Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:15 AM EDT

PDB ID	:	1RIB / pdb_00001rib
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
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:

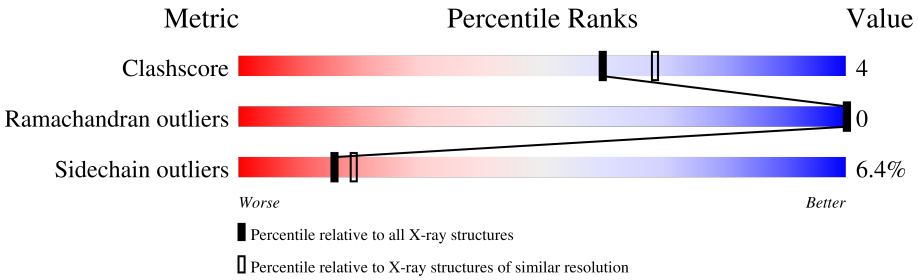
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	73% 15% • 9%
1	B	375	66% 18% 5% • 9%

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.

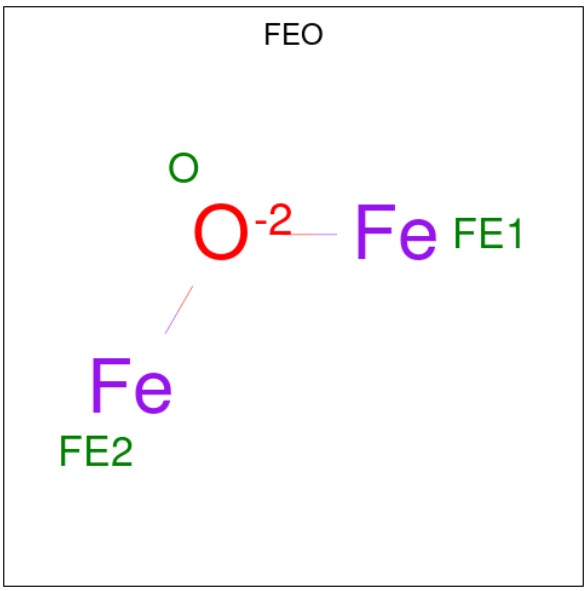
- Molecule 1 is a protein called RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

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 (CCD ID: FEO) (formula: Fe_2O).



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

- Molecule 3 is water.

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

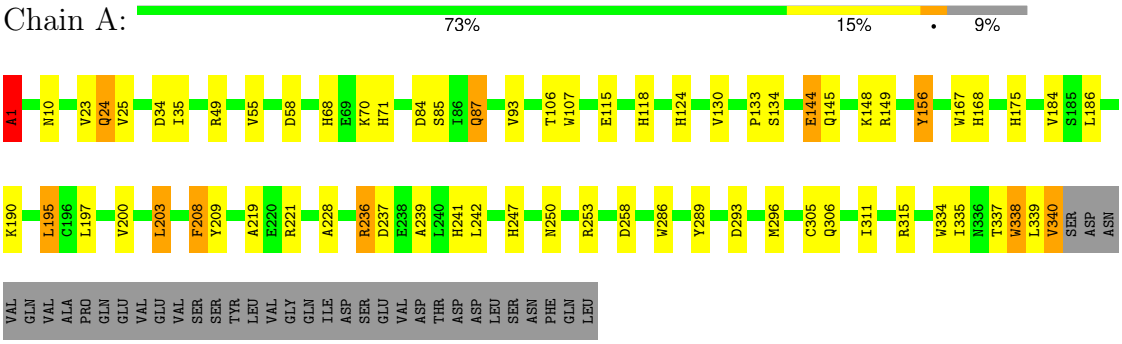
3 Residue-property plots (i)

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. 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. 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.

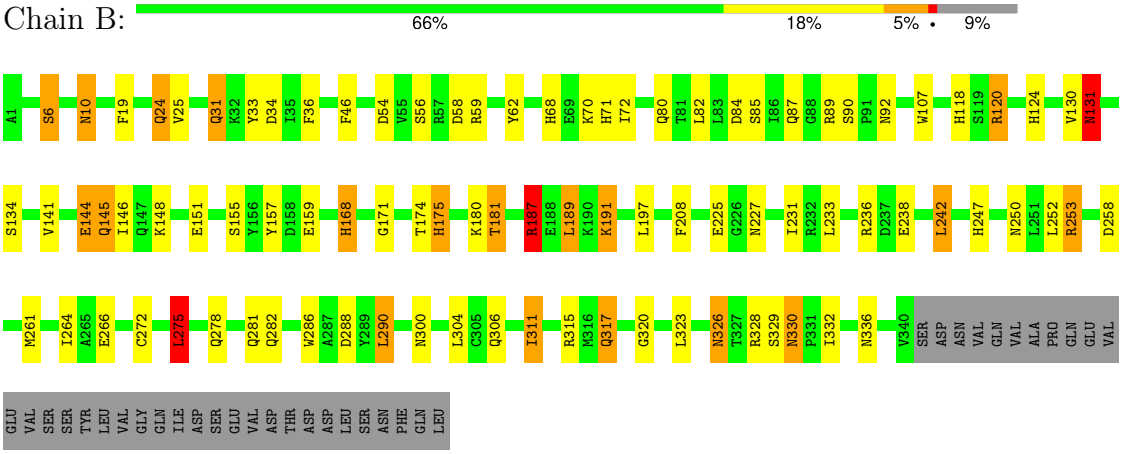
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain A:



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain B:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.00	13/2848 (0.5%)	1.73	45/3864 (1.2%)
1	B	0.93	8/2848 (0.3%)	1.76	57/3864 (1.5%)
All	All	0.97	21/5696 (0.4%)	1.74	102/7728 (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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	ALA	N-CA	-13.74	1.20	1.46
1	A	168	HIS	CD2-NE2	-7.41	1.29	1.37
1	B	118	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	68	HIS	CD2-NE2	-6.60	1.30	1.37
1	B	175	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	124	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	175	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	68	HIS	CD2-NE2	-6.41	1.30	1.37
1	A	247	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	241	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	71	HIS	CD2-NE2	-6.09	1.31	1.37
1	B	124	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	71	HIS	CD2-NE2	-5.99	1.31	1.37
1	B	168	HIS	CD2-NE2	-5.96	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	HIS	CG-ND1	-5.73	1.31	1.38
1	A	118	HIS	CD2-NE2	-5.73	1.31	1.37
1	B	25	VAL	CA-CB	5.63	1.61	1.54
1	B	247	HIS	CD2-NE2	-5.51	1.31	1.37
1	A	1	ALA	CA-C	5.29	1.64	1.52
1	A	71	HIS	CG-ND1	-5.25	1.32	1.38
1	A	247	HIS	CG-ND1	-5.09	1.32	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	ALA	CA-C-O	-11.20	101.77	120.80
1	A	1	ALA	N-CA-CB	-10.53	94.61	110.40
1	B	250	ASN	OD1-CG-ND2	-9.27	113.33	122.60
1	A	87	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	B	258	ASP	CA-CB-CG	8.63	121.23	112.60
1	B	326	ASN	CA-CB-CG	8.62	121.22	112.60
1	B	131	ASN	N-CA-C	8.51	123.02	112.47
1	B	85	SER	N-CA-C	-8.47	102.00	111.14
1	A	247	HIS	CA-CB-CG	-8.42	105.38	113.80
1	B	282	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	B	36	PHE	CA-CB-CG	-7.55	106.25	113.80
1	B	247	HIS	CB-CG-CD2	-7.22	121.81	131.20
1	A	107	TRP	CG-CD2-CE3	7.12	141.02	133.90
1	A	23	VAL	CA-C-N	-7.04	112.01	122.56
1	A	23	VAL	C-N-CA	-7.04	112.01	122.56
1	B	131	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	B	330	ASN	CB-CG-ND2	6.97	126.85	116.40
1	B	89	ARG	N-CA-C	6.94	118.63	111.14
1	B	300	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	306	GLN	OE1-CD-NE2	-6.90	115.70	122.60
1	B	329	SER	N-CA-C	-6.89	100.32	110.52
1	B	330	ASN	OD1-CG-ND2	-6.88	115.72	122.60
1	A	334	TRP	CG-CD2-CE3	6.71	140.61	133.90
1	B	134	SER	N-CA-C	6.70	120.32	111.75
1	B	54	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	10	ASN	CA-CB-CG	6.55	119.15	112.60
1	B	80	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	B	68	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	149	ARG	CA-CB-CG	6.39	126.87	114.10
1	B	278	GLN	OE1-CD-NE2	-6.36	116.25	122.60
1	A	340	VAL	N-CA-CB	-6.33	100.74	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	A	339	LEU	O-C-N	6.23	131.25	123.15
1	A	168	HIS	CB-CG-CD2	-6.22	123.12	131.20
1	A	293	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	115	GLU	CA-C-O	-6.11	112.94	119.97
1	B	281	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	A	236	ARG	CB-CG-CD	-6.09	97.30	111.30
1	B	118	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	A	34	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	191	LYS	CB-CA-C	-5.99	101.48	110.88
1	B	145	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	B	68	HIS	CA-CB-CG	5.89	119.69	113.80
1	A	49	ARG	CA-C-N	5.85	125.32	119.24
1	A	49	ARG	C-N-CA	5.85	125.32	119.24
1	B	208	PHE	CA-CB-CG	-5.83	107.97	113.80
1	A	124	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	B	144	GLU	N-CA-C	5.78	118.32	111.33
1	B	191	LYS	CA-CB-CG	5.77	125.64	114.10
1	A	258	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	167	TRP	CE2-CD2-CE3	5.75	124.55	118.80
1	B	58	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	281	GLN	CG-CD-NE2	5.74	125.01	116.40
1	A	156	TYR	CA-CB-CG	5.73	124.22	113.90
1	B	92	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	B	131	ASN	CB-CG-ND2	5.72	124.98	116.40
1	A	208	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	286	TRP	CE2-CD2-CG	-5.68	100.39	107.20
1	B	71	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	B	146	ILE	CA-C-N	5.60	128.56	120.38
1	B	146	ILE	C-N-CA	5.60	128.56	120.38
1	B	247	HIS	CB-CG-ND1	5.57	131.05	122.70
1	B	329	SER	CA-CB-OG	5.53	122.17	111.10
1	A	144	GLU	CA-CB-CG	5.53	125.16	114.10
1	B	90	SER	N-CA-C	5.51	121.98	109.81
1	A	286	TRP	CB-CG-CD1	-5.50	118.65	126.90
1	B	286	TRP	CB-CG-CD1	-5.48	118.68	126.90
1	A	118	HIS	CB-CG-CD2	-5.47	124.08	131.20
1	B	180	LYS	CB-CG-CD	-5.45	98.75	111.30
1	B	10	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	237	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	286	TRP	CG-CD2-CE3	5.43	139.33	133.90
1	A	334	TRP	CB-CG-CD1	-5.40	118.80	126.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	337	THR	CA-CB-OG1	-5.38	101.53	109.60
1	B	120	ARG	N-CA-CB	-5.38	101.94	110.28
1	A	93	VAL	CG1-CB-CG2	-5.35	99.04	110.80
1	A	106	THR	CA-CB-OG1	-5.32	101.61	109.60
1	A	258	ASP	N-CA-C	-5.30	102.97	109.65
1	B	141	VAL	N-CA-C	5.30	116.07	110.72
1	A	35	ILE	CA-C-O	-5.26	115.58	121.05
1	B	187	ARG	CA-CB-CG	5.22	124.54	114.10
1	B	33	TYR	CA-C-O	5.20	125.95	120.33
1	A	338	TRP	CE2-CD2-CG	-5.19	100.98	107.20
1	B	10	ASN	CB-CG-ND2	5.18	124.17	116.40
1	A	228	ALA	N-CA-C	5.17	116.92	111.28
1	A	107	TRP	CB-CG-CD1	-5.17	119.15	126.90
1	B	107	TRP	CG-CD2-CE3	5.16	139.06	133.90
1	B	275	LEU	CA-CB-CG	5.16	134.36	116.30
1	B	56	SER	N-CA-C	5.13	121.73	110.80
1	A	85	SER	N-CA-C	-5.12	105.59	111.07
1	B	326	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	A	107	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	334	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	247	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	B	332	ILE	CA-C-N	5.07	124.86	119.28
1	B	332	ILE	C-N-CA	5.07	124.86	119.28
1	B	336	ASN	CA-CB-CG	-5.06	107.54	112.60
1	B	90	SER	CA-C-N	5.04	124.48	119.24
1	B	90	SER	C-N-CA	5.04	124.48	119.24
1	B	247	HIS	CA-CB-CG	-5.04	108.76	113.80
1	B	330	ASN	CA-CB-CG	5.03	117.63	112.60
1	B	130	VAL	CB-CA-C	-5.00	105.93	110.63

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 (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	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:A:221:ARG:HH21	1:A:296:MET:HE2	1.66	0.60
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:LYS:HE3	1:A:70:LYS:HB2	1.87	0.42
1:A:311:ILE:HD12	1:A:311:ILE:HA	1.88	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: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:A:186:LEU:HG	1:A:190:LYS:HE3	2.03	0.41
1:B:238:GLU:HG3	3:B:800:HOH:O	2.21	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%)	28	39
1	B	306/339 (90%)	279 (91%)	27 (9%)	9	10
All	All	612/678 (90%)	573 (94%)	39 (6%)	16	19

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	130	VAL
1	A	133	PRO
1	A	134	SER
1	A	148	LYS
1	A	195	LEU
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	82	LEU
1	B	131	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	225	GLU
1	B	233	LEU
1	B	242	LEU
1	B	253	ARG
1	B	266	GLU
1	B	275	LEU
1	B	288	ASP
1	B	290	LEU
1	B	304	LEU
1	B	311	ILE
1	B	317	GLN
1	B	326	ASN
1	B	330	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	68	HIS
1	A	145	GLN
1	A	147	GLN
1	A	168	HIS
1	A	201	ASN
1	A	227	ASN
1	A	317	GLN
1	B	128	ASN
1	B	131	ASN
1	B	145	GLN
1	B	168	HIS
1	B	175	HIS
1	B	201	ASN
1	B	306	GLN
1	B	330	ASN
1	B	336	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

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	B	402	1,3	0,2,2	-	-	-		
2	FEO	A	401	1,3	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

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.