



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:41 AM UTC

PDB ID : 1PEM / pdb_00001pem
Title : Ribonucleotide Reductase Protein R1E from Salmonella typhimurium
Authors : Uppsten, M.; Farnegardh, M.; Jordan, A.; Eliasson, R.; Eklund, H.; Uhlin, U.
Deposited on : 2003-05-22
Resolution : 2.99 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

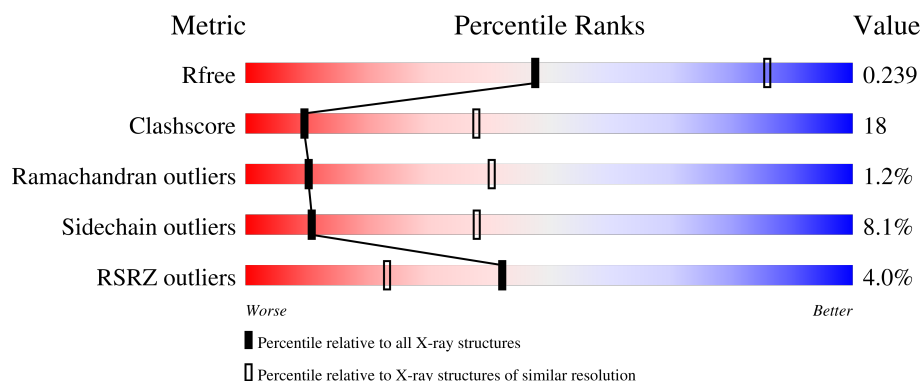
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	714	4% 61% 28% 5% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5447 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.

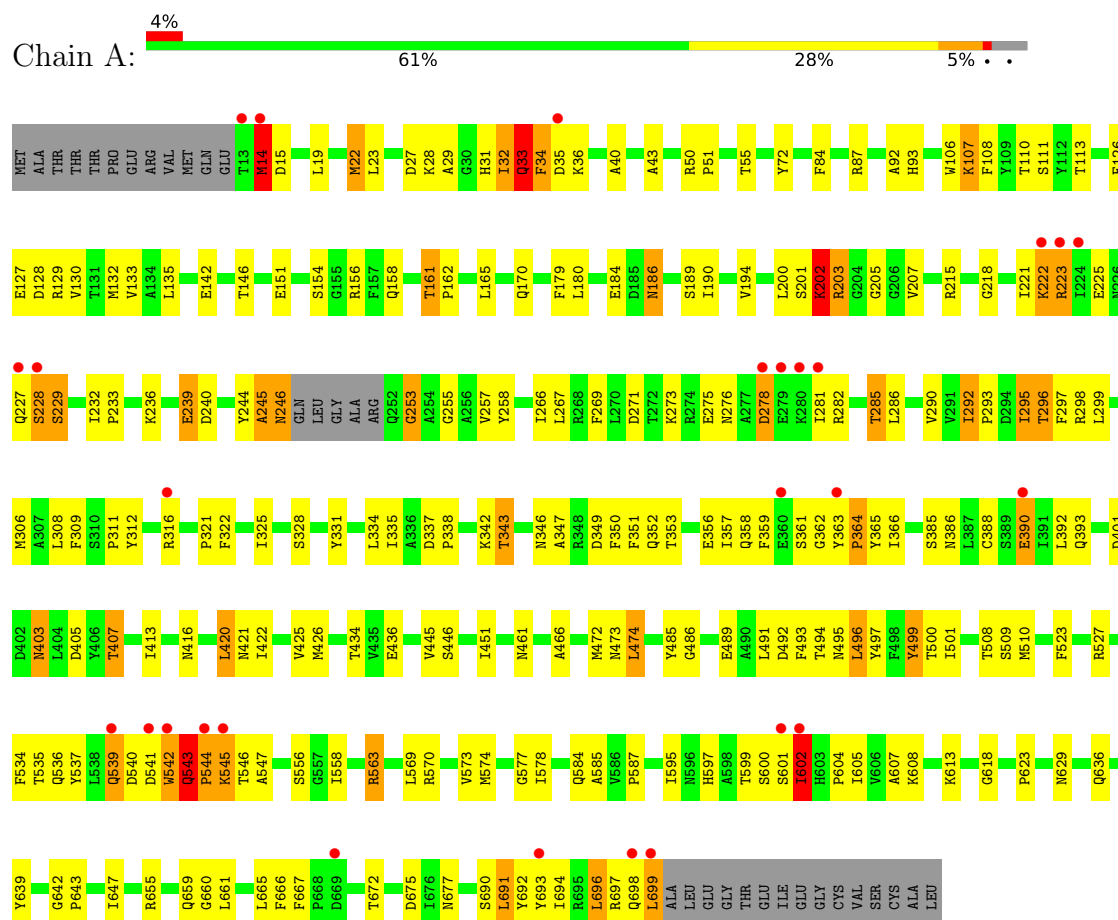
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	682	5447	3454	960	1011	22	0	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: Ribonucleoside-diphosphate reductase 2 alpha chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.08Å 99.08Å 290.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.99 19.96 – 2.99	Depositor EDS
% Data completeness (in resolution range)	20.0 (19.96-2.99) 99.4 (19.96-2.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.57 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.218 , 0.243 0.214 , 0.239	Depositor DCC
R_{free} test set	1518 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5447	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

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	0.93	7/5572 (0.1%)	1.24	39/7544 (0.5%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	ASP	N-CA	9.14	1.58	1.46
1	A	239	GLU	C-N	-7.43	1.23	1.33
1	A	544	PRO	CA-C	-7.08	1.44	1.52
1	A	540	ASP	CA-C	6.11	1.61	1.53
1	A	545	LYS	N-CA	-5.95	1.39	1.46
1	A	292	ILE	CA-CB	-5.84	1.50	1.54
1	A	597	HIS	CA-C	-5.42	1.48	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ILE	N-CA-C	13.65	124.15	111.45
1	A	540	ASP	N-CA-C	-13.53	89.75	110.17
1	A	540	ASP	CA-C-N	12.86	144.86	121.70
1	A	540	ASP	C-N-CA	12.86	144.86	121.70
1	A	15	ASP	N-CA-C	11.89	127.66	108.63
1	A	543	GLN	N-CA-C	9.62	124.06	110.20
1	A	540	ASP	CA-C-O	-9.34	109.74	121.88
1	A	540	ASP	O-C-N	-9.30	110.72	122.43
1	A	545	LYS	N-CA-C	-9.08	101.46	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	N-CA-C	8.68	122.86	111.75
1	A	542	TRP	CA-CB-CG	-8.11	98.19	113.60
1	A	362	GLY	N-CA-C	-7.75	104.60	114.37
1	A	33	GLN	CA-C-N	7.68	130.91	120.38
1	A	33	GLN	C-N-CA	7.68	130.91	120.38
1	A	694	ILE	N-CA-C	-7.62	94.43	107.24
1	A	539	GLN	N-CA-C	-7.56	99.62	110.59
1	A	544	PRO	CA-C-O	6.91	128.53	121.27
1	A	281	ILE	N-CA-C	-6.84	95.11	109.34
1	A	642	GLY	CA-C-N	6.57	126.51	119.28
1	A	642	GLY	C-N-CA	6.57	126.51	119.28
1	A	696	LEU	N-CA-C	-6.50	100.28	110.36
1	A	542	TRP	N-CA-C	6.14	123.89	110.80
1	A	278	ASP	N-CA-C	6.08	118.91	109.60
1	A	540	ASP	CB-CA-C	5.98	123.57	111.60
1	A	407	THR	N-CA-C	-5.89	106.13	113.55
1	A	228	SER	N-CA-C	-5.70	98.67	110.80
1	A	499	TYR	N-CA-C	-5.62	105.16	111.28
1	A	15	ASP	N-CA-CB	-5.61	101.02	109.88
1	A	445	VAL	N-CA-C	-5.48	105.18	110.72
1	A	14	MET	N-CA-C	5.39	122.28	110.80
1	A	194	VAL	N-CA-C	-5.39	105.12	110.62
1	A	608	LYS	N-CA-C	-5.26	104.98	111.40
1	A	364	PRO	CB-CA-C	-5.21	98.99	112.00
1	A	34	PHE	N-CA-C	5.20	117.62	111.33
1	A	276	ASN	N-CA-C	5.14	119.42	113.20
1	A	92	ALA	N-CA-C	-5.04	105.43	111.03
1	A	158	GLN	O-C-N	5.04	124.29	121.27
1	A	146	THR	N-CA-C	-5.02	105.89	111.36
1	A	285	THR	N-CA-C	5.00	119.25	112.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	MET	Peptide

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	5447	0	5332	191	0
All	All	5447	0	5332	191	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 18.

All (191) 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:542:TRP:CE3	1:A:542:TRP:HA	1.71	1.10
1:A:392:LEU:HD12	1:A:659:GLN:O	1.67	0.94
1:A:542:TRP:HA	1:A:542:TRP:HE3	1.16	0.93
1:A:273:LYS:NZ	1:A:363:TYR:CE1	2.41	0.89
1:A:363:TYR:HB3	1:A:364:PRO:HA	1.54	0.87
1:A:542:TRP:CE3	1:A:542:TRP:CA	2.58	0.86
1:A:358:GLN:HA	1:A:363:TYR:O	1.78	0.83
1:A:179:PHE:C	1:A:180:LEU:HD12	2.05	0.81
1:A:602:ILE:CG1	1:A:602:ILE:O	2.29	0.81
1:A:295:ILE:HG12	1:A:296:THR:N	1.96	0.79
1:A:605:ILE:HD12	1:A:607:ALA:O	1.82	0.79
1:A:229:SER:HB2	1:A:233:PRO:HG2	1.63	0.79
1:A:543:GLN:HB3	1:A:544:PRO:HD3	1.63	0.79
1:A:543:GLN:HB3	1:A:544:PRO:CD	2.14	0.77
1:A:232:ILE:HB	1:A:233:PRO:HD3	1.67	0.77
1:A:535:THR:O	1:A:539:GLN:HG2	1.89	0.73
1:A:495:ASN:HD21	1:A:542:TRP:HZ3	1.37	0.72
1:A:584:GLN:O	1:A:659:GLN:HB2	1.90	0.71
1:A:202:LYS:HG2	1:A:202:LYS:O	1.91	0.71
1:A:699:LEU:H	1:A:699:LEU:CD1	2.03	0.70
1:A:543:GLN:CB	1:A:544:PRO:CD	2.69	0.70
1:A:485:TYR:CZ	1:A:604:PRO:HD3	2.26	0.70
1:A:403:ASN:HD22	1:A:403:ASN:N	1.91	0.69
1:A:602:ILE:O	1:A:602:ILE:HG13	1.91	0.69
1:A:474:LEU:HB3	1:A:602:ILE:HA	1.75	0.69
1:A:295:ILE:CG1	1:A:296:THR:N	2.54	0.68
1:A:273:LYS:NZ	1:A:363:TYR:CD1	2.62	0.68
1:A:496:LEU:HD11	1:A:542:TRP:O	1.95	0.67
1:A:180:LEU:HD12	1:A:180:LEU:N	2.11	0.65
1:A:23:LEU:CD1	1:A:623:PRO:HD3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:THR:HG22	1:A:547:ALA:H	1.62	0.64
1:A:31:HIS:HB3	1:A:629:ASN:OD1	1.99	0.63
1:A:295:ILE:O	1:A:298:ARG:N	2.31	0.63
1:A:353:THR:O	1:A:357:ILE:HG12	1.99	0.62
1:A:699:LEU:CD1	1:A:699:LEU:N	2.61	0.62
1:A:14:MET:HE1	1:A:43:ALA:HA	1.79	0.62
1:A:126:PHE:O	1:A:130:VAL:HG23	1.99	0.62
1:A:699:LEU:N	1:A:699:LEU:HD12	2.15	0.62
1:A:346:ASN:ND2	1:A:349:ASP:OD1	2.32	0.61
1:A:72:TYR:CD1	1:A:132:MET:HE2	2.34	0.61
1:A:293:PRO:HG2	1:A:296:THR:HG22	1.82	0.61
1:A:492:ASP:OD1	1:A:545:LYS:HE3	2.01	0.61
1:A:50:ARG:HB2	1:A:51:PRO:HD3	1.82	0.61
1:A:541:ASP:O	1:A:541:ASP:CG	2.44	0.61
1:A:546:THR:HG22	1:A:547:ALA:N	2.16	0.60
1:A:403:ASN:ND2	1:A:405:ASP:H	1.99	0.60
1:A:643:PRO:O	1:A:647:ILE:HG13	2.01	0.60
1:A:108:PHE:CE1	1:A:113:THR:HB	2.37	0.60
1:A:386:ASN:ND2	1:A:388:CYS:H	2.00	0.59
1:A:363:TYR:CE2	1:A:693:TYR:HE2	2.21	0.59
1:A:308:LEU:HB2	1:A:343:THR:HG23	1.83	0.59
1:A:331:TYR:O	1:A:335:ILE:HG13	2.02	0.59
1:A:639:TYR:CE2	1:A:666:PHE:HB3	2.38	0.58
1:A:401:ASP:HB3	1:A:403:ASN:HD21	1.68	0.58
1:A:537:TYR:HA	1:A:542:TRP:HE1	1.69	0.58
1:A:186:ASN:ND2	1:A:189:SER:H	2.02	0.58
1:A:202:LYS:O	1:A:202:LYS:CG	2.52	0.57
1:A:523:PHE:CZ	1:A:577:GLY:HA2	2.39	0.57
1:A:309:PHE:CE2	1:A:334:LEU:HB3	2.40	0.57
1:A:295:ILE:O	1:A:297:PHE:N	2.37	0.57
1:A:273:LYS:NZ	1:A:363:TYR:HE1	1.97	0.56
1:A:697:ARG:HE	1:A:698:GLN:H	1.51	0.56
1:A:180:LEU:HB2	1:A:413:ILE:HB	1.87	0.56
1:A:31:HIS:CB	1:A:629:ASN:OD1	2.54	0.55
1:A:258:TYR:CZ	1:A:385:SER:HB3	2.42	0.55
1:A:358:GLN:CA	1:A:363:TYR:O	2.52	0.55
1:A:536:GLN:HE22	1:A:655:ARG:HG2	1.72	0.54
1:A:14:MET:CE	1:A:43:ALA:HA	2.37	0.54
1:A:295:ILE:O	1:A:296:THR:C	2.48	0.54
1:A:295:ILE:C	1:A:297:PHE:N	2.66	0.54
1:A:699:LEU:H	1:A:699:LEU:HD13	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASP:HB3	1:A:403:ASN:ND2	2.23	0.54
1:A:393:GLN:HB2	1:A:413:ILE:HD13	1.90	0.53
1:A:661:LEU:N	1:A:661:LEU:HD12	2.23	0.53
1:A:489:GLU:HG2	1:A:546:THR:HG21	1.90	0.53
1:A:496:LEU:O	1:A:499:TYR:HB3	2.09	0.53
1:A:543:GLN:CB	1:A:544:PRO:HD3	2.31	0.53
1:A:232:ILE:HB	1:A:233:PRO:CD	2.38	0.53
1:A:403:ASN:N	1:A:403:ASN:ND2	2.55	0.52
1:A:665:LEU:HD22	1:A:665:LEU:N	2.24	0.52
1:A:266:ILE:HG23	1:A:267:LEU:N	2.25	0.52
1:A:335:ILE:HA	1:A:342:LYS:HE2	1.91	0.52
1:A:556:SER:HB3	1:A:558:ILE:HG12	1.92	0.52
1:A:106:TRP:O	1:A:110:THR:OG1	2.28	0.52
1:A:295:ILE:HD12	1:A:331:TYR:CD2	2.45	0.52
1:A:351:PHE:HB3	1:A:677:ASN:HD21	1.74	0.51
1:A:570:ARG:HG2	1:A:574:MET:HE2	1.91	0.51
1:A:236:LYS:O	1:A:240:ASP:OD1	2.29	0.51
1:A:244:TYR:C	1:A:246:ASN:H	2.17	0.51
1:A:660:GLY:C	1:A:661:LEU:HD12	2.36	0.51
1:A:697:ARG:NE	1:A:698:GLN:H	2.08	0.51
1:A:509:SER:OG	1:A:578:ILE:HG23	2.11	0.50
1:A:32:ILE:O	1:A:33:GLN:HB3	2.12	0.50
1:A:32:ILE:O	1:A:33:GLN:CB	2.59	0.50
1:A:388:CYS:HA	1:A:692:TYR:CE1	2.47	0.50
1:A:510:MET:HA	1:A:578:ILE:HD13	1.94	0.50
1:A:221:ILE:HG22	1:A:222:LYS:HB2	1.94	0.49
1:A:201:SER:C	1:A:203:ARG:H	2.20	0.49
1:A:536:GLN:NE2	1:A:655:ARG:HG2	2.26	0.49
1:A:322:PHE:O	1:A:325:ILE:HG12	2.13	0.49
1:A:485:TYR:CE1	1:A:604:PRO:HD3	2.48	0.49
1:A:14:MET:HE3	1:A:43:ALA:HB1	1.94	0.49
1:A:293:PRO:HD2	1:A:296:THR:HG21	1.95	0.49
1:A:161:THR:N	1:A:162:PRO:HD2	2.28	0.48
1:A:293:PRO:HB2	1:A:328:SER:OG	2.13	0.48
1:A:129:ARG:O	1:A:133:VAL:HG23	2.13	0.48
1:A:201:SER:O	1:A:203:ARG:N	2.46	0.48
1:A:349:ASP:O	1:A:353:THR:HG23	2.14	0.48
1:A:446:SER:OG	1:A:461:ASN:ND2	2.43	0.48
1:A:472:MET:HA	1:A:601:SER:HA	1.96	0.48
1:A:245:ALA:O	1:A:246:ASN:C	2.57	0.47
1:A:486:GLY:O	1:A:491:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ALA:O	1:A:350:PHE:HB3	2.13	0.47
1:A:563:ARG:HE	1:A:563:ARG:HB3	1.57	0.47
1:A:186:ASN:HD21	1:A:189:SER:H	1.60	0.47
1:A:205:GLY:HA3	1:A:253:GLY:HA3	1.96	0.47
1:A:403:ASN:ND2	1:A:403:ASN:H	2.13	0.47
1:A:690:SER:O	1:A:691:LEU:HD13	2.14	0.47
1:A:186:ASN:ND2	1:A:186:ASN:C	2.73	0.47
1:A:239:GLU:OE2	1:A:285:THR:HB	2.15	0.47
1:A:403:ASN:ND2	1:A:403:ASN:C	2.71	0.47
1:A:585:ALA:HB2	1:A:659:GLN:NE2	2.29	0.47
1:A:19:LEU:HB2	1:A:40:ALA:HB2	1.97	0.47
1:A:93:HIS:HE1	1:A:128:ASP:OD1	1.97	0.47
1:A:543:GLN:H	1:A:543:GLN:HG3	1.37	0.47
1:A:602:ILE:O	1:A:602:ILE:HG12	2.12	0.46
1:A:290:VAL:HG12	1:A:292:ILE:HG13	1.97	0.46
1:A:474:LEU:CB	1:A:602:ILE:HA	2.45	0.46
1:A:222:LYS:O	1:A:223:ARG:HG2	2.16	0.46
1:A:22:MET:HE3	1:A:36:LYS:NZ	2.30	0.46
1:A:218:GLY:H	1:A:228:SER:HB3	1.80	0.46
1:A:365:TYR:O	1:A:366:ILE:HD13	2.16	0.46
1:A:22:MET:HE2	1:A:36:LYS:HD2	1.97	0.46
1:A:541:ASP:O	1:A:542:TRP:CE3	2.69	0.46
1:A:613:LYS:HA	1:A:618:GLY:O	2.16	0.46
1:A:390:GLU:H	1:A:390:GLU:HG3	1.54	0.45
1:A:534:PHE:O	1:A:535:THR:C	2.57	0.45
1:A:569:LEU:O	1:A:573:VAL:HG23	2.16	0.45
1:A:84:PHE:CE1	1:A:142:GLU:HB3	2.51	0.45
1:A:335:ILE:O	1:A:342:LYS:HE2	2.17	0.45
1:A:32:ILE:HG21	1:A:34:PHE:CE1	2.52	0.45
1:A:393:GLN:HE22	1:A:466:ALA:HB1	1.81	0.45
1:A:19:LEU:O	1:A:22:MET:HB2	2.17	0.45
1:A:87:ARG:HH11	1:A:87:ARG:HG3	1.82	0.45
1:A:403:ASN:HD22	1:A:403:ASN:H	1.65	0.45
1:A:393:GLN:HE22	1:A:466:ALA:CB	2.30	0.44
1:A:605:ILE:HD12	1:A:607:ALA:C	2.39	0.44
1:A:222:LYS:O	1:A:223:ARG:CG	2.66	0.44
1:A:321:PRO:O	1:A:322:PHE:C	2.60	0.44
1:A:667:PHE:HB2	1:A:696:LEU:HD12	1.99	0.44
1:A:356:GLU:O	1:A:359:PHE:HB3	2.17	0.44
1:A:27:ASP:O	1:A:29:ALA:N	2.51	0.44
1:A:696:LEU:HD12	1:A:696:LEU:HA	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:TYR:CD2	1:A:666:PHE:HB3	2.53	0.43
1:A:436:GLU:HG3	1:A:508:THR:HG23	2.00	0.43
1:A:666:PHE:CD1	1:A:666:PHE:N	2.86	0.43
1:A:346:ASN:O	1:A:347:ALA:C	2.62	0.43
1:A:422:ILE:HG23	1:A:497:TYR:CE1	2.53	0.43
1:A:363:TYR:CB	1:A:364:PRO:HA	2.34	0.43
1:A:672:THR:O	1:A:675:ASP:HB2	2.18	0.43
1:A:186:ASN:C	1:A:186:ASN:HD22	2.27	0.43
1:A:151:GLU:OE1	1:A:434:THR:HG23	2.18	0.43
1:A:258:TYR:OH	1:A:385:SER:HB3	2.19	0.42
1:A:266:ILE:O	1:A:269:PHE:HB3	2.20	0.42
1:A:365:TYR:CD2	1:A:692:TYR:O	2.73	0.42
1:A:358:GLN:HG2	1:A:363:TYR:C	2.43	0.42
1:A:493:PHE:O	1:A:494:THR:C	2.62	0.42
1:A:180:LEU:N	1:A:180:LEU:CD1	2.81	0.42
1:A:215:ARG:HA	1:A:311:PRO:HG2	2.02	0.42
1:A:295:ILE:HD11	1:A:299:LEU:HD11	2.01	0.42
1:A:337:ASP:HA	1:A:338:PRO:HD3	1.86	0.42
1:A:34:PHE:O	1:A:35:ASP:C	2.58	0.42
1:A:309:PHE:CD1	1:A:309:PHE:N	2.87	0.42
1:A:201:SER:C	1:A:203:ARG:N	2.78	0.42
1:A:426:MET:HE2	1:A:493:PHE:HE1	1.85	0.42
1:A:595:ILE:HD13	1:A:595:ILE:HG21	1.76	0.42
1:A:72:TYR:CG	1:A:132:MET:HE2	2.56	0.41
1:A:154:SER:OG	1:A:156:ARG:HB2	2.20	0.41
1:A:207:VAL:O	1:A:255:GLY:HA2	2.20	0.41
1:A:473:ASN:HA	1:A:599:THR:OG1	2.20	0.41
1:A:312:TYR:CZ	1:A:316:ARG:HD2	2.56	0.41
1:A:605:ILE:O	1:A:605:ILE:HG13	2.21	0.41
1:A:393:GLN:NE2	1:A:466:ALA:HB1	2.36	0.41
1:A:500:THR:O	1:A:501:ILE:C	2.63	0.41
1:A:267:LEU:HA	1:A:267:LEU:HD23	1.77	0.40
1:A:420:LEU:HD13	1:A:425:VAL:HG21	2.03	0.40
1:A:451:ILE:O	1:A:451:ILE:HG22	2.20	0.40
1:A:107:LYS:HE2	1:A:111:SER:OG	2.21	0.40
1:A:403:ASN:HD22	1:A:403:ASN:C	2.25	0.40
1:A:23:LEU:HD11	1:A:623:PRO:HD3	2.03	0.40
1:A:421:ASN:OD1	1:A:421:ASN:C	2.64	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	678/714 (95%)	616 (91%)	54 (8%)	8 (1%)	10	40

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	202	LYS
1	A	33	GLN
1	A	28	LYS
1	A	600	SER
1	A	245	ALA
1	A	253	GLY
1	A	602	ILE

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	571/596 (96%)	525 (92%)	46 (8%)	11	38

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	55	THR
1	A	107	LYS

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Mol	Chain	Res	Type
1	A	127	GLU
1	A	135	LEU
1	A	161	THR
1	A	165	LEU
1	A	170	GLN
1	A	184	GLU
1	A	186	ASN
1	A	190	ILE
1	A	200	LEU
1	A	202	LYS
1	A	203	ARG
1	A	222	LYS
1	A	223	ARG
1	A	227	GLN
1	A	229	SER
1	A	246	ASN
1	A	257	VAL
1	A	271	ASP
1	A	275	GLU
1	A	278	ASP
1	A	282	ARG
1	A	286	LEU
1	A	295	ILE
1	A	296	THR
1	A	306	MET
1	A	343	THR
1	A	352	GLN
1	A	361	SER
1	A	390	GLU
1	A	403	ASN
1	A	407	THR
1	A	416	ASN
1	A	420	LEU
1	A	474	LEU
1	A	496	LEU
1	A	527	ARG
1	A	543	GLN
1	A	563	ARG
1	A	587	PRO
1	A	602	ILE
1	A	636	GLN
1	A	691	LEU

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Mol	Chain	Res	Type
1	A	699	LEU

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	38	GLN
1	A	186	ASN
1	A	195	ASN
1	A	226	ASN
1	A	227	GLN
1	A	303	ASN
1	A	393	GLN
1	A	403	ASN
1	A	424	HIS
1	A	461	ASN
1	A	465	HIS
1	A	495	ASN
1	A	507	HIS
1	A	536	GLN
1	A	581	GLN
1	A	582	ASN
1	A	677	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 ⓘ

There are no ligands in this entry.

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, 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	682/714 (95%)	0.18	27 (3%) 42 23	40, 53, 82, 111	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ASP	7.1
1	A	280	LYS	4.8
1	A	281	ILE	4.5
1	A	223	ARG	4.5
1	A	699	LEU	4.5
1	A	698	GLN	4.0
1	A	545	LYS	3.8
1	A	224	ILE	3.7
1	A	222	LYS	3.5
1	A	693	TYR	3.5
1	A	542	TRP	3.4
1	A	539	GLN	3.3
1	A	279	GLU	3.2
1	A	13	THR	3.0
1	A	363	TYR	3.0
1	A	14	MET	3.0
1	A	227	GLN	2.9
1	A	228	SER	2.8
1	A	544	PRO	2.6
1	A	601	SER	2.5
1	A	35	ASP	2.4
1	A	669	ASP	2.4
1	A	278	ASP	2.3
1	A	390	GLU	2.3
1	A	602	ILE	2.1
1	A	360	GLU	2.1
1	A	316	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 oligosaccharides 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.