



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:36 AM UTC

PDB ID : 1R1R / pdb_00001r1r
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 ⓘ 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

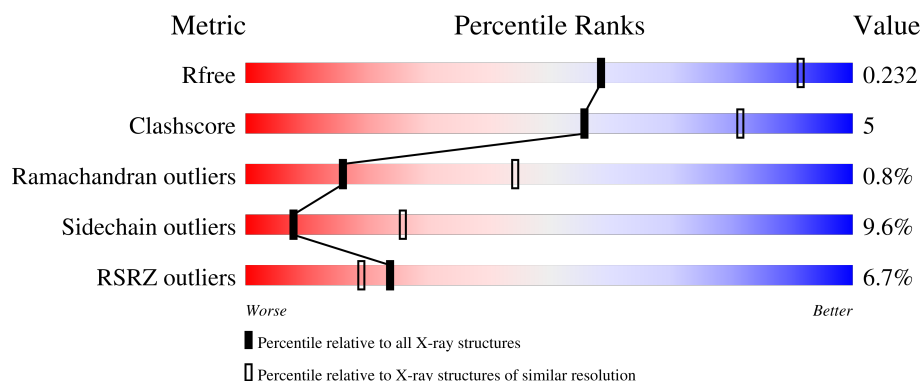
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 $\leq 5\%$. 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	761	4% 76% 18% ...
1	B	761	6% 76% 18% ...
1	C	761	9% 76% 18% ...
2	D	20	15% 60% 20% 20%
2	E	20	20% 60% 20% 20%

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Mol	Chain	Length	Quality of chain
2	F	20	
2	P	20	

2 Entry composition

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
1	A	734	Total	C	N	O	S	0	0	0
			5844	3712	1004	1104	24			
1	B	734	Total	C	N	O	S	0	0	0
			5844	3712	1004	1104	24			
1	C	734	Total	C	N	O	S	0	0	0
			5844	3712	1004	1104	24			

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
2	D	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	E	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	F	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	P	3	Total	C	N	O	0	0	0
			27	20	3	4			

- Molecule 3 is water.

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

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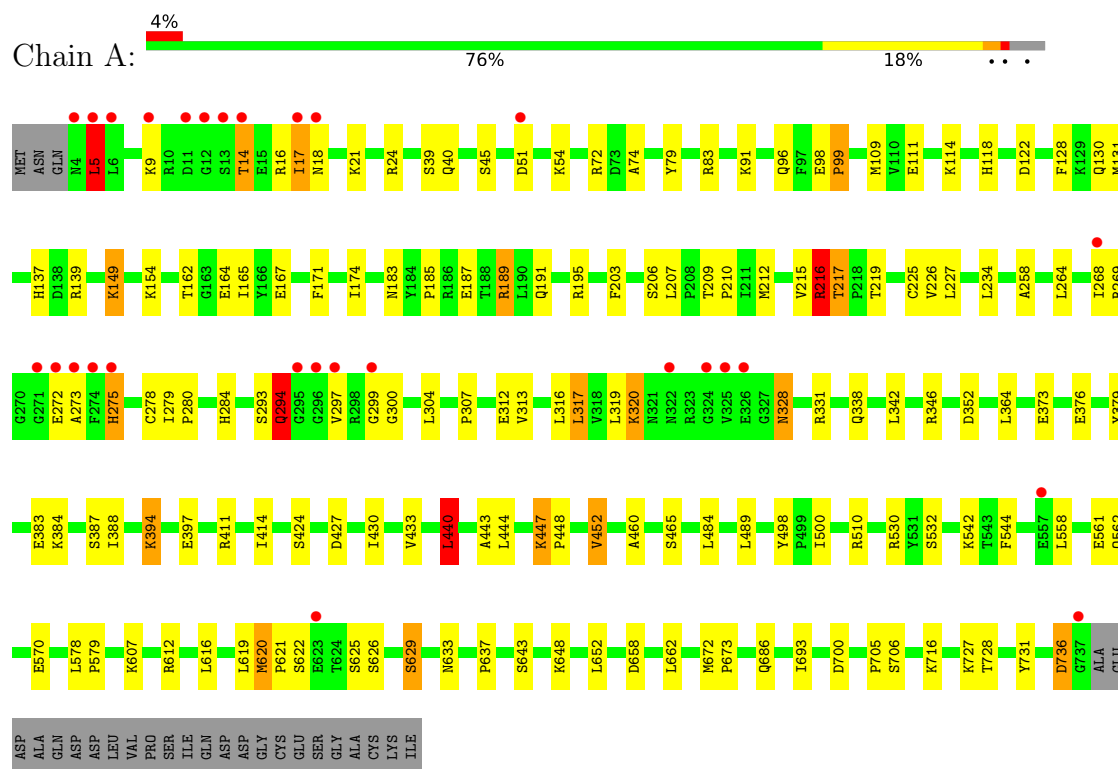
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	104	Total 104	O 104	0	0
3	C	104	Total 104	O 104	0	0

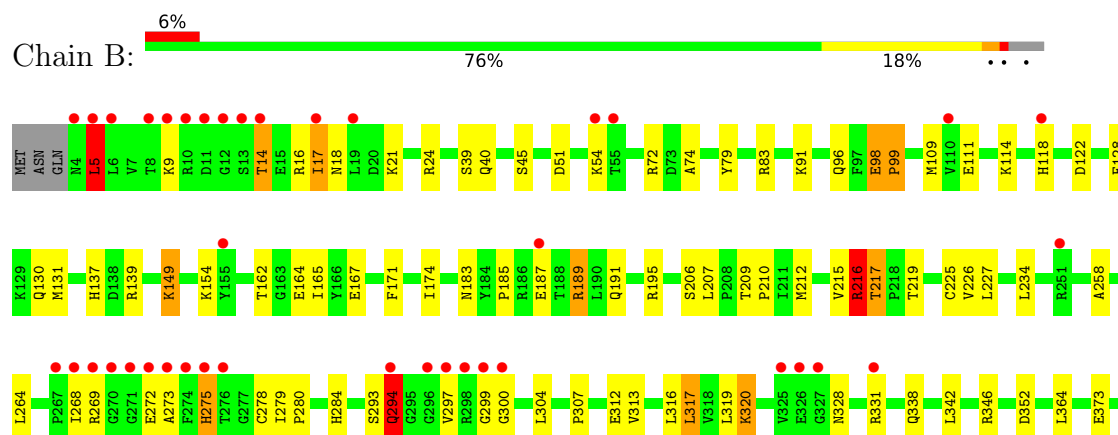
3 Residue-property plots

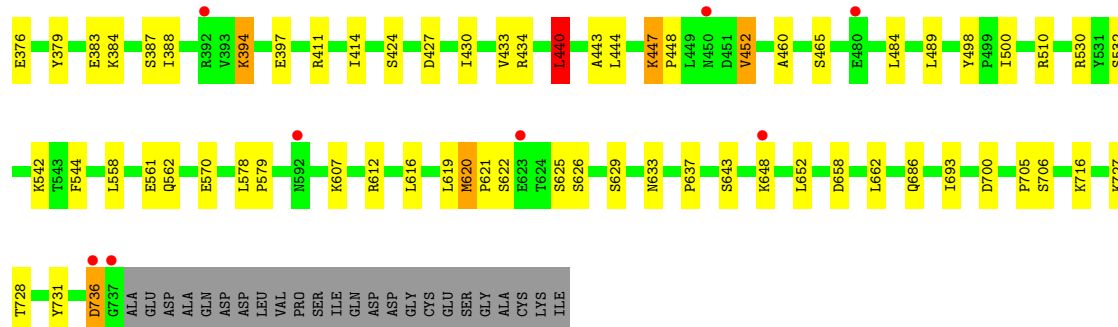
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

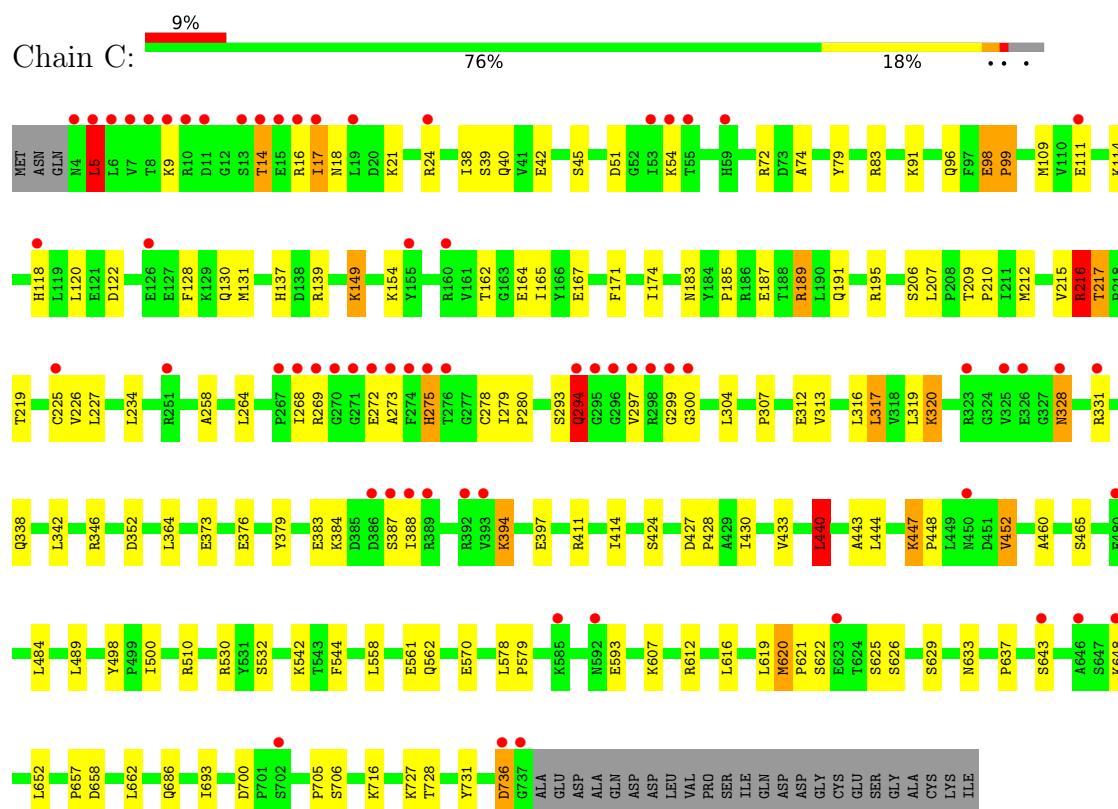


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

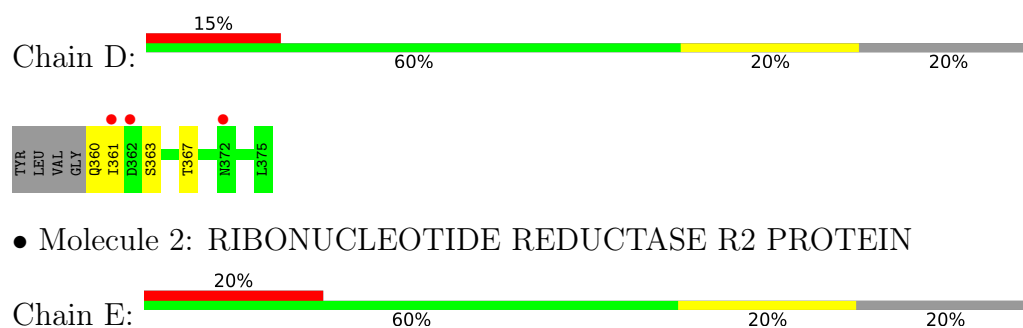




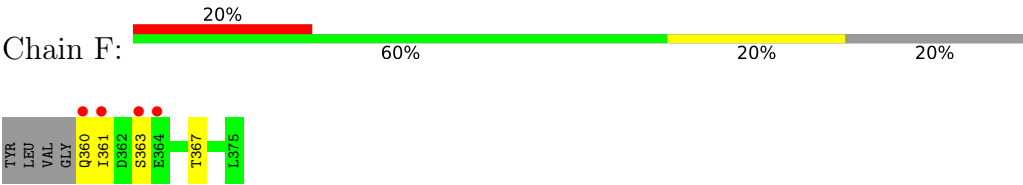
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



4 Data and refinement statistics

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) 95.7 (20.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.88Å)	Xtriage
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.210 , 0.245 0.217 , 0.232	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 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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	0.41	0/5972	1.23	34/8088 (0.4%)
1	B	0.41	0/5972	1.23	34/8088 (0.4%)
1	C	0.41	0/5972	1.23	38/8088 (0.5%)
2	D	0.36	0/129	0.99	0/173
2	E	0.37	0/129	0.99	0/173
2	F	0.36	0/129	0.99	0/173
2	P	0.74	0/27	1.93	0/36
All	All	0.41	0/18330	1.23	106/24819 (0.4%)

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	736	ASP	CA-CB-CG	12.26	124.86	112.60
1	A	736	ASP	CA-CB-CG	12.24	124.84	112.60
1	C	736	ASP	CA-CB-CG	12.23	124.83	112.60
1	C	99	PRO	N-CA-CB	9.38	108.10	103.22
1	B	99	PRO	N-CA-CB	9.37	108.09	103.22
1	A	99	PRO	N-CA-CB	9.30	108.06	103.22
1	B	532	SER	N-CA-C	7.52	122.21	112.89
1	C	532	SER	N-CA-C	7.52	122.21	112.89
1	A	532	SER	N-CA-C	7.49	122.17	112.89
1	B	500	ILE	CA-C-N	6.83	126.34	119.24
1	B	500	ILE	C-N-CA	6.83	126.34	119.24
1	C	500	ILE	CA-C-N	6.81	126.33	119.24
1	C	500	ILE	C-N-CA	6.81	126.33	119.24
1	A	500	ILE	CA-C-N	6.80	126.31	119.24
1	A	500	ILE	C-N-CA	6.80	126.31	119.24
1	C	278	CYS	N-CA-C	6.55	118.21	111.14
1	B	278	CYS	N-CA-C	6.53	118.19	111.14
1	A	278	CYS	N-CA-C	6.48	118.14	111.14
1	B	14	THR	N-CA-C	6.32	119.80	109.76
1	C	14	THR	N-CA-C	6.28	119.75	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	THR	N-CA-C	6.28	119.75	109.76
1	A	299	GLY	CA-C-O	-6.25	117.01	121.88
1	B	299	GLY	CA-C-O	-6.21	117.03	121.88
1	C	299	GLY	CA-C-O	-6.21	117.04	121.88
1	A	500	ILE	CA-C-O	6.07	123.27	119.51
1	B	500	ILE	CA-C-O	6.01	123.23	119.51
1	A	440	LEU	N-CA-C	6.00	119.92	112.24
1	C	500	ILE	CA-C-O	5.96	123.21	119.51
1	B	440	LEU	N-CA-C	5.96	119.87	112.24
1	C	440	LEU	N-CA-C	5.95	119.85	112.24
1	C	217	THR	CA-C-N	5.90	125.58	119.56
1	C	217	THR	C-N-CA	5.90	125.58	119.56
1	A	217	THR	CA-C-N	5.88	125.56	119.56
1	A	217	THR	C-N-CA	5.88	125.56	119.56
1	B	217	THR	CA-C-N	5.83	125.51	119.56
1	B	217	THR	C-N-CA	5.83	125.51	119.56
1	B	331	ARG	N-CA-C	5.71	118.44	111.82
1	A	331	ARG	N-CA-C	5.68	118.40	111.82
1	C	331	ARG	N-CA-C	5.68	118.41	111.82
1	B	448	PRO	N-CA-CB	5.67	108.36	103.31
1	C	448	PRO	N-CA-CB	5.64	108.33	103.31
1	A	448	PRO	N-CA-CB	5.63	108.32	103.31
1	B	98	GLU	CA-C-N	5.61	123.70	119.66
1	B	98	GLU	C-N-CA	5.61	123.70	119.66
1	B	452	VAL	N-CA-CB	5.61	117.48	110.47
1	C	452	VAL	N-CA-CB	5.59	117.45	110.47
1	A	452	VAL	N-CA-CB	5.57	117.43	110.47
1	A	98	GLU	CA-C-N	5.56	123.67	119.66
1	A	98	GLU	C-N-CA	5.56	123.67	119.66
1	B	498	TYR	CA-C-N	5.56	125.09	119.19
1	B	498	TYR	C-N-CA	5.56	125.09	119.19
1	B	637	PRO	N-CA-CB	5.56	106.11	103.22
1	C	498	TYR	CA-C-N	5.56	125.08	119.19
1	C	498	TYR	C-N-CA	5.56	125.08	119.19
1	C	98	GLU	CA-C-N	5.54	123.65	119.66
1	C	98	GLU	C-N-CA	5.54	123.65	119.66
1	A	498	TYR	CA-C-N	5.54	125.06	119.19
1	A	498	TYR	C-N-CA	5.54	125.06	119.19
1	A	637	PRO	N-CA-CB	5.53	106.10	103.22
1	B	447	LYS	CA-C-N	5.53	125.45	119.76
1	B	447	LYS	C-N-CA	5.53	125.45	119.76
1	C	637	PRO	N-CA-CB	5.50	106.08	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	LYS	CA-C-N	5.48	125.41	119.76
1	A	447	LYS	C-N-CA	5.48	125.41	119.76
1	C	447	LYS	CA-C-N	5.46	125.38	119.76
1	C	447	LYS	C-N-CA	5.46	125.38	119.76
1	C	427	ASP	CA-C-N	5.39	125.06	119.56
1	C	427	ASP	C-N-CA	5.39	125.06	119.56
1	B	427	ASP	CA-C-N	5.35	125.02	119.56
1	B	427	ASP	C-N-CA	5.35	125.02	119.56
1	A	185	PRO	N-CA-CB	5.35	107.96	103.25
1	A	427	ASP	CA-C-N	5.34	125.01	119.56
1	A	427	ASP	C-N-CA	5.34	125.01	119.56
1	C	185	PRO	N-CA-CB	5.33	107.94	103.25
1	B	185	PRO	N-CA-CB	5.33	107.94	103.25
1	C	700	ASP	CA-C-N	5.33	125.15	119.28
1	C	700	ASP	C-N-CA	5.33	125.15	119.28
1	C	544	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	544	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	700	ASP	CA-C-N	5.32	125.13	119.28
1	B	700	ASP	C-N-CA	5.32	125.13	119.28
1	B	544	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	700	ASP	CA-C-N	5.31	125.12	119.28
1	A	700	ASP	C-N-CA	5.31	125.12	119.28
1	C	620	MET	CA-C-N	5.29	125.27	120.03
1	C	620	MET	C-N-CA	5.29	125.27	120.03
1	B	620	MET	CA-C-N	5.29	125.27	120.03
1	B	620	MET	C-N-CA	5.29	125.27	120.03
1	A	620	MET	CA-C-N	5.27	125.25	120.03
1	A	620	MET	C-N-CA	5.27	125.25	120.03
1	C	444	LEU	CA-C-N	5.22	124.98	119.76
1	C	444	LEU	C-N-CA	5.22	124.98	119.76
1	A	444	LEU	CA-C-N	5.17	124.93	119.76
1	A	444	LEU	C-N-CA	5.17	124.93	119.76
1	B	74	ALA	CA-C-N	5.10	124.71	119.56
1	B	74	ALA	C-N-CA	5.10	124.71	119.56
1	C	74	ALA	CA-C-N	5.08	124.69	119.56
1	C	74	ALA	C-N-CA	5.08	124.69	119.56
1	A	74	ALA	CA-C-N	5.05	124.66	119.56
1	A	74	ALA	C-N-CA	5.05	124.66	119.56
1	C	593	GLU	CA-C-N	5.03	125.24	120.31
1	C	593	GLU	C-N-CA	5.03	125.24	120.31
1	C	428	PRO	N-CA-CB	5.01	108.49	103.48
1	C	657	PRO	N-CA-CB	5.00	107.69	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	LEU	CA-C-N	5.00	124.90	119.85
1	B	444	LEU	C-N-CA	5.00	124.90	119.85

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	5844	0	5770	56	0
1	B	5844	0	5770	55	0
1	C	5844	0	5770	56	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	166	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 5.

All (166) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.70	0.73
1:B:207:LEU:HB2	1:B:212:MET:HE3	1.73	0.71
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.73	0.71
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.73	0.71
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:293:SER:O	1:B:294:GLN:C	2.56	0.48
1:C:293:SER:O	1:C:294:GLN:C	2.57	0.48
1:A:79:TYR:O	1:A:83:ARG:HG3	2.14	0.48
1:A:293:SER:O	1:A:294:GLN:C	2.56	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: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:109:MET:HE3	1:A:114:LYS:HB2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:MET:HE3	1:B:114:LYS:HB2	1.98	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:C:128:PHE:HA	1:C:131:MET:HE3	1.99	0.45
1:A:620:MET:HB2	1:A:621:PRO:HD2	1.99	0.45
1:B:128:PHE:HA	1:B:131:MET:HE3	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:109:MET:HE3	1:C:114:LYS:HB2	1.98	0.45
1:A:128:PHE:HA	1:A:131:MET:HE3	1.99	0.44
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 ⓘ

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	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	16	44
1	B	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	16	44
1	C	732/761 (96%)	697 (95%)	29 (4%)	6 (1%)	16	44
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
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%)	16	44

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 ⓘ

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%)	571 (91%)	58 (9%)	8	27
1	B	629/651 (97%)	571 (91%)	58 (9%)	8	27
1	C	629/651 (97%)	571 (91%)	58 (9%)	8	27
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%)	1751 (90%)	187 (10%)	8	26

All (187) 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	72	ARG
1	A	91	LYS
1	A	96	GLN
1	A	111	GLU
1	A	118	HIS
1	A	130	GLN
1	A	139	ARG
1	A	149	LYS
1	A	154	LYS

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	183	ASN
1	A	187	GLU
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
1	A	328	ASN
1	A	364	LEU
1	A	373	GLU
1	A	384	LYS
1	A	387	SER
1	A	388	ILE
1	A	394	LYS
1	A	414	ILE
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	542	LYS
1	A	607	LYS
1	A	616	LEU
1	A	625	SER
1	A	626	SER
1	A	629	SER
1	A	643	SER
1	A	648	LYS
1	A	716	LYS
1	A	736	ASP
2	D	360	GLN
2	D	361	ILE
2	D	363	SER
2	D	367	THR

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Mol	Chain	Res	Type
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	72	ARG
1	B	91	LYS
1	B	96	GLN
1	B	111	GLU
1	B	118	HIS
1	B	130	GLN
1	B	139	ARG
1	B	149	LYS
1	B	154	LYS
1	B	165	ILE
1	B	183	ASN
1	B	187	GLU
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	328	ASN
1	B	364	LEU
1	B	373	GLU
1	B	384	LYS
1	B	387	SER
1	B	388	ILE
1	B	394	LYS
1	B	414	ILE

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Mol	Chain	Res	Type
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	542	LYS
1	B	607	LYS
1	B	616	LEU
1	B	625	SER
1	B	626	SER
1	B	629	SER
1	B	643	SER
1	B	648	LYS
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
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	72	ARG
1	C	91	LYS
1	C	96	GLN
1	C	111	GLU
1	C	118	HIS
1	C	130	GLN
1	C	139	ARG
1	C	149	LYS
1	C	154	LYS
1	C	165	ILE
1	C	183	ASN

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Mol	Chain	Res	Type
1	C	187	GLU
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	328	ASN
1	C	364	LEU
1	C	373	GLU
1	C	384	LYS
1	C	387	SER
1	C	388	ILE
1	C	394	LYS
1	C	414	ILE
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	542	LYS
1	C	607	LYS
1	C	616	LEU
1	C	625	SER
1	C	626	SER
1	C	629	SER
1	C	643	SER
1	C	648	LYS
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 (27)

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	416	ASN
1	A	661	HIS
1	A	696	ASN
1	A	733	ASN
2	D	360	GLN
1	B	18	ASN
1	B	35	ASN
1	B	46	HIS
1	B	250	GLN
1	B	275	HIS
1	B	328	ASN
1	B	416	ASN
1	B	661	HIS
2	E	360	GLN
1	C	18	ASN
1	C	46	HIS
1	C	250	GLN
1	C	275	HIS
1	C	328	ASN
1	C	416	ASN
1	C	661	HIS
2	F	360	GLN

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	734/761 (96%)	-0.13	28 (3%)	44	36	10, 24, 77, 108	0
1	B	734/761 (96%)	0.58	47 (6%)	25	20	10, 24, 77, 108	0
1	C	734/761 (96%)	0.63	65 (8%)	15	13	10, 24, 77, 108	0
2	D	16/20 (80%)	1.25	3 (18%)	3	3	45, 82, 91, 97	0
2	E	16/20 (80%)	1.83	4 (25%)	2	1	45, 82, 91, 97	0
2	F	16/20 (80%)	1.68	4 (25%)	2	1	45, 82, 91, 97	0
2	P	3/20 (15%)	2.52	1 (33%)	1	1	30, 30, 37, 43	0
All	All	2253/2363 (95%)	0.39	152 (6%)	24	19	10, 25, 83, 108	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ALA	7.0
1	B	273	ALA	6.9
1	C	273	ALA	6.6
1	C	274	PHE	6.4
1	A	296	GLY	6.1
2	P	3	VAL	5.6
1	C	4	ASN	5.5
1	C	271	GLY	5.1
1	C	297	VAL	5.0
1	C	326	GLU	5.0
1	C	275	HIS	5.0
1	C	8	THR	5.0
1	B	300	GLY	4.8
1	C	296	GLY	4.8
1	B	623	GLU	4.8
1	A	13	SER	4.6
1	B	271	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	17	ILE	4.6
1	B	274	PHE	4.5
1	C	272	GLU	4.4
1	C	736	ASP	4.4
1	C	126	GLU	4.4
1	A	297	VAL	4.3
1	C	13	SER	4.3
1	C	11	ASP	4.3
1	C	623	GLU	4.3
1	A	274	PHE	4.2
1	C	160	ARG	4.1
2	E	360	GLN	4.1
1	C	294	GLN	4.1
1	C	10	ARG	4.1
1	C	14	THR	4.1
1	B	5	LEU	4.0
2	F	361	ILE	4.0
1	A	271	GLY	3.8
1	C	111	GLU	3.8
1	C	5	LEU	3.8
1	B	325	VAL	3.7
1	A	6	LEU	3.7
1	C	269	ARG	3.7
1	A	11	ASP	3.6
1	A	17	ILE	3.6
1	A	12	GLY	3.6
1	B	297	VAL	3.5
1	C	298	ARG	3.5
1	C	480	GLU	3.5
1	B	294	GLN	3.4
1	B	272	GLU	3.4
1	A	9	LYS	3.4
1	A	5	LEU	3.3
1	A	268	ILE	3.3
1	B	268	ILE	3.2
1	A	275	HIS	3.2
1	A	299	GLY	3.2
1	C	268	ILE	3.2
2	E	361	ILE	3.2
1	C	267	PRO	3.2
1	C	19	LEU	3.1
1	C	54	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	9	LYS	3.1
1	C	387	SER	3.1
1	A	623	GLU	3.1
1	A	4	ASN	3.1
2	E	363	SER	3.0
1	C	251	ARG	3.0
1	B	10	ARG	3.0
1	C	53	ILE	3.0
1	A	272	GLU	3.0
1	B	8	THR	3.0
1	C	16	ARG	3.0
1	C	392	ARG	2.9
1	A	737	GLY	2.9
2	E	364	GLU	2.9
1	C	276	THR	2.9
1	B	269	ARG	2.9
1	B	270	GLY	2.9
1	B	296	GLY	2.9
2	F	364	GLU	2.9
2	D	372	ASN	2.9
1	C	55	THR	2.9
1	C	299	GLY	2.9
1	C	737	GLY	2.9
1	C	592	ASN	2.8
1	C	295	GLY	2.8
1	C	389	ARG	2.8
1	B	17	ILE	2.8
1	B	11	ASP	2.8
1	A	325	VAL	2.8
1	B	155	TYR	2.7
1	B	275	HIS	2.7
1	B	12	GLY	2.7
1	B	737	GLY	2.7
1	C	6	LEU	2.7
1	C	9	LYS	2.7
1	B	592	ASN	2.7
1	C	225	CYS	2.7
1	B	4	ASN	2.7
1	C	118	HIS	2.7
1	C	325	VAL	2.7
1	A	14	THR	2.6
1	B	736	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	323	ARG	2.6
1	C	270	GLY	2.6
1	B	14	THR	2.6
1	B	326	GLU	2.6
1	B	118	HIS	2.6
1	C	24	ARG	2.6
1	A	322	ASN	2.6
1	C	155	TYR	2.5
2	D	361	ILE	2.5
1	C	59	HIS	2.5
2	F	360	GLN	2.5
1	B	187	GLU	2.5
1	B	648	LYS	2.5
1	B	13	SER	2.4
1	A	295	GLY	2.4
1	C	643	SER	2.4
1	B	251	ARG	2.3
1	B	55	THR	2.3
1	C	300	GLY	2.3
1	A	324	GLY	2.3
2	D	362	ASP	2.3
1	B	19	LEU	2.3
1	C	648	LYS	2.3
1	B	450	ASN	2.2
1	C	15	GLU	2.2
1	B	299	GLY	2.2
1	C	386	ASP	2.2
1	B	267	PRO	2.2
1	B	6	LEU	2.2
1	C	585	LYS	2.2
1	C	331	ARG	2.2
1	B	276	THR	2.2
1	C	646	ALA	2.2
1	B	392	ARG	2.1
1	C	7	VAL	2.1
1	B	327	GLY	2.1
1	B	331	ARG	2.1
1	C	450	ASN	2.1
1	B	298	ARG	2.1
1	A	557	GLU	2.1
2	F	363	SER	2.1
1	A	51	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	702	SER	2.0
1	C	393	VAL	2.0
1	A	326	GLU	2.0
1	B	54	LYS	2.0
1	B	110	VAL	2.0
1	A	18	ASN	2.0
1	C	328	ASN	2.0
1	C	388	ILE	2.0
1	B	480	GLU	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.