:VAL:CG1	1:A:233:LEU:HD11	2.29	0.61
1:A:197[B]:VAL:HG11	1:A:233:LEU:HD11	1.82	0.61
1:A:267:LEU:HD13	1:B:267:LEU:CD1	2.32	0.60
1:D:217:GLN:NE2	4:D:468:HOH:O	2.35	0.59
1:B:195:PHE:CE2	1:B:197[B]:VAL:HG22	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:CD1	1:B:267:LEU:HD13	2.32	0.59
1:D:45:LEU:O	1:D:265:LYS:HE3	2.03	0.59
1:C:201:LEU:HD11	1:C:218:ALA:HA	1.86	0.58
1:B:279:ILE:O	1:B:279:ILE:HG22	2.02	0.58
1:C:45:LEU:O	1:C:265:LYS:HE3	2.04	0.57
1:B:199:HIS:HB2	1:B:236:GLU:OE2	2.06	0.55
1:B:45:LEU:O	1:B:265:LYS:HE3	2.06	0.55
1:D:62:SER:HB3	1:D:65:SER:OG	2.05	0.55
1:C:39:VAL:O	1:C:43:ARG:HG3	2.08	0.54
1:A:62:SER:HB3	1:A:65:SER:OG	2.07	0.54
1:D:214:ARG:HH21	1:D:216:ALA:H	1.54	0.54
1:B:52:LYS:HE2	1:B:234:PHE:CZ	2.43	0.53
1:B:114:PHE:HE2	1:D:118:GLN:HG2	1.74	0.52
1:B:204:ARG:CG	1:B:204:ARG:NH2	2.73	0.52
1:A:236:GLU:O	1:A:237:SER:OG	2.28	0.51
1:B:180:GLY:HA3	4:B:324:HOH:O	2.11	0.50
1:A:254:LEU:HD23	1:A:255:HIS:NE2	2.27	0.50
1:A:267:LEU:HD13	1:B:267:LEU:HD13	1.95	0.48
1:A:235:LEU:HD13	1:A:237:SER:HA	1.96	0.47
1:A:254:LEU:HD23	1:A:255:HIS:CD2	2.48	0.47
1:C:100:GLN:O	1:C:104:GLU:HG3	2.14	0.47
1:A:267:LEU:CD1	1:B:267:LEU:CD1	2.92	0.46
1:D:180:GLY:HA3	4:D:440:HOH:O	2.15	0.46
1:B:93[B]:VAL:CG1	1:B:98:GLN:HB2	2.47	0.45
1:A:254:LEU:O	1:A:254:LEU:HG	2.17	0.45
1:B:63:ILE:HA	1:D:119:THR:HG21	1.99	0.45
1:A:20:GLY:HA2	1:A:235:LEU:O	2.18	0.44
1:A:45:LEU:O	1:A:265:LYS:HE3	2.16	0.44
1:B:141:SER:OG	1:B:144[A]:GLN:HG3	2.18	0.44
1:B:140:LEU:HG	1:B:144[A]:GLN:HB2	1.99	0.44
1:B:59[B]:ASN:OD1	1:B:59[B]:ASN:O	2.36	0.44
1:B:93[B]:VAL:HG13	1:B:98:GLN:HB2	2.00	0.44
1:B:22:ILE:HG23	1:B:34:THR:HG21	2.00	0.43
1:C:20:GLY:HA2	1:C:235:LEU:O	2.17	0.43
1:B:13:ASN:HD21	1:B:229:ARG:NH2	2.03	0.43
1:B:201:LEU:HD11	1:B:218:ALA:HA	2.00	0.43
1:C:141:SER:OG	1:C:144:GLN:HG3	2.18	0.43
1:D:37:HIS:HD2	1:D:254:LEU:HG	1.82	0.43
1:A:180:GLY:HA3	4:A:427:HOH:O	2.18	0.43
1:D:267:LEU:C	1:D:267:LEU:HD23	2.39	0.42
1:C:140:LEU:HG	1:C:144:GLN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HG22	1:D:119:THR:HG23	2.03	0.41
1:A:56:ASP:OD1	1:A:67:ARG:CZ	2.69	0.41
1:A:140:LEU:HG	1:A:144:GLN:HB2	2.03	0.40
1:A:197[B]:VAL:CG1	1:A:233:LEU:CD1	2.97	0.40
1:B:151:LYS:HD3	4:B:386:HOH:O	2.22	0.40
1:D:57:LYS:HD2	1:D:57:LYS:HA	1.91	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	249/280 (89%)	244 (98%)	4 (2%)	1 (0%)	39	19
1	B	252/280 (90%)	245 (97%)	6 (2%)	1 (0%)	39	19
1	C	254/280 (91%)	249 (98%)	4 (2%)	1 (0%)	39	19
1	D	254/280 (91%)	250 (98%)	3 (1%)	1 (0%)	39	19
All	All	1009/1120 (90%)	988 (98%)	17 (2%)	4 (0%)	39	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	229	ARG
1	B	229	ARG
1	A	229	ARG
1	C	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	218/236 (92%)	213 (98%)	5 (2%)	58	33
1	B	222/236 (94%)	217 (98%)	5 (2%)	58	33
1	C	222/236 (94%)	218 (98%)	4 (2%)	66	46
1	D	220/236 (93%)	212 (96%)	8 (4%)	42	16
All	All	882/944 (93%)	860 (98%)	22 (2%)	57	30

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	67	ARG
1	A	73	GLU
1	A	165	ARG
1	A	186	GLN
1	B	13	ASN
1	B	80	LYS
1	B	204	ARG
1	B	255	HIS
1	B	277	LEU
1	C	165	ARG
1	C	202	GLN
1	C	252	LEU
1	C	277	LEU
1	D	118	GLN
1	D	127	LYS
1	D	154[A]	GLU
1	D	154[B]	GLU
1	D	165	ARG
1	D	205	ASP
1	D	214	ARG
1	D	255	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN

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Mol	Chain	Res	Type
1	A	23	ASN
1	A	118	GLN
1	B	13	ASN
1	B	138	GLN
1	B	173	ASN
1	B	199	HIS
1	B	217	GLN
1	C	97	HIS
1	C	100	GLN
1	C	186	GLN
1	D	23	ASN
1	D	37	HIS
1	D	186	GLN
1	D	274	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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	253/280 (90%)	0.81	36 (14%) 4 5	21, 35, 66, 80	1 (0%)
1	B	253/280 (90%)	0.40	11 (4%) 39 45	21, 29, 48, 75	0
1	C	257/280 (91%)	0.47	16 (6%) 24 29	21, 29, 48, 85	0
1	D	259/280 (92%)	1.00	43 (16%) 2 4	21, 36, 67, 75	0
All	All	1022/1120 (91%)	0.67	106 (10%) 8 11	21, 32, 64, 85	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	LEU	11.8
1	D	277	LEU	9.1
1	A	66	TYR	8.3
1	C	278	THR	8.1
1	C	255	HIS	7.4
1	D	206	ALA	7.0
1	C	254	LEU	6.3
1	B	279	ILE	6.2
1	A	61	SER	6.0
1	C	203	THR	6.0
1	B	256	LEU	5.8
1	D	66	TYR	5.5
1	B	255	HIS	5.5
1	C	202	GLN	5.4
1	D	72	GLU	5.4
1	A	202	GLN	5.0
1	D	253	PRO	5.0
1	A	254	LEU	4.9
1	C	238	HIS	4.9
1	C	277	LEU	4.8
1	D	205	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	252	LEU	4.5
1	B	202	GLN	4.4
1	C	237	SER	4.4
1	C	253	PRO	4.3
1	A	237	SER	4.3
1	D	252	LEU	4.2
1	D	71	LEU	4.1
1	D	105	VAL	4.0
1	D	73	GLU	4.0
1	D	27	SER	3.8
1	D	76	LYS	3.8
1	D	104	GLU	3.8
1	B	277	LEU	3.7
1	A	67	ARG	3.7
1	A	27	SER	3.7
1	D	254	LEU	3.7
1	A	69	VAL	3.6
1	D	203	THR	3.6
1	A	71	LEU	3.6
1	D	75	LEU	3.6
1	A	30	SER	3.6
1	D	80	LYS	3.5
1	D	33	GLN	3.5
1	D	28	LEU	3.4
1	A	76	LYS	3.4
1	A	73	GLU	3.3
1	A	276	ILE	3.3
1	C	204	ARG	3.2
1	D	69	VAL	3.2
1	B	278	THR	3.2
1	B	270	LEU	3.1
1	A	216	ALA	3.1
1	A	235	LEU	3.1
1	D	63	ILE	3.0
1	A	64	HIS	3.0
1	D	276	ILE	2.9
1	D	233	LEU	2.9
1	D	267	LEU	2.9
1	A	29	ASP	2.9
1	A	256	LEU	2.8
1	A	72	GLU	2.8
1	A	75	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	79	GLU	2.8
1	A	33	GLN	2.8
1	A	31	THR	2.8
1	D	61	SER	2.8
1	D	213	GLY	2.7
1	D	100	GLN	2.7
1	A	97	HIS	2.6
1	B	114	PHE	2.6
1	D	255	HIS	2.6
1	C	251	ALA	2.5
1	D	238	HIS	2.5
1	D	215	ARG	2.5
1	A	77	ILE	2.4
1	D	29	ASP	2.4
1	D	30	SER	2.4
1	A	80	LYS	2.4
1	A	55	PHE	2.4
1	A	255	HIS	2.4
1	D	261	LEU	2.3
1	B	7	ASP	2.3
1	D	172	ASP	2.3
1	D	223	LEU	2.3
1	A	56	ASP	2.3
1	A	22	ILE	2.3
1	B	204	ARG	2.3
1	C	33	GLN	2.3
1	A	37	HIS	2.2
1	B	37	HIS	2.2
1	A	203	THR	2.2
1	D	31	THR	2.2
1	D	214	ARG	2.2
1	D	201	LEU	2.2
1	D	55	PHE	2.1
1	A	26	GLU	2.1
1	A	197[A]	VAL	2.1
1	C	65[A]	SER	2.1
1	C	270	LEU	2.1
1	A	204	ARG	2.1
1	D	74	GLY	2.1
1	D	237	SER	2.1
1	D	186	GLN	2.0
1	C	256	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	68	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	CL	C	301	1/1	0.96	0.06	-1.32	41,41,41,41	0
2	CL	A	301	1/1	0.97	0.08	-1.76	34,34,34,34	0
3	NA	C	302	1/1	0.97	0.06	-1.92	26,26,26,26	0
2	CL	D	301	1/1	0.94	0.08	-2.19	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.