



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:29 AM UTC

PDB ID : 1R2F / pdb_00001r2f
Title : RIBONUCLEOTIDE REDUCTASE R2F PROTEIN FROM SALMONELLA
TYPHIMURIUM
Authors : Eklund, H.; Eriksson, M.
Deposited on : 1998-08-24
Resolution : 2.10 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

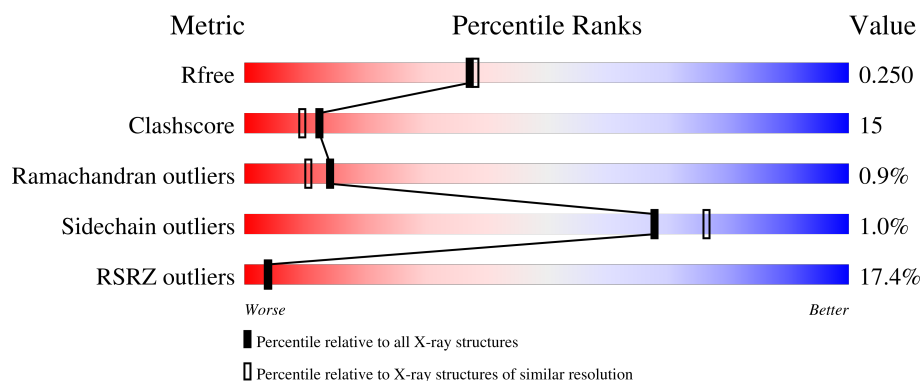
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

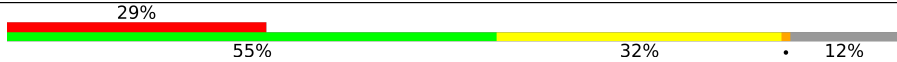
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	
1	B	319	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4924 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 PROTEIN (RIBONUCLEOTIDE REDUCTASE R2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2268	1471	364	425	8			
1	B	281	Total	C	N	O	S	0	0	0
			2255	1463	362	422	8			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	266	Total	O	0	0
			266	266		
3	B	131	Total	O	0	0
			131	131		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.49Å 71.74Å 96.07Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-2.10) 93.0 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.247 0.223 , 0.250	Depositor DCC
R_{free} test set	2196 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4924	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% 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: FE

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	0.44	1/2324 (0.0%)	0.88	8/3166 (0.3%)
1	B	0.37	0/2310	0.84	1/3146 (0.0%)
All	All	0.41	1/4634 (0.0%)	0.87	9/6312 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	MET	SD-CE	-6.09	1.64	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	N-CA-C	7.61	120.46	111.71
1	A	72	ILE	N-CA-C	6.88	116.89	110.42
1	A	113	CYS	N-CA-C	6.38	119.89	110.46
1	A	163	TYR	N-CA-C	6.28	120.04	112.38
1	A	72	ILE	CB-CA-C	-5.83	104.34	111.87
1	A	164	SER	N-CA-C	-5.52	105.81	112.54
1	A	181	THR	N-CA-C	-5.35	105.53	111.36
1	A	149	LYS	N-CA-C	-5.04	106.40	112.54
1	B	164	SER	N-CA-C	-5.02	106.25	112.38

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	2268	0	2247	51	0
1	B	2255	0	2235	89	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	266	0	0	3	0
3	B	131	0	0	0	0
All	All	4924	0	4482	139	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 15.

All (139) 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:A:97:MET:HA	1:A:97:MET:HE2	1.32	1.06
1:B:131:LEU:HA	1:B:134:LYS:HZ3	1.41	0.84
1:A:97:MET:HA	1:A:97:MET:CE	2.11	0.81
1:B:108:ILE:HD11	1:B:184:LEU:HD23	1.66	0.75
1:B:167:TRP:NE1	1:B:282:ILE:HD13	2.04	0.73
1:B:138:ILE:HD11	1:B:161:LEU:CD1	2.21	0.71
1:B:188:ILE:O	1:B:192:GLU:HG2	1.90	0.71
1:A:96:PHE:CD2	1:A:97:MET:HE3	2.26	0.70
1:A:216:GLU:O	1:A:220:LEU:HD13	1.91	0.69
1:A:279:ASN:C	1:A:279:ASN:HD22	2.00	0.68
1:B:254:LEU:HD12	1:B:255:CYS:N	2.08	0.68
1:A:25:ARG:HH11	1:A:25:ARG:HB2	1.61	0.66
1:A:96:PHE:CE2	1:A:97:MET:HE3	2.31	0.66
1:A:97:MET:HE1	1:A:100:VAL:HG21	1.78	0.65
1:B:152:ILE:HD11	1:B:203:TYR:CZ	2.31	0.65
1:B:168:LEU:HB3	1:B:169:PRO:HD3	1.78	0.65
1:A:201:TYR:CZ	1:A:205:ILE:HD11	2.31	0.64
1:A:215:ARG:HB2	1:A:215:ARG:NH1	2.12	0.64
1:B:131:LEU:HA	1:B:134:LYS:NZ	2.13	0.64
1:B:129:PRO:HB2	1:B:130:PRO:HD3	1.79	0.63
1:A:279:ASN:ND2	1:A:281:ALA:H	1.96	0.63
1:B:247:VAL:HG12	1:B:251:LYS:HE3	1.79	0.63
1:A:279:ASN:HD22	1:A:280:PRO:N	1.97	0.62
1:B:42:ILE:N	1:B:43:PRO:HD2	2.15	0.61
1:B:138:ILE:HD11	1:B:161:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:SER:OG	1:B:52:GLU:HG3	2.00	0.61
1:A:215:ARG:HB2	1:A:215:ARG:HH11	1.65	0.60
1:A:212:ALA:HA	1:A:215:ARG:NH1	2.17	0.60
1:B:259:ASN:HD21	1:B:271:PHE:H	1.49	0.60
1:B:170:MET:HG3	1:B:286:LEU:HD21	1.84	0.59
1:B:133:ARG:HB3	1:B:232:ASN:HD21	1.68	0.58
1:A:207:LEU:HD22	1:A:215:ARG:HG2	1.86	0.57
1:B:39:SER:O	1:B:42:ILE:HG13	2.04	0.57
1:B:55:LEU:O	1:B:59:VAL:HG23	2.05	0.57
1:B:167:TRP:HE1	1:B:282:ILE:HD13	1.67	0.57
1:A:215:ARG:HH11	1:A:215:ARG:CB	2.19	0.56
1:B:148:LEU:HD12	1:B:210:LEU:HD11	1.87	0.56
1:A:77:SER:OG	1:A:150:LYS:HD3	2.06	0.56
1:A:73:ALA:O	1:A:77:SER:HB2	2.05	0.56
1:A:234:ILE:O	1:A:238:GLU:HG3	2.06	0.56
1:B:25:ARG:HH11	1:B:25:ARG:HG3	1.71	0.55
3:A:559:HOH:O	1:B:79:MET:HE1	2.06	0.55
1:B:230:TYR:O	1:B:234:ILE:HG12	2.07	0.54
1:B:259:ASN:O	1:B:263:MET:HG2	2.08	0.54
1:B:279:ASN:HD22	1:B:280:PRO:CD	2.21	0.54
1:A:130:PRO:HA	1:A:232:ASN:HD21	1.74	0.53
1:B:46:GLN:HA	1:B:46:GLN:OE1	2.08	0.53
1:B:167:TRP:HE1	1:B:282:ILE:CD1	2.21	0.53
1:B:230:TYR:HE1	1:B:254:LEU:HD13	1.74	0.53
1:B:131:LEU:C	1:B:131:LEU:HD13	2.33	0.53
1:B:148:LEU:CD1	1:B:210:LEU:HD11	2.39	0.52
1:A:184:LEU:C	1:A:184:LEU:HD23	2.35	0.52
1:A:42:ILE:O	1:A:46:GLN:HG2	2.09	0.52
1:A:279:ASN:HD22	1:A:281:ALA:H	1.56	0.52
1:B:247:VAL:CG1	1:B:251:LYS:HE3	2.40	0.52
1:B:40:ASN:HB2	1:B:180:ASN:OD1	2.11	0.51
1:A:234:ILE:HG23	1:A:251:LYS:HE2	1.92	0.51
1:B:128:ASN:HD22	1:B:131:LEU:HB2	1.77	0.50
1:B:274:GLU:HG3	1:B:275:MET:HG3	1.94	0.50
1:B:57:ILE:HG22	1:B:121:ALA:CB	2.42	0.49
1:B:87:GLU:HG3	1:B:202:LYS:HE3	1.95	0.49
1:B:22:VAL:HG21	1:B:198:TYR:CD1	2.47	0.49
1:B:117:GLU:O	1:B:120:ALA:HB3	2.13	0.49
1:A:25:ARG:HB2	1:A:25:ARG:NH1	2.26	0.48
1:B:253:PHE:O	1:B:256:TYR:HB3	2.13	0.48
1:B:128:ASN:HD22	1:B:131:LEU:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:CE	1:A:100:VAL:HG21	2.44	0.48
1:A:129:PRO:HB2	1:A:130:PRO:HD3	1.96	0.48
1:A:231:ASP:OD2	1:A:235:ARG:NH1	2.44	0.48
1:A:188:ILE:O	1:A:192:GLU:HG2	2.13	0.48
1:B:103:ARG:C	1:B:103:ARG:HD3	2.39	0.48
1:B:18:LYS:HD2	1:B:201:TYR:CD2	2.50	0.47
1:B:246:TRP:O	1:B:248:ASN:N	2.48	0.47
1:B:213:ILE:O	1:B:217:GLU:HG3	2.14	0.47
1:B:253:PHE:HA	1:B:278:VAL:CG2	2.45	0.47
1:B:53:GLN:O	1:B:57:ILE:HG13	2.15	0.47
1:B:279:ASN:HD22	1:B:280:PRO:HD2	1.78	0.47
1:B:36:VAL:HA	1:B:37:PRO:HD3	1.78	0.46
1:B:111:THR:O	1:B:111:THR:HG22	2.14	0.46
1:B:133:ARG:NH1	1:B:136:GLN:NE2	2.63	0.46
1:A:128:ASN:ND2	1:A:130:PRO:HD2	2.30	0.46
1:B:170:MET:SD	1:B:285:ALA:O	2.73	0.46
1:A:57:ILE:HG22	1:A:121:ALA:CB	2.45	0.46
1:A:156:PHE:O	1:A:160:PHE:HB3	2.16	0.46
1:A:72:ILE:O	1:A:76:PRO:HG3	2.15	0.46
1:A:133:ARG:NH1	1:A:136:GLN:OE1	2.48	0.46
1:A:53:GLN:O	1:A:57:ILE:HG13	2.16	0.46
1:B:39:SER:C	1:B:41:ASP:H	2.24	0.45
1:B:246:TRP:O	1:B:247:VAL:C	2.59	0.45
1:B:94:ILE:O	1:B:98:GLU:HG2	2.16	0.45
1:B:163:TYR:H	1:B:163:TYR:HD1	1.65	0.45
1:B:55:LEU:CD1	1:B:240:LEU:HG	2.47	0.45
1:B:244:THR:HB	1:B:246:TRP:CE3	2.51	0.45
1:B:253:PHE:HA	1:B:278:VAL:HG21	1.97	0.45
1:B:172:PHE:HD2	1:B:178:LEU:HD12	1.82	0.45
1:B:18:LYS:NZ	1:B:197:TYR:OH	2.49	0.45
1:A:94:ILE:O	1:A:98:GLU:HG2	2.16	0.44
1:B:163:TYR:HB3	1:B:253:PHE:CE2	2.52	0.44
1:B:166:PHE:C	1:B:169:PRO:HD2	2.42	0.44
1:A:13:LYS:HE2	1:B:119:ASP:OD1	2.16	0.44
1:B:33:PRO:HG2	1:B:34:GLU:OE1	2.17	0.44
1:B:163:TYR:HA	1:B:166:PHE:HB2	1.99	0.44
1:A:164:SER:HB3	1:A:254:LEU:HD21	1.99	0.44
1:A:181:THR:O	1:A:185:ILE:HG12	2.18	0.44
1:B:168:LEU:HD11	1:B:172:PHE:CZ	2.52	0.44
1:B:25:ARG:HG3	1:B:25:ARG:NH1	2.33	0.44
1:B:167:TRP:CH2	1:B:246:TRP:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:TYR:HE1	1:B:254:LEU:CD1	2.31	0.43
1:B:66:LEU:HB2	1:B:162:PHE:HE1	1.82	0.43
1:A:279:ASN:C	1:A:279:ASN:ND2	2.72	0.43
1:B:111:THR:O	1:B:112:LEU:HD23	2.19	0.43
1:B:279:ASN:HD22	1:B:279:ASN:C	2.26	0.43
1:B:18:LYS:HD2	1:B:201:TYR:CE2	2.54	0.43
1:B:163:TYR:CD1	1:B:163:TYR:N	2.87	0.43
1:A:129:PRO:HD2	1:A:130:PRO:HD3	2.01	0.42
1:B:279:ASN:HD22	1:B:280:PRO:N	2.17	0.42
1:A:82:ALA:HB1	1:A:87:GLU:HB3	2.01	0.42
1:A:207:LEU:O	1:A:215:ARG:HD3	2.19	0.42
1:B:246:TRP:O	1:B:249:ASP:N	2.50	0.42
1:A:212:ALA:HA	1:A:215:ARG:CZ	2.49	0.42
1:B:65:LEU:HD23	1:B:131:LEU:HD11	2.01	0.42
1:B:139:LEU:O	1:B:143:VAL:HG22	2.20	0.42
1:B:166:PHE:O	1:B:169:PRO:HD2	2.19	0.42
1:A:146:GLU:HA	1:A:147:PRO:HD2	1.81	0.42
1:A:186:ARG:NH1	1:A:285:ALA:O	2.53	0.42
1:B:65:LEU:CD2	1:B:131:LEU:HD11	2.49	0.42
1:B:237:THR:HG23	1:B:250:VAL:HG11	2.02	0.41
1:B:103:ARG:HD3	1:B:103:ARG:O	2.20	0.41
1:A:18:LYS:HE2	1:A:18:LYS:HB2	1.95	0.41
1:A:18:LYS:HD2	1:A:201:TYR:CD2	2.55	0.41
1:B:104:SER:O	1:B:107:SER:HB2	2.21	0.41
1:B:167:TRP:NE1	1:B:282:ILE:CD1	2.77	0.41
1:B:137:ILE:HG21	1:B:229:LEU:HD21	2.02	0.41
1:B:148:LEU:HD21	1:B:206:ALA:CB	2.51	0.41
1:B:172:PHE:CD2	1:B:178:LEU:HD12	2.56	0.41
1:A:40:ASN:ND2	3:A:420:HOH:O	2.54	0.40
1:A:136:GLN:HG2	3:A:591:HOH:O	2.21	0.40
1:B:122:TYR:O	1:B:125:SER:HB3	2.21	0.40
1:A:18:LYS:HD2	1:A:201:TYR:CE2	2.57	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	281/319 (88%)	276 (98%)	4 (1%)	1 (0%)	30	28
1	B	279/319 (88%)	265 (95%)	10 (4%)	4 (1%)	9	5
All	All	560/638 (88%)	541 (97%)	14 (2%)	5 (1%)	14	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	GLY
1	B	247	VAL
1	B	40	ASN
1	B	242	ALA
1	A	74	GLY

5.3.2 Protein sidechains [i](#)

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	243/275 (88%)	240 (99%)	3 (1%)	63	72
1	B	241/275 (88%)	239 (99%)	2 (1%)	73	81
All	All	484/550 (88%)	479 (99%)	5 (1%)	68	76

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	MET
1	A	127	GLU
1	A	279	ASN
1	B	34	GLU
1	B	116	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	29	ASN
1	A	40	ASN
1	A	46	GLN
1	A	53	GLN
1	A	71	ASN
1	A	128	ASN
1	A	132	GLN
1	A	208	GLN
1	A	232	ASN
1	A	264	ASN
1	A	279	ASN
1	B	29	ASN
1	B	40	ASN
1	B	53	GLN
1	B	71	ASN
1	B	114	GLN
1	B	128	ASN
1	B	132	GLN
1	B	136	GLN
1	B	180	ASN
1	B	208	GLN
1	B	232	ASN
1	B	259	ASN
1	B	279	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 4 ligands modelled in this entry, 4 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	283/319 (88%)	0.17	5 (1%) 67 70	23, 30, 43, 45	0
1	B	281/319 (88%)	1.48	93 (33%) 1 1	27, 55, 73, 81	0
All	All	564/638 (88%)	0.83	98 (17%) 4 4	23, 37, 69, 81	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	TRP	4.7
1	B	112	LEU	4.3
1	B	254	LEU	4.3
1	B	45	TRP	4.2
1	A	145	ASP	4.1
1	B	171	TYR	4.0
1	B	263	MET	3.9
1	B	284	ALA	3.9
1	B	239	ALA	3.8
1	B	113	CYS	3.8
1	B	240	LEU	3.7
1	B	270	LEU	3.7
1	B	269	ALA	3.6
1	B	47	THR	3.6
1	B	248	ASN	3.5
1	B	136	GLN	3.5
1	B	242	ALA	3.4
1	B	285	ALA	3.4
1	B	111	THR	3.4
1	A	243	GLU	3.4
1	B	243	GLU	3.4
1	B	118	VAL	3.3
1	B	244	THR	3.3
1	B	51	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	ARG	3.2
1	B	44	ALA	3.2
1	B	262	LEU	3.1
1	B	249	ASP	3.1
1	B	267	TYR	3.1
1	B	79	MET	3.1
1	B	169	PRO	3.0
1	B	116	LYS	3.0
1	B	236	TYR	3.0
1	B	246	TRP	3.0
1	B	241	TYR	3.0
1	B	253	PHE	3.0
1	B	138	ILE	2.9
1	B	109	PHE	2.8
1	B	215	ARG	2.8
1	B	178	LEU	2.8
1	B	135	ALA	2.8
1	B	124	TRP	2.8
1	B	256	TYR	2.8
1	B	234	ILE	2.8
1	B	283	LEU	2.7
1	B	60	PHE	2.7
1	B	182	ALA	2.7
1	B	271	PHE	2.7
1	B	238	GLU	2.7
1	B	42	ILE	2.7
1	B	282	ILE	2.6
1	B	275	MET	2.6
1	B	252	ALA	2.6
1	B	131	LEU	2.6
1	B	272	PRO	2.6
1	B	224	ASP	2.6
1	B	56	THR	2.6
1	B	122	TYR	2.5
1	B	245	GLY	2.5
1	B	258	ALA	2.5
1	B	125	SER	2.5
1	B	226	LEU	2.5
1	B	261	ALA	2.5
1	B	110	SER	2.5
1	B	121	ALA	2.5
1	B	62	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	264	ASN	2.5
1	B	48	LEU	2.4
1	B	220	LEU	2.4
1	B	235	ARG	2.4
1	B	255	CYS	2.4
1	B	40	ASN	2.4
1	B	57	ILE	2.3
1	B	274	GLU	2.3
1	B	129	PRO	2.3
1	B	120	ALA	2.3
1	B	221	PHE	2.2
1	B	279	ASN	2.2
1	B	145	ASP	2.2
1	B	207	LEU	2.2
1	B	117	GLU	2.2
1	A	175	ARG	2.2
1	B	172	PHE	2.2
1	B	281	ALA	2.2
1	A	288	PRO	2.1
1	B	277	ASP	2.2
1	B	162	PHE	2.1
1	B	265	LEU	2.1
1	A	12	ASN	2.1
1	B	37	PRO	2.1
1	B	181	THR	2.1
1	B	54	GLN	2.1
1	B	185	ILE	2.1
1	B	163	TYR	2.1
1	B	260	LYS	2.1
1	B	157	LEU	2.1
1	B	164	SER	2.1
1	B	231	ASP	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	FE	B	403	1/1	0.98	0.03	43,43,43,43	0
2	FE	B	402	1/1	0.99	0.03	43,43,43,43	1
2	FE	A	400	1/1	0.99	0.05	32,32,32,32	0
2	FE	A	401	1/1	1.00	0.05	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.