



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:38 PM UTC

PDB ID : 1PFR / pdb_00001pfr
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

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

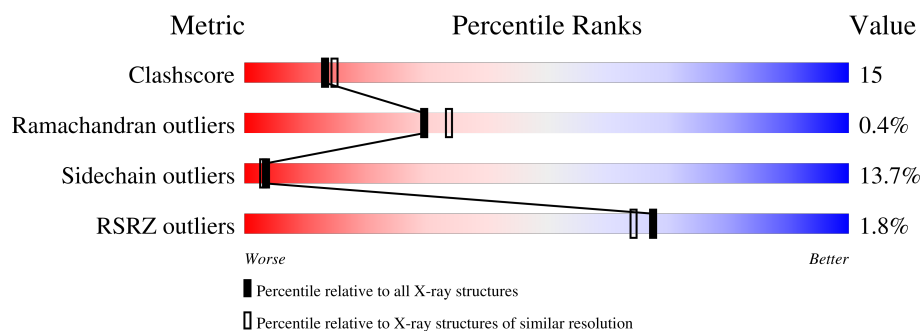
1 Overall quality at a glance

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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	340	3% 59% 31% 9% .
1	B	340	% 61% 31% 7% .

2 Entry composition [i](#)

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 mutation	UNP P69924
B	211	ALA	SER	engineered mutation	UNP P69924

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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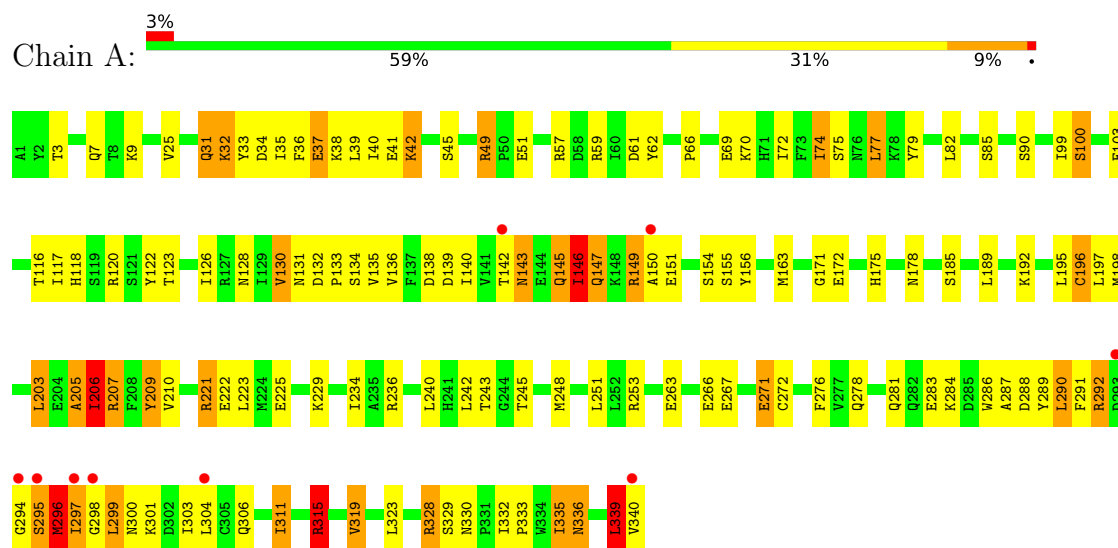
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	107	Total 107	O 107	0	0

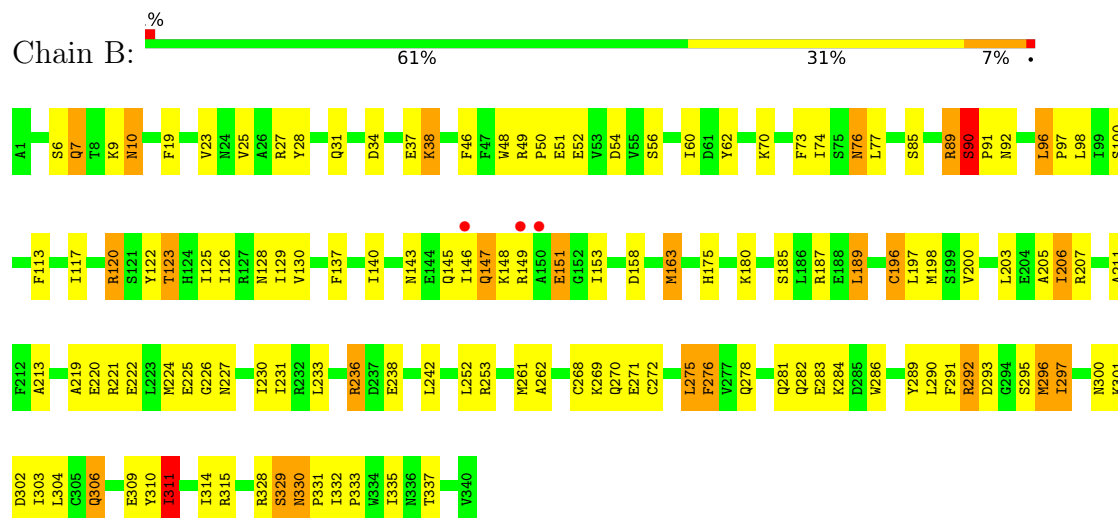
3 Residue-property plots

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: PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE



• Molecule 1: PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE



4 Data and refinement statistics

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 15.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (15.00-2.20) 88.3 (15.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.18Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.179 , (Not available) 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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: 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	0.90	3/2852 (0.1%)	1.49	42/3868 (1.1%)
1	B	0.82	0/2852	1.51	32/3868 (0.8%)
All	All	0.86	3/5704 (0.1%)	1.50	74/7736 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	MET	CG-SD	-12.20	1.50	1.80
1	A	297	ILE	C-O	12.07	1.38	1.24
1	A	299	LEU	N-CA	5.77	1.53	1.45

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	SER	N-CA-C	9.72	125.88	113.25
1	B	296	MET	N-CA-C	-9.41	95.83	110.42
1	A	339	LEU	N-CA-C	8.57	123.16	110.48
1	A	221	ARG	N-CA-C	-8.22	103.35	112.72
1	B	329	SER	N-CA-C	-7.96	99.05	110.59
1	A	140	ILE	N-CA-C	7.88	117.91	110.74
1	B	140	ILE	N-CA-C	-7.87	105.51	112.12
1	B	23	VAL	CB-CA-C	-7.80	99.70	111.33
1	A	209	TYR	N-CA-C	7.62	120.55	111.33
1	B	226	GLY	N-CA-C	-7.60	103.30	112.49
1	B	56	SER	N-CA-C	7.45	120.34	111.33
1	A	90	SER	N-CA-C	7.39	122.86	113.25
1	B	158	ASP	N-CA-C	7.30	118.88	111.07
1	A	207	ARG	N-CA-C	7.29	121.08	111.75
1	A	40	ILE	CB-CA-C	-7.15	102.66	112.02
1	A	32	LYS	N-CA-C	-7.12	102.93	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	SER	N-CA-C	-6.93	103.80	111.36
1	A	99	ILE	N-CA-C	6.81	118.47	109.21
1	B	205	ALA	N-CA-C	6.79	118.68	111.28
1	B	123	THR	N-CA-C	-6.70	103.45	111.69
1	A	117	ILE	N-CA-C	-6.67	104.02	110.42
1	A	298	GLY	O-C-N	-6.63	115.05	122.28
1	B	311	ILE	CB-CA-C	6.59	121.32	112.22
1	A	315	ARG	N-CA-C	6.59	118.46	111.28
1	B	292	ARG	N-CA-C	-6.49	103.70	111.69
1	A	85	SER	N-CA-C	-6.44	104.19	111.14
1	A	145	GLN	CA-C-N	-6.38	112.39	120.56
1	A	145	GLN	C-N-CA	-6.38	112.39	120.56
1	B	37	GLU	N-CA-C	-6.18	104.62	111.36
1	B	302	ASP	N-CA-C	6.15	117.98	111.28
1	A	25	VAL	CB-CA-C	-6.14	103.16	111.15
1	A	72	ILE	CB-CA-C	-6.09	103.81	112.22
1	A	311	ILE	N-CA-C	6.07	116.24	110.53
1	B	180	LYS	N-CA-C	6.01	119.62	109.76
1	A	196	CYS	N-CA-C	-5.81	104.86	111.14
1	B	23	VAL	N-CA-C	5.81	116.56	109.30
1	A	319	VAL	CG1-CB-CG2	5.80	123.57	110.80
1	B	230	ILE	CB-CA-C	-5.80	104.21	112.22
1	A	291	PHE	CB-CA-C	5.78	120.03	111.88
1	A	292	ARG	N-CA-C	5.70	122.93	110.80
1	B	137	PHE	N-CA-C	5.62	118.17	111.71
1	B	128	ASN	N-CA-C	5.61	119.99	113.20
1	A	37	GLU	N-CA-C	-5.56	104.85	111.69
1	A	100	SER	N-CA-C	5.55	120.76	112.94
1	A	155	SER	N-CA-C	5.55	117.77	111.11
1	B	52	GLU	N-CA-C	5.53	119.65	113.02
1	B	262	ALA	N-CA-C	-5.51	105.36	111.36
1	B	306	GLN	N-CA-C	-5.47	105.39	111.36
1	A	36	PHE	N-CA-C	5.46	117.99	111.71
1	B	225	GLU	N-CA-C	5.44	119.63	112.89
1	A	171	GLY	N-CA-C	-5.42	103.93	112.61
1	A	205	ALA	N-CA-C	5.40	118.33	111.69
1	A	303	ILE	N-CA-C	-5.38	105.25	110.42
1	A	206	ILE	N-CA-C	5.37	120.51	109.34
1	A	136	VAL	CB-CA-C	-5.33	105.06	112.04
1	A	336	ASN	N-CA-C	5.33	117.83	111.71
1	B	147	GLN	N-CA-C	5.31	122.11	110.80
1	A	90	SER	CA-C-O	5.28	123.49	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ILE	CB-CA-C	-5.27	105.12	112.02
1	A	236	ARG	CB-CG-CD	-5.26	99.19	111.30
1	A	319	VAL	CA-CB-CG2	5.26	119.35	110.40
1	B	206	ILE	N-CA-C	5.25	120.25	109.34
1	B	89	ARG	N-CA-C	5.22	119.55	112.04
1	A	77	LEU	N-CA-C	-5.18	105.53	111.07
1	B	253	ARG	CB-CA-C	-5.17	102.21	110.79
1	B	27	ARG	N-CA-C	-5.16	101.52	109.52
1	A	251	LEU	N-CA-C	-5.16	105.73	111.36
1	B	6	SER	N-CA-C	-5.14	102.68	110.28
1	B	130	VAL	N-CA-CB	5.12	118.17	112.34
1	A	172	GLU	N-CA-CB	-5.10	102.54	110.04
1	A	198	MET	N-CA-C	-5.08	105.92	111.82
1	A	222	GLU	N-CA-C	5.07	118.58	111.74
1	A	175	HIS	N-CA-CB	-5.05	103.40	111.43
1	B	268	CYS	N-CA-C	5.04	119.27	113.18

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	2788	0	2733	88	0
1	B	2788	0	2731	79	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	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 15.

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:205:ALA:HB1	1:A:315:ARG:HG2	1.42	1.01
1:A:163:MET:HE2	1:A:189:LEU:HD13	1.58	0.84
1:B:221:ARG:HH21	1:B:296:MET:HE3	1.43	0.83
1:B:163:MET:HE2	1:B:189:LEU:HG	1.62	0.80
1:A:205:ALA:HB1	1:A:315:ARG:CG	2.11	0.79
1:B:221:ARG:HH21	1:B:296:MET:CE	1.96	0.77
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:B:143:ASN:CG	1:B:146:ILE:HD12	2.10	0.75
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
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: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: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:275:LEU:C	1:B:275:LEU:HD12	2.22	0.63
1:A:323:LEU:N	1:A:323:LEU:HD23	2.13	0.63
1:B:291:PHE:CD2	1:B:295:SER:HA	2.33	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:A:288:ASP:O	1:A:289:TYR:C	2.42	0.61
1:B:221:ARG:NH2	1:B:296:MET:HE3	2.13	0.60
1:A:163:MET:HE3	4:A:701:HOH:O	2.03	0.59
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:296:MET:HE2	1:B:297:ILE:O	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:116:THR:O	1:A:120:ARG:HG3	2.06	0.56
1:B:76:ASN:HD21	1:B:211:ALA:HA	1.71	0.56
1:A:242:LEU:C	1:A:242:LEU:HD23	2.32	0.55
1:A:292:ARG:C	1:A:294:GLY:H	2.14	0.55
1:B:10:ASN:H	1:B:10:ASN:HD22	1.55	0.54
1:B:149:ARG:NH1	1:B:149:ARG:HG2	2.22	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:B:300:ASN:CG	1:B:303:ILE:HD12	2.33	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
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:B:203:LEU:HD23	1:B:203:LEU:C	2.36	0.51
1:A:49:ARG:HD2	1:A:51:GLU:OE1	2.10	0.51
1:A:149:ARG:O	1:A:149:ARG:NE	2.43	0.51
1:A:163:MET:HB3	1:A:189:LEU:HD13	1.91	0.51
1:A:134:SER:O	1:A:138:ASP:HB2	2.11	0.51
1:B:149:ARG:NH2	1:B:286:TRP:CE3	2.79	0.51
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:203:LEU:C	1:A:203:LEU:HD12	2.37	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: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:271:GLU:O	1:A:272:CYS:C	2.55	0.49
1:A:209:TYR:CD1	1:A:209:TYR:N	2.80	0.49
1:A:205:ALA:C	1:A:206:ILE:HD12	2.37	0.49
1:B:236:ARG:HD2	4:B:613:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:130:VAL:CG1	1:A:132:ASP:H	2.25	0.47
1:A:205:ALA:HB1	1:A:315:ARG:CD	2.43	0.47
1:B:73:PHE:CZ	1:B:224:MET:HE2	2.49	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:A:245:THR:HA	1:A:248:MET:HE3	1.96	0.46
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
1:B:331:PRO:C	1:B:333:PRO:HD3	2.41	0.46
1:A:147:GLN:CG	1:B:7:GLN:HE21	2.29	0.46
1:B:296:MET:HE3	1:B:296:MET:HB2	1.63	0.45
1:A:3:THR:HG23	1:A:3:THR:O	2.16	0.45
1:B:125:ILE:HD13	1:B:227:ASN:OD1	2.16	0.45
1:B:219:ALA:O	1:B:220:GLU:C	2.56	0.45
1:A:339:LEU:HD12	1:A:339:LEU:HA	1.72	0.45
1:A:79:TYR:CZ	1:A:149:ARG:CZ	3.00	0.44
1:A:196:CYS:HG	3:A:603:HG:HG	1.60	0.44
1:B:314:ILE:HD12	1:B:314:ILE:HG23	1.63	0.44
1:B:148:LYS:HA	1:B:151:GLU:OE1	2.17	0.44
1:B:149:ARG:HG2	1:B:149:ARG:HH11	1.83	0.44
1:B:330:ASN:HD22	1:B:330:ASN:C	2.26	0.44
1:A:57:ARG:NH1	1:A:61:ASP:OD1	2.50	0.44
1:A:205:ALA:HB1	1:A:315:ARG:HD3	2.00	0.44
1:A:146:ILE:HG22	1:A:147:GLN:N	2.31	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:59:ARG:HB2	1:A:128:ASN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TYR:O	1:B:70:LYS:HE3	2.19	0.43
1:B:48:TRP:CE2	1:B:233:LEU:HB3	2.54	0.43
1:B:303:ILE:O	1:B:306:GLN:HB2	2.19	0.43
1:A:288:ASP:O	1:A:290:LEU:N	2.51	0.42
1:B:221:ARG:O	1:B:222:GLU:HB2	2.19	0.42
1:B:221:ARG:HH21	1:B:296:MET:HE1	1.79	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: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:51:GLU:H	1:B:51:GLU:CD	2.28	0.42
1:B:337:THR:O	1:B:337:THR:HG22	2.19	0.42
1:A:132:ASP:HA	1:A:133:PRO:HD2	1.93	0.42
1:A:205:ALA:O	1:A:315:ARG:HD3	2.20	0.42
1:A:253:ARG:O	1:A:253:ARG:HG3	2.18	0.41
1:A:66:PRO:HG2	1:A:69:GLU:CD	2.45	0.41
1:A:143:ASN:CG	1:A:146:ILE:HD12	2.45	0.41
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:A:284:LYS:O	1:A:287:ALA:HB3	2.21	0.41
1:B:90:SER:O	1:B:91:PRO:C	2.62	0.41
1:B:292:ARG:HG2	1:B:293:ASP:H	1.79	0.41
1:A:118:HIS:CD2	1:A:234:ILE:HG12	2.56	0.41
1:B:92:ASN:O	1:B:96:LEU:HB2	2.21	0.41
1:B:286:TRP:O	1:B:289:TYR:HB3	2.21	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:N	1:B:149:ARG:HD3	2.37	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:145:GLN:HG3	1:B:289:TYR:CE1	2.56	0.40
1:B:198:MET:HG2	1:B:272:CYS:SG	2.62	0.40
1:A:283:GLU:O	1:A:286:TRP:HB3	2.21	0.40
1:A:287:ALA:CB	1:A:304:LEU:CD2	3.00	0.40
1:A:335:ILE:CG2	1:A:336:ASN:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	21	23
1	B	338/340 (99%)	327 (97%)	10 (3%)	1 (0%)	36	42
All	All	676/680 (99%)	647 (96%)	26 (4%)	3 (0%)	30	34

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

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%)	262 (86%)	44 (14%)	3	2
1	B	306/306 (100%)	266 (87%)	40 (13%)	4	3
All	All	612/612 (100%)	528 (86%)	84 (14%)	3	3

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	9	LYS
1	A	31	GLN

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Mol	Chain	Res	Type
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	130	VAL
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	197	LEU
1	A	203	LEU
1	A	206	ILE
1	A	210	VAL
1	A	271	GLU
1	A	276	PHE
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	332	ILE
1	A	335	ILE
1	A	339	LEU
1	B	7	GLN

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Mol	Chain	Res	Type
1	B	10	ASN
1	B	25	VAL
1	B	31	GLN
1	B	38	LYS
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	123	THR
1	B	129	ILE
1	B	151	GLU
1	B	163	MET
1	B	185	SER
1	B	187	ARG
1	B	189	LEU
1	B	196	CYS
1	B	197	LEU
1	B	236	ARG
1	B	238	GLU
1	B	242	LEU
1	B	269	LYS
1	B	270	GLN
1	B	271	GLU
1	B	275	LEU
1	B	276	PHE
1	B	278	GLN
1	B	281	GLN
1	B	284	LYS
1	B	290	LEU
1	B	297	ILE
1	B	301	LYS
1	B	304	LEU
1	B	311	ILE
1	B	329	SER
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	7	GLN
1	A	63	GLN
1	A	80	GLN
1	A	131	ASN
1	A	168	HIS
1	A	227	ASN
1	A	306	GLN
1	A	326	GLN
1	B	7	GLN
1	B	10	ASN
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 [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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	340/340 (100%)	-0.34	9 (2%) 57 54	10, 25, 55, 75	0
1	B	340/340 (100%)	-0.38	3 (0%) 81 79	9, 25, 56, 73	0
All	All	680/680 (100%)	-0.36	12 (1%) 67 64	9, 25, 56, 75	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	SER	4.4
1	A	297	ILE	3.6
1	A	293	ASP	3.5
1	A	142	THR	2.9
1	B	149	ARG	2.8
1	A	294	GLY	2.7
1	A	340	VAL	2.4
1	A	150	ALA	2.3
1	B	150	ALA	2.3
1	B	146	ILE	2.1
1	A	298	GLY	2.1
1	A	304	LEU	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 oligosaccharides 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
3	HG	A	604	1/1	0.81	0.21	38,38,38,38	1
3	HG	B	608	1/1	0.96	0.04	20,20,20,20	1
3	HG	B	607	1/1	0.98	0.13	18,18,18,18	1
2	FE	A	501	1/1	0.99	0.07	33,33,33,33	0
2	FE	B	503	1/1	0.99	0.02	26,26,26,26	0
3	HG	A	603	1/1	0.99	0.04	31,31,31,31	1
2	FE	A	502	1/1	1.00	0.05	33,33,33,33	0
2	FE	B	504	1/1	1.00	0.01	26,26,26,26	0
3	HG	B	605	1/1	1.00	0.02	38,38,38,38	0
3	HG	B	606	1/1	1.00	0.03	25,25,25,25	1
3	HG	A	601	1/1	1.00	0.02	33,33,33,33	0
3	HG	A	602	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.