



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 02:30 PM EDT

PDB ID : 1YFD
Title : Crystal structure of the Y122H mutant of ribonucleotide reductase R2 protein from *E. coli*
Authors : Kolberg, M.; Logan, D.T.; Bleifuss, G.; Poetsch, S.; Sjoeborg, B.M.; Graeslund, A.; Lubitz, W.; Lassmann, G.; Lendzian, F.
Deposited on : 2004-12-31
Resolution : 1.90 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

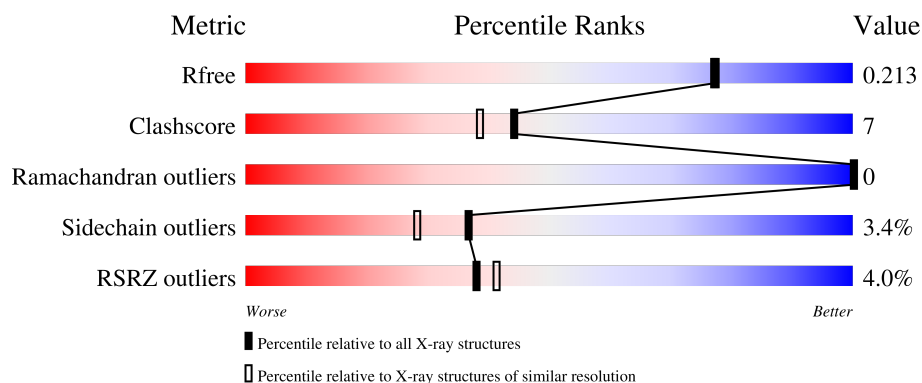
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	375	<div> <div>2%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	B	375	<div> <div>5%</div> <div>76%</div> <div>13%</div> <div>9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6035 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 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2786	1781	466	526	13			
1	B	341	Total	C	N	O	S	0	0	0
			2792	1784	467	528	13			

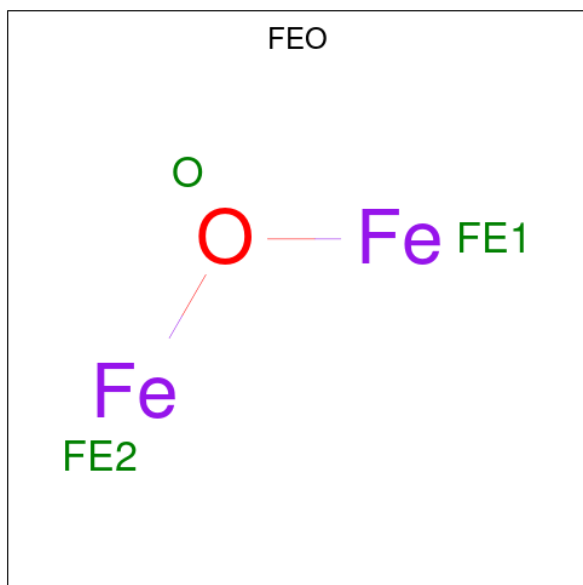
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	HIS	TYR	engineered mutation	UNP P69924
B	122	HIS	TYR	engineered mutation	UNP P69924

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Hg	0	0
			4	4		
2	B	9	Total	Hg	0	0
			9	9		

- Molecule 3 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	O	0	0
			3	2	1		
3	B	1	Total	Fe	O	0	0
			3	2	1		

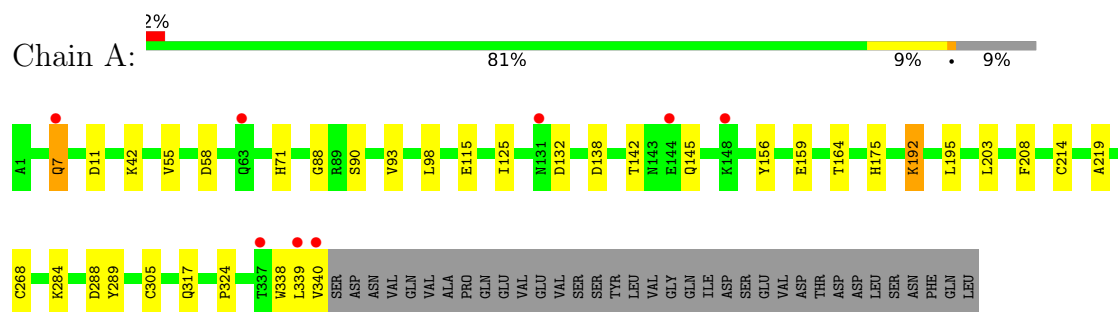
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		
4	B	218	Total	O	0	0
			218	218		

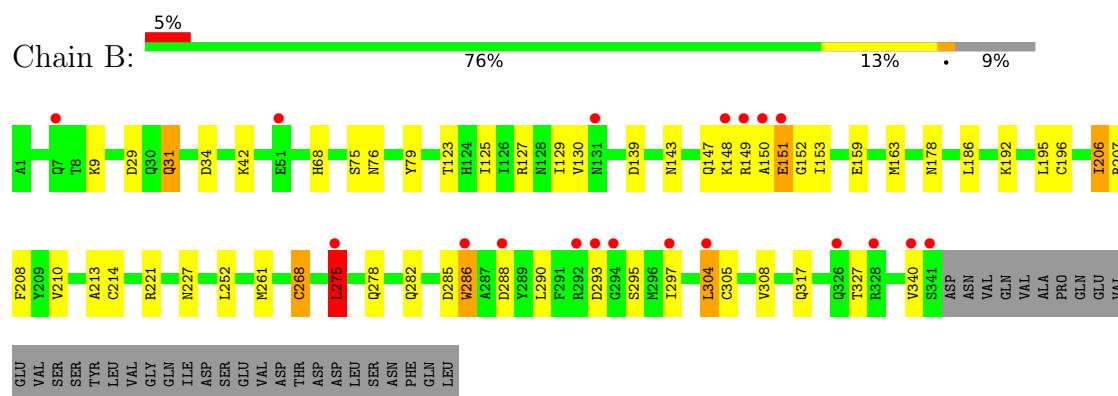
3 Residue-property plots [i](#)

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 1 beta chain



- Molecule 1: Ribonucleoside-diphosphate reductase 1 beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.04Å 84.74Å 115.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.46 – 1.90 19.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.46-1.90) 99.2 (19.38-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.173 , 0.206 0.181 , 0.213	Depositor DCC
R_{free} test set	2312 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6035	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, FEO

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	0.59	0/2850	0.77	4/3866 (0.1%)
1	B	0.58	1/2856 (0.0%)	0.82	8/3874 (0.2%)
All	All	0.58	1/5706 (0.0%)	0.79	12/7740 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	LEU	CG-CD1	6.67	1.76	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	LEU	CB-CG-CD1	12.96	133.03	111.00
1	B	304	LEU	CA-CB-CG	7.66	132.92	115.30
1	B	304	LEU	CB-CG-CD2	-6.53	99.89	111.00
1	B	285	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	275	LEU	CA-CB-CG	6.05	129.22	115.30
1	A	288	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	11	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	132	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	29	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	275	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	288	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	58	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2786	0	2730	24	0
1	B	2792	0	2733	54	0
2	A	4	0	0	2	0
2	B	9	0	0	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	220	0	0	3	0
4	B	218	0	0	12	0
All	All	6035	0	5463	73	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 7.

All (73) 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:B:304:LEU:CG	1:B:304:LEU:CD1	1.76	1.57
1:A:305:CYS:HB2	4:A:806:HOH:O	1.43	1.17
1:B:196:CYS:SG	2:B:602:HG:HG	1.72	1.07
1:B:125:ILE:HD13	1:B:227:ASN:HD22	1.23	1.03
1:B:214:CYS:SG	2:B:607:HG:HG	1.91	0.88
1:B:125:ILE:HD12	4:B:812:HOH:O	1.80	0.80
1:B:304:LEU:CD1	1:B:304:LEU:CD2	2.60	0.79
1:B:125:ILE:HD13	1:B:227:ASN:ND2	1.97	0.78
1:B:149:ARG:NH2	1:B:286:TRP:CE3	2.51	0.78
1:B:304:LEU:CD1	1:B:304:LEU:HG	2.08	0.77
1:B:149:ARG:HD3	1:B:286:TRP:HB2	1.67	0.76
1:B:150:ALA:HB1	1:B:153:ILE:HD12	1.74	0.69
1:A:214:CYS:SG	2:A:606:HG:HG	2.14	0.66
1:A:175:HIS:HD2	1:B:178:ASN:HD21	1.44	0.66
1:B:252:LEU:HD22	1:B:261:MET:HG2	1.77	0.66
1:A:305:CYS:SG	2:A:609:HG:HG	2.14	0.65
1:B:210:VAL:HG21	1:B:308:VAL:HG22	1.78	0.65
1:A:268:CYS:SG	4:A:745:HOH:O	2.35	0.65
1:B:286:TRP:CZ3	1:B:290:LEU:HD21	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ALA:HB3	4:B:745:HOH:O	1.98	0.63
1:A:7:GLN:H	1:A:7:GLN:CD	2.02	0.62
1:A:142:THR:HG23	1:B:9:LYS:HE3	1.81	0.61
1:A:156:TYR:OH	1:A:195:LEU:HB2	2.01	0.60
1:A:175:HIS:CD2	1:B:178:ASN:HD21	2.20	0.59
1:A:159:GLU:OE1	1:A:192:LYS:NZ	2.35	0.59
1:B:123:THR:O	1:B:127:ARG:HG3	2.03	0.57
1:B:149:ARG:CZ	1:B:286:TRP:CE3	2.86	0.57
1:A:7:GLN:NE2	4:A:663:HOH:O	2.22	0.57
1:B:139:ASP:O	1:B:143:ASN:HB2	2.07	0.55
1:A:138:ASP:HB3	1:B:9:LYS:HE2	1.88	0.55
1:A:98:LEU:HD21	1:A:164:THR:HG23	1.89	0.54
1:B:76:ASN:ND2	4:B:777:HOH:O	2.40	0.53
1:B:163:MET:HE3	1:B:192:LYS:HG3	1.91	0.53
1:A:284:LYS:HE2	1:A:305:CYS:SG	2.49	0.53
1:B:163:MET:CE	1:B:192:LYS:HG3	2.38	0.53
1:A:156:TYR:CE2	1:A:192:LYS:HD2	2.45	0.52
1:B:207:ARG:HH22	1:B:282:GLN:NE2	2.08	0.52
1:B:207:ARG:HH12	1:B:282:GLN:HE21	1.58	0.51
1:B:286:TRP:HD1	4:B:807:HOH:O	1.92	0.51
1:B:305:CYS:HB2	4:B:785:HOH:O	2.11	0.51
1:A:90:SER:HA	1:A:93:VAL:HG22	1.94	0.49
1:B:213:ALA:HB3	1:B:304:LEU:HD12	1.95	0.49
1:B:268:CYS:HB2	4:B:752:HOH:O	2.12	0.48
1:B:68:HIS:HE1	1:B:295:SER:O	1.97	0.48
1:A:142:THR:CG2	1:B:9:LYS:HE3	2.44	0.47
1:A:219:ALA:HB1	1:A:338:TRP:CH2	2.49	0.47
1:B:150:ALA:C	4:B:745:HOH:O	2.53	0.47
1:B:152:GLY:N	4:B:638:HOH:O	2.36	0.46
1:B:340:VAL:HG22	4:B:634:HOH:O	2.16	0.46
1:A:203:LEU:C	1:A:203:LEU:HD23	2.36	0.46
1:A:71:HIS:HE1	1:A:289:TYR:O	1.99	0.45
1:B:207:ARG:HH22	1:B:282:GLN:HE22	1.64	0.45
1:B:149:ARG:HD3	1:B:286:TRP:CB	2.43	0.45
1:B:206:ILE:HG13	1:B:207:ARG:N	2.27	0.45
1:B:195:LEU:HD21	4:B:752:HOH:O	2.16	0.45
1:B:275:LEU:HB2	4:B:739:HOH:O	2.16	0.45
1:B:31:GLN:HG3	1:B:34:ASP:HA	1.99	0.45
1:B:129:ILE:HG13	1:B:130:VAL:HG13	1.99	0.45
1:B:207:ARG:HH12	1:B:282:GLN:NE2	2.14	0.45
1:B:79:TYR:CZ	1:B:149:ARG:HG2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:HD3	1:B:297:ILE:HB	1.99	0.44
1:B:31:GLN:CG	1:B:34:ASP:HA	2.48	0.44
1:B:147:GLN:O	1:B:151:GLU:HB2	2.18	0.44
1:B:149:ARG:NH2	1:B:286:TRP:CZ3	2.85	0.43
1:B:159:GLU:OE1	1:B:192:LYS:NZ	2.48	0.43
1:B:75:SER:HB3	1:B:286:TRP:CH2	2.53	0.43
1:B:210:VAL:CG2	1:B:308:VAL:HG22	2.48	0.43
1:A:340:VAL:HG12	1:A:340:VAL:O	2.19	0.42
1:B:149:ARG:CZ	1:B:286:TRP:CD2	3.03	0.41
1:A:7:GLN:CD	1:A:7:GLN:N	2.74	0.41
1:A:55:VAL:HG11	1:A:125:ILE:HD13	2.03	0.40
1:B:327:THR:HA	4:B:735:HOH:O	2.21	0.40
1:A:88:GLY:HA2	1:A:115:GLU:HB2	2.04	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	338/375 (90%)	331 (98%)	7 (2%)	0	100	100
1	B	339/375 (90%)	333 (98%)	6 (2%)	0	100	100
All	All	677/750 (90%)	664 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	307/340 (90%)	299 (97%)	8 (3%)	46	39
1	B	308/340 (91%)	295 (96%)	13 (4%)	30	20
All	All	615/680 (90%)	594 (97%)	21 (3%)	37	28

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	42	LYS
1	A	145	GLN
1	A	192	LYS
1	A	208	PHE
1	A	317	GLN
1	A	324	PRO
1	A	339	LEU
1	B	31	GLN
1	B	42	LYS
1	B	148	LYS
1	B	151	GLU
1	B	186	LEU
1	B	206	ILE
1	B	208	PHE
1	B	268	CYS
1	B	275	LEU
1	B	278	GLN
1	B	286	TRP
1	B	293	ASP
1	B	317	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	71	HIS
1	A	145	GLN
1	A	147	GLN
1	A	175	HIS
1	A	201	ASN

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Mol	Chain	Res	Type
1	A	250	ASN
1	A	306	GLN
1	A	317	GLN
1	B	12	GLN
1	B	63	GLN
1	B	68	HIS
1	B	76	ASN
1	B	80	GLN
1	B	128	ASN
1	B	227	ASN
1	B	282	GLN
1	B	306	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FEO	A	501	4,1	0,2,2	-	-	-		
3	FEO	B	502	4,1	0,2,2	-	-	-		

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 [i](#)

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	340/375 (90%)	-0.10	8 (2%) 59 62	7, 16, 30, 35	0
1	B	341/375 (90%)	0.12	19 (5%) 24 27	7, 18, 34, 42	0
All	All	681/750 (90%)	0.01	27 (3%) 38 41	7, 16, 32, 42	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	340	VAL	8.2
1	A	340	VAL	6.9
1	B	148	LYS	6.5
1	B	341	SER	4.6
1	B	286	TRP	3.7
1	B	304	LEU	3.6
1	B	151	GLU	3.5
1	A	63	GLN	3.5
1	B	288	ASP	3.3
1	B	293	ASP	3.2
1	B	292	ARG	2.8
1	B	131	ASN	2.7
1	A	7	GLN	2.7
1	B	297	ILE	2.7
1	B	326	GLN	2.6
1	B	275	LEU	2.6
1	B	51	GLU	2.5
1	B	7	GLN	2.4
1	A	148	LYS	2.4
1	A	337	THR	2.3
1	A	131	ASN	2.3
1	B	328	ARG	2.2
1	B	294	GLY	2.1
1	B	149	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	144	GLU	2.1
1	A	339	LEU	2.1
1	B	150	ALA	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 monosaccharides 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	HG	B	610	1/1	0.97	0.05	24,24,24,24	1
2	HG	B	603	1/1	0.98	0.04	20,20,20,20	1
2	HG	B	608	1/1	0.98	0.05	20,20,20,20	1
2	HG	A	609	1/1	0.98	0.04	21,21,21,21	1
2	HG	B	602	1/1	0.99	0.12	31,31,31,31	1
2	HG	A	606	1/1	0.99	0.05	15,15,15,15	1
2	HG	B	611	1/1	0.99	0.03	20,20,20,20	1
2	HG	B	612	1/1	0.99	0.04	24,24,24,24	1
2	HG	B	613	1/1	0.99	0.03	27,27,27,27	1
3	FEO	A	501	3/3	0.99	0.04	12,12,12,13	0
2	HG	B	604	1/1	1.00	0.02	14,14,14,14	1
2	HG	B	607	1/1	1.00	0.04	15,15,15,15	1
2	HG	A	601	1/1	1.00	0.01	13,13,13,13	0
2	HG	A	605	1/1	1.00	0.02	14,14,14,14	0
3	FEO	B	502	3/3	1.00	0.03	10,10,11,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.