Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:31 PM GMT

PDB ID	:	1PFR
Title	:	RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 BETA CHAIN
Authors	:	Logan, D.T.; Su, X.D.; Aberg, A.; Regnstrom, K.; Hajdu, J.; Eklund, H.; Nordlund, P.
Deposited on	:	1996-12-03
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 (i) symbol.

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

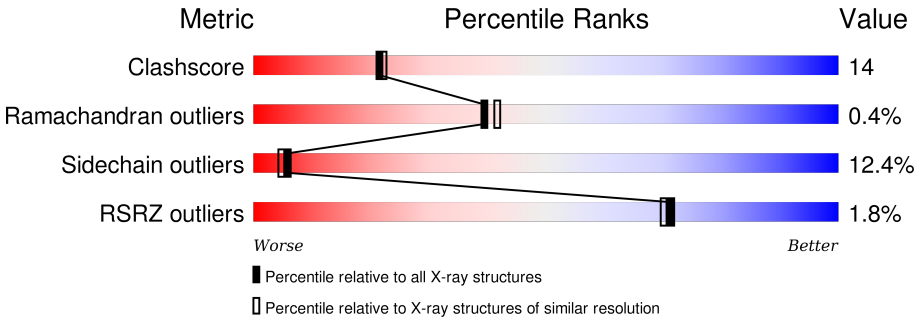
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 <=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	340	3% 66% 27% 6%
1	B	340	% 68% 26% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HG	B	607	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5807 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 R2 OF RIBONUCLEOTIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2788	1784	464	527	13			
1	B	340	Total	C	N	O	S	0	0	0
			2788	1784	464	527	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	ALA	SER	ENGINEERED	UNP P69924
B	211	ALA	SER	ENGINEERED	UNP P69924

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		

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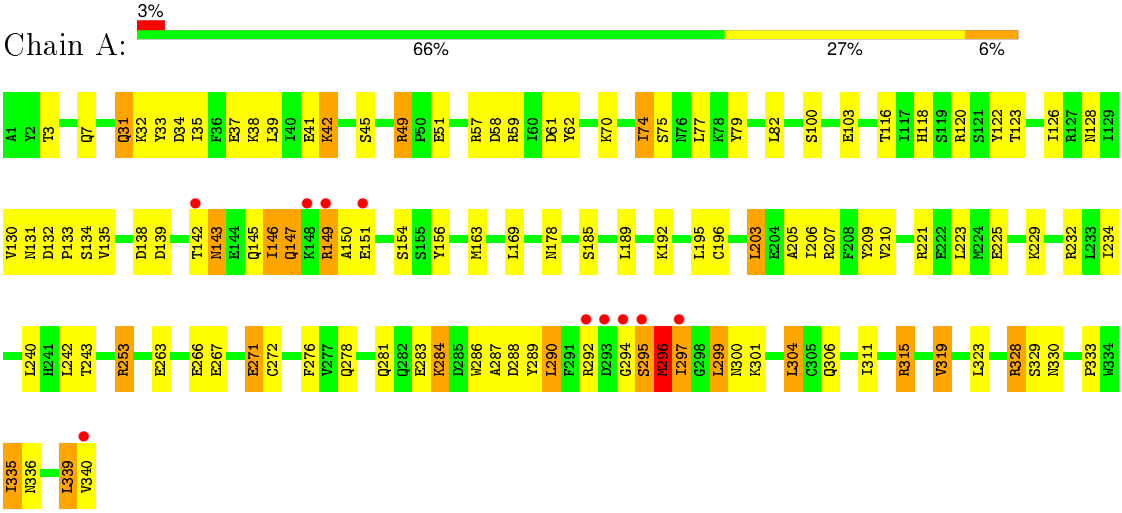
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	107	Total	O	0	0
			107	107		

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 errors 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.

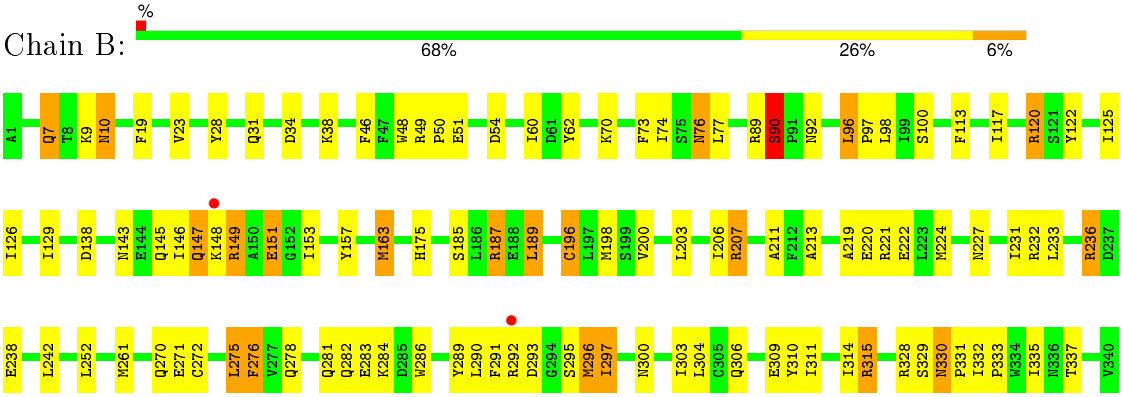
- Molecule 1: PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE

Chain A:



- Molecule 1: PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE

Chain B:



4 Data and refinement statistics (i)

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)	15.00 – 2.20 16.82 – 2.18	Depositor EDS
% Data completeness (in resolution range)	89.0 (15.00-2.20) 87.9 (16.82-2.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.18Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.179 , (Not available) 0.173 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 87.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 34219 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5807	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FE, HG

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	0.71	2/2852 (0.1%)	1.14	7/3868 (0.2%)
1	B	0.65	0/2852	1.17	9/3868 (0.2%)
All	All	0.68	2/5704 (0.0%)	1.16	16/7736 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	MET	CG-SD	-11.88	1.50	1.81
1	A	297	ILE	C-O	7.94	1.38	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	VAL	CG1-CB-CG2	7.92	123.57	110.90
1	A	58	ASP	CB-CG-OD1	7.87	125.38	118.30
1	B	236	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	207	ARG	NE-CZ-NH1	-7.13	116.74	120.30
1	B	232	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	304	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	A	299	LEU	CA-CB-CG	6.17	129.50	115.30
1	B	23	VAL	CB-CA-C	-6.16	99.70	111.40
1	B	138	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	319	VAL	CA-CB-CG2	5.63	119.35	110.90
1	B	296	MET	N-CA-C	-5.62	95.83	111.00
1	B	90	SER	N-CA-C	5.51	125.88	111.00
1	A	284	LYS	CD-CE-NZ	-5.20	99.73	111.70
1	B	315	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	187	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	169	LEU	CB-CG-CD1	-5.05	102.41	111.00

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	2788	0	2733	87	0
1	B	2788	0	2731	73	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
4	A	112	0	0	4	0
4	B	107	0	0	2	0
All	All	5807	0	5464	153	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 14.

All (153) 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:221:ARG:HH21	1:B:296:MET:HE3	1.08	1.09
1:A:205:ALA:HB1	1:A:315:ARG:HG2	1.42	1.01
1:A:163:MET:HE2	1:A:189:LEU:HD13	1.59	0.85
1:B:163:MET:HE2	1:B:189:LEU:HG	1.56	0.85
1:A:205:ALA:HB1	1:A:315:ARG:CG	2.11	0.79
1:B:221:ARG:NH2	1:B:296:MET:HE3	1.94	0.78
1:A:32:LYS:HD3	1:A:33:TYR:CE2	2.20	0.77
1:A:132:ASP:O	1:A:135:VAL:HG22	1.85	0.76
1:A:178:ASN:HD21	1:B:175:HIS:HD2	1.35	0.74
1:A:205:ALA:CB	1:A:315:ARG:HG2	2.16	0.74
1:B:292:ARG:HG2	1:B:293:ASP:N	2.02	0.74
1:A:306:GLN:HG2	1:A:328:ARG:HH21	1.51	0.74
1:B:291:PHE:HD2	1:B:295:SER:HA	1.52	0.72
1:A:203:LEU:HA	1:A:207:ARG:HG3	1.70	0.72
1:B:227:ASN:O	1:B:231:ILE:HG12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:CG	1:B:146:ILE:HD12	2.10	0.71
1:A:300:ASN:O	1:A:304:LEU:HD13	1.91	0.69
1:A:178:ASN:HD21	1:B:175:HIS:CD2	2.10	0.69
1:A:163:MET:HE3	4:A:701:HOH:O	1.92	0.69
1:B:46:PHE:CD2	1:B:236:ARG:HD3	2.29	0.68
1:A:130:VAL:HG12	1:A:132:ASP:H	1.59	0.67
1:B:221:ARG:HH21	1:B:296:MET:CE	1.96	0.66
1:B:311:ILE:O	1:B:315:ARG:HG2	1.96	0.66
1:A:145:GLN:O	1:A:149:ARG:HG3	1.96	0.65
1:B:330:ASN:ND2	1:B:332:ILE:H	1.93	0.65
1:B:291:PHE:CD2	1:B:295:SER:HA	2.33	0.63
1:A:323:LEU:HD23	1:A:323:LEU:N	2.13	0.63
1:A:139:ASP:O	1:A:143:ASN:HB2	1.99	0.62
1:B:19:PHE:CE1	1:B:98:LEU:HD22	2.33	0.62
1:A:263:GLU:O	1:A:267:GLU:HG2	2.00	0.62
1:B:49:ARG:HB3	1:B:51:GLU:OE1	2.02	0.59
1:A:253:ARG:NH1	1:A:266:GLU:HG2	2.18	0.59
1:B:275:LEU:HD12	1:B:275:LEU:C	2.22	0.59
1:A:205:ALA:CB	1:A:206:ILE:HD12	2.33	0.58
1:A:74:ILE:HG22	1:A:75:SER:N	2.18	0.58
1:A:130:VAL:HG13	4:A:693:HOH:O	2.04	0.57
1:A:62:TYR:CZ	1:A:70:LYS:HG2	2.40	0.57
1:B:46:PHE:CE2	1:B:236:ARG:HD3	2.40	0.57
1:B:77:LEU:HD13	4:B:665:HOH:O	2.04	0.57
1:A:221:ARG:HB2	1:A:223:LEU:HD12	1.87	0.57
1:A:287:ALA:CB	1:A:304:LEU:HD23	2.34	0.56
1:B:330:ASN:HD22	1:B:331:PRO:N	2.03	0.56
1:A:288:ASP:O	1:A:289:TYR:C	2.42	0.56
1:B:76:ASN:HD21	1:B:211:ALA:HA	1.71	0.56
1:A:116:THR:O	1:A:120:ARG:HG3	2.06	0.56
1:B:149:ARG:NH1	1:B:149:ARG:HG2	2.22	0.54
1:B:10:ASN:H	1:B:10:ASN:HD22	1.55	0.54
1:A:296:MET:HG2	1:A:297:ILE:H	1.72	0.54
1:B:207:ARG:HH22	1:B:282:GLN:NE2	2.06	0.54
1:B:309:GLU:OE1	1:B:328:ARG:NH2	2.41	0.54
1:B:196:CYS:O	1:B:200:VAL:HG23	2.08	0.54
1:A:205:ALA:HA	1:A:242:LEU:HD12	1.90	0.53
1:A:31:GLN:HG3	1:A:34:ASP:HA	1.90	0.53
1:A:122:TYR:O	1:A:126:ILE:HG13	2.09	0.53
1:A:39:LEU:HD22	1:A:240:LEU:HD22	1.91	0.52
1:B:300:ASN:ND2	1:B:303:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HH12	1:A:266:GLU:HG2	1.74	0.52
1:B:207:ARG:HH22	1:B:282:GLN:HE22	1.57	0.52
1:A:330:ASN:ND2	1:A:333:PRO:HA	2.25	0.52
1:B:149:ARG:O	1:B:153:ILE:HD12	2.10	0.51
1:A:196:CYS:HG	3:A:603:HG:HG	1.53	0.51
1:A:49:ARG:HD2	1:A:51:GLU:OE1	2.10	0.51
1:A:149:ARG:NE	1:A:149:ARG:O	2.43	0.51
1:A:163:MET:HB3	1:A:189:LEU:HD13	1.91	0.51
1:A:292:ARG:C	1:A:294:GLY:H	2.14	0.51
1:B:149:ARG:NH2	1:B:286:TRP:CE3	2.79	0.51
1:A:134:SER:O	1:A:138:ASP:HB2	2.11	0.51
1:A:163:MET:HE2	1:A:189:LEU:CD1	2.37	0.50
1:A:149:ARG:NH1	1:A:286:TRP:CD2	2.80	0.50
1:B:34:ASP:OD2	1:B:38:LYS:HE3	2.11	0.50
1:B:332:ILE:N	1:B:333:PRO:HD3	2.25	0.50
1:A:123:THR:HG21	1:B:28:TYR:HB2	1.94	0.50
1:B:283:GLU:O	1:B:286:TRP:HB3	2.11	0.50
1:A:242:LEU:C	1:A:242:LEU:HD23	2.32	0.50
1:A:340:VAL:HG12	1:A:340:VAL:OXT	2.12	0.50
1:A:242:LEU:HD23	1:A:243:THR:N	2.27	0.49
1:A:209:TYR:N	1:A:209:TYR:CD1	2.80	0.49
1:B:236:ARG:HD2	4:B:613:HOH:O	2.12	0.49
1:B:221:ARG:HD3	1:B:297:ILE:CG1	2.43	0.49
1:A:79:TYR:CD2	1:A:149:ARG:NH1	2.81	0.49
1:B:252:LEU:HD22	1:B:261:MET:HG3	1.93	0.49
1:B:300:ASN:CG	1:B:303:ILE:HD12	2.33	0.48
1:B:213:ALA:HA	1:B:335:ILE:HD11	1.94	0.48
1:A:263:GLU:HB3	4:A:684:HOH:O	2.13	0.48
1:B:289:TYR:O	1:B:292:ARG:HD3	2.13	0.48
1:A:62:TYR:CE1	1:A:70:LYS:HG2	2.49	0.48
1:A:225:GLU:O	1:A:229:LYS:HG3	2.13	0.48
1:B:50:PRO:HG2	1:B:120:ARG:HG2	1.95	0.48
1:B:206:ILE:HD12	1:B:276:PHE:HE1	1.79	0.48
1:B:96:LEU:CB	1:B:97:PRO:HD3	2.44	0.47
1:A:163:MET:HB3	1:A:163:MET:HE2	1.86	0.47
1:A:205:ALA:HB1	1:A:315:ARG:CD	2.43	0.47
1:A:130:VAL:CG1	1:A:132:ASP:H	2.25	0.47
1:A:147:GLN:HE21	1:B:7:GLN:HG3	1.80	0.47
1:B:221:ARG:HD3	1:B:297:ILE:HG12	1.96	0.47
1:B:113:PHE:CZ	1:B:117:ILE:HD11	2.51	0.46
1:B:310:TYR:CZ	1:B:330:ASN:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:HD23	1:B:203:LEU:C	2.36	0.46
1:A:147:GLN:CG	1:B:7:GLN:HE21	2.29	0.46
1:A:203:LEU:HD12	1:A:203:LEU:C	2.37	0.45
1:A:3:THR:HG23	1:A:3:THR:O	2.16	0.45
1:A:205:ALA:C	1:A:206:ILE:HD12	2.37	0.45
1:B:125:ILE:HD13	1:B:227:ASN:OD1	2.16	0.45
1:A:146:ILE:HG22	1:A:147:GLN:N	2.31	0.45
1:A:271:GLU:O	1:A:272:CYS:C	2.55	0.45
1:A:339:LEU:HA	1:A:339:LEU:HD12	1.72	0.45
1:A:79:TYR:CZ	1:A:149:ARG:CZ	3.00	0.44
1:B:314:ILE:HG23	1:B:314:ILE:HD12	1.63	0.44
1:B:149:ARG:HH11	1:B:149:ARG:HG2	1.83	0.44
1:B:148:LYS:HA	1:B:151:GLU:OE1	2.17	0.44
1:A:205:ALA:HB1	1:A:315:ARG:HD3	2.00	0.44
1:A:57:ARG:NH1	1:A:61:ASP:OD1	2.50	0.44
1:A:287:ALA:HB1	1:A:304:LEU:CD2	2.48	0.44
1:A:205:ALA:HB3	1:A:206:ILE:HD12	1.99	0.43
1:A:335:ILE:HG23	1:A:336:ASN:N	2.32	0.43
1:A:253:ARG:O	1:A:253:ARG:HG3	2.18	0.43
1:A:59:ARG:HB2	1:A:128:ASN:O	2.19	0.43
1:B:221:ARG:O	1:B:222:GLU:HB2	2.19	0.43
1:A:32:LYS:N	1:A:103:GLU:OE2	2.49	0.43
1:B:10:ASN:HD22	1:B:10:ASN:N	2.17	0.43
1:B:62:TYR:O	1:B:70:LYS:HE3	2.19	0.43
1:B:303:ILE:O	1:B:306:GLN:HB2	2.19	0.43
1:B:48:TRP:CE2	1:B:233:LEU:HB3	2.54	0.43
1:A:288:ASP:O	1:A:290:LEU:N	2.51	0.42
1:A:149:ARG:NH2	1:A:283:GLU:OE2	2.53	0.42
1:B:206:ILE:CD1	1:B:276:PHE:HE1	2.32	0.42
1:A:79:TYR:CE2	1:A:149:ARG:NH2	2.87	0.42
1:B:73:PHE:CZ	1:B:224:MET:HE2	2.54	0.42
1:A:37:GLU:OE2	1:A:41:GLU:OE2	2.36	0.42
1:A:39:LEU:CD2	1:A:240:LEU:HD22	2.48	0.42
1:B:337:THR:HG22	1:B:337:THR:O	2.19	0.42
1:A:205:ALA:O	1:A:315:ARG:HD3	2.20	0.42
1:A:132:ASP:HA	1:A:133:PRO:HD2	1.93	0.42
1:A:178:ASN:ND2	1:B:175:HIS:HD2	2.11	0.41
1:A:42:LYS:HB3	1:A:240:LEU:HD11	2.03	0.41
1:B:89:ARG:HG3	1:B:90:SER:N	2.35	0.41
1:B:331:PRO:C	1:B:333:PRO:HD3	2.41	0.41
1:A:284:LYS:O	1:A:287:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HG2	1:B:293:ASP:H	1.79	0.41
1:B:286:TRP:O	1:B:289:TYR:HB3	2.21	0.41
1:B:92:ASN:O	1:B:96:LEU:HB2	2.21	0.41
1:A:118:HIS:CD2	1:A:234:ILE:HG12	2.56	0.41
1:A:138:ASP:O	1:B:9:LYS:NZ	2.54	0.41
1:A:156:TYR:HD2	4:A:636:HOH:O	2.05	0.41
1:B:149:ARG:HD3	1:B:149:ARG:N	2.37	0.40
1:B:145:GLN:HG3	1:B:289:TYR:CE1	2.56	0.40
1:A:79:TYR:HE1	1:A:150:ALA:HB2	1.86	0.40
1:B:122:TYR:O	1:B:126:ILE:HD12	2.22	0.40
1:B:198:MET:HG2	1:B:272:CYS:SG	2.62	0.40
1:A:287:ALA:CB	1:A:304:LEU:CD2	3.00	0.40
1:A:283:GLU:O	1:A:286:TRP:HB3	2.21	0.40
1:A:335:ILE:CG2	1:A:336:ASN:N	2.84	0.40
1:B:219:ALA:O	1:B:220:GLU:C	2.56	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	338/340 (99%)	320 (95%)	16 (5%)	2 (1%)	30	29
1	B	338/340 (99%)	327 (97%)	10 (3%)	1 (0%)	46	50
All	All	676/680 (99%)	647 (96%)	26 (4%)	3 (0%)	39	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	A	143	ASN
1	B	147	GLN

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	306/306 (100%)	265 (87%)	41 (13%)	5 4
1	B	306/306 (100%)	271 (89%)	35 (11%)	7 6
All	All	612/612 (100%)	536 (88%)	76 (12%)	6 5

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	31	GLN
1	A	35	ILE
1	A	38	LYS
1	A	42	LYS
1	A	45	SER
1	A	49	ARG
1	A	74	ILE
1	A	77	LEU
1	A	82	LEU
1	A	100	SER
1	A	131	ASN
1	A	142	THR
1	A	146	ILE
1	A	147	GLN
1	A	149	ARG
1	A	151	GLU
1	A	154	SER
1	A	185	SER
1	A	192	LYS
1	A	195	LEU
1	A	203	LEU
1	A	210	VAL
1	A	232	ARG
1	A	253	ARG
1	A	271	GLU
1	A	276	PHE

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Mol	Chain	Res	Type
1	A	278	GLN
1	A	281	GLN
1	A	290	LEU
1	A	295	SER
1	A	296	MET
1	A	299	LEU
1	A	301	LYS
1	A	311	ILE
1	A	315	ARG
1	A	319	VAL
1	A	328	ARG
1	A	329	SER
1	A	335	ILE
1	A	339	LEU
1	B	7	GLN
1	B	10	ASN
1	B	31	GLN
1	B	54	ASP
1	B	60	ILE
1	B	74	ILE
1	B	76	ASN
1	B	90	SER
1	B	96	LEU
1	B	100	SER
1	B	120	ARG
1	B	129	ILE
1	B	147	GLN
1	B	149	ARG
1	B	151	GLU
1	B	157	TYR
1	B	163	MET
1	B	185	SER
1	B	187	ARG
1	B	189	LEU
1	B	196	CYS
1	B	238	GLU
1	B	242	LEU
1	B	270	GLN
1	B	271	GLU
1	B	275	LEU
1	B	276	PHE
1	B	278	GLN

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Mol	Chain	Res	Type
1	B	281	GLN
1	B	284	LYS
1	B	290	LEU
1	B	297	ILE
1	B	304	LEU
1	B	329	SER
1	B	330	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	63	GLN
1	A	80	GLN
1	A	131	ASN
1	A	326	GLN
1	B	7	GLN
1	B	10	ASN
1	B	21	GLN
1	B	76	ASN
1	B	128	ASN
1	B	175	HIS
1	B	282	GLN
1	B	326	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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, 95^{th} 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	340/340 (100%)	-0.55	10 (2%) 55 54	10, 25, 55, 75	0
1	B	340/340 (100%)	-0.60	2 (0%) 90 90	9, 25, 56, 73	0
All	All	680/680 (100%)	-0.57	12 (1%) 71 70	9, 25, 56, 75	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	GLY	7.4
1	A	297	ILE	6.3
1	A	293	ASP	5.1
1	A	295	SER	4.2
1	A	340	VAL	4.2
1	A	292	ARG	3.9
1	A	149	ARG	3.2
1	A	148	LYS	3.1
1	B	148	LYS	2.2
1	A	142	THR	2.2
1	A	151	GLU	2.1
1	B	292	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	HG	B	607	1/1	0.98	0.18	2.48	18,18,18,18	1
3	HG	B	608	1/1	0.98	0.04	-2.13	20,20,20,20	1
2	FE	A	501	1/1	0.99	0.03	-2.54	33,33,33,33	0
2	FE	B	504	1/1	1.00	0.04	-2.98	26,26,26,26	0
2	FE	B	503	1/1	0.99	0.04	-3.13	26,26,26,26	0
2	FE	A	502	1/1	0.99	0.03	-3.34	33,33,33,33	0
3	HG	A	603	1/1	0.98	0.04	-3.34	31,31,31,31	1
3	HG	A	601	1/1	1.00	0.02	-3.50	33,33,33,33	0
3	HG	B	605	1/1	1.00	0.04	-4.12	38,38,38,38	0
3	HG	B	606	1/1	0.99	0.02	-4.56	25,25,25,25	1
3	HG	A	602	1/1	1.00	0.02	-6.59	37,37,37,37	0
3	HG	A	604	1/1	0.77	0.18	-	38,38,38,38	1

6.5 Other polymers

There are no such residues in this entry.