



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:41 am BST

PDB ID : 4N83
Title : X-ray crystal structure of Streptococcus sanguinis dimanganese(II)-NrdF
Authors : Boal, A.K.; Rosenzweig, A.C.
Deposited on : 2013-10-16
Resolution : 2.65 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
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

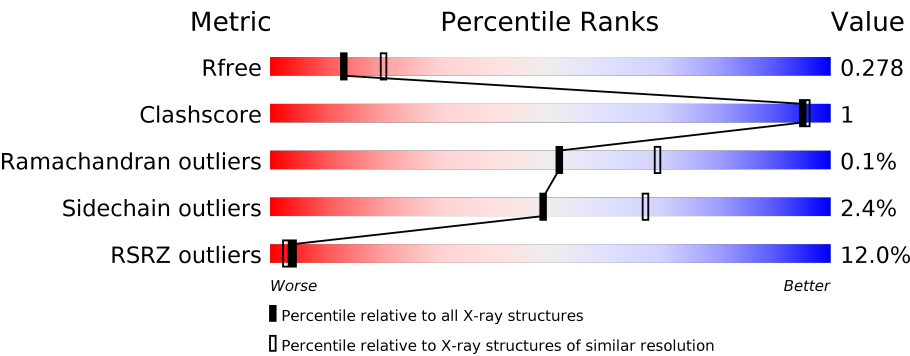
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	A	319	<div><div>37%</div><div><div></div><div>87%</div><div>11%</div></div></div>
1	B	319	<div><div>%</div><div><div></div><div>82%</div><div>7%</div><div>11%</div></div></div>
1	C	319	<div><div>2%</div><div><div></div><div>85%</div><div>11%</div></div></div>
1	D	319	<div><div>5%</div><div><div></div><div>85%</div><div>11%</div></div></div>
1	E	319	<div><div>11%</div><div><div></div><div>84%</div><div>11%</div></div></div>
1	F	319	<div><div>%</div><div><div></div><div>86%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	319	<div><div></div><div>28%</div><div></div><div>85%</div><div></div><div>11%</div></div>
1	H	319	<div>%<div><div></div><div></div><div>84%</div><div></div><div>11%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18705 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 Ribonucleoside-diphosphate reductase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2336	1508	366	458	4			
1	B	284	Total	C	N	O	S	0	0	0
			2329	1504	365	456	4			
1	C	284	Total	C	N	O	S	0	0	0
			2329	1504	365	456	4			
1	D	284	Total	C	N	O	S	0	0	0
			2329	1504	365	456	4			
1	E	284	Total	C	N	O	S	0	0	0
			2329	1504	365	456	4			
1	F	284	Total	C	N	O	S	0	0	0
			2329	1504	365	456	4			
1	G	283	Total	C	N	O	S	0	0	0
			2322	1500	364	454	4			
1	H	283	Total	C	N	O	S	0	0	0
			2322	1500	364	454	4			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0

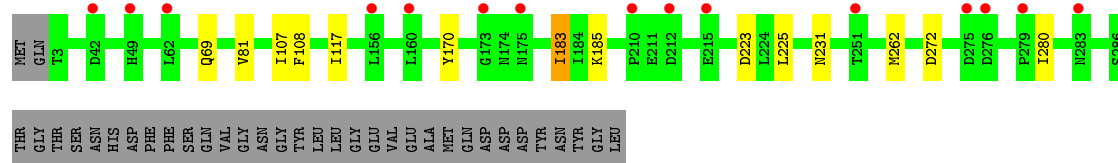
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	27	Total 27	O 27	0	0
3	C	7	Total 7	O 7	0	0
3	D	2	Total 2	O 2	0	0
3	E	3	Total 3	O 3	0	0
3	F	4	Total 4	O 4	0	0
3	H	20	Total 20	O 20	0	0


- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

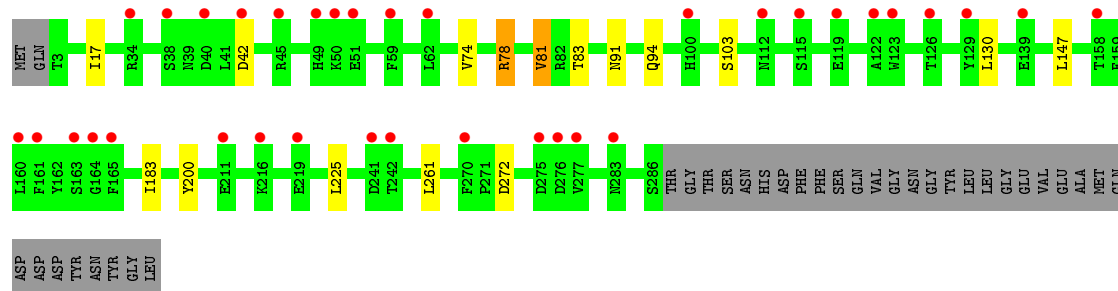


Chain D: 




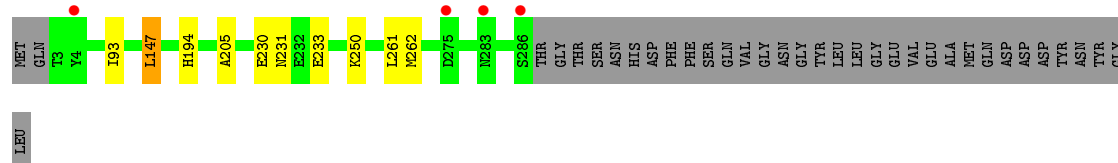
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain E: 




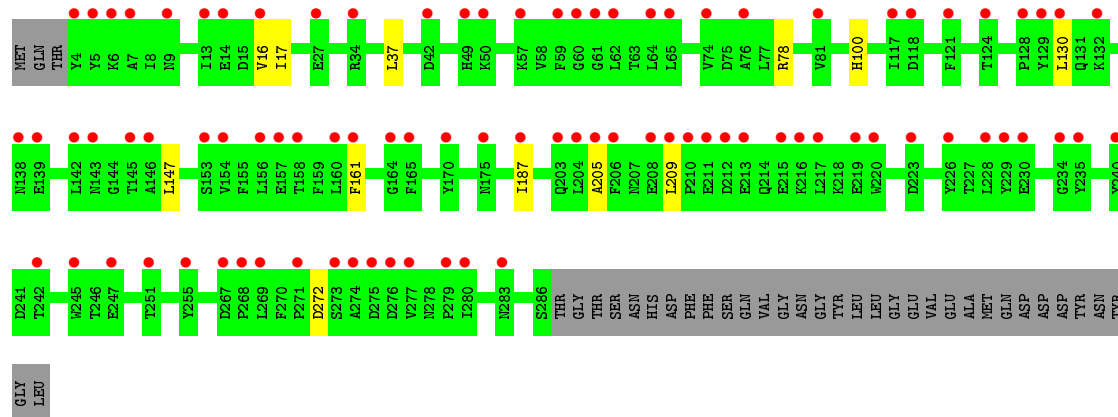
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain F: 

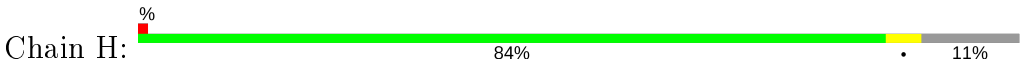


- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain G: 



- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.66Å 80.22Å 166.37Å 90.00° 105.91° 90.00°	Depositor
Resolution (Å)	29.90 – 2.65 29.88 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.5 (29.90-2.65) 86.7 (29.88-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.235 , 0.278 0.236 , 0.278	Depositor DCC
R_{free} test set	3799 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18705	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.93% 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: MN

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	0.28	0/2391	0.39	0/3246
1	B	0.31	0/2384	0.47	0/3236
1	C	0.31	0/2384	0.48	0/3236
1	D	0.28	0/2384	0.43	0/3236
1	E	0.28	0/2384	0.43	0/3236
1	F	0.30	0/2384	0.47	0/3236
1	G	0.28	0/2377	0.41	0/3226
1	H	0.31	0/2377	0.46	0/3226
All	All	0.29	0/19065	0.44	0/25878

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	2336	0	2264	4	0
1	B	2329	0	2257	9	0
1	C	2329	0	2257	5	0
1	D	2329	0	2257	5	0
1	E	2329	0	2257	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2329	0	2257	5	0
1	G	2322	0	2250	3	0
1	H	2322	0	2250	7	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	1	0	0	0	0
3	B	27	0	0	0	0
3	C	7	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	H	20	0	0	1	0
All	All	18705	0	18049	43	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 1.

All (43) 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:E:103:SER:HB2	1:E:183:ILE:HD11	1.72	0.71
1:D:107:ILE:HD11	1:D:183:ILE:HD11	1.82	0.62
1:B:180:VAL:O	1:B:183:ILE:HG22	2.03	0.59
1:B:147:LEU:HD11	1:B:205:ALA:HB3	1.90	0.54
1:A:146:ALA:O	1:A:147:LEU:HB2	2.08	0.53
1:H:59:PHE:CE1	1:H:184:ILE:HD11	2.44	0.52
1:G:147:LEU:HD11	1:G:205:ALA:HB3	1.92	0.52
1:F:233:GLU:HB2	1:F:250:LYS:HE2	1.92	0.51
1:E:78:ARG:NH2	1:E:91:ASN:OD1	2.43	0.51
1:B:74:VAL:HG11	1:B:94:GLN:HB2	1.93	0.50
1:F:93:ILE:HG23	1:F:194:HIS:CE1	2.47	0.50
1:F:230:GLU:O	1:F:233:GLU:HG2	2.13	0.49
1:B:50:LYS:HE2	1:B:242:THR:HB	1.94	0.49
1:A:147:LEU:HD23	1:A:217:LEU:HD22	1.96	0.48
1:C:69:GLN:HE21	1:C:69:GLN:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:LYS:HD2	1:H:160:LEU:HD13	1.96	0.47
1:B:225:LEU:HD12	1:B:261:LEU:HD11	1.98	0.46
1:E:17:ILE:HD13	1:E:200:TYR:CZ	2.51	0.46
1:D:107:ILE:CD1	1:D:183:ILE:HD11	2.45	0.46
1:D:170:TYR:CE1	1:D:280:ILE:HD11	2.50	0.46
1:D:69:GLN:HA	1:D:69:GLN:HE21	1.81	0.45
1:A:156:LEU:HD12	1:A:160:LEU:HD11	1.98	0.45
1:B:73:GLY:HA2	1:B:141:TYR:CE2	2.52	0.45
1:C:32:ASP:N	1:C:32:ASP:OD2	2.48	0.45
1:G:16:VAL:HG23	1:G:17:ILE:HD12	1.99	0.44
1:H:39:ASN:HD22	1:H:39:ASN:N	2.15	0.44
1:C:235:TYR:O	1:C:238:SER:HB3	2.18	0.44
1:G:100:HIS:CD2	1:G:187:ILE:HG12	2.53	0.43
1:F:233:GLU:HB2	1:F:250:LYS:CE	2.47	0.43
1:E:81:VAL:HG13	1:E:83:THR:O	2.19	0.43
1:E:74:VAL:HG11	1:E:94:GLN:HB2	2.01	0.43
1:B:39:ASN:HD22	1:B:39:ASN:N	2.17	0.43
1:F:147:LEU:HD11	1:F:205:ALA:HB3	1.99	0.43
1:H:84:ALA:HA	3:H:520:HOH:O	2.19	0.43
1:H:247:GLU:O	1:H:251:THR:HG23	2.19	0.43
1:C:160:LEU:HD11	1:C:228:LEU:HD13	2.01	0.43
1:B:125:ASN:HD21	1:H:7:ALA:H	1.65	0.43
1:D:108:PHE:HB3	1:D:117:ILE:HG12	2.01	0.42
1:A:221:MET:HE2	1:A:261:LEU:HD23	2.02	0.41
1:E:103:SER:CB	1:E:183:ILE:HD11	2.45	0.41
1:H:65:LEU:HD11	1:H:133:LYS:HE3	2.02	0.41
1:B:59:PHE:CE1	1:B:184:ILE:HD11	2.56	0.40
1:C:35:ILE:N	1:C:35:ILE:HD12	2.36	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	283/319 (89%)	274 (97%)	8 (3%)	1 (0%)	34	48
1	B	282/319 (88%)	274 (97%)	7 (2%)	1 (0%)	34	48
1	C	282/319 (88%)	277 (98%)	5 (2%)	0	100	100
1	D	282/319 (88%)	278 (99%)	4 (1%)	0	100	100
1	E	282/319 (88%)	273 (97%)	9 (3%)	0	100	100
1	F	282/319 (88%)	275 (98%)	7 (2%)	0	100	100
1	G	281/319 (88%)	274 (98%)	7 (2%)	0	100	100
1	H	281/319 (88%)	274 (98%)	7 (2%)	0	100	100
All	All	2255/2552 (88%)	2199 (98%)	54 (2%)	2 (0%)	51	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	B	285	ILE

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	256/284 (90%)	254 (99%)	2 (1%)	81	89
1	B	255/284 (90%)	246 (96%)	9 (4%)	36	52
1	C	255/284 (90%)	247 (97%)	8 (3%)	40	57
1	D	255/284 (90%)	247 (97%)	8 (3%)	40	57
1	E	255/284 (90%)	247 (97%)	8 (3%)	40	57
1	F	255/284 (90%)	251 (98%)	4 (2%)	62	78
1	G	254/284 (89%)	248 (98%)	6 (2%)	49	67
1	H	254/284 (89%)	250 (98%)	4 (2%)	62	78
All	All	2039/2272 (90%)	1990 (98%)	49 (2%)	49	67

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	161	PHE
1	B	16	VAL
1	B	42	ASP
1	B	75	ASP
1	B	81	VAL
1	B	132	LYS
1	B	147	LEU
1	B	248	GLU
1	B	261	LEU
1	B	273	SER
1	C	32	ASP
1	C	42	ASP
1	C	113	THR
1	C	211	GLU
1	C	243	VAL
1	C	261	LEU
1	C	262	MET
1	C	272	ASP
1	D	81	VAL
1	D	183	ILE
1	D	185	LYS
1	D	223	ASP
1	D	225	LEU
1	D	231	ASN
1	D	262	MET
1	D	272	ASP
1	E	42	ASP
1	E	78	ARG
1	E	81	VAL
1	E	130	LEU
1	E	147	LEU
1	E	225	LEU
1	E	261	LEU
1	E	272	ASP
1	F	147	LEU
1	F	231	ASN
1	F	261	LEU
1	F	262	MET
1	G	37	LEU
1	G	78	ARG
1	G	130	LEU
1	G	161	PHE

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Mol	Chain	Res	Type
1	G	209	LEU
1	G	272	ASP
1	H	32	ASP
1	H	53	ASP
1	H	238	SER
1	H	272	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	39	ASN
1	A	69	GLN
1	A	266	GLN
1	B	11	ASN
1	B	39	ASN
1	B	112	ASN
1	B	125	ASN
1	B	214	GLN
1	B	263	ASN
1	C	11	ASN
1	C	28	GLN
1	C	39	ASN
1	C	69	GLN
1	C	112	ASN
1	C	179	ASN
1	C	214	GLN
1	C	263	ASN
1	C	283	ASN
1	D	28	GLN
1	D	39	ASN
1	D	69	GLN
1	D	214	GLN
1	D	231	ASN
1	D	263	ASN
1	D	266	GLN
1	E	11	ASN
1	E	39	ASN
1	E	69	GLN
1	E	266	GLN
1	F	69	GLN
1	G	11	ASN

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Mol	Chain	Res	Type
1	G	39	ASN
1	G	100	HIS
1	G	231	ASN
1	G	263	ASN
1	G	266	GLN
1	H	11	ASN
1	H	39	ASN
1	H	69	GLN
1	H	263	ASN

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](#)

Of 16 ligands modelled in this entry, 16 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

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	285/319 (89%)	1.92	119 (41%) 0 0	58, 111, 135, 141	0
1	B	284/319 (89%)	-0.17	2 (0%) 87 87	11, 15, 30, 38	0
1	C	284/319 (89%)	-0.17	6 (2%) 63 59	12, 21, 43, 62	0
1	D	284/319 (89%)	0.32	15 (5%) 26 23	14, 49, 71, 86	0
1	E	284/319 (89%)	0.74	35 (12%) 4 2	20, 64, 95, 112	0
1	F	284/319 (89%)	-0.00	4 (1%) 75 73	13, 29, 58, 76	0
1	G	283/319 (88%)	1.57	89 (31%) 0 0	52, 87, 113, 133	0
1	H	283/319 (88%)	-0.15	2 (0%) 87 87	11, 16, 35, 39	0
All	All	2271/2552 (88%)	0.51	272 (11%) 4 3	11, 37, 116, 141	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	PRO	8.1
1	A	161	PHE	7.4
1	A	53	ASP	7.2
1	G	5	TYR	7.2
1	A	284	GLY	6.8
1	A	240	TYR	6.7
1	G	271	PRO	6.5
1	A	279	PRO	6.4
1	G	212	ASP	6.1
1	G	276	ASP	5.9
1	A	165	PHE	5.9
1	G	226	TYR	5.4
1	G	13	ILE	5.3
1	A	175	ASN	5.2
1	G	161	PHE	5.2
1	A	139	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	238	SER	4.9
1	A	276	ASP	4.9
1	A	135	GLU	4.8
1	A	65	LEU	4.8
1	E	126	THR	4.8
1	A	272	ASP	4.8
1	A	62	LEU	4.7
1	A	46	LYS	4.7
1	A	156	LEU	4.7
1	G	206	PHE	4.5
1	A	178	ALA	4.5
1	A	113	THR	4.5
1	G	277	VAL	4.4
1	A	275	ASP	4.4
1	A	162	TYR	4.4
1	G	156	LEU	4.3
1	G	267	ASP	4.3
1	E	49	HIS	4.3
1	A	244	GLY	4.3
1	A	146	ALA	4.2
1	A	153	SER	4.2
1	G	4	TYR	4.2
1	A	166	PHE	4.2
1	E	62	LEU	4.1
1	G	216	LYS	4.1
1	G	209	LEU	4.1
1	G	251	THR	4.1
1	A	268	PRO	4.0
1	A	121	PHE	4.0
1	A	159	PHE	4.0
1	G	124	THR	4.0
1	G	62	LEU	3.9
1	G	268	PRO	3.9
1	A	255	TYR	3.9
1	A	283	ASN	3.9
1	A	119	GLU	3.9
1	A	36	PRO	3.9
1	A	137	ILE	3.9
1	G	235	TYR	3.9
1	G	142	LEU	3.9
1	G	121	PHE	3.9
1	G	139	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	220	TRP	3.8
1	A	143	ASN	3.8
1	A	129	TYR	3.8
1	A	4	TYR	3.7
1	A	211	GLU	3.7
1	A	280	ILE	3.7
1	G	160	LEU	3.7
1	A	204	LEU	3.7
1	A	45	ARG	3.7
1	E	211	GLU	3.7
1	A	210	PRO	3.6
1	G	230	GLU	3.6
1	A	38	SER	3.6
1	A	42	ASP	3.6
1	G	65	LEU	3.6
1	D	62	LEU	3.6
1	G	219	GLU	3.5
1	G	50	LYS	3.5
1	G	145	THR	3.5
1	A	229	TYR	3.5
1	A	287	THR	3.4
1	A	208	GLU	3.4
1	A	126	THR	3.4
1	A	145	THR	3.4
1	A	34	ARG	3.4
1	E	165	PHE	3.4
1	G	132	LYS	3.4
1	A	230	GLU	3.4
1	A	249	VAL	3.3
1	A	141	TYR	3.3
1	A	110	THR	3.3
1	G	129	TYR	3.3
1	A	49	HIS	3.3
1	G	130	LEU	3.3
1	E	242	THR	3.3
1	A	206	PHE	3.3
1	G	275	ASP	3.3
1	G	245	TRP	3.2
1	A	219	GLU	3.2
1	A	66	ASP	3.2
1	G	242	THR	3.2
1	G	49	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	207	ASN	3.2
1	A	248	GLU	3.1
1	A	163	SER	3.1
1	A	239	LEU	3.1
1	G	215	GLU	3.1
1	A	281	VAL	3.1
1	G	280	ILE	3.1
1	G	283	ASN	3.1
1	A	271	PRO	3.1
1	A	245	TRP	3.0
1	G	153	SER	3.0
1	A	5	TYR	3.0
1	D	215	GLU	3.0
1	G	217	LEU	3.0
1	A	252	PHE	3.0
1	E	51	GLU	3.0
1	G	247	GLU	3.0
1	A	222	TYR	3.0
1	A	212	ASP	3.0
1	G	204	LEU	3.0
1	F	286	SER	3.0
1	A	262	MET	3.0
1	G	154	VAL	3.0
1	A	251	THR	2.9
1	D	279	PRO	2.9
1	E	38	SER	2.9
1	C	3	THR	2.9
1	E	119	GLU	2.9
1	D	42	ASP	2.9
1	E	161	PHE	2.9
1	G	213	GLU	2.9
1	G	229	TYR	2.9
1	A	155	PHE	2.8
1	A	223	ASP	2.8
1	A	50	LYS	2.8
1	G	211	GLU	2.8
1	D	49	HIS	2.8
1	E	45	ARG	2.8
1	E	241	ASP	2.8
1	D	173	GLY	2.8
1	E	276	ASP	2.8
1	A	158	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	115	SER	2.8
1	E	275	ASP	2.8
1	A	61	GLY	2.8
1	A	282	MET	2.7
1	G	273	SER	2.7
1	A	254	ARG	2.7
1	C	286	SER	2.7
1	C	275	ASP	2.7
1	G	175	ASN	2.7
1	G	27	GLU	2.7
1	A	116	GLU	2.7
1	G	170	TYR	2.7
1	A	154	VAL	2.7
1	D	156	LEU	2.7
1	H	280	ILE	2.7
1	C	42	ASP	2.7
1	G	16	VAL	2.7
1	A	273	SER	2.7
1	G	128	PRO	2.6
1	A	6	LYS	2.6
1	E	112	ASN	2.6
1	E	283	ASN	2.6
1	G	143	ASN	2.6
1	G	57	LYS	2.6
1	E	122	ALA	2.6
1	A	209	LEU	2.6
1	A	216	LYS	2.5
1	E	216	LYS	2.5
1	G	279	PRO	2.5
1	G	146	ALA	2.5
1	A	164	GLY	2.5
1	A	237	GLU	2.5
1	D	210	PRO	2.5
1	G	205	ALA	2.5
1	E	277	VAL	2.5
1	G	117	ILE	2.5
1	A	177	LEU	2.5
1	G	64	LEU	2.5
1	A	55	VAL	2.5
1	G	76	ALA	2.5
1	G	14	GLU	2.5
1	F	283	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	210	PRO	2.5
1	A	69	GLN	2.5
1	G	165	PHE	2.5
1	G	158	THR	2.5
1	A	123	TRP	2.5
1	D	283	ASN	2.5
1	G	138	ASN	2.5
1	A	242	THR	2.4
1	G	228	LEU	2.4
1	A	202	PHE	2.4
1	A	47	LEU	2.4
1	A	269	LEU	2.4
1	E	160	LEU	2.4
1	B	34	ARG	2.4
1	A	157	GLU	2.4
1	G	274	ALA	2.4
1	E	164	GLY	2.4
1	A	140	ILE	2.4
1	A	15	ASP	2.4
1	E	42	ASP	2.4
1	G	9	ASN	2.4
1	E	50	LYS	2.4
1	G	6	LYS	2.4
1	G	187	ILE	2.4
1	A	39	ASN	2.4
1	C	262	MET	2.4
1	A	215	GLU	2.4
1	A	241	ASP	2.3
1	C	212	ASP	2.3
1	G	61	GLY	2.3
1	A	148	GLU	2.3
1	G	157	GLU	2.3
1	E	100	HIS	2.3
1	G	7	ALA	2.3
1	A	127	ASN	2.3
1	A	33	THR	2.3
1	E	139	GLU	2.3
1	G	118	ASP	2.3
1	G	203	GLN	2.3
1	D	276	ASP	2.3
1	G	60	GLY	2.3
1	A	30	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	2.3
1	D	175	ASN	2.3
1	E	129	TYR	2.3
1	G	240	TYR	2.3
1	E	270	PHE	2.3
1	E	115	SER	2.2
1	G	34	ARG	2.2
1	G	59	PHE	2.2
1	A	174	ASN	2.2
1	A	122	ALA	2.2
1	D	275	ASP	2.2
1	E	34	ARG	2.2
1	D	160	LEU	2.2
1	E	59	PHE	2.2
1	A	48	SER	2.2
1	A	70	SER	2.2
1	G	208	GLU	2.2
1	G	234	GLY	2.2
1	F	275	ASP	2.2
1	G	223	ASP	2.2
1	A	117	ILE	2.1
1	A	205	ALA	2.1
1	D	251	THR	2.1
1	A	261	LEU	2.1
1	H	279	PRO	2.1
1	E	123	TRP	2.1
1	G	42	ASP	2.1
1	G	81	VAL	2.1
1	A	236	THR	2.1
1	E	163	SER	2.1
1	A	60	GLY	2.1
1	E	40	ASP	2.1
1	G	164	GLY	2.1
1	A	59	PHE	2.1
1	A	37	LEU	2.1
1	A	228	LEU	2.1
1	G	74	VAL	2.1
1	G	255	TYR	2.1
1	A	152	ALA	2.1
1	G	269	LEU	2.0
1	B	280	ILE	2.0
1	E	219	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	4	TYR	2.0
1	A	7	ALA	2.0
1	D	212	ASP	2.0
1	E	158	THR	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	MN	G	402	1/1	0.61	0.23	95,95,95,95	0
2	MN	A	402	1/1	0.85	0.20	91,91,91,91	0
2	MN	A	401	1/1	0.88	0.18	72,72,72,72	0
2	MN	E	402	1/1	0.94	0.18	50,50,50,50	0
2	MN	D	401	1/1	0.96	0.18	37,37,37,37	0
2	MN	E	401	1/1	0.97	0.13	41,41,41,41	0
2	MN	F	402	1/1	0.97	0.13	24,24,24,24	0
2	MN	D	402	1/1	0.97	0.14	33,33,33,33	0
2	MN	C	401	1/1	0.98	0.13	16,16,16,16	0
2	MN	F	401	1/1	0.99	0.13	23,23,23,23	0
2	MN	C	402	1/1	0.99	0.11	25,25,25,25	0
2	MN	H	401	1/1	0.99	0.10	8,8,8,8	0
2	MN	H	402	1/1	0.99	0.10	11,11,11,11	0
2	MN	B	402	1/1	0.99	0.10	9,9,9,9	0
2	MN	G	401	1/1	0.99	0.19	64,64,64,64	0
2	MN	B	401	1/1	1.00	0.11	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.