



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:27 am GMT

PDB ID : 1RIB
Title : STRUCTURE AND FUNCTION OF THE ESCHERICHIA COLI RIBONUCLEOTIDE REDUCTASE PROTEIN R2
Authors : Eklund, H.
Deposited on : 1993-01-19
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

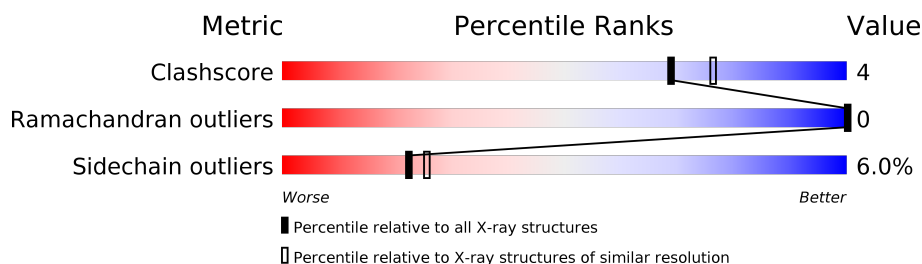
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5899 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.

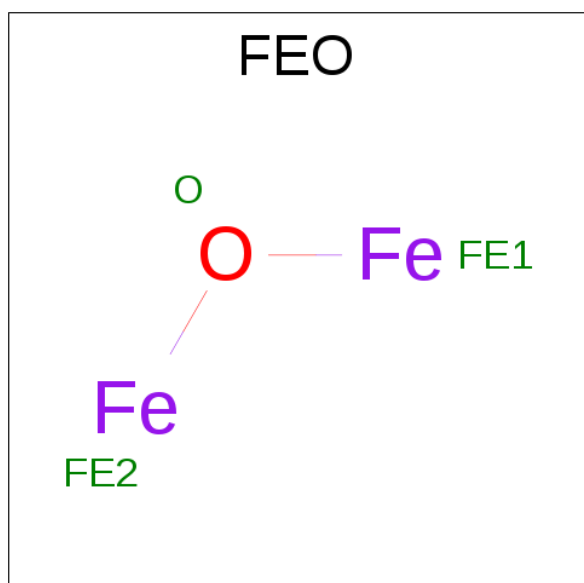
- Molecule 1 is a protein called RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2784	1782	463	526	13			
1	B	340	Total	C	N	O	S	0	0	0
			2784	1782	463	526	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	GLN	CONFLICT	UNP P69924
A	24	GLN	ASN	CONFLICT	UNP P69924
A	326	ASN	GLN	CONFLICT	UNP P69924
B	7	ALA	GLN	CONFLICT	UNP P69924
B	24	GLN	ASN	CONFLICT	UNP P69924
B	326	ASN	GLN	CONFLICT	UNP P69924

- Molecule 2 is MU-OXO-DIIRON (three-letter code: FEO) (formula: Fe₂O).



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

- Molecule 3 is water.

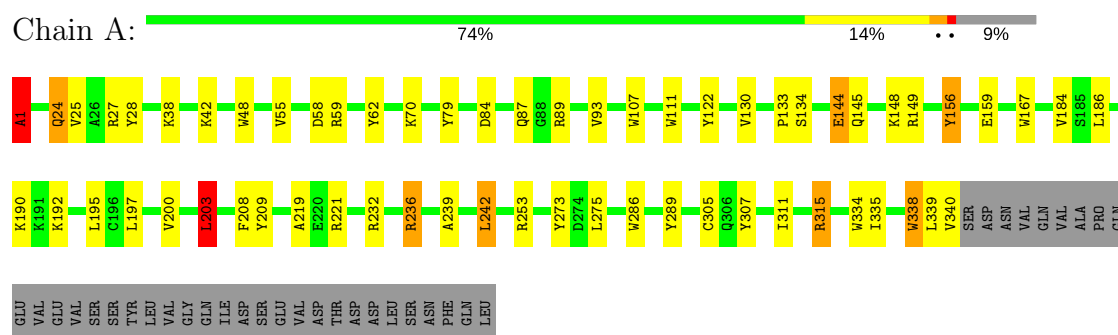
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total 161	O 161	0	0
3	B	164	Total 164	O 164	0	0

3 Residue-property plots [i](#)

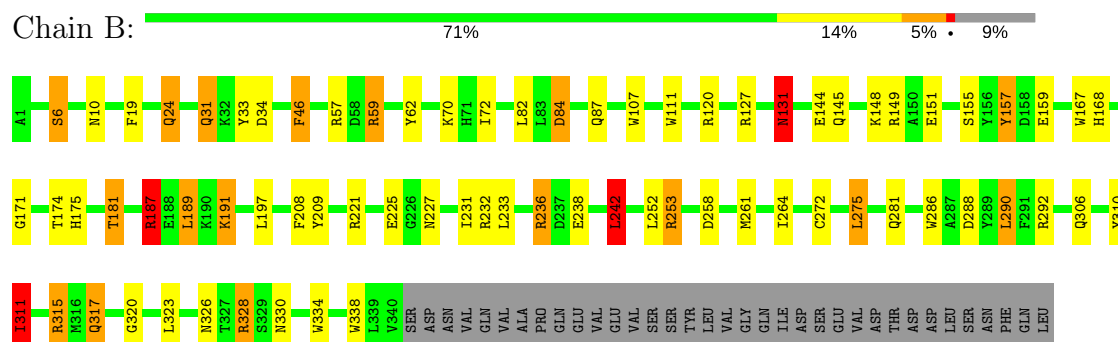
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.30Å 85.50Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5899	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.83	2/2848 (0.1%)	1.52	56/3864 (1.4%)
1	B	0.77	0/2848	1.50	44/3864 (1.1%)
All	All	0.80	2/5696 (0.0%)	1.51	100/7728 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ALA	N-CA	-13.10	1.20	1.46
1	A	1	ALA	CA-CB	-5.04	1.41	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ALA	N-CA-CB	-11.07	94.61	110.10
1	B	236	ARG	NE-CZ-NH2	-10.63	114.98	120.30
1	A	286	TRP	CD1-CG-CD2	9.34	113.77	106.30
1	A	338	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	A	1	ALA	CA-C-O	-8.73	101.77	120.10
1	B	236	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	A	286	TRP	CE2-CD2-CG	-8.64	100.39	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	A	167	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	B	275	LEU	CA-CB-CG	8.29	134.36	115.30
1	A	28	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	107	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	A	338	TRP	CE2-CD2-CG	-7.91	100.98	107.30
1	A	203	LEU	CA-CB-CG	7.90	133.48	115.30
1	A	107	TRP	CE2-CD2-CG	-7.77	101.09	107.30
1	B	286	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	334	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	107	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	B	59	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	B	310	TYR	CB-CG-CD2	-7.54	116.48	121.00
1	B	338	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	334	TRP	CG-CD2-CE3	7.46	140.61	133.90
1	A	93	VAL	CG1-CB-CG2	-7.41	99.04	110.90
1	B	187	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	286	TRP	CE2-CD2-CG	-7.36	101.42	107.30
1	A	236	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	334	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	307	TYR	CB-CG-CD2	-7.13	116.72	121.00
1	B	111	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	A	1	ALA	CA-C-N	7.00	132.60	117.20
1	B	107	TRP	CD1-CG-CD2	6.97	111.87	106.30
1	B	167	TRP	CD1-CG-CD2	6.95	111.86	106.30
1	B	107	TRP	CE2-CD2-CG	-6.91	101.77	107.30
1	A	27	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	127	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	242	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	48	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	B	334	TRP	CD1-CG-CD2	6.71	111.66	106.30
1	A	315	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	A	232	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	111	TRP	CD1-CG-CD2	6.49	111.49	106.30
1	A	236	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	167	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	A	286	TRP	CB-CG-CD1	-6.43	118.65	127.00
1	B	286	TRP	CB-CG-CD1	-6.40	118.68	127.00
1	B	57	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	334	TRP	CB-CG-CD1	-6.31	118.80	127.00
1	A	149	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	122	TYR	CB-CG-CD2	-6.27	117.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	TRP	CE2-CD2-CG	-6.26	102.30	107.30
1	B	242	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	89	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	48	TRP	CD1-CG-CD2	6.24	111.30	106.30
1	A	89	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	167	TRP	CE2-CD2-CG	-6.13	102.39	107.30
1	A	149	ARG	CA-CB-CG	6.12	126.87	113.40
1	A	107	TRP	CB-CG-CD1	-6.04	119.15	127.00
1	A	286	TRP	CG-CD2-CE3	6.03	139.33	133.90
1	A	79	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	B	111	TRP	CE2-CD2-CG	-5.93	102.55	107.30
1	A	273	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	232	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	27	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	57	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	328	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	221	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	221	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	107	TRP	CG-CD2-CE3	5.74	139.06	133.90
1	A	338	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	B	338	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	A	156	TYR	CA-CB-CG	5.69	124.22	113.40
1	B	59	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	59	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	292	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	315	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	311	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	B	191	LYS	CA-CB-CG	5.57	125.64	113.40
1	B	157	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	A	167	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	A	236	ARG	CB-CG-CD	-5.50	97.30	111.60
1	A	62	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	107	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	B	286	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B	149	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	144	GLU	CA-CB-CG	5.34	125.16	113.40
1	A	339	LEU	O-C-N	5.34	131.25	122.70
1	B	187	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	258	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	286	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	232	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	338	TRP	CG-CD1-NE1	-5.30	104.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	TYR	CB-CG-CD1	-5.26	117.85	121.00
1	B	84	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	130	VAL	CA-CB-CG2	-5.20	103.11	110.90
1	B	33	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	111	TRP	CE2-CD2-CG	-5.13	103.19	107.30
1	A	275	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	82	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	187	ARG	CA-CB-CG	5.06	124.54	113.40
1	B	46	PHE	CB-CG-CD2	-5.06	117.26	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	156	TYR	Sidechain
1	B	131	ASN	Peptide
1	B	157	TYR	Sidechain

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	2784	0	2731	20	0
1	B	2784	0	2731	27	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	161	0	0	7	0
3	B	164	0	0	6	0
All	All	5899	0	5462	47	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 4.

All (47) 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:305:CYS:SG	3:A:668:HOH:O	2.48	0.71
1:A:209:TYR:OH	1:A:340:VAL:HG21	1.96	0.65
1:B:306:GLN:HG3	1:B:328:ARG:HD3	1.81	0.62
1:B:252:LEU:HD22	1:B:261:MET:HG3	1.84	0.58
1:B:317:GLN:HB2	1:B:323:LEU:HD21	1.85	0.58
1:A:311:ILE:O	1:A:315:ARG:HG2	2.04	0.56
1:B:6:SER:O	1:B:24:GLN:HG2	2.05	0.56
1:B:62:TYR:O	1:B:70:LYS:HE3	2.05	0.56
1:A:239:ALA:HB2	1:A:340:VAL:HG13	1.89	0.55
1:A:200:VAL:HG13	3:A:520:HOH:O	2.07	0.54
1:A:203:LEU:HG	3:A:520:HOH:O	2.09	0.53
1:B:168:HIS:HD2	3:B:539:HOH:O	1.91	0.53
1:B:155:SER:O	1:B:159:GLU:HG3	2.10	0.51
1:A:236:ARG:HD3	3:A:727:HOH:O	2.09	0.51
1:B:272:CYS:O	1:B:275:LEU:HB3	2.10	0.51
1:B:174:THR:HG22	1:B:181:THR:HG22	1.93	0.51
1:A:1:ALA:HB3	3:A:589:HOH:O	2.12	0.50
1:B:19:PHE:HE1	1:B:189:LEU:HD13	1.76	0.50
1:B:120:ARG:HD3	3:B:511:HOH:O	2.11	0.49
1:A:84:ASP:HA	1:A:87:GLN:HB2	1.96	0.48
1:A:144:GLU:HG2	3:A:810:HOH:O	2.14	0.48
1:B:31:GLN:HG3	1:B:34:ASP:HA	1.95	0.48
1:B:19:PHE:CE1	1:B:189:LEU:HD13	2.49	0.47
1:A:219:ALA:HB1	1:A:338:TRP:CH2	2.50	0.46
1:B:227:ASN:O	1:B:231:ILE:HG12	2.15	0.46
1:A:145:GLN:HG2	1:A:289:TYR:HB2	1.98	0.45
1:B:187:ARG:HD3	1:B:264:ILE:HD11	1.99	0.45
1:A:184:VAL:HG13	3:A:774:HOH:O	2.16	0.44
1:B:236:ARG:HD2	3:B:572:HOH:O	2.16	0.44
1:A:195:LEU:HD13	1:A:195:LEU:HA	1.86	0.44
1:B:311:ILE:O	1:B:315:ARG:HG2	2.18	0.44
1:A:55:VAL:O	1:A:58:ASP:HB2	2.18	0.43
1:B:84:ASP:HA	1:B:87:GLN:HB2	2.01	0.42
1:B:171:GLY:O	1:B:175:HIS:HE1	2.02	0.42
1:B:145:GLN:NE2	1:B:145:GLN:HA	2.34	0.42
1:B:168:HIS:HE1	3:B:565:HOH:O	2.01	0.42
1:B:46:PHE:CD2	1:B:236:ARG:HD3	2.55	0.42
1:A:311:ILE:HA	1:A:311:ILE:HD12	1.88	0.42
1:A:70:LYS:HB2	1:A:70:LYS:HE3	1.87	0.42
1:B:253:ARG:HH12	1:B:320:GLY:HA3	1.85	0.42
1:B:59:ARG:HH21	1:B:131:ASN:HB2	1.83	0.41
1:A:159:GLU:HB3	1:A:192:LYS:HZ2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:HD12	3:B:800:HOH:O	2.20	0.41
1:A:24:GLN:HG2	1:A:25:VAL:N	2.36	0.41
1:B:238:GLU:HG3	3:B:800:HOH:O	2.21	0.41
1:A:186:LEU:HG	1:A:190:LYS:HE3	2.03	0.41
1:B:72:ILE:HG23	1:B:290:LEU:HG	2.03	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	338/375 (90%)	332 (98%)	6 (2%)	0	100	100
All	All	676/750 (90%)	663 (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	306/339 (90%)	294 (96%)	12 (4%)	37	46
1	B	306/339 (90%)	281 (92%)	25 (8%)	13	13
All	All	612/678 (90%)	575 (94%)	37 (6%)	22	25

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	38	LYS
1	A	42	LYS
1	A	133	PRO
1	A	134	SER
1	A	148	LYS
1	A	197	LEU
1	A	203	LEU
1	A	208	PHE
1	A	242	LEU
1	A	253	ARG
1	A	335	ILE
1	B	6	SER
1	B	10	ASN
1	B	24	GLN
1	B	31	GLN
1	B	131	ASN
1	B	144	GLU
1	B	148	LYS
1	B	151	GLU
1	B	181	THR
1	B	187	ARG
1	B	189	LEU
1	B	191	LYS
1	B	197	LEU
1	B	208	PHE
1	B	225	GLU
1	B	233	LEU
1	B	242	LEU
1	B	253	ARG
1	B	281	GLN
1	B	288	ASP
1	B	290	LEU
1	B	311	ILE
1	B	317	GLN
1	B	326	ASN
1	B	330	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	145	GLN
1	A	201	ASN
1	A	227	ASN
1	B	10	ASN
1	B	131	ASN
1	B	145	GLN
1	B	168	HIS
1	B	175	HIS
1	B	330	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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	FEO	A	401	1,3	0,2,2	0.00	-	0,1,1	0.00	-
2	FEO	B	402	1,3	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FEO	A	401	1,3	-	0/0/0/0	0/0/0/0
2	FEO	B	402	1,3	-	0/0/0/0	0/0/0/0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.