



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:56 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

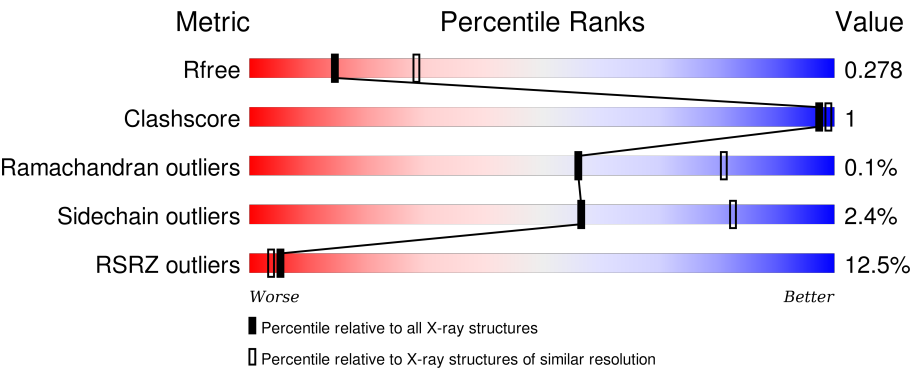
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 $\leq 5\%$. 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>39%</div><div><div></div><div>87%</div><div></div><div>11%</div></div></div>
1	B	319	<div><div>%</div><div><div></div><div>82%</div><div></div><div>7%</div><div>11%</div></div></div>
1	C	319	<div><div>2%</div><div><div></div><div>85%</div><div></div><div>11%</div></div></div>
1	D	319	<div><div>5%</div><div><div></div><div>85%</div><div></div><div>11%</div></div></div>
1	E	319	<div><div>12%</div><div><div></div><div>84%</div><div></div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	319	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>86%</div><div>11%</div></div><div><div></div><div></div><div></div></div></div>
1	G	319	<div><div><div></div><div></div><div></div></div><div><div>29%</div><div>85%</div><div>11%</div></div><div><div></div><div></div><div></div></div></div>
1	H	319	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>84%</div><div>11%</div></div><div><div></div><div></div><div></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

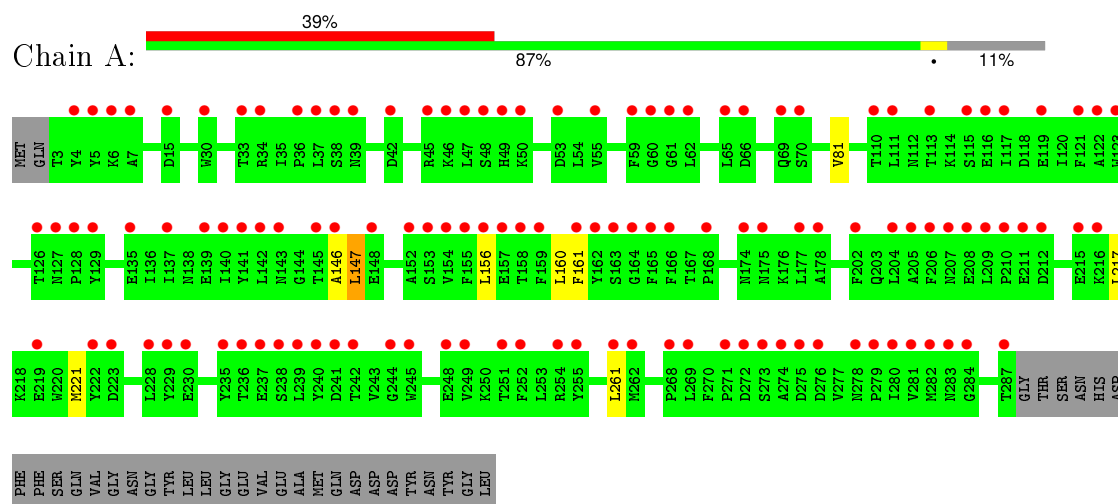
- Molecule 3 is water.

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

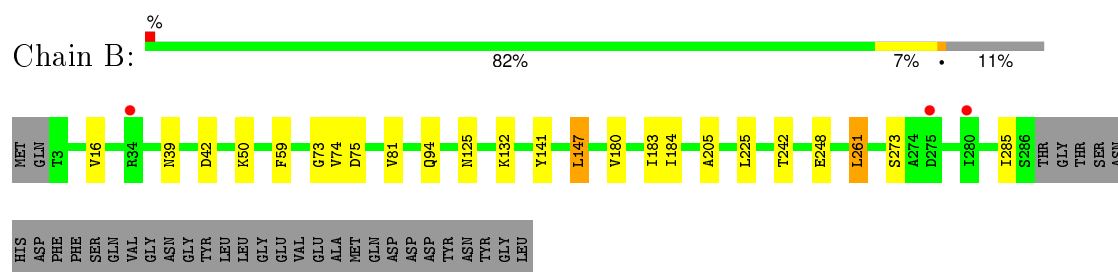
3 Residue-property plots [i](#)

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.

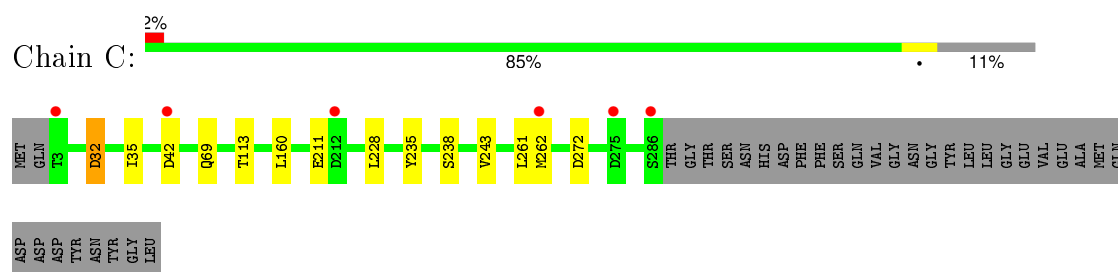
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



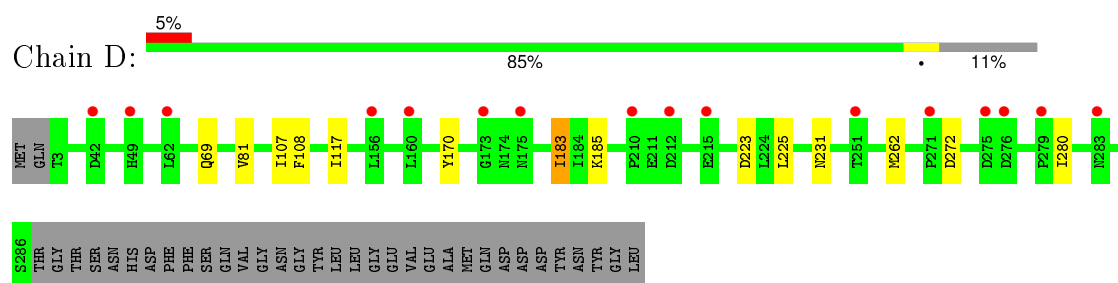
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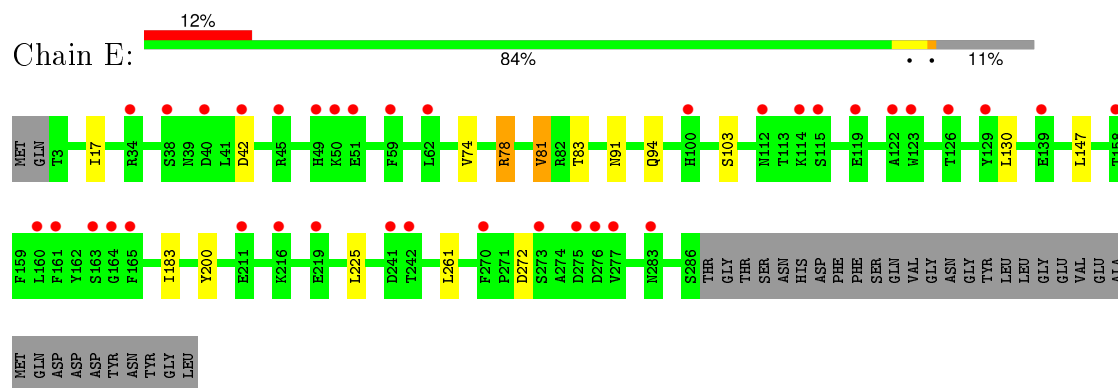
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



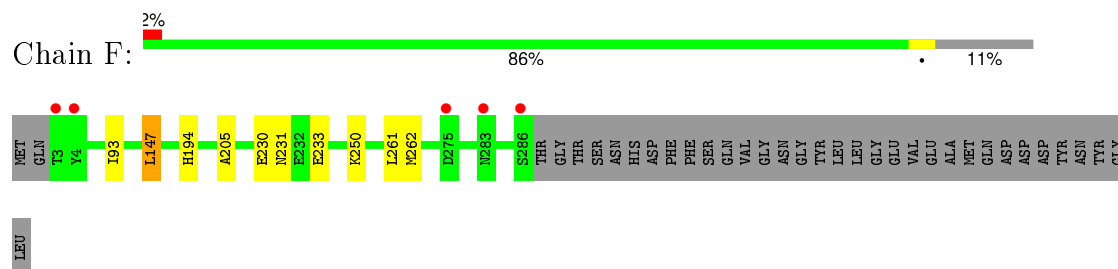
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



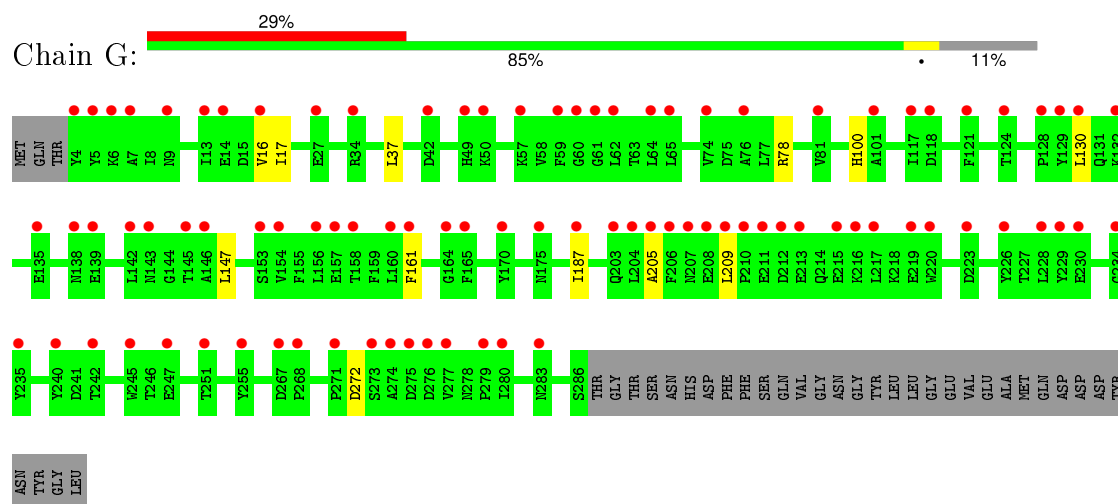
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



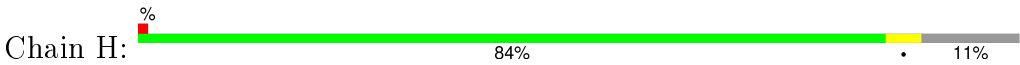
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



- 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 (5.32%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 75270 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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 [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	283/319 (89%)	274 (97%)	8 (3%)	1 (0%)	39	65
1	B	282/319 (88%)	274 (97%)	7 (2%)	1 (0%)	39	65
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%)	56	81

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%)	86	95
1	B	255/284 (90%)	246 (96%)	9 (4%)	43	71
1	C	255/284 (90%)	247 (97%)	8 (3%)	47	75
1	D	255/284 (90%)	247 (97%)	8 (3%)	47	75
1	E	255/284 (90%)	247 (97%)	8 (3%)	47	75
1	F	255/284 (90%)	251 (98%)	4 (2%)	70	89
1	G	254/284 (89%)	248 (98%)	6 (2%)	57	82
1	H	254/284 (89%)	250 (98%)	4 (2%)	70	89
All	All	2039/2272 (90%)	1990 (98%)	49 (2%)	57	82

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%)	1.97	124 (43%) 0 0	58, 111, 135, 141	0
1	B	284/319 (89%)	-0.13	3 (1%) 82 82	11, 15, 30, 38	0
1	C	284/319 (89%)	-0.14	6 (2%) 67 66	12, 21, 43, 62	0
1	D	284/319 (89%)	0.36	16 (5%) 28 25	14, 49, 71, 86	0
1	E	284/319 (89%)	0.79	37 (13%) 5 3	20, 64, 95, 112	0
1	F	284/319 (89%)	0.03	5 (1%) 71 70	13, 29, 58, 76	0
1	G	283/319 (88%)	1.63	91 (32%) 1 0	52, 87, 113, 133	0
1	H	283/319 (88%)	-0.12	3 (1%) 82 82	11, 16, 35, 39	0
All	All	2271/2552 (88%)	0.55	285 (12%) 5 4	11, 37, 116, 141	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	PRO	8.2
1	A	161	PHE	7.5
1	A	53	ASP	7.3
1	G	5	TYR	7.2
1	A	284	GLY	6.9
1	A	240	TYR	6.9
1	G	271	PRO	6.8
1	A	279	PRO	6.7
1	G	212	ASP	6.3
1	G	276	ASP	6.2
1	A	165	PHE	5.9
1	G	226	TYR	5.5
1	G	13	ILE	5.3
1	A	139	GLU	5.3
1	A	175	ASN	5.3
1	G	161	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	276	ASP	5.0
1	A	135	GLU	5.0
1	E	126	THR	4.9
1	A	46	LYS	4.9
1	A	238	SER	4.8
1	A	65	LEU	4.8
1	A	272	ASP	4.8
1	A	156	LEU	4.8
1	G	206	PHE	4.7
1	A	62	LEU	4.7
1	A	178	ALA	4.7
1	A	275	ASP	4.6
1	G	277	VAL	4.6
1	A	113	THR	4.5
1	A	162	TYR	4.5
1	G	267	ASP	4.4
1	G	4	TYR	4.4
1	G	156	LEU	4.4
1	A	146	ALA	4.4
1	A	153	SER	4.3
1	G	216	LYS	4.3
1	E	49	HIS	4.3
1	G	209	LEU	4.3
1	A	121	PHE	4.2
1	A	244	GLY	4.2
1	A	268	PRO	4.2
1	E	62	LEU	4.2
1	A	166	PHE	4.1
1	G	124	THR	4.1
1	G	142	LEU	4.1
1	A	283	ASN	4.1
1	G	251	THR	4.1
1	A	143	ASN	4.0
1	A	36	PRO	4.0
1	G	220	TRP	4.0
1	G	121	PHE	4.0
1	G	268	PRO	4.0
1	G	62	LEU	4.0
1	G	139	GLU	3.9
1	A	159	PHE	3.9
1	A	211	GLU	3.9
1	A	280	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	4	TYR	3.9
1	A	119	GLU	3.9
1	E	211	GLU	3.8
1	A	204	LEU	3.8
1	G	235	TYR	3.8
1	A	137	ILE	3.8
1	G	219	GLU	3.8
1	A	45	ARG	3.8
1	G	160	LEU	3.8
1	G	230	GLU	3.7
1	A	229	TYR	3.7
1	A	255	TYR	3.7
1	A	110	THR	3.7
1	A	210	PRO	3.7
1	G	145	THR	3.7
1	A	38	SER	3.7
1	A	129	TYR	3.6
1	E	242	THR	3.6
1	D	62	LEU	3.6
1	G	65	LEU	3.6
1	A	42	ASP	3.6
1	G	50	LYS	3.5
1	A	230	GLU	3.5
1	A	145	THR	3.5
1	A	141	TYR	3.5
1	A	219	GLU	3.5
1	A	287	THR	3.5
1	A	208	GLU	3.5
1	A	34	ARG	3.4
1	G	132	LYS	3.4
1	E	165	PHE	3.4
1	A	126	THR	3.4
1	A	66	ASP	3.4
1	G	245	TRP	3.3
1	G	129	TYR	3.3
1	G	215	GLU	3.3
1	A	212	ASP	3.3
1	G	275	ASP	3.3
1	A	49	HIS	3.3
1	G	130	LEU	3.3
1	G	242	THR	3.3
1	A	249	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	206	PHE	3.2
1	A	262	MET	3.2
1	E	51	GLU	3.2
1	G	49	HIS	3.2
1	A	281	VAL	3.2
1	A	239	LEU	3.2
1	G	217	LEU	3.2
1	G	283	ASN	3.2
1	A	163	SER	3.1
1	G	247	GLU	3.1
1	G	280	ILE	3.1
1	A	248	GLU	3.1
1	F	286	SER	3.1
1	G	153	SER	3.1
1	A	245	TRP	3.1
1	C	3	THR	3.1
1	G	204	LEU	3.1
1	A	207	ASN	3.0
1	A	271	PRO	3.0
1	G	154	VAL	3.0
1	D	215	GLU	3.0
1	D	279	PRO	3.0
1	A	223	ASP	3.0
1	A	5	TYR	3.0
1	A	222	TYR	3.0
1	D	42	ASP	3.0
1	E	241	ASP	3.0
1	E	276	ASP	3.0
1	E	119	GLU	3.0
1	E	38	SER	3.0
1	A	252	PHE	3.0
1	G	211	GLU	3.0
1	E	275	ASP	2.9
1	D	49	HIS	2.9
1	D	173	GLY	2.9
1	A	282	MET	2.9
1	G	213	GLU	2.9
1	E	161	PHE	2.9
1	G	170	TYR	2.9
1	A	251	THR	2.9
1	A	115	SER	2.9
1	G	143	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	45	ARG	2.8
1	G	27	GLU	2.8
1	A	155	PHE	2.8
1	A	50	LYS	2.8
1	A	158	THR	2.8
1	C	275	ASP	2.8
1	A	61	GLY	2.8
1	G	229	TYR	2.8
1	E	283	ASN	2.8
1	G	16	VAL	2.7
1	G	175	ASN	2.7
1	G	273	SER	2.7
1	C	42	ASP	2.7
1	C	286	SER	2.7
1	A	216	LYS	2.7
1	E	112	ASN	2.7
1	D	156	LEU	2.7
1	A	154	VAL	2.7
1	E	42	ASP	2.7
1	A	254	ARG	2.7
1	G	279	PRO	2.7
1	A	273	SER	2.7
1	G	210	PRO	2.7
1	G	57	LYS	2.6
1	G	205	ALA	2.6
1	A	15	ASP	2.6
1	E	122	ALA	2.6
1	E	216	LYS	2.6
1	E	50	LYS	2.6
1	A	209	LEU	2.6
1	H	280	ILE	2.6
1	D	210	PRO	2.6
1	E	277	VAL	2.6
1	G	128	PRO	2.6
1	A	116	GLU	2.6
1	A	6	LYS	2.6
1	G	138	ASN	2.6
1	G	146	ALA	2.6
1	A	215	GLU	2.6
1	A	237	GLU	2.6
1	A	177	LEU	2.5
1	A	140	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	76	ALA	2.5
1	A	242	THR	2.5
1	F	283	ASN	2.5
1	G	14	GLU	2.5
1	G	9	ASN	2.5
1	G	64	LEU	2.5
1	A	69	GLN	2.5
1	A	241	ASP	2.5
1	G	117	ILE	2.5
1	G	187	ILE	2.5
1	A	164	GLY	2.5
1	A	157	GLU	2.5
1	G	165	PHE	2.5
1	E	160	LEU	2.5
1	C	262	MET	2.5
1	A	123	TRP	2.5
1	D	283	ASN	2.5
1	G	228	LEU	2.5
1	G	158	THR	2.5
1	B	34	ARG	2.5
1	A	269	LEU	2.5
1	E	164	GLY	2.5
1	D	175	ASN	2.5
1	A	55	VAL	2.4
1	A	202	PHE	2.4
1	C	212	ASP	2.4
1	A	47	LEU	2.4
1	G	6	LYS	2.4
1	E	139	GLU	2.4
1	G	223	ASP	2.4
1	A	142	LEU	2.4
1	G	157	GLU	2.4
1	A	39	ASN	2.4
1	A	127	ASN	2.4
1	E	100	HIS	2.4
1	E	115	SER	2.4
1	G	118	ASP	2.4
1	E	270	PHE	2.3
1	G	61	GLY	2.3
1	G	34	ARG	2.3
1	A	33	THR	2.3
1	D	276	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	203	GLN	2.3
1	A	148	GLU	2.3
1	G	7	ALA	2.3
1	D	275	ASP	2.3
1	G	59	PHE	2.3
1	G	274	ALA	2.3
1	G	240	TYR	2.3
1	G	208	GLU	2.3
1	A	30	TRP	2.3
1	E	129	TYR	2.3
1	G	60	GLY	2.3
1	A	261	LEU	2.3
1	A	174	ASN	2.3
1	E	40	ASP	2.2
1	F	275	ASP	2.2
1	A	122	ALA	2.2
1	D	160	LEU	2.2
1	A	70	SER	2.2
1	E	59	PHE	2.2
1	E	219	GLU	2.2
1	A	117	ILE	2.2
1	A	48	SER	2.2
1	G	42	ASP	2.2
1	E	34	ARG	2.2
1	A	37	LEU	2.2
1	G	234	GLY	2.2
1	A	205	ALA	2.2
1	A	236	THR	2.1
1	A	59	PHE	2.1
1	A	228	LEU	2.1
1	A	60	GLY	2.1
1	H	279	PRO	2.1
1	G	255	TYR	2.1
1	A	152	ALA	2.1
1	B	275	ASP	2.1
1	E	163	SER	2.1
1	G	164	GLY	2.1
1	G	101	ALA	2.1
1	E	273	SER	2.1
1	A	111	LEU	2.1
1	B	280	ILE	2.1
1	D	212	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	7	ALA	2.1
1	F	3	THR	2.1
1	G	74	VAL	2.1
1	G	81	VAL	2.1
1	A	235	TYR	2.1
1	F	4	TYR	2.1
1	E	158	THR	2.0
1	E	123	TRP	2.0
1	G	135	GLU	2.0
1	A	278	ASN	2.0
1	E	114	LYS	2.0
1	H	212	ASP	2.0
1	A	274	ALA	2.0
1	D	251	THR	2.0
1	G	207	ASN	2.0
1	A	168	PRO	2.0
1	D	271	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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MN	D	401	1/1	0.96	0.18	-0.83	37,37,37,37	0
2	MN	G	402	1/1	0.62	0.23	-0.95	95,95,95,95	0
2	MN	A	402	1/1	0.85	0.20	-1.08	91,91,91,91	0
2	MN	C	401	1/1	0.98	0.13	-1.30	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	D	402	1/1	0.97	0.14	-1.40	33,33,33,33	0
2	MN	A	401	1/1	0.88	0.18	-1.41	72,72,72,72	0
2	MN	F	401	1/1	0.99	0.13	-1.76	23,23,23,23	0
2	MN	G	401	1/1	0.99	0.19	-1.87	64,64,64,64	0
2	MN	F	402	1/1	0.97	0.13	-2.10	24,24,24,24	0
2	MN	B	402	1/1	0.99	0.11	-2.14	9,9,9,9	0
2	MN	E	402	1/1	0.94	0.19	-2.16	50,50,50,50	0
2	MN	B	401	1/1	1.00	0.11	-2.51	5,5,5,5	0
2	MN	E	401	1/1	0.98	0.13	-2.62	41,41,41,41	0
2	MN	C	402	1/1	0.99	0.11	-3.11	25,25,25,25	0
2	MN	H	401	1/1	0.99	0.10	-3.47	8,8,8,8	0
2	MN	H	402	1/1	0.99	0.10	-4.79	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.