



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 PM UTC

PDB ID : 3STE / pdb_00003ste
Title : Crystal structure of a mutant (Q202A) of 3-deoxy-D-manno-octulosonate 8-phosphate synthase (KDO8PS) from *Neisseria meningitidis*
Authors : Allison, T.M.; Jameson, G.B.; Gloyne, B.J.; Parker, E.J.
Deposited on : 2011-07-09
Resolution : 2.05 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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

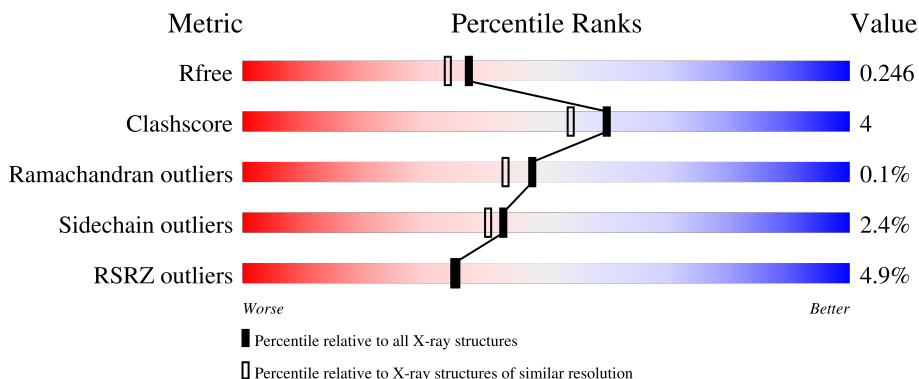
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
1	B	280	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div>
1	C	280	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div>
1	D	280	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8275 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
			Total	C	N	O	S			
1	A	250	1892	1214	320	347	11	0	0	0
1	B	249	1944	1253	325	355	11	0	5	0
1	C	253	1962	1264	329	358	11	0	3	0
1	D	254	1941	1247	325	358	11	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	GLN	engineered mutation	UNP Q9JZ55
B	202	ALA	GLN	engineered mutation	UNP Q9JZ55
C	202	ALA	GLN	engineered mutation	UNP Q9JZ55
D	202	ALA	GLN	engineered mutation	UNP Q9JZ55

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

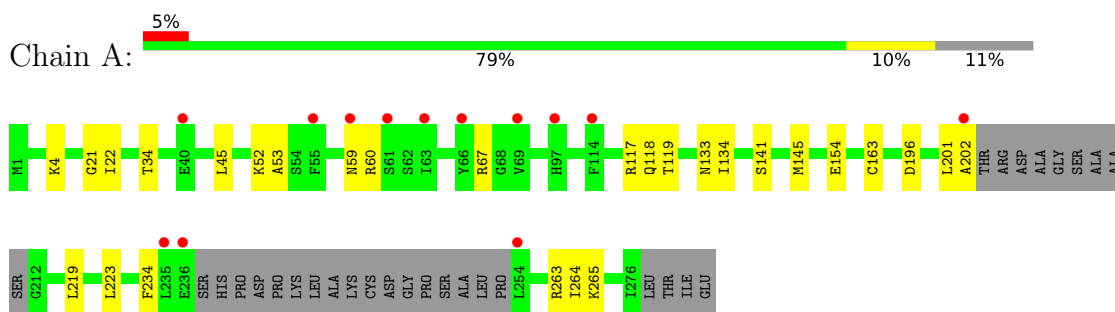
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total 114	O 114	0	0
4	B	142	Total 142	O 142	0	0
4	C	151	Total 151	O 151	0	0
4	D	127	Total 127	O 127	0	0

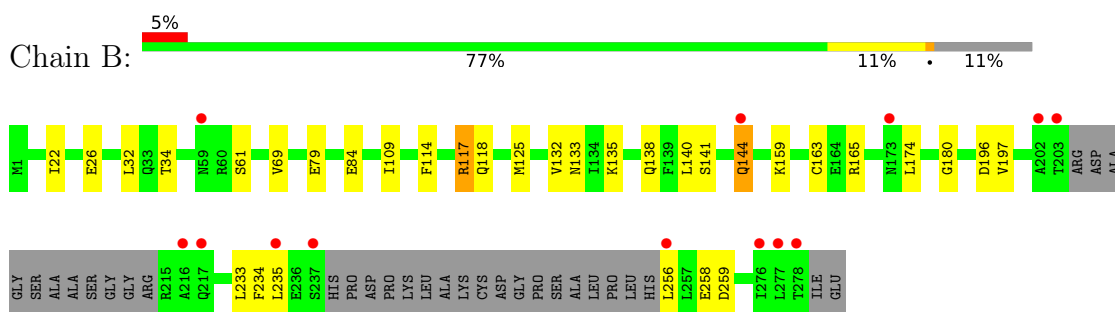
3 Residue-property plots [i](#)

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.

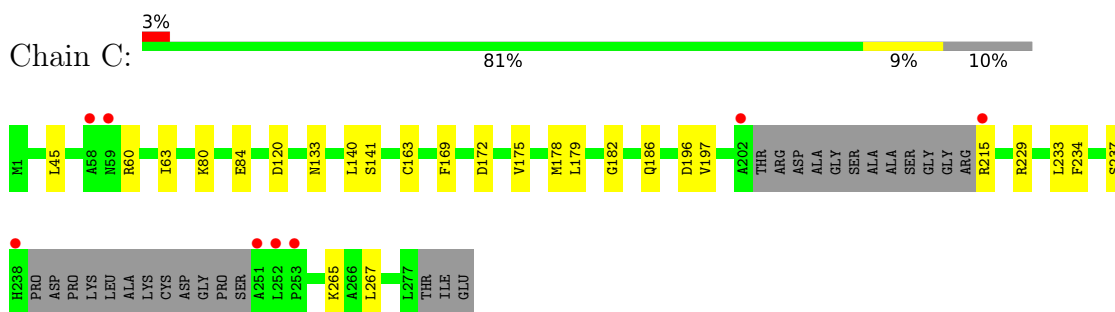
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



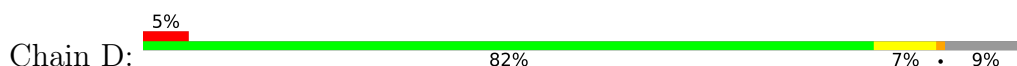
- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase

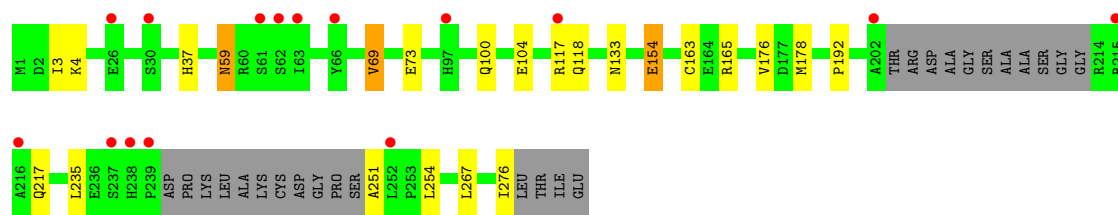


- Molecule 1: 2-dehydro-3-deoxyphosphooctonate aldolase



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.00Å 85.71Å 163.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.60 – 2.05 30.60 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.60-2.05) 98.9 (30.60-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.05Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.247 0.204 , 0.246	Depositor DCC
R_{free} test set	3606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.150	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.014 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8275	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA

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	0.60	0/1923	0.78	0/2601
1	B	0.64	0/1984	0.78	0/2680
1	C	0.63	0/2001	0.76	0/2705
1	D	0.58	0/1978	0.74	0/2677
All	All	0.61	0/7886	0.76	0/10663

There are no bond length outliers.

There are no bond angle outliers.

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	1892	0	1919	18	0
1	B	1944	0	2014	22	0
1	C	1962	0	2024	21	0
1	D	1941	0	1979	19	0
2	C	1	0	0	0	0
3	C	1	0	0	0	0
4	A	114	0	0	0	0
4	B	142	0	0	2	0
4	C	151	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	127	0	0	1	0
All	All	8275	0	7936	67	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 (67) 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:109[A]:ILE:HG22	1:B:125:MET:HE3	1.35	1.04
1:B:114:PHE:HB3	1:D:117:ARG:HH21	1.31	0.94
1:B:109[A]:ILE:CG2	1:B:125:MET:HE3	2.10	0.82
1:A:133:ASN:HD21	1:A:163:CYS:HB2	1.45	0.81
1:A:22:ILE:HG23	1:A:34:THR:HG21	1.69	0.75
1:B:196:ASP:HA	1:B:234:PHE:HB3	1.71	0.72
1:B:133:ASN:HD21	1:B:163:CYS:HB2	1.57	0.69
1:C:267[A]:LEU:CD1	1:D:267:LEU:HD13	2.27	0.65
1:C:267[A]:LEU:HD13	1:D:267:LEU:CD1	2.29	0.63
1:B:256:LEU:HD23	1:B:259:ASP:H	1.64	0.63
1:A:196:ASP:HA	1:A:234:PHE:HB3	1.81	0.62
1:D:69:VAL:HG13	1:D:73:GLU:HB3	1.82	0.61
1:C:267[A]:LEU:CD1	1:D:267:LEU:CD1	2.80	0.59
1:B:180:GLY:HA3	4:B:367:HOH:O	2.01	0.58
1:B:109[B]:ILE:HD12	1:B:125:MET:HG2	1.87	0.56
1:D:133:ASN:HD21	1:D:163:CYS:HB2	1.70	0.56
1:A:59:ASN:C	1:A:59:ASN:ND2	2.64	0.56
1:D:251:ALA:HB2	4:D:377:HOH:O	2.06	0.55
1:C:215:ARG:NH1	4:C:452:HOH:O	2.39	0.55
1:C:196:ASP:HA	1:C:234:PHE:HB3	1.87	0.55
1:A:59:ASN:C	1:A:59:ASN:HD22	2.16	0.54
1:C:80:LYS:NZ	1:C:84:GLU:OE1	2.40	0.54
1:C:182:GLY:O	1:C:186:GLN:HG2	2.06	0.54
1:A:141:SER:HB2	1:C:172:ASP:OD1	2.10	0.52
1:A:223:LEU:CD2	1:A:264:ILE:HD13	2.40	0.52
1:C:267[A]:LEU:HD11	1:D:267:LEU:HD13	1.91	0.52
1:C:133:ASN:HD21	1:C:163:CYS:HB2	1.74	0.52
1:A:21:GLY:HA3	1:A:52:LYS:O	2.11	0.51
1:A:134:ILE:HG22	1:A:145:MET:HE1	1.93	0.50
1:D:235:LEU:C	1:D:235:LEU:HD12	2.36	0.50
1:C:140:LEU:HD23	1:C:141:SER:O	2.12	0.49
1:B:22:ILE:HG23	1:B:34:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:SER:OG	1:B:144:GLN:NE2	2.44	0.49
1:D:154:GLU:O	1:D:154:GLU:HG3	2.10	0.48
1:B:138:GLN:NE2	1:B:174:LEU:HD21	2.30	0.47
1:D:37:HIS:CD2	1:D:254:LEU:HG	2.50	0.47
1:A:45:LEU:O	1:A:265:LYS:HE3	2.15	0.46
1:C:267[A]:LEU:HD13	1:D:267:LEU:HD11	1.96	0.46
1:A:59:ASN:HD22	1:A:60:ARG:N	2.12	0.46
1:B:22:ILE:CG2	1:B:34:THR:HG21	2.46	0.46
1:B:135:LYS:NZ	1:B:196:ASP:OD2	2.47	0.46
1:A:52:LYS:HG2	1:A:53:ALA:N	2.32	0.45
1:B:26:GLU:O	1:B:69:VAL:CG1	2.64	0.45
1:A:201:LEU:O	1:A:202:ALA:HB3	2.17	0.45
1:C:178:MET:HE3	1:D:178:MET:HG3	2.00	0.44
1:B:125:MET:CE	1:B:132:VAL:HG13	2.47	0.44
1:C:197[B]:VAL:CG1	1:C:233:LEU:HD11	2.47	0.44
1:B:32:LEU:HD22	1:B:84:GLU:OE1	2.17	0.44
1:D:100:GLN:O	1:D:104:GLU:HG2	2.18	0.44
1:D:3:ILE:HD12	1:D:192:PRO:HG2	1.99	0.44
1:B:117:ARG:O	1:D:59:ASN:HB3	2.18	0.43
1:D:176:VAL:CG1	1:D:178:MET:HE2	2.48	0.43
1:B:197[B]:VAL:CG2	1:B:233:LEU:HD11	2.49	0.43
1:D:176:VAL:HG12	1:D:178:MET:HE2	2.00	0.43
1:B:125:MET:HE2	1:B:132:VAL:HG13	2.01	0.42
1:C:179:LEU:HD22	1:D:217:GLN:HB3	2.01	0.42
1:A:223:LEU:HD23	1:A:264:ILE:HD13	2.01	0.42
1:C:45:LEU:O	1:C:265:LYS:HE3	2.20	0.42
1:A:154:GLU:HG2	1:C:63:ILE:HD11	2.00	0.42
1:B:197[A]:VAL:HG12	1:B:235:LEU:HD23	2.02	0.42
1:C:169:PHE:HB2	1:C:175:VAL:HG12	2.02	0.41
1:B:79:GLU:HG2	4:B:528:HOH:O	2.20	0.41
1:C:120:ASP:HB2	4:C:384:HOH:O	2.21	0.41
1:A:119:THR:CG2	1:C:63:ILE:HA	2.51	0.41
1:A:219:LEU:HD21	1:A:263:ARG:HD3	2.02	0.41
1:A:119:THR:HG21	1:C:63:ILE:HA	2.03	0.40
1:B:256:LEU:HD21	1:B:258:GLU:HB3	2.03	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	244/280 (87%)	240 (98%)	4 (2%)	0	100	100
1	B	248/280 (89%)	241 (97%)	7 (3%)	0	100	100
1	C	250/280 (89%)	246 (98%)	3 (1%)	1 (0%)	30	22
1	D	249/280 (89%)	246 (99%)	3 (1%)	0	100	100
All	All	991/1120 (88%)	973 (98%)	17 (2%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	205/235 (87%)	201 (98%)	4 (2%)	48	48
1	B	216/235 (92%)	209 (97%)	7 (3%)	34	29
1	C	218/235 (93%)	216 (99%)	2 (1%)	70	75
1	D	214/235 (91%)	207 (97%)	7 (3%)	33	28
All	All	853/940 (91%)	833 (98%)	20 (2%)	43	42

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	67	ARG
1	A	117	ARG
1	A	118	GLN
1	B	61	SER
1	B	117	ARG
1	B	118	GLN
1	B	140	LEU
1	B	144	GLN
1	B	159	LYS
1	B	165	ARG
1	C	60	ARG
1	C	237	SER
1	D	4	LYS
1	D	59	ASN
1	D	69	VAL
1	D	118	GLN
1	D	154	GLU
1	D	165	ARG
1	D	276	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	94	HIS
1	A	110	GLN
1	A	133	ASN
1	B	23	ASN
1	B	98	GLN
1	B	110	GLN
1	B	133	ASN
1	B	138	GLN
1	C	64	HIS
1	C	110	GLN
1	C	133	ASN
1	C	144	GLN
1	C	274	GLN
1	D	23	ASN
1	D	37	HIS
1	D	110	GLN
1	D	133	ASN
1	D	144	GLN

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Mol	Chain	Res	Type
1	D	147	ASN
1	D	153	HIS
1	D	217	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	250/280 (89%)	0.32	13 (5%) 33 33	20, 40, 75, 93	1 (0%)
1	B	249/280 (88%)	0.07	13 (5%) 33 33	15, 32, 51, 77	6 (2%)
1	C	253/280 (90%)	-0.08	8 (3%) 50 50	12, 32, 55, 72	3 (1%)
1	D	254/280 (90%)	0.21	15 (5%) 28 28	22, 39, 69, 95	1 (0%)
All	All	1006/1120 (89%)	0.13	49 (4%) 35 35	12, 35, 66, 95	11 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	4.6
1	A	236	GLU	4.0
1	D	66	TYR	4.0
1	B	216	ALA	3.7
1	B	144	GLN	3.6
1	A	63	ILE	3.6
1	B	173	ASN	3.6
1	B	217[A]	GLN	3.5
1	B	235	LEU	3.5
1	D	202	ALA	3.4
1	A	254	LEU	3.4
1	B	237	SER	3.3
1	D	62	SER	3.2
1	B	256	LEU	3.2
1	C	59	ASN	3.2
1	A	66	TYR	3.1
1	D	215	ARG	3.0
1	A	202	ALA	2.9
1	B	203	THR	2.8
1	A	59	ASN	2.8
1	D	239	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	202	ALA	2.7
1	D	117	ARG	2.7
1	D	61	SER	2.7
1	C	251	ALA	2.6
1	D	30[A]	SER	2.6
1	B	278	THR	2.6
1	B	59	ASN	2.5
1	A	114	PHE	2.5
1	C	238	HIS	2.4
1	D	63	ILE	2.4
1	B	277	LEU	2.3
1	A	97	HIS	2.3
1	A	69	VAL	2.3
1	C	202	ALA	2.3
1	C	252	LEU	2.3
1	D	252	LEU	2.3
1	D	238	HIS	2.2
1	A	40	GLU	2.2
1	D	97	HIS	2.1
1	C	215	ARG	2.1
1	A	55	PHE	2.1
1	A	61	SER	2.1
1	C	58	ALA	2.1
1	D	26	GLU	2.0
1	D	216	ALA	2.1
1	B	276	ILE	2.0
1	D	237	SER	2.0
1	C	253	PRO	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 oligosaccharides 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
2	CL	C	281	1/1	0.93	0.09	49,49,49,49	0
3	NA	C	282	1/1	0.98	0.09	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.