



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:39 am BST

PDB ID : 1ZG1
Title : NarL complexed to nirB promoter non-palindromic tail-to-tail DNA site
Authors : Maris, A.E.; Kaczor-Grzeskowiak, M.; Ma, Z.; Kopka, M.L.; Gunsalus, R.P.;
Dickerson, R.E.
Deposited on : 2005-04-20
Resolution : 2.30 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 : 2.11
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) : 2.11

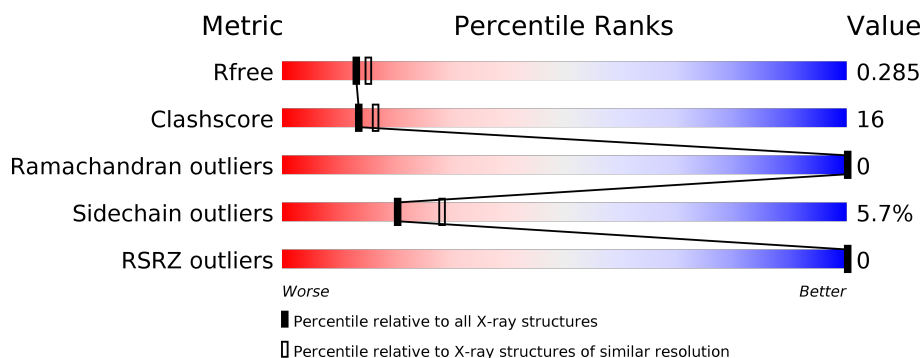
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	C	20	<div> <div>45%</div> <div>55%</div> </div>
1	H	20	<div> <div>65%</div> <div>35%</div> </div>
2	D	20	<div> <div>65%</div> <div>35%</div> </div>
2	G	20	<div> <div>50%</div> <div>50%</div> </div>
3	A	82	<div> <div>50%</div> <div>28%</div> <div>•</div> <div>20%</div> </div>
3	B	82	<div> <div>51%</div> <div>28%</div> <div>•</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	82	 48% 32% 20%
3	F	82	 55% 23% 20%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3954 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 DNA chain called 5'-D(*CP*GP*TP*AP*CP*TP*CP*CP*TP*TP*AP*AP*TP*GP*GP*GP*TP*AP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	0	0
			406	195	72	120	19			
1	H	20	Total	C	N	O	P	0	0	0
			406	195	72	120	19			

- Molecule 2 is a DNA chain called 5'-D(*CP*GP*TP*AP*CP*CP*CP*AP*TP*TP*AP*AP*GP*GP*AP*GP*TP*AP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	P	0	0	0
			408	195	78	116	19			
2	G	20	Total	C	N	O	P	0	0	0
			408	195	78	116	19			

- Molecule 3 is a protein called Nitrate/nitrite response regulator protein narL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	66	Total	C	N	O	Se	4	0	0
			548	347	107	91	3			
3	B	66	Total	C	N	O	Se	0	0	0
			548	347	107	91	3			
3	E	66	Total	C	N	O	Se	4	0	0
			548	347	107	91	3			
3	F	66	Total	C	N	O	Se	0	0	0
			548	347	107	91	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	MSE	-	EXPRESSION TAG	UNP P0AF28
A	136	ARG	-	EXPRESSION TAG	UNP P0AF28

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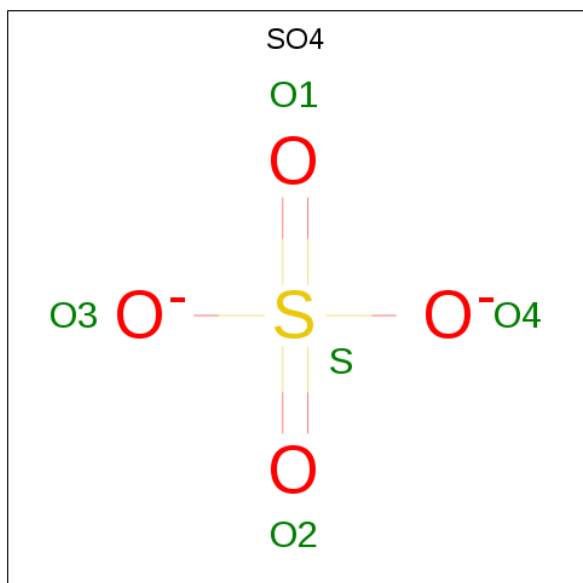
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	EXPRESSION TAG	UNP P0AF28
A	138	SER	-	EXPRESSION TAG	UNP P0AF28
A	139	HIS	-	EXPRESSION TAG	UNP P0AF28
A	140	HIS	-	EXPRESSION TAG	UNP P0AF28
A	141	HIS	-	EXPRESSION TAG	UNP P0AF28
A	142	HIS	-	EXPRESSION TAG	UNP P0AF28
A	143	HIS	-	EXPRESSION TAG	UNP P0AF28
A	144	HIS	-	EXPRESSION TAG	UNP P0AF28
A	145	GLY	-	EXPRESSION TAG	UNP P0AF28
A	146	SER	-	EXPRESSION TAG	UNP P0AF28
A	175	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
A	194	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
A	198	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
B	135	MSE	-	EXPRESSION TAG	UNP P0AF28
B	136	ARG	-	EXPRESSION TAG	UNP P0AF28
B	137	GLY	-	EXPRESSION TAG	UNP P0AF28
B	138	SER	-	EXPRESSION TAG	UNP P0AF28
B	139	HIS	-	EXPRESSION TAG	UNP P0AF28
B	140	HIS	-	EXPRESSION TAG	UNP P0AF28
B	141	HIS	-	EXPRESSION TAG	UNP P0AF28
B	142	HIS	-	EXPRESSION TAG	UNP P0AF28
B	143	HIS	-	EXPRESSION TAG	UNP P0AF28
B	144	HIS	-	EXPRESSION TAG	UNP P0AF28
B	145	GLY	-	EXPRESSION TAG	UNP P0AF28
B	146	SER	-	EXPRESSION TAG	UNP P0AF28
B	175	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
B	194	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
B	198	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
E	135	MSE	-	EXPRESSION TAG	UNP P0AF28
E	136	ARG	-	EXPRESSION TAG	UNP P0AF28
E	137	GLY	-	EXPRESSION TAG	UNP P0AF28
E	138	SER	-	EXPRESSION TAG	UNP P0AF28
E	139	HIS	-	EXPRESSION TAG	UNP P0AF28
E	140	HIS	-	EXPRESSION TAG	UNP P0AF28
E	141	HIS	-	EXPRESSION TAG	UNP P0AF28
E	142	HIS	-	EXPRESSION TAG	UNP P0AF28
E	143	HIS	-	EXPRESSION TAG	UNP P0AF28
E	144	HIS	-	EXPRESSION TAG	UNP P0AF28
E	145	GLY	-	EXPRESSION TAG	UNP P0AF28
E	146	SER	-	EXPRESSION TAG	UNP P0AF28
E	175	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
E	194	MSE	MET	MODIFIED RESIDUE	UNP P0AF28

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Chain	Residue	Modelled	Actual	Comment	Reference
E	198	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
F	135	MSE	-	EXPRESSION TAG	UNP P0AF28
F	136	ARG	-	EXPRESSION TAG	UNP P0AF28
F	137	GLY	-	EXPRESSION TAG	UNP P0AF28
F	138	SER	-	EXPRESSION TAG	UNP P0AF28
F	139	HIS	-	EXPRESSION TAG	UNP P0AF28
F	140	HIS	-	EXPRESSION TAG	UNP P0AF28
F	141	HIS	-	EXPRESSION TAG	UNP P0AF28
F	142	HIS	-	EXPRESSION TAG	UNP P0AF28
F	143	HIS	-	EXPRESSION TAG	UNP P0AF28
F	144	HIS	-	EXPRESSION TAG	UNP P0AF28
F	145	GLY	-	EXPRESSION TAG	UNP P0AF28
F	146	SER	-	EXPRESSION TAG	UNP P0AF28
F	175	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
F	194	MSE	MET	MODIFIED RESIDUE	UNP P0AF28
F	198	MSE	MET	MODIFIED RESIDUE	UNP P0AF28

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

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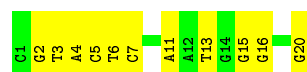
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

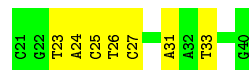
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	17	Total	O	0	0
			17	17		
5	D	11	Total	O	0	0
			11	11		
5	G	11	Total	O	0	0
			11	11		
5	H	11	Total	O	0	0
			11	11		
5	A	11	Total	O	0	0
			11	11		
5	B	8	Total	O	0	0
			8	8		
5	E	11	Total	O	0	0
			11	11		
5	F	9	Total	O	0	0
			9	9		

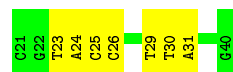
● Molecule 1: 5'-D(*CP*GP*TP*AP*CP*TP*CP*CP*TP*TP*AP*AP*TP*GP*GP*GP*TP*A
P*CP*G)-3'



- Molecule 1: 5'-D(*CP*GP*TP*AP*CP*TP*CP*CP*TP*TP*AP*AP*TP*GP*GP*GP*TP*AP*CP*G)-3'



- Molecule 2: 5'-D(*CP*GP*TP*AP*CP*CP*CP*AP*TP*TP*AP*AP*GP*GP*AP*GP*TP*A
P*CP*G)-3'

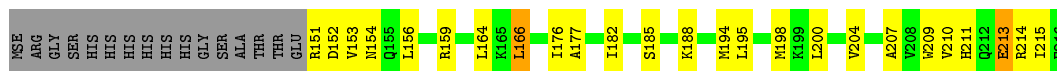


- Molecule 2: 5'-D(*CP*GP*TP*AP*CP*CP*CP*AP*TP*TP*AP*AP*GP*GP*AP*GP*TP*A
P*CP*G)-3'



- Molecule 3: Nitrate/nitrite response regulator protein narX

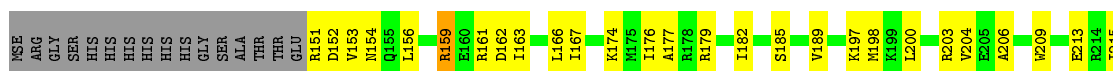




- Molecule 3: Nitrate/nitrite response regulator protein narL



- Molecule 3: Nitrate/nitrite response regulator protein narL



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- Molecule 3: Nitrate/nitrite response regulator protein narL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.58Å 52.82Å 84.97Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	9.00 – 2.30 24.46 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (9.00-2.30) 97.1 (24.46-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.257 , 0.286 0.256 , 0.285	Depositor DCC
R_{free} test set	1600 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.789	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3954	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7126e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: SO4

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	C	0.42	0/454	0.80	0/699
1	H	0.43	0/454	0.79	0/699
2	D	0.39	0/458	0.79	0/705
2	G	0.38	0/458	0.77	0/705
3	A	0.37	0/552	0.56	0/732
3	B	0.36	0/552	0.58	0/732
3	E	0.36	0/552	0.59	0/732
3	F	0.34	0/552	0.54	0/732
All	All	0.38	0/4032	0.68	0/5736

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	C	406	0	228	12	0
1	H	406	0	228	7	0
2	D	408	0	226	7	0
2	G	408	0	226	11	0
3	A	548	0	596	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	548	0	596	16	0
3	E	548	0	596	22	0
3	F	548	0	596	17	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	A	11	0	0	0	0
5	B	8	0	0	0	0
5	C	17	0	0	0	0
5	D	11	0	0	0	0
5	E	11	0	0	0	0
5	F	9	0	0	0	0
5	G	11	0	0	0	0
5	H	11	0	0	0	0
All	All	3954	0	3292	112	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 16.

All (112) 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)
3:A:153:VAL:HA	3:A:198:MSE:HE1	1.22	1.12
3:A:194:MSE:HE2	3:A:198:MSE:HG3	1.51	0.92
3:F:164:LEU:HD13	3:F:194:MSE:HE3	1.52	0.91
2:G:6:DC:H2''	2:G:7:DC:H5'	1.52	0.90
2:G:6:DC:C2'	2:G:7:DC:H5'	2.02	0.88
3:F:194:MSE:HE2	3:F:198:MSE:HG3	1.58	0.86
3:A:164:LEU:HD13	3:A:194:MSE:HE3	1.58	0.83
3:A:153:VAL:HA	3:A:198:MSE:CE	2.11	0.79
3:A:156:LEU:HG	3:A:198:MSE:HE2	1.68	0.76
3:A:156:LEU:CG	3:A:198:MSE:HE2	2.20	0.72
3:A:156:LEU:CD1	3:A:198:MSE:HE2	2.22	0.70
2:D:29:DT:H2''	2:D:30:DT:H5'	1.74	0.67
3:B:153:VAL:HG21	3:B:215:ILE:HG23	1.77	0.67
3:A:198:MSE:HE3	3:A:209:TRP:HH2	1.60	0.66
1:C:6:DT:C2'	1:C:7:DC:H5'	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:164:LEU:HD13	3:F:194:MSE:CE	2.24	0.65
3:B:153:VAL:HG21	3:B:215:ILE:CG2	2.26	0.65
3:E:153:VAL:HG12	3:E:161:ARG:HD3	1.80	0.64
3:A:152:ASP:OD2	3:A:154:ASN:HB2	1.98	0.63
3:B:198:MSE:HE2	3:B:198:MSE:HA	1.80	0.63
3:A:156:LEU:HD11	3:A:198:MSE:HE2	1.80	0.63
3:A:198:MSE:HE3	3:A:209:TRP:CH2	2.33	0.63
3:A:210:VAL:HA	3:A:215:ILE:HD12	1.82	0.62
3:A:164:LEU:HD13	3:A:194:MSE:CE	2.29	0.61
3:B:153:VAL:HG22	3:B:209:TRP:CH2	2.35	0.61
3:F:201:LYS:HD2	3:F:205:GLU:OE2	2.01	0.61
3:A:214:ARG:HG3	3:A:214:ARG:HH21	1.67	0.59
3:B:152:ASP:OD2	3:B:154:ASN:HB2	2.03	0.59
3:A:153:VAL:CA	3:A:198:MSE:HE1	2.15	0.58
3:F:198:MSE:HE2	3:F:198:MSE:HA	1.86	0.58
3:F:166:LEU:HD12	3:F:176:ILE:HG23	1.87	0.57
3:E:200:LEU:HD13	3:E:206:ALA:HA	1.87	0.56
2:G:9:DT:H2''	2:G:10:DT:H5'	1.88	0.55
3:F:177:ALA:HB1	3:F:182:ILE:O	2.07	0.54
1:H:26:DT:C2'	1:H:27:DC:H5'	2.38	0.54
3:E:151:ARG:HH21	3:E:200:LEU:HD23	1.71	0.54
3:E:198:MSE:HA	3:E:198:MSE:HE2	1.88	0.54
1:C:6:DT:H2''	1:C:7:DC:H5'	1.90	0.53
1:H:26:DT:H2''	1:H:27:DC:H5'	1.91	0.52
3:A:166:LEU:HD23	3:A:176:ILE:HG23	1.92	0.52
3:E:204:VAL:HG22	3:F:204:VAL:HG22	1.91	0.52
3:B:164:LEU:HD13	3:B:216:PHE:HE2	1.74	0.52
2:G:3:DT:H2''	2:G:4:DA:H5'	1.92	0.51
2:G:4:DA:C2	2:G:5:DC:C2	2.98	0.51
1:C:11:DA:C2	2:D:31:DA:C2	2.99	0.51
3:E:159:ARG:O	3:E:163:ILE:HD12	2.11	0.50
3:E:153:VAL:HG13	3:E:156:LEU:HD12	1.93	0.50
1:C:5:DC:H3'	1:C:6:DT:H71	1.94	0.50
3:A:198:MSE:CE	3:A:209:TRP:HH2	2.25	0.50
3:A:177:ALA:HB1	3:A:182:ILE:O	2.13	0.49
3:E:166:LEU:HD12	3:E:176:ILE:HG23	1.94	0.49
1:H:33:DT:H72	3:F:188:LYS:HD3	1.95	0.49
3:E:177:ALA:HB1	3:E:182:ILE:O	2.13	0.49
1:C:13:DT:H72	3:A:188:LYS:HD3	1.95	0.48
2:G:11:DA:C2	1:H:31:DA:C2	3.02	0.48
2:G:9:DT:H2''	2:G:10:DT:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:THR:OG1	3:B:160:GLU:HG3	2.13	0.48
3:B:159:ARG:O	3:B:162:ASP:HB2	2.14	0.48
3:B:166:LEU:HD12	3:B:176:ILE:HG23	1.96	0.47
3:A:207:ALA:O	3:A:211:HIS:HD2	1.97	0.47
2:D:29:DT:H2''	2:D:30:DT:C5'	2.42	0.46
1:H:25:DC:H3'	1:H:26:DT:H71	1.97	0.46
3:A:164:LEU:CD1	3:A:194:MSE:HE3	2.39	0.46
3:F:197:LYS:O	3:F:198:MSE:HE2	2.16	0.46
1:C:15:DG:H2'	1:C:16:DG:H8	1.80	0.46
2:D:25:DC:H2'	2:D:26:DC:C6	2.51	0.45
3:B:168:ALA:O	3:B:211:HIS:HE1	1.99	0.45
3:E:153:VAL:HG21	3:E:215:ILE:HG21	1.99	0.45
1:H:23:DT:H2''	1:H:24:DA:H5'	1.99	0.45
3:E:151:ARG:HE	3:E:200:LEU:HD21	1.82	0.45
1:C:20:DG:C8	1:C:20:DG:H5''	2.52	0.45
2:D:23:DT:H2''	2:D:24:DA:H5'	1.98	0.45
1:C:4:DA:C2	1:C:5:DC:C2	3.04	0.45
2:D:25:DC:H5	3:A:185:SER:HB3	1.82	0.45
3:E:174:LYS:NZ	3:E:174:LYS:HB2	2.32	0.44
3:B:153:VAL:HG12	3:B:161:ARG:HD3	2.00	0.44
3:F:164:LEU:CD1	3:F:194:MSE:HE3	2.36	0.44
3:A:151:ARG:NH1	3:A:200:LEU:CD2	2.81	0.44
3:A:204:VAL:HG22	3:B:204:VAL:HG22	2.00	0.44
3:A:209:TRP:CE2	3:A:215:ILE:HD11	2.52	0.44
1:C:20:DG:H8	1:C:20:DG:H5''	1.82	0.44
3:E:153:VAL:HG22	3:E:209:TRP:CH2	2.52	0.44
3:E:167:ILE:CD1	3:E:203:ARG:NH2	2.81	0.44
3:B:153:VAL:HG22	3:B:209:TRP:HH2	1.79	0.43
3:B:197:LYS:O	3:B:198:MSE:HE2	2.18	0.43
2:D:24:DA:C2	2:D:25:DC:C2	3.06	0.43
3:E:151:ARG:NH2	3:E:200:LEU:HD23	2.33	0.43
2:G:17:DT:H2''	2:G:18:DA:C5'	2.49	0.43
3:E:167:ILE:HD13	3:E:203:ARG:NH2	2.34	0.43
3:F:156:LEU:HD21	3:F:198:MSE:HG2	2.01	0.43
1:H:24:DA:C2	1:H:25:DC:C2	3.07	0.43
3:E:152:ASP:OD2	3:E:154:ASN:HB2	2.19	0.42
2:G:6:DC:H2'	2:G:7:DC:H5'	1.96	0.42
3:B:177:ALA:HB1	3:B:182:ILE:O	2.19	0.42
1:C:13:DT:C7	3:A:188:LYS:HE2	2.50	0.42
1:C:2:DG:H2'	1:C:3:DT:H71	2.01	0.42
3:E:159:ARG:O	3:E:162:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:204:VAL:O	3:F:208:VAL:HG23	2.19	0.42
1:C:15:DG:H2'	1:C:16:DG:C8	2.55	0.42
3:F:213:GLU:HB3	3:F:215:ILE:CD1	2.50	0.42
3:A:151:ARG:HD3	3:A:198:MSE:O	2.19	0.42
3:F:159:ARG:O	3:F:162:ASP:HB2	2.20	0.42
2:G:5:DC:H5	3:F:185:SER:HB3	1.85	0.41
2:G:9:DT:H2'	2:G:10:DT:C6	2.56	0.41
3:B:153:VAL:HG21	3:B:215:ILE:HG21	2.01	0.41
3:E:185:SER:O	3:E:189:VAL:HG23	2.21	0.41
3:A:166:LEU:HD12	3:A:166:LEU:HA	1.90	0.40
3:E:151:ARG:NE	3:E:200:LEU:HD21	2.36	0.40
3:F:200:LEU:HD12	3:F:200:LEU:HA	1.91	0.40
3:E:159:ARG:HA	3:E:159:ARG:HD3	1.97	0.40
3:A:213:GLU:O	3:A:214:ARG:C	2.59	0.40
3:E:197:LYS:O	3:E:198:MSE:HE2	2.21	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	
3	A	64/82 (78%)	63 (98%)	1 (2%)	0	100	100
3	B	64/82 (78%)	64 (100%)	0	0	100	100
3	E	64/82 (78%)	63 (98%)	1 (2%)	0	100	100
3	F	64/82 (78%)	64 (100%)	0	0	100	100
All	All	256/328 (78%)	254 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	A	61/70 (87%)	57 (93%)	4 (7%)	16	22
3	B	61/70 (87%)	57 (93%)	4 (7%)	16	22
3	E	61/70 (87%)	58 (95%)	3 (5%)	25	35
3	F	61/70 (87%)	58 (95%)	3 (5%)	25	35
All	All	244/280 (87%)	230 (94%)	14 (6%)	20	28

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	159	ARG
3	A	166	LEU
3	A	195	LEU
3	A	213	GLU
3	B	164	LEU
3	B	179	ARG
3	B	200	LEU
3	B	213	GLU
3	E	159	ARG
3	E	179	ARG
3	E	213	GLU
3	F	195	LEU
3	F	200	LEU
3	F	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	212	GLN
3	B	154	ASN
3	F	154	ASN
3	F	212	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	SO4	G	304	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	E	307	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	B	306	-	4,4,4	0.29	0	6,6,6	0.07	0
4	SO4	A	301	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	A	305	-	4,4,4	0.28	0	6,6,6	0.04	0
4	SO4	C	302	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	B	309	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	H	303	-	4,4,4	0.28	0	6,6,6	0.07	0
4	SO4	F	308	-	4,4,4	0.26	0	6,6,6	0.07	0

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 [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	C	20/20 (100%)	-0.75	0 100 100	32, 48, 60, 62	0
1	H	20/20 (100%)	-0.71	0 100 100	31, 48, 57, 61	0
2	D	20/20 (100%)	-0.75	0 100 100	33, 46, 58, 59	0
2	G	20/20 (100%)	-0.77	0 100 100	34, 47, 59, 61	0
3	A	63/82 (76%)	-0.34	0 100 100	29, 41, 60, 69	1 (1%)
3	B	63/82 (76%)	-0.36	0 100 100	29, 40, 60, 70	0
3	E	63/82 (76%)	-0.33	0 100 100	29, 40, 61, 72	1 (1%)
3	F	63/82 (76%)	-0.33	0 100 100	29, 41, 61, 74	0
All	All	332/408 (81%)	-0.44	0 100 100	29, 43, 61, 74	2 (0%)

There are no RSRZ outliers to report.

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. 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(\AA^2)	Q<0.9
4	SO4	H	303	5/5	0.85	0.25	91,92,92,93	0
4	SO4	C	302	5/5	0.88	0.21	92,92,93,93	0
4	SO4	B	309	5/5	0.93	0.16	108,108,109,109	0
4	SO4	B	306	5/5	0.95	0.17	82,82,82,82	0
4	SO4	G	304	5/5	0.95	0.14	85,85,86,87	0
4	SO4	A	301	5/5	0.96	0.16	87,88,88,88	0
4	SO4	A	305	5/5	0.97	0.08	83,83,84,84	0
4	SO4	E	307	5/5	0.98	0.13	75,75,76,76	0
4	SO4	F	308	5/5	0.98	0.15	85,85,85,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.