



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:20 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 wwPDB X-ray Structure Validation Summary 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

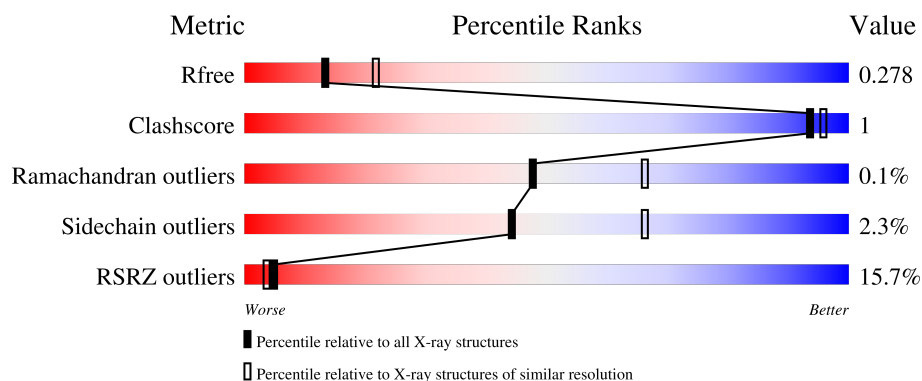
1 Overall quality at a glance

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

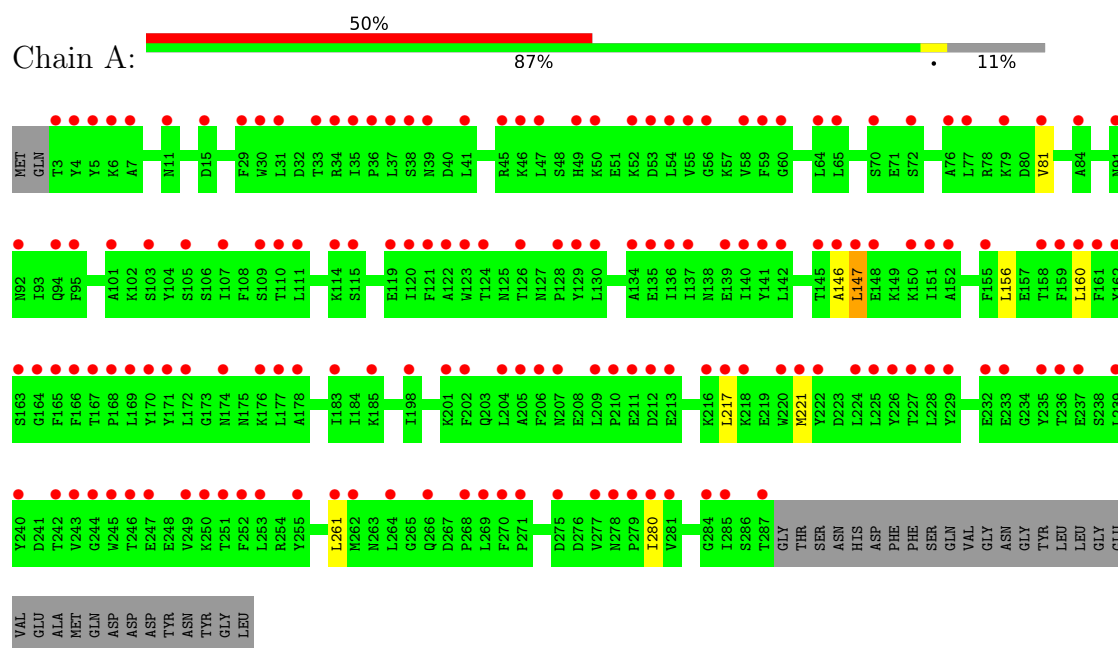
- Molecule 3 is water.

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

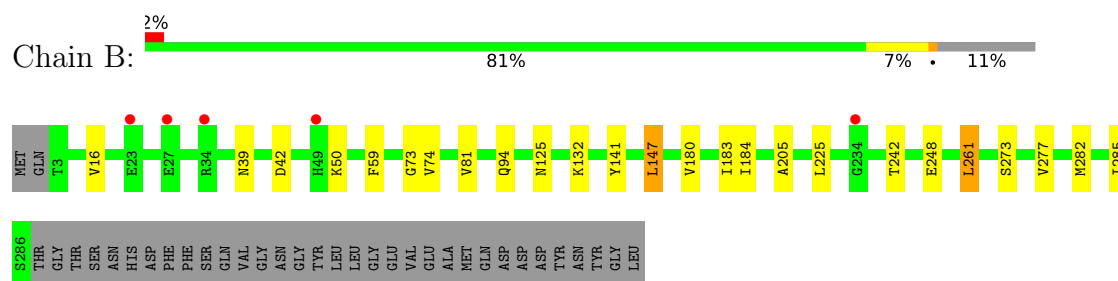
3 Residue-property plots

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.

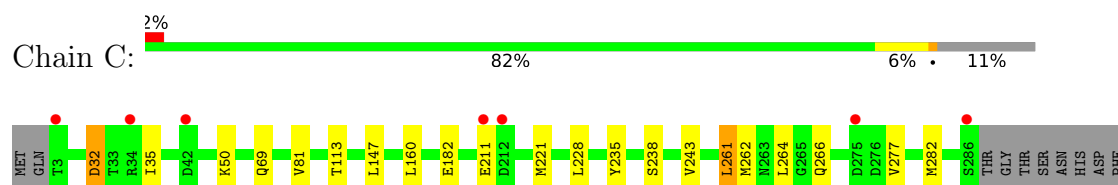
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



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 V78 V81 R82 T83 N91 Q94 S103 I107 L111 N112 T113 K114 S115 W123 T126 Y129 L130 E139 L147 Y170 Y171 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 ALA MET GLN ASP

ASP TYR ASN TYR GLY LEU

• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta

Chain G: 34% 85% 11%

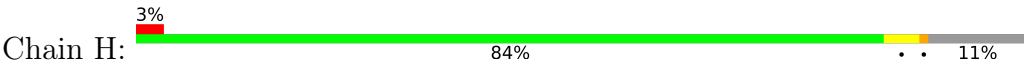
MET GLN THR Y4 Y5 K6 A7 T8 N9 N10 N11 N12 N13 E14 V16 D15 I17 D18 K19 L37 L43 H49 K50 K57 L65 L68 Q69 S70 V74 D75 L76 A77 L77 R78 K79 D80 W81 R82 T83 A84 A88 V89 H100 F121 A122 W123 N125 N126 N127 P128

Y129 L130 K132 I136 I137 N138 E139 N140 Y141 N142 N143 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
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
GLU
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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2039/2272 (90%)	1992 (98%)	47 (2%)	44 66

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	130	LEU
1	F	147	LEU
1	E	147	LEU
1	E	261	LEU
1	F	261	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	263	ASN
1	G	28	GLN
1	F	11	ASN
1	F	112	ASN
1	G	100	HIS

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

The worst 5 of 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

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

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.