Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 11:20 AM EDT

PDB ID	:	1R1R
Title	:	RIBONUCLEOTIDE REDUCTASE R1 PROTEIN MUTANT Y730F WITH A REDUCED ACTIVE SITE FROM ESCHERICHIA COLI
Authors	:	Eriksson, M.; Eklund, H.
Deposited on	:	1997-07-15
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

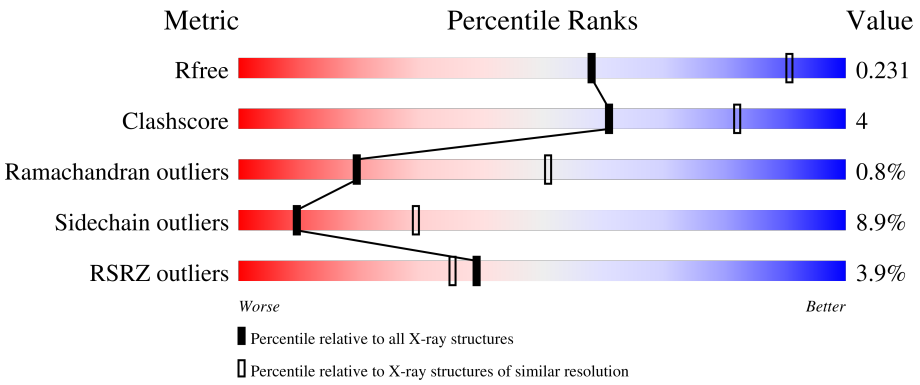
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	761	4% 79% 16%
1	B	761	4% 79% 16%
1	C	761	3% 79% 16%
2	D	20	15% 60% 20% 20%
2	E	20	15% 60% 20% 20%

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Mol	Chain	Length	Quality of chain
2	F	20	5% 60% 20% 20%
2	P	20	5% 5% 5% 85%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18258 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
			Total	C	N	O	S			
1	A	734	5844	3712	1004	1104	24	0	0	0
1	B	734	5844	3712	1004	1104	24	0	0	0
1	C	734	5844	3712	1004	1104	24	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	PHE	TYR	engineered mutation	UNP P00452
B	730	PHE	TYR	engineered mutation	UNP P00452
C	730	PHE	TYR	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	16	129	77	19	33	0	0	0
2	E	16	129	77	19	33	0	0	0
2	F	16	129	77	19	33	0	0	0
2	P	3	27	20	3	4	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	104	104	104	0	0

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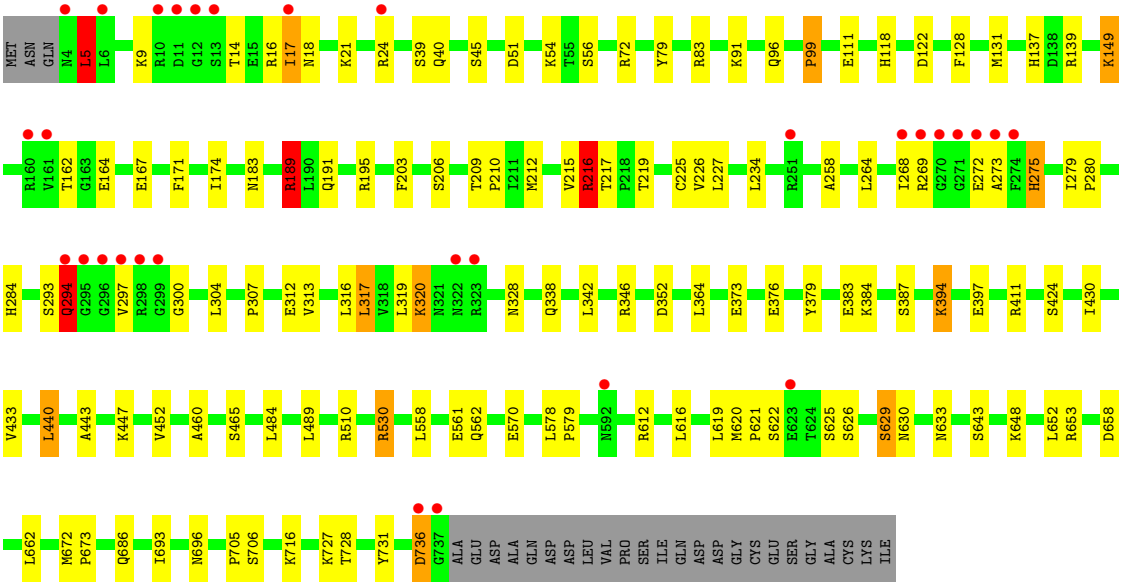
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	104	104	104	0	0
			Total	O		
3	C	104	104	104	0	0

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 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.

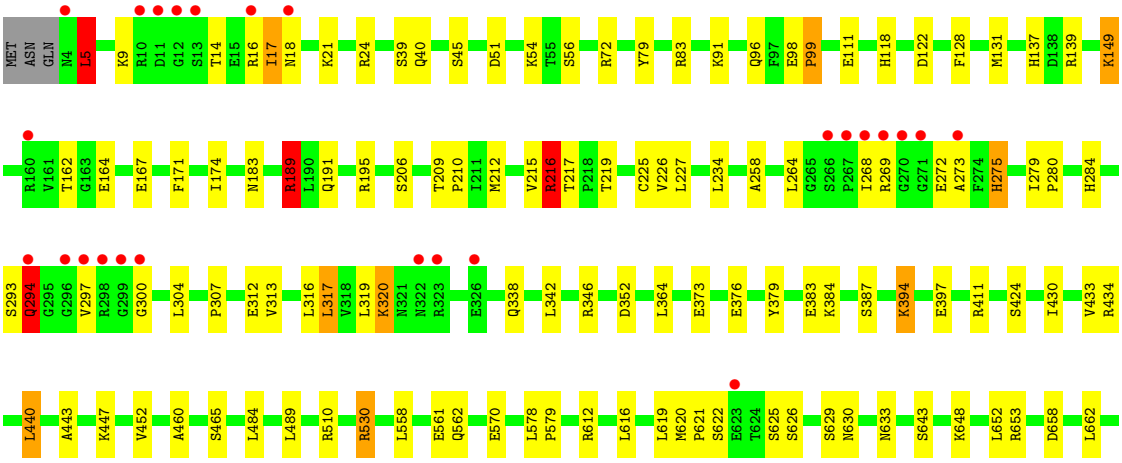
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

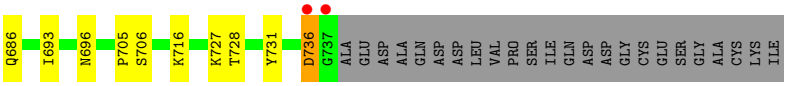
Chain A:



• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

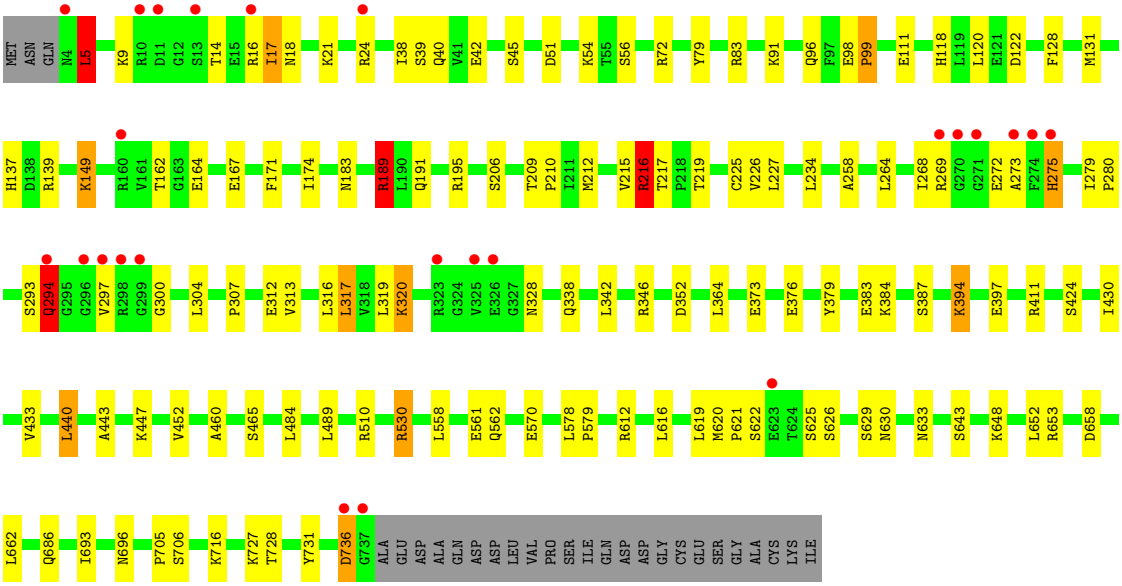
Chain B:





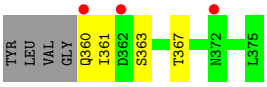
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain C:



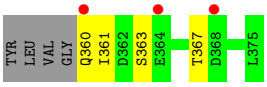
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D:



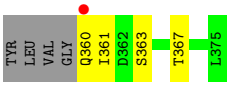
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E:



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F:



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain P:

Y1
L2
V3
GLY
GLN
ILE
ASP
SER
GLU
VAL
ASP
THR
ASP
ASP
LEU
SER
ASN
PHE
GLN
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	227.82Å 227.82Å 343.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.90) 96.1 (20.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 2.88Å)	Xtriage
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.210 , 0.245 0.216 , 0.231	Depositor DCC
R_{free} test set	2008 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18258	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.36	0/5972	0.88	5/8088 (0.1%)
1	B	0.36	0/5972	0.88	5/8088 (0.1%)
1	C	0.36	0/5972	0.88	5/8088 (0.1%)
2	D	0.36	0/129	0.75	0/173
2	E	0.36	0/129	0.75	0/173
2	F	0.36	0/129	0.75	0/173
2	P	0.72	0/27	1.81	1/36 (2.8%)
All	All	0.36	0/18330	0.88	16/24819 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	653	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	653	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	653	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	653	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	653	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	653	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	P	2	LEU	CA-CB-CG	5.87	128.79	115.30
1	A	530	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	189	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	189	ARG	CD-NE-CZ	5.42	131.18	123.60
1	B	530	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	530	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	189	ARG	CD-NE-CZ	5.40	131.16	123.60
1	B	736	ASP	CA-CB-CG	5.21	124.86	113.40
1	A	736	ASP	CA-CB-CG	5.20	124.84	113.40
1	C	736	ASP	CA-CB-CG	5.19	124.83	113.40

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	5844	0	5770	54	0
1	B	5844	0	5770	53	0
1	C	5844	0	5770	54	0
2	D	129	0	111	0	0
2	E	129	0	111	0	0
2	F	129	0	111	0	0
2	P	27	0	31	1	0
3	A	104	0	0	0	0
3	B	104	0	0	0	0
3	C	104	0	0	0	0
All	All	18258	0	17674	160	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 (160) 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:394:LYS:HB3	1:A:397:GLU:HG3	1.68	0.76
1:C:215:VAL:O	1:C:216:ARG:HB3	1.85	0.76
1:B:394:LYS:HB3	1:B:397:GLU:HG3	1.68	0.75
1:C:394:LYS:HB3	1:C:397:GLU:HG3	1.68	0.75
1:A:215:VAL:O	1:A:216:ARG:HB3	1.85	0.75
1:B:215:VAL:O	1:B:216:ARG:HB3	1.85	0.74
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.70	0.73
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.70	0.73
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.70	0.73
1:A:149:LYS:HG2	1:A:652:LEU:HD21	1.74	0.69
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.75	0.69
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.75	0.68
1:B:149:LYS:HG2	1:B:652:LEU:HD21	1.74	0.68
1:C:149:LYS:HG2	1:C:652:LEU:HD21	1.74	0.68
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.77	0.67
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.77	0.67
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.77	0.66
1:A:5:LEU:HD22	1:A:17:ILE:HG13	1.79	0.64
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.80	0.63
1:B:561:GLU:HG2	1:B:562:GLN:HG3	1.81	0.63
1:C:5:LEU:HD22	1:C:17:ILE:HG13	1.79	0.63
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.80	0.63
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.81	0.63
1:B:5:LEU:HD22	1:B:17:ILE:HG13	1.79	0.62
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.82	0.62
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.82	0.62
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.80	0.62
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.82	0.62
1:A:561:GLU:HG2	1:A:562:GLN:HG3	1.81	0.61
1:A:279:ILE:HD12	1:A:319:LEU:HD21	1.83	0.60
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.83	0.60
1:B:279:ILE:HD12	1:B:319:LEU:HD21	1.84	0.59
1:A:5:LEU:O	1:A:17:ILE:HB	2.03	0.59
1:B:5:LEU:O	1:B:17:ILE:HB	2.03	0.59
1:C:279:ILE:HD12	1:C:319:LEU:HD21	1.84	0.59
1:C:5:LEU:O	1:C:17:ILE:HB	2.02	0.59
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.84	0.59
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.84	0.58
1:B:342:LEU:HD13	1:B:376:GLU:HG3	1.86	0.58
1:C:342:LEU:HD13	1:C:376:GLU:HG3	1.86	0.56
1:A:342:LEU:HD13	1:A:376:GLU:HG3	1.86	0.56
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.88	0.56
1:B:578:LEU:HB3	1:B:579:PRO:HD2	1.88	0.55
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.88	0.55
1:C:167:GLU:OE2	1:C:216:ARG:NH1	2.41	0.54
1:A:167:GLU:OE2	1:A:216:ARG:NH1	2.41	0.53
1:B:167:GLU:OE2	1:B:216:ARG:NH1	2.41	0.53
1:B:430:ILE:HG21	1:B:570:GLU:HG2	1.89	0.53
1:A:430:ILE:HG21	1:A:570:GLU:HG2	1.90	0.53
1:C:430:ILE:HG21	1:C:570:GLU:HG2	1.90	0.53
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.44	0.52
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.91	0.52
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.91	0.52
1:C:264:LEU:HD12	1:C:275:HIS:O	2.10	0.52
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.91	0.52
1:A:264:LEU:HD12	1:A:275:HIS:O	2.10	0.51
1:B:264:LEU:HD12	1:B:275:HIS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ILE:HB	1:B:275:HIS:CD2	2.47	0.50
1:C:268:ILE:HB	1:C:275:HIS:CD2	2.47	0.50
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.93	0.50
1:B:234:LEU:HG	1:B:272:GLU:HB3	1.94	0.50
1:C:234:LEU:HG	1:C:272:GLU:HB3	1.94	0.50
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.93	0.50
1:A:234:LEU:HG	1:A:272:GLU:HB3	1.93	0.49
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.93	0.49
1:A:268:ILE:HB	1:A:275:HIS:CD2	2.47	0.48
1:A:128:PHE:HA	1:A:131:MET:HE3	1.96	0.48
1:A:79:TYR:O	1:A:83:ARG:HG3	2.14	0.48
1:C:79:TYR:O	1:C:83:ARG:HG3	2.14	0.47
1:C:268:ILE:HB	1:C:275:HIS:HD2	1.79	0.47
1:B:79:TYR:O	1:B:83:ARG:HG3	2.14	0.47
1:B:128:PHE:HA	1:B:131:MET:HE3	1.97	0.47
1:C:128:PHE:HA	1:C:131:MET:HE3	1.97	0.47
1:C:622:SER:O	1:C:633:ASN:HB3	2.15	0.47
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.48	0.47
1:A:18:ASN:ND2	1:A:21:LYS:HG3	2.31	0.46
1:B:622:SER:O	1:B:633:ASN:HB3	2.15	0.46
1:C:18:ASN:ND2	1:C:21:LYS:HG3	2.31	0.46
1:B:268:ILE:HB	1:B:275:HIS:HD2	1.79	0.46
1:B:18:ASN:ND2	1:B:21:LYS:HG3	2.31	0.46
1:C:510:ARG:NH2	1:C:570:GLU:OE1	2.48	0.46
1:C:705:PRO:O	1:C:706:SER:HB2	2.16	0.46
1:A:622:SER:O	1:A:633:ASN:HB3	2.15	0.46
1:B:705:PRO:O	1:B:706:SER:HB2	2.15	0.46
1:A:705:PRO:O	1:A:706:SER:HB2	2.15	0.46
1:A:122:ASP:O	1:A:189:ARG:NH2	2.49	0.45
1:A:268:ILE:HB	1:A:275:HIS:HD2	1.80	0.45
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.97	0.45
1:B:510:ARG:NH2	1:B:570:GLU:OE1	2.48	0.45
1:B:122:ASP:O	1:B:189:ARG:NH2	2.49	0.45
1:C:122:ASP:O	1:C:189:ARG:NH2	2.49	0.45
1:A:620:MET:HB2	1:A:621:PRO:HD2	1.99	0.45
1:B:620:MET:HB2	1:B:621:PRO:HD2	1.99	0.45
1:C:212:MET:O	1:C:216:ARG:NH2	2.50	0.45
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.98	0.44
1:B:686:GLN:NE2	1:B:727:LYS:HE3	2.33	0.44
1:C:620:MET:HB2	1:C:621:PRO:HD2	1.99	0.44
1:C:686:GLN:NE2	1:C:727:LYS:HE3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.97	0.44
1:B:17:ILE:HD13	1:B:18:ASN:N	2.33	0.44
1:B:212:MET:O	1:B:216:ARG:NH2	2.50	0.44
1:B:293:SER:O	1:B:294:GLN:C	2.56	0.44
1:A:217:THR:OG1	1:A:219:THR:HG22	2.18	0.44
1:C:217:THR:OG1	1:C:219:THR:HG22	2.18	0.44
1:A:212:MET:O	1:A:216:ARG:NH2	2.50	0.43
1:C:293:SER:O	1:C:294:GLN:C	2.57	0.43
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.33	0.43
1:A:328:ASN:HD22	1:A:328:ASN:HA	1.64	0.43
1:C:312:GLU:O	1:C:316:LEU:HG	2.19	0.43
1:A:17:ILE:HD13	1:A:18:ASN:N	2.33	0.43
1:A:162:THR:OG1	1:A:164:GLU:HG3	2.18	0.43
1:A:293:SER:O	1:A:294:GLN:C	2.56	0.43
1:B:312:GLU:O	1:B:316:LEU:HG	2.19	0.43
1:B:162:THR:OG1	1:B:164:GLU:HG3	2.18	0.43
1:B:217:THR:OG1	1:B:219:THR:HG22	2.18	0.43
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.49	0.43
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.49	0.42
1:C:17:ILE:HD13	1:C:18:ASN:N	2.33	0.42
1:C:346:ARG:HD2	1:C:352:ASP:O	2.19	0.42
1:A:379:TYR:O	1:A:383:GLU:HG3	2.19	0.42
1:B:379:TYR:O	1:B:383:GLU:HG3	2.19	0.42
1:A:312:GLU:O	1:A:316:LEU:HG	2.19	0.42
1:C:162:THR:OG1	1:C:164:GLU:HG3	2.18	0.42
1:C:191:GLN:O	1:C:195:ARG:HG3	2.20	0.42
1:C:328:ASN:HD22	1:C:328:ASN:HA	1.64	0.42
1:A:171:PHE:HA	1:A:174:ILE:HG22	2.02	0.42
1:B:346:ARG:HD2	1:B:352:ASP:O	2.19	0.42
1:A:346:ARG:HD2	1:A:352:ASP:O	2.19	0.42
1:B:98:GLU:HA	1:B:99:PRO:HD3	1.91	0.42
1:C:379:TYR:O	1:C:383:GLU:HG3	2.19	0.42
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.49	0.42
1:B:191:GLN:O	1:B:195:ARG:HG3	2.20	0.42
1:C:209:THR:N	1:C:210:PRO:CD	2.83	0.42
1:C:171:PHE:HA	1:C:174:ILE:HG22	2.02	0.41
1:B:209:THR:HB	1:B:210:PRO:HD3	2.02	0.41
1:B:209:THR:N	1:B:210:PRO:CD	2.83	0.41
1:C:209:THR:HB	1:C:210:PRO:HD3	2.02	0.41
1:C:307:PRO:HA	1:C:338:GLN:HB2	2.02	0.41
1:A:672:MET:HA	1:A:673:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:HA	1:B:174:ILE:HG22	2.02	0.41
1:B:440:LEU:HD12	1:B:728:THR:HB	2.02	0.41
1:A:191:GLN:O	1:A:195:ARG:HG3	2.20	0.41
1:A:209:THR:HB	1:A:210:PRO:HD3	2.02	0.41
1:C:98:GLU:HA	1:C:99:PRO:HD3	1.92	0.41
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.56	0.41
1:C:440:LEU:HD12	1:C:728:THR:HB	2.02	0.41
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.56	0.41
1:A:209:THR:N	1:A:210:PRO:CD	2.83	0.41
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.09	0.41
1:A:307:PRO:HA	1:A:338:GLN:HB2	2.02	0.41
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.56	0.41
1:A:203:PHE:HB3	1:A:629:SER:HB3	2.03	0.41
1:B:307:PRO:HA	1:B:338:GLN:HB2	2.02	0.41
1:B:434:ARG:HH11	1:B:434:ARG:HD3	1.75	0.41
1:A:320:LYS:HE2	1:A:411:ARG:HB2	2.03	0.40
1:A:440:LEU:HD12	1:A:728:THR:HB	2.03	0.40
1:C:320:LYS:HE2	1:C:411:ARG:HB2	2.03	0.40
1:B:320:LYS:HE2	1:B:411:ARG:HB2	2.03	0.40
1:C:38:ILE:O	1:C:42:GLU:HG3	2.22	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	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	19	51
1	B	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	19	51
1	C	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	19	51
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	F	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	P	1/20 (5%)	0	1 (100%)	0	100	100
All	All	2239/2363 (95%)	2130 (95%)	91 (4%)	18 (1%)	19	51

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	B	294	GLN
1	C	294	GLN
1	A	216	ARG
1	A	273	ALA
1	B	216	ARG
1	B	273	ALA
1	C	216	ARG
1	C	273	ALA
1	A	5	LEU
1	A	300	GLY
1	B	5	LEU
1	B	300	GLY
1	C	5	LEU
1	C	300	GLY
1	A	731	TYR
1	B	731	TYR
1	C	731	TYR

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	629/651 (97%)	576 (92%)	53 (8%)	11	31
1	B	629/651 (97%)	576 (92%)	53 (8%)	11	31
1	C	629/651 (97%)	576 (92%)	53 (8%)	11	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	16/19 (84%)	12 (75%)	4 (25%)	0	2
2	E	16/19 (84%)	12 (75%)	4 (25%)	0	2
2	F	16/19 (84%)	12 (75%)	4 (25%)	0	2
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1938/2029 (96%)	1766 (91%)	172 (9%)	9	29

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	14	THR
1	A	16	ARG
1	A	17	ILE
1	A	24	ARG
1	A	39	SER
1	A	40	GLN
1	A	45	SER
1	A	51	ASP
1	A	54	LYS
1	A	56	SER
1	A	72	ARG
1	A	91	LYS
1	A	96	GLN
1	A	99	PRO
1	A	111	GLU
1	A	118	HIS
1	A	139	ARG
1	A	149	LYS
1	A	183	ASN
1	A	189	ARG
1	A	206	SER
1	A	216	ARG
1	A	225	CYS
1	A	226	VAL
1	A	269	ARG
1	A	275	HIS
1	A	294	GLN
1	A	297	VAL
1	A	317	LEU
1	A	320	LYS

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Mol	Chain	Res	Type
1	A	364	LEU
1	A	373	GLU
1	A	384	LYS
1	A	387	SER
1	A	394	LYS
1	A	424	SER
1	A	440	LEU
1	A	447	LYS
1	A	452	VAL
1	A	484	LEU
1	A	530	ARG
1	A	616	LEU
1	A	625	SER
1	A	626	SER
1	A	629	SER
1	A	630	ASN
1	A	643	SER
1	A	648	LYS
1	A	696	ASN
1	A	716	LYS
1	A	736	ASP
2	D	360	GLN
2	D	361	ILE
2	D	363	SER
2	D	367	THR
1	B	5	LEU
1	B	9	LYS
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	24	ARG
1	B	39	SER
1	B	40	GLN
1	B	45	SER
1	B	51	ASP
1	B	54	LYS
1	B	56	SER
1	B	72	ARG
1	B	91	LYS
1	B	96	GLN
1	B	99	PRO
1	B	111	GLU

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Mol	Chain	Res	Type
1	B	118	HIS
1	B	139	ARG
1	B	149	LYS
1	B	183	ASN
1	B	189	ARG
1	B	206	SER
1	B	216	ARG
1	B	225	CYS
1	B	226	VAL
1	B	269	ARG
1	B	275	HIS
1	B	294	GLN
1	B	297	VAL
1	B	317	LEU
1	B	320	LYS
1	B	364	LEU
1	B	373	GLU
1	B	384	LYS
1	B	387	SER
1	B	394	LYS
1	B	424	SER
1	B	440	LEU
1	B	447	LYS
1	B	452	VAL
1	B	484	LEU
1	B	530	ARG
1	B	616	LEU
1	B	625	SER
1	B	626	SER
1	B	629	SER
1	B	630	ASN
1	B	643	SER
1	B	648	LYS
1	B	696	ASN
1	B	716	LYS
1	B	736	ASP
2	E	360	GLN
2	E	361	ILE
2	E	363	SER
2	E	367	THR
1	C	5	LEU
1	C	9	LYS

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Mol	Chain	Res	Type
1	C	14	THR
1	C	16	ARG
1	C	17	ILE
1	C	24	ARG
1	C	39	SER
1	C	40	GLN
1	C	45	SER
1	C	51	ASP
1	C	54	LYS
1	C	56	SER
1	C	72	ARG
1	C	91	LYS
1	C	96	GLN
1	C	99	PRO
1	C	111	GLU
1	C	118	HIS
1	C	139	ARG
1	C	149	LYS
1	C	183	ASN
1	C	189	ARG
1	C	206	SER
1	C	216	ARG
1	C	225	CYS
1	C	226	VAL
1	C	269	ARG
1	C	275	HIS
1	C	294	GLN
1	C	297	VAL
1	C	317	LEU
1	C	320	LYS
1	C	364	LEU
1	C	373	GLU
1	C	384	LYS
1	C	387	SER
1	C	394	LYS
1	C	424	SER
1	C	440	LEU
1	C	447	LYS
1	C	452	VAL
1	C	484	LEU
1	C	530	ARG
1	C	616	LEU

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Mol	Chain	Res	Type
1	C	625	SER
1	C	626	SER
1	C	629	SER
1	C	630	ASN
1	C	643	SER
1	C	648	LYS
1	C	696	ASN
1	C	716	LYS
1	C	736	ASP
2	F	360	GLN
2	F	361	ILE
2	F	363	SER
2	F	367	THR
2	P	2	LEU

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	18	ASN
1	A	46	HIS
1	A	250	GLN
1	A	275	HIS
1	A	328	ASN
1	A	596	HIS
1	A	630	ASN
1	A	661	HIS
2	D	360	GLN
1	B	18	ASN
1	B	46	HIS
1	B	250	GLN
1	B	275	HIS
1	B	328	ASN
1	B	596	HIS
1	B	630	ASN
1	B	661	HIS
1	C	18	ASN
1	C	46	HIS
1	C	250	GLN
1	C	275	HIS
1	C	328	ASN
1	C	596	HIS
1	C	630	ASN

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Mol	Chain	Res	Type
1	C	661	HIS

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)

There are no ligands in this entry.

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 (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	734/761 (96%)	-0.42	30 (4%)	37	32	10, 24, 77, 108	0
1	B	734/761 (96%)	-0.02	27 (3%)	41	37	10, 24, 77, 108	0
1	C	734/761 (96%)	-0.08	24 (3%)	46	41	10, 24, 77, 108	0
2	D	16/20 (80%)	0.75	3 (18%)	1	0	45, 82, 91, 97	0
2	E	16/20 (80%)	0.82	3 (18%)	1	0	45, 82, 91, 97	0
2	F	16/20 (80%)	0.93	1 (6%)	20	16	45, 82, 91, 97	0
2	P	3/20 (15%)	0.37	0	100	100	30, 30, 37, 43	0
All	All	2253/2363 (95%)	-0.15	88 (3%)	39	35	10, 25, 83, 108	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	GLY	6.9
1	A	297	VAL	6.7
1	A	296	GLY	6.4
1	C	4	ASN	5.8
1	C	297	VAL	5.5
1	B	294	GLN	5.4
1	C	737	GLY	5.3
1	A	270	GLY	5.2
1	A	12	GLY	5.1
1	B	296	GLY	5.0
1	B	10	ARG	5.0
1	B	297	VAL	4.9
1	B	269	ARG	4.9
1	C	298	ARG	4.8
1	C	296	GLY	4.8
1	A	11	ASP	4.8
2	F	360	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	737	GLY	4.5
1	A	4	ASN	4.4
1	A	299	GLY	4.3
1	A	273	ALA	4.2
1	C	294	GLN	4.2
1	C	736	ASP	4.1
1	A	271	GLY	4.0
1	C	269	ARG	3.9
1	A	298	ARG	3.8
1	A	323	ARG	3.8
1	B	273	ALA	3.8
2	E	360	GLN	3.8
1	B	11	ASP	3.8
1	A	269	ARG	3.7
1	C	10	ARG	3.6
1	A	294	GLN	3.6
1	C	274	PHE	3.5
1	C	270	GLY	3.5
1	A	13	SER	3.5
1	B	323	ARG	3.5
1	B	4	ASN	3.4
1	B	12	GLY	3.4
1	C	11	ASP	3.3
1	A	322	ASN	3.3
1	B	322	ASN	3.2
1	C	273	ALA	3.2
1	C	271	GLY	3.1
2	D	360	GLN	3.1
1	C	299	GLY	3.1
1	A	736	ASP	3.1
1	B	270	GLY	3.1
1	B	736	ASP	3.0
1	A	10	ARG	3.0
1	C	16	ARG	3.0
1	B	271	GLY	3.0
1	B	268	ILE	3.0
2	D	372	ASN	2.9
1	B	326	GLU	2.8
1	A	24	ARG	2.8
1	A	274	PHE	2.7
1	A	6	LEU	2.7
1	C	13	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	298	ARG	2.6
1	A	592	ASN	2.6
1	C	275	HIS	2.6
1	B	267	PRO	2.6
1	A	17	ILE	2.5
1	A	160	ARG	2.5
1	A	623	GLU	2.5
1	C	323	ARG	2.5
1	B	299	GLY	2.4
1	C	325	VAL	2.4
1	B	16	ARG	2.4
1	C	160	ARG	2.4
1	A	268	ILE	2.4
1	B	623	GLU	2.4
1	A	295	GLY	2.3
1	B	266	SER	2.3
1	B	160	ARG	2.3
1	C	623	GLU	2.3
2	E	368	ASP	2.2
1	C	326	GLU	2.2
1	B	18	ASN	2.2
1	B	13	SER	2.2
1	A	272	GLU	2.1
2	E	364	GLU	2.1
1	A	161	VAL	2.1
1	C	24	ARG	2.1
2	D	362	ASP	2.0
1	B	300	GLY	2.0
1	A	251	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.