



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:22 PM UTC

PDB ID : 4N83 / pdb_00004n83
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 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
Xtriage (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

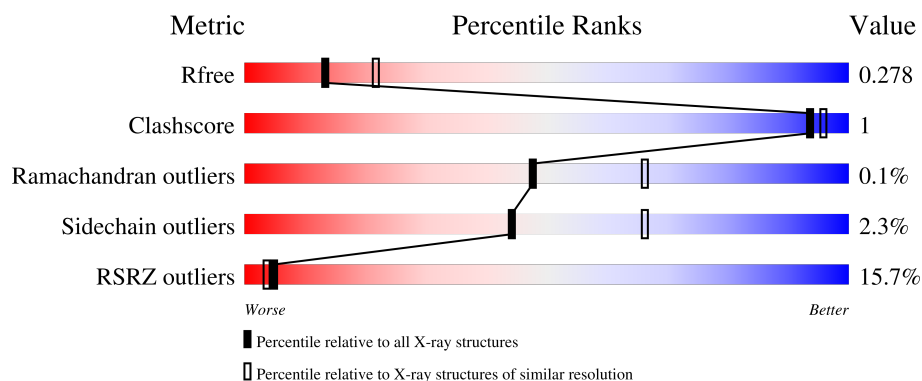
1 Overall quality at a glance

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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	319	50% 87% 11%
1	B	319	2% 81% 7% 11%
1	C	319	2% 82% 6% 11%
1	D	319	4% 85% 11%
1	E	319	16% 83% 5% 11%

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Mol	Chain	Length	Quality of chain
1	F	319	3% 86% 11%
1	G	319	34% 85% 11%
1	H	319	3% 84% 11%

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 (CCD ID: MN) (formula: Mn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Mn 2	0	0
2	H	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

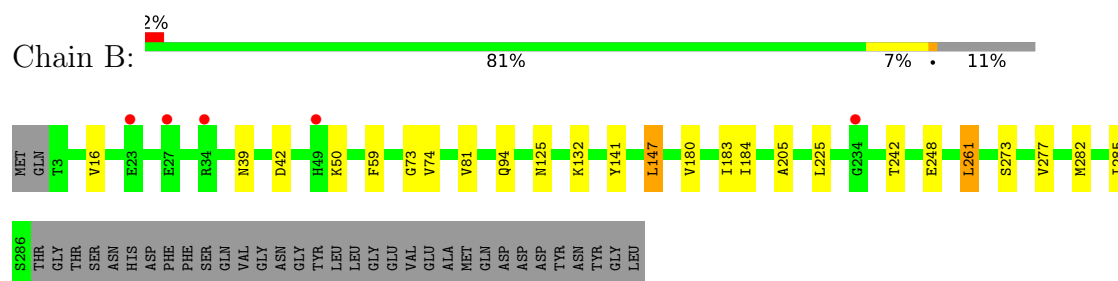
3 Residue-property plots

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.

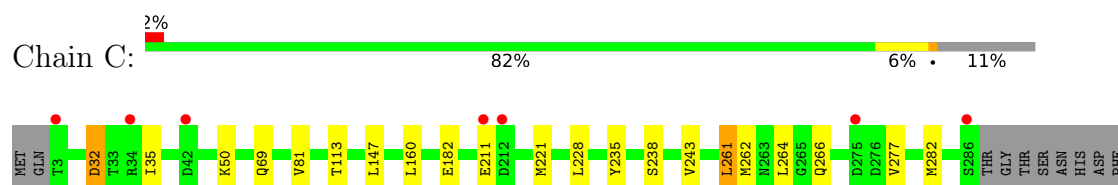
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



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PHE
SER
GLN
VAL
GLY
ASN
GLY
TYR
LEU
LEU
GLY
GLU
VAL
GLU
ALA
MET
GLN
ASP
ASP
TYR
ASN
TYR
GLY
LEU

• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain D: 4% 85% 11%

MET GLN T3 R34 L41 D42 R45 H49 Q69 V81 I107 F108 K114 I117 E139 Y170 G173 I183 I184 K185 E211 E215 D223 L224 L225 M262 I280 S286 THR GLY THR SER ASN HIS ASP PHE PHE SER GLN VAL GLY

ASN GLY TYR LEU GLY VAL ALA MET GLN ASP ASP TYR ASN TYR GLY LEU

• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain E: 16% 83% 5% 11%

MET GLN T3 I17 L37 S38 N39 D40 L41 R45 R46 H49 K50 E51 V55 V58 V74 R78 V81 R82 T83 N91 Q94 S103 I107 L111 N112 T113 K114 S115 W123 T126 Y129 L130 E139 L147 Y170 Y171 L172 G173

N174 N175 K176 L177 A178 I183 I188 Y200 E211 D212 L225 Y226 N231 S238 L239 Y240 D241 T242 V243 G244 W245 T246 E247 E248 V249 L253 N258 L261 M262 P268 L269 F270 A274 V281 S286 THR GLY THR SER ASN HIS ASP PHE PHE SER GLN

VAL GLY ASN GLY TYR LEU GLY VAL ALA MET GLN ASP ASP TYR ASN TYR GLY LEU

• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain F: 3% 86% 11%

MET GLN T3 Y4 V81 I93 L147 H194 A206 Q214 E215 E230 N231 E232 E233 S238 K250 L261 M262 K282 S286 THR GLY THR SER ASN HIS ASP PHE PHE SER GLN VAL GLY ASN GLY TYR LEU LEU GLY VAL GLU VAL GLU ALA MET GLN ASP

ASP TYR ASN TYR GLY LEU

• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain G: 34% 85% 11%

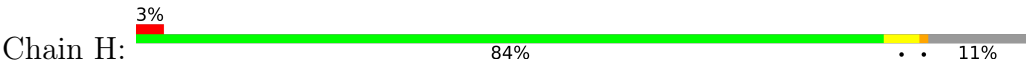
MET GLN THR Y4 Y5 K6 A7 T8 N9 N10 N11 N12 N13 E14 V16 I17 D18 K19 L37 L49 H49 K50 K57 L65 L68 Q69 S70 V74 D75 L76 A77 L77 R78 K79 D80 W81 R82 T83 A84 A88 V89 H100 F121 A122 W123 K124 N125 T126 N127 P128

Y129 L130 K132 I136 I137 N138 E139 N231 Y141 N142 N143 N144 G144 T145 A146 L147 K150 I151 A152 S153 V154 F155 T158 F165 F166 L169 I182 L186 I187 S192 G195 T196 Y197 F202 Q203 L204 A205 F206 L209 P210 D212 E215 K216 L217 W220 M221

Y222 D223 L224 L225 Y226 T227 L228 Y229 E230 N231 E232 Y235 T236 L239 Y240 D241 T242 V243 W245 T246 E247 E248 V249 K250 T251 Y255 N256 A257 L261 L264 D267 P268 L269 F270 P271 A274 D275 D276 V277 N278 P279 I280 G284 I285 S286 THR GLY THR SER ASN HIS

ASP
PHE
PHE
SER
GLN
VAL
GLY
ASN
GLY
TYR
LEU
LEU
GLY
GLU
VAL
GLU
ALA
MET
GLN
ASP
ASP
ASP
TYR
ASN
TYR
GLY
LEU

● Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



MET GLN THR Y4 A7 E27 R34 N39 H49 D53 F59 L65 A84 K133 L160 I184 D212 G234 S238 E247 T251 D267 V277 N278 P279 I280 V281 M282 S286 THR GLY THR SER ASN HIS ASP PHE PHE SER GLN

VAL GLY ASN GLY TYR LEU LEU GLY VAL GLU ALA MET GLN ASP ASP ASP TYR ASN TYR GLY LEU

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 29.90 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.5 (29.90-2.65) 86.6 (29.90-2.65)	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 (4.38%)	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 , 38.2	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	0.39	0/2391	0.68	0/3246
1	B	0.44	0/2384	0.72	0/3236
1	C	0.42	0/2384	0.72	0/3236
1	D	0.40	0/2384	0.72	0/3236
1	E	0.39	0/2384	0.69	0/3236
1	F	0.41	0/2384	0.74	0/3236
1	G	0.40	0/2377	0.70	0/3226
1	H	0.43	0/2377	0.72	0/3226
All	All	0.41	0/19065	0.71	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	10	0
1	C	2329	0	2257	9	0
1	D	2329	0	2257	5	0
1	E	2329	0	2257	7	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	4	0
1	H	2322	0	2250	8	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	51	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 (51) 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:C:221:MET:HE2	1:C:261:LEU:HD12	1.90	0.54
1:H:277:VAL:HB	1:H:282:MET:HE3	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:C:221:MET:HE1	1:C:266:GLN:HG3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:221:MET:HE1	1:G:261:LEU:HD23	1.95	0.48
1:C:69:GLN:HE21	1:C:69:GLN:HA	1.79	0.47
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:HE21	1:D:69:GLN:HA	1.81	0.45
1:C:221:MET:HE3	1:C:264:LEU:HD13	1.98	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:OD2	1:C:32:ASP:N	2.48	0.45
1:G:16:VAL:HG23	1:G:17:ILE:HD12	1.99	0.44
1:H:39:ASN:N	1:H:39:ASN:HD22	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:N	1:B:39:ASN:HD22	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:C:277:VAL:HB	1:C:282:MET:HE3	2.02	0.42
1:D:108:PHE:HB3	1:D:117:ILE:HG12	2.01	0.42
1:A:221:MET:HE2	1:A:261:LEU:HD23	2.01	0.41
1:E:103:SER:CB	1:E:183:ILE:HD11	2.45	0.41
1:E:245:TRP:O	1:E:246:THR:C	2.63	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
1:B:277:VAL:HB	1:B:282:MET:HE3	2.04	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%)	30	45
1	B	282/319 (88%)	274 (97%)	7 (2%)	1 (0%)	30	45
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%)	48	66

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%)	73	85
1	B	255/284 (90%)	247 (97%)	8 (3%)	35	56
1	C	255/284 (90%)	245 (96%)	10 (4%)	28	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	255/284 (90%)	249 (98%)	6 (2%)	43	65
1	E	255/284 (90%)	247 (97%)	8 (3%)	35	56
1	F	255/284 (90%)	250 (98%)	5 (2%)	48	69
1	G	254/284 (89%)	250 (98%)	4 (2%)	55	74
1	H	254/284 (89%)	250 (98%)	4 (2%)	55	74
All	All	2039/2272 (90%)	1992 (98%)	47 (2%)	44	66

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	280	ILE
1	B	16	VAL
1	B	42	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	50	LYS
1	C	81	VAL
1	C	113	THR
1	C	147	LEU
1	C	182	GLU
1	C	211	GLU
1	C	243	VAL
1	C	261	LEU
1	C	262	MET
1	D	81	VAL
1	D	183	ILE
1	D	185	LYS
1	D	223	ASP
1	D	225	LEU
1	D	262	MET
1	E	78	ARG
1	E	81	VAL
1	E	130	LEU
1	E	147	LEU

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Mol	Chain	Res	Type
1	E	225	LEU
1	E	231	ASN
1	E	261	LEU
1	E	262	MET
1	F	81	VAL
1	F	147	LEU
1	F	231	ASN
1	F	261	LEU
1	F	262	MET
1	G	37	LEU
1	G	130	LEU
1	G	182	GLU
1	G	209	LEU
1	H	53	ASP
1	H	184	ILE
1	H	238	SER
1	H	251	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	143	ASN
1	A	179	ASN
1	A	194	HIS
1	A	263	ASN
1	B	39	ASN
1	B	125	ASN
1	B	143	ASN
1	B	174	ASN
1	B	194	HIS
1	B	214	GLN
1	B	263	ASN
1	C	39	ASN
1	C	69	GLN
1	C	143	ASN
1	C	214	GLN
1	C	263	ASN
1	C	283	ASN
1	D	28	GLN
1	D	69	GLN
1	D	143	ASN

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Mol	Chain	Res	Type
1	D	214	GLN
1	D	263	ASN
1	E	39	ASN
1	E	49	HIS
1	E	69	GLN
1	E	100	HIS
1	E	179	ASN
1	E	263	ASN
1	F	11	ASN
1	F	28	GLN
1	F	69	GLN
1	F	112	ASN
1	F	179	ASN
1	F	194	HIS
1	G	28	GLN
1	G	39	ASN
1	G	100	HIS
1	G	231	ASN
1	G	263	ASN
1	G	266	GLN
1	H	28	GLN
1	H	39	ASN
1	H	69	GLN
1	H	179	ASN
1	H	194	HIS
1	H	263	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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%)	2.29	160 (56%) 0 0	58, 111, 134, 141	0
1	B	284/319 (89%)	0.08	5 (1%) 67 63	11, 15, 30, 38	0
1	C	284/319 (89%)	0.15	7 (2%) 58 52	12, 21, 43, 62	0
1	D	284/319 (89%)	0.63	12 (4%) 40 32	14, 49, 71, 86	0
1	E	284/319 (89%)	1.15	50 (17%) 4 3	20, 64, 95, 112	0
1	F	284/319 (89%)	0.35	8 (2%) 55 48	13, 29, 58, 76	0
1	G	283/319 (88%)	1.81	107 (37%) 1 0	52, 87, 113, 133	0
1	H	283/319 (88%)	0.12	8 (2%) 55 48	11, 16, 35, 39	0
All	All	2271/2552 (88%)	0.82	357 (15%) 5 4	11, 37, 116, 141	0

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	LEU	5.5
1	A	146	ALA	5.5
1	G	5	TYR	4.9
1	G	4	TYR	4.6
1	A	240	TYR	4.6
1	A	128	PRO	4.5
1	A	145	THR	4.4
1	A	53	ASP	4.3
1	G	251	THR	4.2
1	A	137	ILE	4.2
1	A	253	LEU	4.2
1	E	41	LEU	4.2
1	G	130	LEU	4.2
1	G	6	LYS	4.1
1	A	141	TYR	4.1
1	G	146	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	244	GLY	4.1
1	G	13	ILE	4.1
1	A	166	PHE	4.0
1	A	3	THR	4.0
1	A	245	TRP	4.0
1	A	212	ASP	3.9
1	A	222	TYR	3.9
1	G	269	LEU	3.9
1	A	202	PHE	3.8
1	A	206	PHE	3.8
1	E	231	ASN	3.8
1	G	124	THR	3.8
1	A	37	LEU	3.8
1	A	55	VAL	3.8
1	A	280	ILE	3.7
1	A	252	PHE	3.7
1	A	164	GLY	3.7
1	A	205	ALA	3.7
1	G	90	PHE	3.7
1	A	126	THR	3.7
1	A	243	VAL	3.7
1	A	178	ALA	3.6
1	A	177	LEU	3.6
1	A	228	LEU	3.6
1	A	287	THR	3.6
1	A	225	LEU	3.6
1	E	183	ILE	3.6
1	A	227	THR	3.6
1	A	121	PHE	3.6
1	E	244	GLY	3.5
1	A	271	PRO	3.5
1	A	239	LEU	3.5
1	G	217	LEU	3.5
1	G	76	ALA	3.5
1	A	209	LEU	3.5
1	A	46	LYS	3.5
1	A	65	LEU	3.5
1	E	211	GLU	3.5
1	G	139	GLU	3.5
1	G	10	TRP	3.5
1	A	115	SER	3.4
1	E	115	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	220	TRP	3.4
1	A	285	ILE	3.4
1	A	158	THR	3.4
1	A	70	SER	3.4
1	E	178	ALA	3.4
1	A	226	TYR	3.4
1	A	269	LEU	3.4
1	G	122	ALA	3.4
1	A	135	GLU	3.3
1	E	49	HIS	3.3
1	A	229	TYR	3.3
1	G	226	TYR	3.3
1	G	16	VAL	3.3
1	A	284	GLY	3.3
1	G	121	PHE	3.3
1	A	242	THR	3.3
1	G	242	THR	3.3
1	A	255	TYR	3.3
1	G	235	TYR	3.3
1	A	281	VAL	3.3
1	H	280	ILE	3.3
1	D	49	HIS	3.2
1	A	4	TYR	3.2
1	A	79	LYS	3.2
1	D	286	SER	3.2
1	A	165	PHE	3.2
1	A	249	VAL	3.2
1	D	183	ILE	3.2
1	G	11	ASN	3.2
1	B	234	GLY	3.2
1	G	209	LEU	3.1
1	A	36	PRO	3.1
1	A	5	TYR	3.1
1	G	216	LYS	3.1
1	A	221	MET	3.1
1	A	105	SER	3.1
1	C	286	SER	3.1
1	G	271	PRO	3.1
1	A	123	TRP	3.1
1	G	128	PRO	3.1
1	A	152	ALA	3.1
1	A	159	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	204	LEU	3.0
1	G	228	LEU	3.0
1	A	139	GLU	3.0
1	A	50	LYS	3.0
1	A	251	THR	3.0
1	A	198	ILE	3.0
1	G	78	ARG	3.0
1	G	286	SER	3.0
1	A	49	HIS	3.0
1	G	7	ALA	3.0
1	A	41	LEU	3.0
1	A	210	PRO	3.0
1	G	210	PRO	3.0
1	A	58	VAL	3.0
1	G	206	PHE	3.0
1	A	261	LEU	2.9
1	G	123	TRP	2.9
1	A	147	LEU	2.9
1	E	286	SER	2.9
1	G	153	SER	2.9
1	E	45	ARG	2.9
1	G	231	ASN	2.9
1	A	140	ILE	2.9
1	A	250	LYS	2.9
1	G	277	VAL	2.9
1	A	279	PRO	2.9
1	G	279	PRO	2.9
1	A	39	ASN	2.9
1	A	236	THR	2.9
1	A	34	ARG	2.8
1	A	72	SER	2.8
1	C	42	ASP	2.8
1	A	235	TYR	2.8
1	A	111	LEU	2.8
1	A	211	GLU	2.8
1	G	212	ASP	2.8
1	A	124	THR	2.8
1	A	246	THR	2.8
1	G	89	VAL	2.8
1	A	64	LEU	2.8
1	E	241	ASP	2.8
1	A	7	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	129	TYR	2.8
1	A	6	LYS	2.8
1	A	129	TYR	2.8
1	A	218	LYS	2.7
1	A	136	ILE	2.7
1	A	151	ILE	2.7
1	A	47	LEU	2.7
1	F	238	SER	2.7
1	A	262	MET	2.7
1	A	232	GLU	2.7
1	D	42	ASP	2.7
1	G	126	THR	2.7
1	A	107	ILE	2.7
1	A	30	TRP	2.7
1	E	173	GLY	2.7
1	E	129	TYR	2.7
1	B	27	GLU	2.7
1	G	257	ALA	2.7
1	G	245	TRP	2.7
1	E	242	THR	2.7
1	G	158	THR	2.7
1	G	8	ILE	2.6
1	A	172	LEU	2.6
1	A	56	GLY	2.6
1	A	119	GLU	2.6
1	E	51	GLU	2.6
1	G	195	GLY	2.6
1	G	50	LYS	2.6
1	A	168	PRO	2.6
1	G	267	ASP	2.6
1	G	197	TYR	2.6
1	A	54	LEU	2.6
1	G	243	VAL	2.6
1	A	220	TRP	2.6
1	A	268	PRO	2.6
1	G	227	THR	2.6
1	E	212	ASP	2.6
1	E	107	ILE	2.6
1	G	264	LEU	2.6
1	A	150	LYS	2.6
1	D	215	GLU	2.6
1	A	33	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	120	ILE	2.6
1	A	224	LEU	2.6
1	G	255	TYR	2.6
1	A	52	LYS	2.6
1	D	139	GLU	2.6
1	E	139	GLU	2.6
1	A	92	ASN	2.6
1	A	163	SER	2.5
1	C	3	THR	2.5
1	A	216	LYS	2.5
1	A	148	GLU	2.5
1	G	14	GLU	2.5
1	G	268	PRO	2.5
1	A	91	ASN	2.5
1	A	207	ASN	2.5
1	F	3	THR	2.5
1	G	192	SER	2.5
1	A	77	LEU	2.5
1	A	217	LEU	2.5
1	G	224	LEU	2.5
1	G	230	GLU	2.5
1	G	247	GLU	2.5
1	G	84	ALA	2.5
1	A	103	SER	2.5
1	A	114	LYS	2.5
1	G	151	ILE	2.5
1	G	280	ILE	2.5
1	A	160	LEU	2.5
1	G	68	LEU	2.5
1	F	4	TYR	2.5
1	A	84	ALA	2.5
1	A	155	PHE	2.5
1	A	161	PHE	2.5
1	A	38	SER	2.5
1	A	169	LEU	2.5
1	C	212	ASP	2.5
1	A	233	GLU	2.5
1	G	81	VAL	2.5
1	G	249	VAL	2.5
1	G	88	ALA	2.5
1	A	183	ILE	2.4
1	G	169	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	123	TRP	2.4
1	G	49	HIS	2.4
1	B	23	GLU	2.4
1	F	215	GLU	2.4
1	H	234	GLY	2.4
1	A	170	TYR	2.4
1	G	202	PHE	2.4
1	E	239	LEU	2.4
1	G	204	LEU	2.4
1	E	248	GLU	2.4
1	A	176	LYS	2.4
1	E	46	LYS	2.4
1	G	250	LYS	2.4
1	G	74	VAL	2.4
1	A	29	PHE	2.4
1	A	45	ARG	2.4
1	G	276	ASP	2.4
1	A	277	VAL	2.4
1	G	165	PHE	2.4
1	G	222	TYR	2.4
1	G	274	ALA	2.4
1	G	145	THR	2.4
1	G	138	ASN	2.4
1	A	109	SER	2.4
1	H	212	ASP	2.4
1	G	284	GLY	2.4
1	A	81	VAL	2.4
1	E	274	ALA	2.4
1	G	225	LEU	2.3
1	A	247	GLU	2.3
1	E	55	VAL	2.3
1	A	59	PHE	2.3
1	A	76	ALA	2.3
1	A	130	LEU	2.3
1	E	269	LEU	2.3
1	E	170	TYR	2.3
1	E	112	ASN	2.3
1	G	57	LYS	2.3
1	H	27	GLU	2.3
1	H	34	ARG	2.3
1	E	243	VAL	2.3
1	E	130	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	141	TYR	2.3
1	A	237	GLU	2.3
1	B	34	ARG	2.3
1	F	214	GLN	2.3
1	G	83	THR	2.3
1	G	132	LYS	2.3
1	G	150	LYS	2.3
1	A	11	ASN	2.3
1	E	174	ASN	2.3
1	F	231	ASN	2.3
1	G	143	ASN	2.3
1	A	60	GLY	2.3
1	A	31	LEU	2.3
1	D	41	LEU	2.3
1	A	95	PHE	2.3
1	G	19	LYS	2.2
1	G	240	TYR	2.2
1	A	278	ASN	2.2
1	A	15	ASP	2.2
1	E	111	LEU	2.2
1	D	114	LYS	2.2
1	E	114	LYS	2.2
1	G	12	ALA	2.2
1	G	17	ILE	2.2
1	G	140	ILE	2.2
1	G	239	LEU	2.2
1	E	249	VAL	2.2
1	D	211	GLU	2.2
1	A	171	TYR	2.2
1	A	94	GLN	2.2
1	A	266	GLN	2.2
1	D	173	GLY	2.2
1	E	281	VAL	2.2
1	G	155	PHE	2.2
1	A	162	TYR	2.2
1	B	49	HIS	2.2
1	G	166	PHE	2.2
1	A	122	ALA	2.1
1	G	215	GLU	2.1
1	E	268	PRO	2.1
1	E	176	LYS	2.1
1	E	258	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	278	ASN	2.1
1	G	229	TYR	2.1
1	A	264	LEU	2.1
1	E	37	LEU	2.1
1	E	172	LEU	2.1
1	G	70	SER	2.1
1	G	137	ILE	2.1
1	A	270	PHE	2.1
1	A	213	GLU	2.1
1	E	245	TRP	2.1
1	E	247	GLU	2.1
1	G	79	LYS	2.1
1	A	174	ASN	2.1
1	G	186	LEU	2.1
1	G	136	ILE	2.1
1	H	49	HIS	2.1
1	A	101	ALA	2.1
1	G	232	GLU	2.1
1	D	45	ARG	2.1
1	E	126	THR	2.1
1	E	253	LEU	2.1
1	G	99	VAL	2.1
1	E	270	PHE	2.1
1	E	238	SER	2.1
1	D	34	ARG	2.1
1	G	236	THR	2.1
1	F	282	MET	2.1
1	G	9	ASN	2.1
1	A	35	ILE	2.1
1	E	226	TYR	2.1
1	A	275	ASP	2.0
1	C	275	ASP	2.0
1	H	267	ASP	2.0
1	A	167	THR	2.0
1	G	147	LEU	2.0
1	E	39	ASN	2.0
1	E	188	ILE	2.0
1	E	58	VAL	2.0
1	C	34	ARG	2.0
1	C	211	GLU	2.0
1	A	134	ALA	2.0
1	A	185	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	201	LYS	2.0
1	F	286	SER	2.0
1	A	110	THR	2.0
1	E	262	MET	2.0
1	G	65	LEU	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	MN	G	402	1/1	0.84	0.11	95,95,95,95	0
2	MN	A	402	1/1	0.89	0.09	91,91,91,91	0
2	MN	E	402	1/1	0.93	0.05	50,50,50,50	0
2	MN	A	401	1/1	0.93	0.07	72,72,72,72	0
2	MN	E	401	1/1	0.94	0.05	41,41,41,41	0
2	MN	D	401	1/1	0.95	0.06	37,37,37,37	0
2	MN	D	402	1/1	0.96	0.04	33,33,33,33	0
2	MN	G	401	1/1	0.98	0.04	64,64,64,64	0
2	MN	C	402	1/1	0.98	0.03	25,25,25,25	0
2	MN	B	402	1/1	0.99	0.01	9,9,9,9	0
2	MN	F	401	1/1	0.99	0.02	23,23,23,23	0
2	MN	F	402	1/1	0.99	0.03	24,24,24,24	0
2	MN	C	401	1/1	0.99	0.03	16,16,16,16	0
2	MN	B	401	1/1	0.99	0.02	5,5,5,5	0
2	MN	H	401	1/1	0.99	0.02	8,8,8,8	0
2	MN	H	402	1/1	0.99	0.03	11,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.