



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:10 PM UTC

PDB ID : 2XAW / pdb_00002xaw
Title : Ribonucleotide reductase Y730N02Y and Y731F modified R1 subunit of E. coli
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on : 2010-03-31
Resolution : 3.10 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:

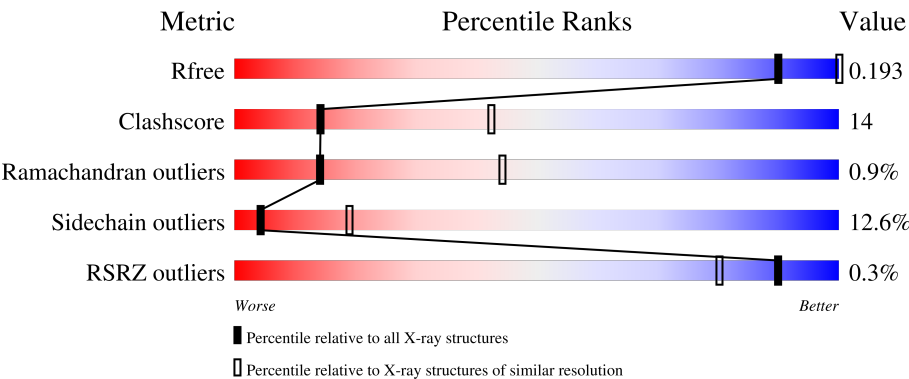
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	63%28%.
1	B	761	63%27%6%.
1	C	761	68%24%. .
2	D	20	30%20%5%45%
2	E	20	5%35%15%5%45%

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Mol	Chain	Length	Quality of chain
2	F	20	35% 25% 40%
2	P	20	5% 5% 5% 85%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18220 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 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5795	3679	995	1097	24			
1	B	727	Total	C	N	O	S	0	0	0
			5795	3679	995	1097	24			
1	C	727	Total	C	N	O	S	0	0	0
			5795	3679	995	1097	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	731	PHE	TYR	engineered mutation	UNP P00452
B	731	PHE	TYR	engineered mutation	UNP P00452
C	731	PHE	TYR	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	0
			89	54	13	22			
2	E	11	Total	C	N	O	0	0	0
			89	54	13	22			
2	F	12	Total	C	N	O	0	0	0
			98	59	14	25			
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	152	Total	O	0	0
			152	152		

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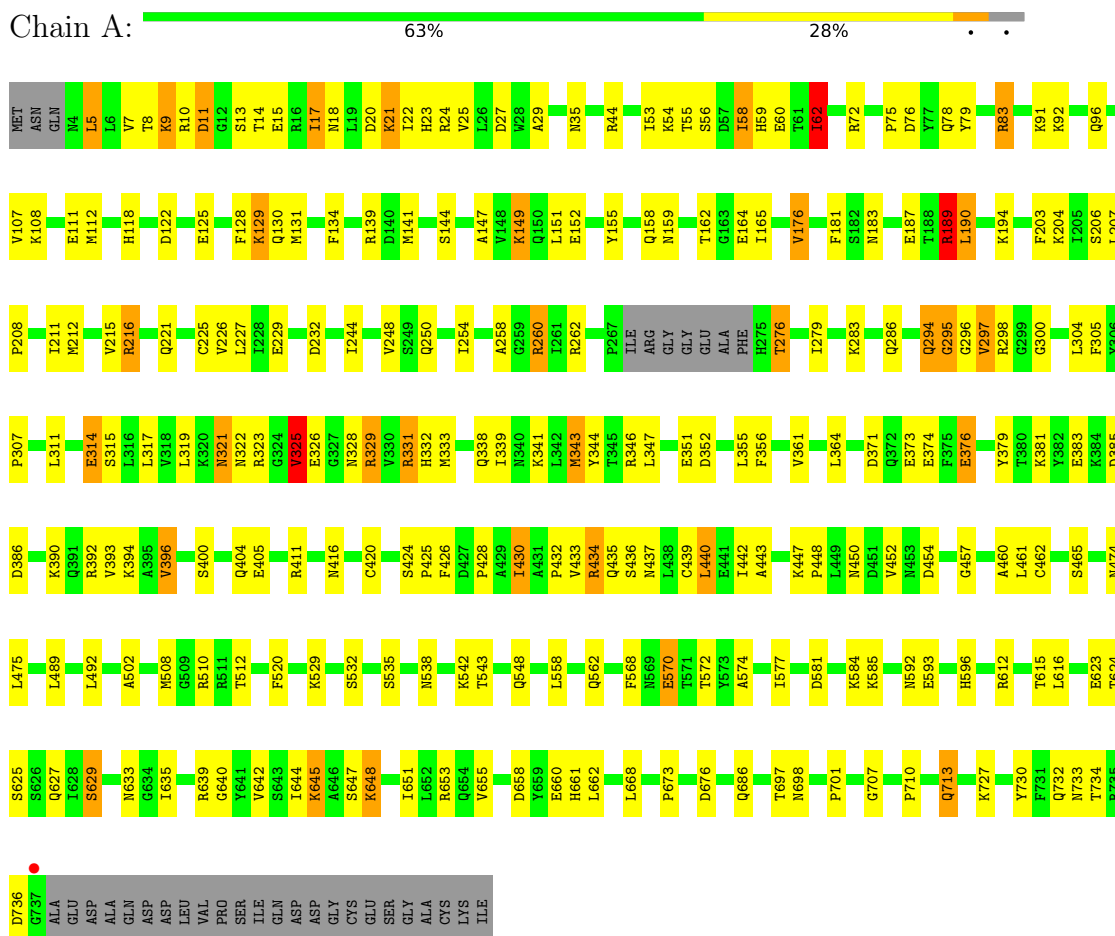
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	179	Total 179	O 179	0	0
3	C	195	Total 195	O 195	0	0
3	D	2	Total 2	O 2	0	0
3	E	1	Total 1	O 1	0	0
3	F	2	Total 2	O 2	0	0
3	P	1	Total 1	O 1	0	0

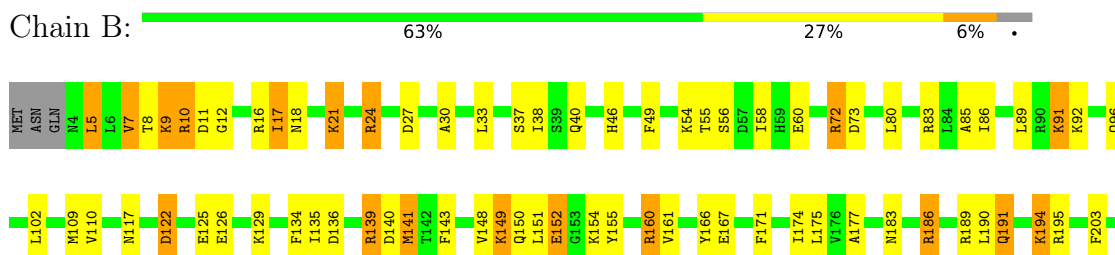
3 Residue-property plots

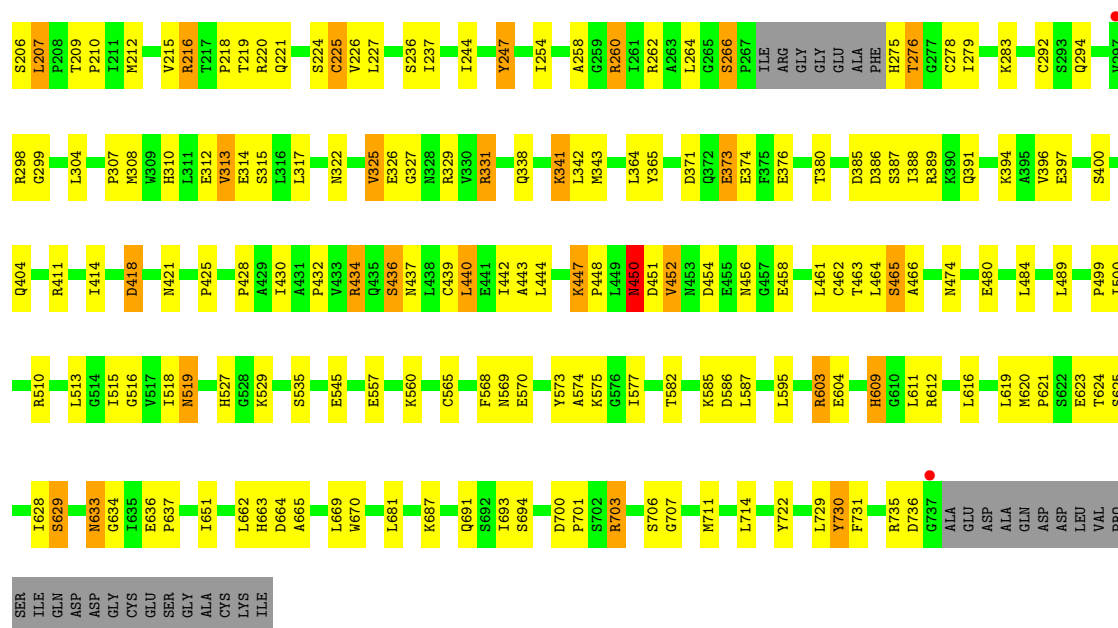
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1 SUBUNIT ALPHA



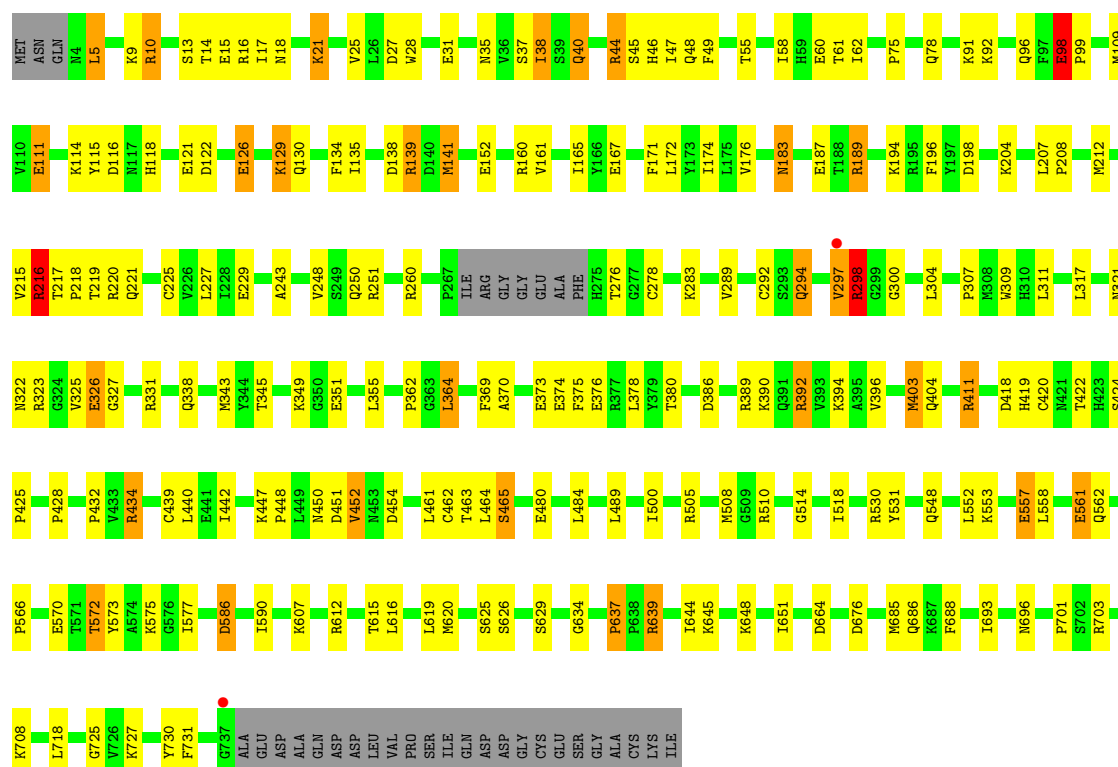
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA





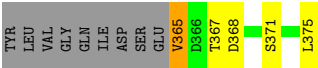
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C: 68% 24%

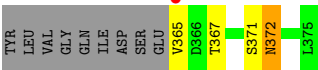
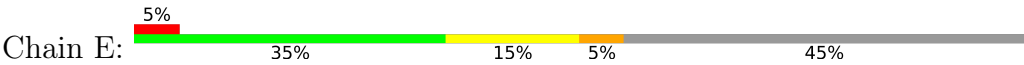


• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

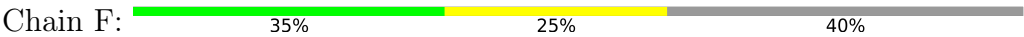
Chain D: 30% 20% 5% 45%



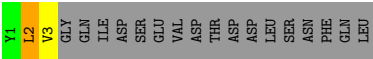
● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	223.89Å 223.89Å 336.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 3.10 168.03 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (169.03-3.10) 97.2 (168.03-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.234 (Not available) , 0.193	Depositor DCC
R_{free} test set	2894 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18220	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NIY

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	0.68	2/5904 (0.0%)	0.99	4/7994 (0.1%)
1	B	0.69	0/5904	0.99	12/7994 (0.2%)
1	C	0.75	2/5904 (0.0%)	1.02	14/7994 (0.2%)
2	D	0.64	0/89	0.86	0/119
2	E	0.67	0/89	1.17	0/119
2	F	0.64	0/98	0.89	0/131
2	P	0.96	0/27	1.48	1/36 (2.8%)
All	All	0.71	4/18015 (0.0%)	1.00	31/24387 (0.1%)

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	VAL	CA-CB	5.60	1.62	1.54
1	A	62	ILE	CA-CB	5.39	1.61	1.54
1	C	99	PRO	CA-C	5.37	1.55	1.52
1	A	325	VAL	CA-CB	5.10	1.59	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	278	CYS	N-CA-C	8.28	121.05	111.11
1	C	620	MET	CA-C-N	-8.01	112.46	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620	MET	C-N-CA	-8.01	112.46	120.31
1	C	411	ARG	N-CA-C	6.90	119.24	110.61
1	C	331	ARG	N-CA-C	6.87	121.25	113.01
1	B	299	GLY	N-CA-C	-6.31	104.70	112.33
1	B	450	ASN	CB-CA-C	-6.23	100.84	110.81
1	A	189	ARG	N-CA-C	5.98	118.28	111.11
1	B	387	SER	N-CA-C	-5.94	105.88	113.01
1	C	298	ARG	N-CA-C	5.87	118.30	108.02
1	C	572	THR	N-CA-C	-5.71	105.57	112.54
1	B	464	LEU	N-CA-C	5.70	118.83	109.72
1	A	295	GLY	N-CA-C	-5.65	99.79	113.18
1	A	676	ASP	N-CA-C	5.59	117.07	110.97
1	C	98	GLU	CA-C-N	-5.55	115.66	119.66
1	C	98	GLU	C-N-CA	-5.55	115.66	119.66
1	C	637	PRO	CA-C-N	5.46	125.38	119.76
1	C	637	PRO	C-N-CA	5.46	125.38	119.76
1	A	176	VAL	N-CA-C	-5.45	105.19	110.42
1	B	219	THR	N-CA-C	5.39	117.50	110.43
1	B	326	GLU	N-CA-C	5.35	117.81	111.33
1	C	452	VAL	CB-CA-C	-5.28	102.63	111.29
1	C	590	ILE	N-CA-C	5.26	119.17	113.43
1	C	189	ARG	N-CA-C	5.24	117.41	111.02
1	B	247	TYR	N-CA-C	5.09	116.64	111.14
2	P	2	LEU	N-CA-C	5.08	118.40	110.32
1	B	703	ARG	N-CA-C	-5.08	105.86	113.89
1	B	209	THR	CA-C-N	-5.01	113.48	119.05
1	B	209	THR	C-N-CA	-5.01	113.48	119.05
1	B	620	MET	CA-C-N	-5.00	114.59	119.99
1	B	620	MET	C-N-CA	-5.00	114.59	119.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	450	ASN	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	5795	0	5714	169	0
1	B	5795	0	5714	180	0
1	C	5795	0	5715	145	0
2	D	89	0	77	1	0
2	E	89	0	77	4	0
2	F	98	0	83	1	0
2	P	27	0	31	1	0
3	A	152	0	0	29	0
3	B	179	0	0	27	0
3	C	195	0	0	36	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	P	1	0	0	0	0
All	All	18220	0	17411	497	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 (497) 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:117:ASN:HB2	3:B:2034:HOH:O	1.41	1.20
1:A:294:GLN:HE21	1:A:294:GLN:HA	0.97	1.12
1:C:126:GLU:HA	1:C:129:LYS:HB2	1.30	1.10
1:B:160:ARG:HE	1:B:160:ARG:HA	0.98	1.08
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.12	1.08
1:B:207:LEU:HB2	1:B:212:MET:HE2	1.37	1.05
1:C:160:ARG:HG3	3:C:2048:HOH:O	1.56	1.03
1:C:404:GLN:HB2	3:C:2119:HOH:O	1.57	1.02
1:B:10:ARG:H	1:B:10:ARG:HD2	1.24	0.99
1:A:79:TYR:O	1:A:83:ARG:HG2	1.63	0.99
1:B:160:ARG:HA	1:B:160:ARG:NE	1.80	0.97
1:A:294:GLN:HA	1:A:294:GLN:NE2	1.78	0.95
1:A:9:LYS:CE	3:A:2002:HOH:O	2.14	0.95
1:C:283:LYS:HG3	3:C:2083:HOH:O	1.64	0.95
1:A:346:ARG:HD2	1:A:352:ASP:O	1.68	0.93
1:C:480:GLU:HB2	3:C:2139:HOH:O	1.70	0.92
1:C:44:ARG:HG2	1:C:44:ARG:HH11	1.35	0.91
1:B:160:ARG:HE	1:B:160:ARG:CA	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:GLN:HG3	1:C:298:ARG:HB2	1.53	0.90
1:B:11:ASP:CG	1:B:12:GLY:H	1.80	0.90
1:A:351:GLU:HB3	3:A:2081:HOH:O	1.73	0.88
1:B:109:MET:HE1	1:B:166:TYR:HB3	1.57	0.86
1:B:314:GLU:HG2	3:B:2073:HOH:O	1.74	0.86
1:C:373:GLU:HG2	3:C:2112:HOH:O	1.75	0.86
1:B:91:LYS:HD3	3:B:2025:HOH:O	1.76	0.85
1:A:215:VAL:O	1:A:216:ARG:HB3	1.75	0.85
1:A:294:GLN:HE21	1:A:294:GLN:CA	1.82	0.85
1:C:251:ARG:HD3	3:C:2073:HOH:O	1.76	0.85
1:C:212:MET:O	1:C:216:ARG:NH2	2.10	0.84
1:A:9:LYS:HE2	3:A:2002:HOH:O	1.70	0.83
1:A:125:GLU:HG2	1:A:129:LYS:HE3	1.58	0.83
1:C:75:PRO:O	1:C:78:GLN:HG2	1.80	0.82
1:B:10:ARG:HD2	1:B:10:ARG:N	1.93	0.81
1:A:221:GLN:OE1	1:A:250:GLN:HG2	1.81	0.81
1:A:376:GLU:HB2	3:A:2085:HOH:O	1.81	0.81
2:E:372:ASN:H	2:E:372:ASN:ND2	1.78	0.81
1:B:225:CYS:HB3	3:B:2113:HOH:O	1.81	0.80
1:C:480:GLU:HB3	3:C:2056:HOH:O	1.80	0.80
1:A:294:GLN:HG3	1:A:295:GLY:H	1.45	0.80
1:B:603:ARG:HG3	1:B:603:ARG:HH11	1.47	0.79
1:C:111:GLU:HG2	3:C:2038:HOH:O	1.82	0.78
1:C:362:PRO:HA	3:C:2106:HOH:O	1.81	0.78
1:C:373:GLU:CG	3:C:2112:HOH:O	2.30	0.78
1:B:10:ARG:H	1:B:10:ARG:CD	1.96	0.78
1:C:46:HIS:HD2	1:C:49:PHE:CE2	2.02	0.77
1:A:425:PRO:HG3	1:A:615:THR:HG22	1.67	0.77
1:B:18:ASN:ND2	1:B:21:LYS:HB2	1.99	0.77
1:C:46:HIS:CD2	1:C:49:PHE:HE2	2.02	0.76
1:A:9:LYS:HE3	1:A:10:ARG:H	1.51	0.76
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.68	0.75
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.01	0.75
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.66	0.75
1:C:10:ARG:HG2	3:C:2010:HOH:O	1.85	0.75
1:B:215:VAL:O	1:B:216:ARG:HB3	1.86	0.75
1:A:322:ASN:O	1:A:323:ARG:HB2	1.86	0.75
1:B:450:ASN:HB2	1:B:454:ASP:HB2	1.69	0.73
1:A:532:SER:HB2	1:A:673:PRO:HD2	1.70	0.73
1:B:203:PHE:HB3	1:B:629:SER:HB3	1.70	0.73
1:C:215:VAL:O	1:C:216:ARG:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:TRP:HZ2	1:C:141:MET:CE	2.02	0.73
1:A:59:HIS:HA	1:A:62:ILE:HD13	1.71	0.73
1:C:326:GLU:OE1	1:C:326:GLU:HA	1.89	0.72
1:C:46:HIS:HD2	1:C:49:PHE:HE2	1.36	0.72
1:A:300:GLY:HA2	3:A:2057:HOH:O	1.88	0.72
1:B:404:GLN:HG2	3:B:2106:HOH:O	1.90	0.72
1:C:349:LYS:HE2	3:C:2101:HOH:O	1.89	0.72
1:C:129:LYS:HE2	3:C:2040:HOH:O	1.89	0.71
1:B:480:GLU:HA	3:B:2049:HOH:O	1.89	0.71
1:A:279:ILE:HG12	1:A:319:LEU:HD21	1.72	0.71
1:B:633:ASN:HB3	3:B:2146:HOH:O	1.91	0.70
1:B:191:GLN:O	1:B:195:ARG:HG3	1.92	0.70
1:C:28:TRP:CZ2	1:C:141:MET:HE3	2.28	0.69
1:C:122:ASP:O	1:C:189:ARG:NH2	2.26	0.69
1:A:393:VAL:HB	3:A:2093:HOH:O	1.91	0.69
2:E:372:ASN:H	2:E:372:ASN:HD22	1.38	0.69
1:B:474:ASN:HB2	3:B:2119:HOH:O	1.93	0.69
1:A:83:ARG:HH11	1:A:83:ARG:CG	1.99	0.68
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.75	0.68
1:C:557:GLU:HB3	3:C:2155:HOH:O	1.94	0.68
1:C:44:ARG:HG2	1:C:44:ARG:NH1	2.07	0.68
1:C:664:ASP:HB2	3:C:2185:HOH:O	1.94	0.68
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.57	0.67
1:B:186:ARG:HB3	3:B:2046:HOH:O	1.92	0.67
1:B:207:LEU:HB2	1:B:212:MET:CE	2.21	0.67
1:B:122:ASP:O	1:B:189:ARG:NH2	2.26	0.67
1:C:167:GLU:OE2	1:C:216:ARG:NH1	2.28	0.66
1:B:582:THR:HA	3:B:2139:HOH:O	1.96	0.66
1:C:696:ASN:OD1	1:C:731:PHE:HB2	1.95	0.66
1:C:126:GLU:CA	1:C:129:LYS:HB2	2.18	0.66
1:A:450:ASN:HB2	1:A:454:ASP:OD2	1.96	0.66
1:A:176:VAL:HG11	1:A:212:MET:HE1	1.78	0.66
1:C:505:ARG:HD2	3:C:2142:HOH:O	1.95	0.66
1:A:639:ARG:HD3	3:A:2150:HOH:O	1.95	0.65
1:C:46:HIS:CD2	1:C:49:PHE:CE2	2.80	0.65
1:A:447:LYS:HE3	3:A:2102:HOH:O	1.96	0.65
1:B:568:PHE:CE2	1:B:574:ALA:HA	2.31	0.65
1:B:11:ASP:CG	1:B:12:GLY:N	2.52	0.65
1:B:621:PRO:HD3	1:B:694:SER:OG	1.97	0.64
1:A:226:VAL:HG12	1:A:461:LEU:HD23	1.79	0.64
1:A:321:ASN:HB3	1:A:405:GLU:OE1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LYS:HG3	1:B:609:HIS:CD2	2.31	0.64
1:C:28:TRP:HZ2	1:C:141:MET:HE3	1.60	0.64
1:A:296:GLY:HA3	3:A:2072:HOH:O	1.96	0.64
1:B:603:ARG:HG3	1:B:603:ARG:NH1	2.12	0.64
1:B:565:CYS:HB3	1:B:612:ARG:O	1.98	0.64
1:C:480:GLU:CB	3:C:2056:HOH:O	2.42	0.64
1:B:109:MET:HE1	1:B:166:TYR:CB	2.26	0.63
1:A:221:GLN:HG2	3:A:2056:HOH:O	1.98	0.63
1:B:633:ASN:N	1:B:633:ASN:HD22	1.94	0.63
1:B:110:VAL:CG1	1:B:117:ASN:HB3	2.29	0.63
1:A:83:ARG:HG3	1:A:83:ARG:NH1	1.91	0.62
1:B:24:ARG:HD2	3:B:2014:HOH:O	1.99	0.62
1:B:260:ARG:HH21	1:B:448:PRO:HG3	1.63	0.62
1:B:136:ASP:HB3	1:B:139:ARG:NH1	2.14	0.62
1:B:298:ARG:HG2	3:B:2071:HOH:O	1.97	0.62
1:B:260:ARG:HD2	1:B:365:TYR:CE2	2.35	0.62
1:C:376:GLU:HG2	3:C:2113:HOH:O	1.98	0.62
1:B:298:ARG:HB3	1:B:298:ARG:NH1	2.16	0.61
1:B:55:THR:HG23	1:B:56:SER:H	1.64	0.61
1:C:183:ASN:HB3	3:C:2053:HOH:O	2.01	0.60
1:C:196:PHE:HZ	1:C:207:LEU:HD11	1.66	0.60
1:B:331:ARG:HD2	3:B:2082:HOH:O	2.01	0.60
1:B:86:ILE:HG21	1:B:140:ASP:HB3	1.82	0.60
1:B:466:ALA:HA	1:B:516:GLY:O	2.00	0.60
1:B:46:HIS:HD2	1:B:49:PHE:CE2	2.20	0.60
1:B:215:VAL:O	1:B:216:ARG:CB	2.50	0.60
1:C:225:CYS:HB2	3:C:2128:HOH:O	2.02	0.60
1:C:392:ARG:NH1	1:C:392:ARG:HB3	2.17	0.60
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.85	0.59
1:A:18:ASN:CG	1:A:21:LYS:HB2	2.28	0.59
1:B:294:GLN:HG2	3:B:2066:HOH:O	2.03	0.59
1:A:260:ARG:HH21	1:A:434:ARG:NH2	2.01	0.59
1:B:266:SER:O	1:B:275:HIS:CD2	2.56	0.59
1:A:108:LYS:O	1:A:112:MET:HG2	2.02	0.58
1:B:376:GLU:HG3	3:B:2093:HOH:O	2.03	0.58
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.28	0.58
1:A:141:MET:HG2	3:A:2010:HOH:O	2.02	0.58
1:A:208:PRO:HG2	1:A:211:ILE:HD12	1.85	0.58
1:A:75:PRO:HD2	3:A:2012:HOH:O	2.04	0.58
1:A:584:LYS:HD2	3:A:2119:HOH:O	2.03	0.58
1:B:298:ARG:HD3	3:B:2068:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:GLU:HA	1:B:400:SER:HB2	1.84	0.58
1:B:283:LYS:NZ	1:B:327:GLY:HA2	2.19	0.58
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.85	0.57
1:B:298:ARG:HB2	3:B:2070:HOH:O	2.04	0.57
1:A:633:ASN:HB3	3:A:2128:HOH:O	2.04	0.57
1:B:443:ALA:O	1:B:444:LEU:HD23	2.04	0.57
1:C:212:MET:HA	1:C:212:MET:HE2	1.86	0.57
1:A:75:PRO:O	1:A:78:GLN:HB2	2.04	0.57
1:C:462:CYS:HB2	1:C:464:LEU:HD21	1.85	0.57
1:A:439:CYS:O	1:A:440:LEU:HB2	2.03	0.57
1:B:568:PHE:HE2	1:B:574:ALA:HA	1.69	0.56
1:C:21:LYS:O	1:C:25:VAL:HG23	2.05	0.56
1:B:700:ASP:OD2	1:B:735:ARG:HD3	2.05	0.56
1:A:532:SER:CB	1:A:673:PRO:HD2	2.36	0.56
1:B:110:VAL:HG13	1:B:117:ASN:HB3	1.88	0.56
1:A:144:SER:O	1:A:147:ALA:HB3	2.05	0.56
1:B:10:ARG:HH21	1:B:91:LYS:HE2	1.71	0.55
1:B:149:LYS:HE3	1:B:152:GLU:OE1	2.05	0.55
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.88	0.55
1:C:644:ILE:HG23	1:C:651:ILE:HG23	1.89	0.55
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.88	0.55
1:B:46:HIS:CD2	1:B:49:PHE:CE2	2.94	0.55
1:A:648:LYS:HG3	3:A:2137:HOH:O	2.07	0.55
1:B:5:LEU:O	1:B:17:ILE:HB	2.06	0.55
1:B:447:LYS:HD2	1:B:456:ASN:O	2.07	0.55
1:A:11:ASP:OD1	1:A:13:SER:OG	2.25	0.55
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.42	0.55
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.88	0.55
1:B:439:CYS:O	1:B:694:SER:HB3	2.06	0.55
1:C:518:ILE:HA	1:C:634:GLY:HA2	1.88	0.55
1:A:331:ARG:HH11	1:A:331:ARG:H	1.54	0.54
1:A:442:ILE:HG13	1:A:462:CYS:HB3	1.89	0.54
1:B:212:MET:O	1:B:216:ARG:NH2	2.38	0.54
1:A:212:MET:O	1:A:216:ARG:NH2	2.40	0.54
1:A:297:VAL:CG2	3:A:2074:HOH:O	2.55	0.54
1:A:510:ARG:HB2	1:A:512:THR:HG23	1.90	0.54
1:C:45:SER:HB2	1:C:61:THR:HG22	1.90	0.54
1:C:98:GLU:OE2	1:C:98:GLU:HA	2.07	0.54
1:B:418:ASP:HB2	3:B:2109:HOH:O	2.07	0.54
1:A:425:PRO:HG2	1:A:426:PHE:CD2	2.43	0.54
1:C:419:HIS:CD2	1:C:725:GLY:HA2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:HIS:HA	1:C:121:GLU:HB2	1.90	0.54
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.37	0.54
1:B:18:ASN:HD22	1:B:21:LYS:HE2	1.70	0.54
1:B:46:HIS:CD2	1:B:49:PHE:HE2	2.25	0.54
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.15	0.54
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.90	0.54
1:B:195:ARG:HD3	3:B:2047:HOH:O	2.07	0.54
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.90	0.54
1:B:10:ARG:HH21	1:B:91:LYS:CE	2.21	0.54
1:C:139:ARG:NH2	1:C:198:ASP:OD1	2.41	0.54
1:A:294:GLN:CG	1:A:295:GLY:H	2.14	0.53
1:B:136:ASP:HB3	1:B:139:ARG:HH11	1.73	0.53
1:B:432:PRO:CG	1:B:434:ARG:HD3	2.37	0.53
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.90	0.53
1:A:508:MET:HE2	1:A:508:MET:HA	1.90	0.53
1:A:181:PHE:O	1:A:189:ARG:HD2	2.08	0.53
1:A:203:PHE:HB3	1:A:629:SER:HB3	1.89	0.53
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.89	0.53
1:B:283:LYS:HZ1	1:B:327:GLY:HA2	1.74	0.53
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.44	0.53
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.91	0.53
1:A:710:PRO:HG2	1:A:713:GLN:HB2	1.91	0.53
1:C:321:ASN:HA	3:C:2120:HOH:O	2.08	0.53
1:C:28:TRP:CZ2	1:C:141:MET:CE	2.88	0.52
1:A:29:ALA:O	1:A:83:ARG:NH1	2.41	0.52
1:B:396:VAL:HG23	3:B:2103:HOH:O	2.08	0.52
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.92	0.52
1:C:18:ASN:ND2	1:C:21:LYS:HB2	2.25	0.52
1:B:236:SER:O	1:B:237:ILE:C	2.52	0.52
1:A:627:GLN:OE1	1:A:645:LYS:HE3	2.10	0.52
1:C:298:ARG:HB3	1:C:298:ARG:CZ	2.40	0.52
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.45	0.52
1:B:27:ASP:HA	1:B:38:ILE:HD11	1.92	0.52
1:C:172:LEU:HD23	1:C:172:LEU:C	2.35	0.52
1:C:464:LEU:HA	1:C:514:GLY:O	2.10	0.51
1:A:648:LYS:HD2	1:A:648:LYS:N	2.25	0.51
1:A:212:MET:HE2	1:A:212:MET:HA	1.92	0.51
1:A:420:CYS:HA	1:A:727:LYS:HD3	1.92	0.51
1:A:432:PRO:HG2	1:A:434:ARG:HD3	1.92	0.51
1:B:499:PRO:O	1:B:500:ILE:HG13	2.10	0.51
1:B:439:CYS:O	1:B:440:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:CYS:O	1:C:424:SER:HB2	2.11	0.51
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.46	0.51
1:A:344:TYR:O	1:A:347:LEU:HB3	2.11	0.51
1:B:700:ASP:OD2	1:B:735:ARG:CD	2.59	0.51
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.93	0.51
1:A:648:LYS:HD2	1:A:648:LYS:H	1.75	0.51
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.92	0.51
1:B:210:PRO:HG3	1:B:224:SER:HB3	1.93	0.51
1:A:648:LYS:HD3	3:A:2136:HOH:O	2.10	0.50
1:B:527:HIS:O	1:B:529:LYS:HE2	2.12	0.50
1:C:176:VAL:HG11	1:C:212:MET:HE1	1.92	0.50
1:B:55:THR:HG23	1:B:56:SER:N	2.26	0.50
1:C:28:TRP:HZ2	1:C:141:MET:HE1	1.74	0.50
1:A:54:LYS:HE3	3:A:2001:HOH:O	2.11	0.50
1:A:568:PHE:CE2	1:A:574:ALA:HA	2.46	0.50
1:B:308:MET:O	1:B:313:VAL:HG21	2.11	0.50
1:C:44:ARG:NH1	1:C:44:ARG:CG	2.73	0.50
1:C:373:GLU:HG3	3:C:2112:HOH:O	2.04	0.50
1:A:8:THR:HB	1:A:54:LYS:HA	1.93	0.50
1:A:328:ASN:O	1:A:329:ARG:HD3	2.12	0.50
1:B:310:HIS:O	1:B:313:VAL:HB	2.11	0.50
1:B:312:GLU:HG2	3:B:2075:HOH:O	2.11	0.50
1:C:138:ASP:O	1:C:141:MET:HB2	2.12	0.50
1:A:5:LEU:HB3	1:A:17:ILE:HG21	1.94	0.50
1:A:660:GLU:HG3	1:A:661:HIS:N	2.26	0.50
1:B:373:GLU:HA	1:B:376:GLU:HB2	1.94	0.49
1:B:46:HIS:HA	1:B:49:PHE:CD2	2.46	0.49
1:C:221:GLN:OE1	1:C:250:GLN:HG2	2.12	0.49
1:C:373:GLU:HB2	3:C:2111:HOH:O	2.12	0.49
1:A:356:PHE:CD1	1:A:361:VAL:HG11	2.47	0.49
1:A:21:LYS:O	1:A:25:VAL:HG23	2.13	0.49
1:B:298:ARG:HB3	1:B:298:ARG:HH11	1.76	0.49
1:B:109:MET:CE	1:B:166:TYR:HB3	2.35	0.49
1:A:58:ILE:O	1:A:62:ILE:HG23	2.13	0.49
1:B:329:ARG:HB3	1:B:331:ARG:HD3	1.94	0.49
1:B:568:PHE:CE2	1:B:574:ALA:CA	2.95	0.49
1:C:21:LYS:HD3	3:C:2011:HOH:O	2.13	0.49
1:C:91:LYS:HB3	3:C:2007:HOH:O	2.12	0.49
1:A:343:MET:HE2	1:A:343:MET:HA	1.95	0.49
1:C:304:LEU:HD23	1:C:304:LEU:C	2.37	0.49
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:CD1	1:A:131:MET:CE	2.96	0.48
1:A:331:ARG:HH11	1:A:331:ARG:CG	2.26	0.48
1:B:637:PRO:HG2	1:B:669:LEU:HD12	1.95	0.48
1:C:298:ARG:HB3	1:C:298:ARG:NH1	2.29	0.48
2:F:369:ASP:O	2:F:370:LEU:C	2.56	0.48
1:A:311:LEU:HA	1:A:355:LEU:HB3	1.94	0.48
1:C:243:ALA:HA	1:C:500:ILE:HD11	1.95	0.48
1:C:369:PHE:CD1	1:C:434:ARG:HB3	2.49	0.48
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.95	0.48
1:A:260:ARG:HH21	1:A:434:ARG:HH22	1.60	0.48
1:B:529:LYS:HD2	1:B:535:SER:O	2.13	0.48
1:A:396:VAL:CG1	2:D:365:VAL:HG11	2.43	0.48
1:B:342:LEU:HD12	1:B:376:GLU:HG2	1.96	0.48
1:A:426:PHE:O	1:A:428:PRO:HD3	2.13	0.48
1:A:229:GLU:O	1:A:448:PRO:HA	2.13	0.48
1:A:314:GLU:HB2	3:A:2078:HOH:O	2.13	0.48
1:B:266:SER:O	1:B:275:HIS:HD2	1.95	0.48
1:A:430:ILE:HD12	1:A:570:GLU:HA	1.95	0.47
1:B:633:ASN:N	1:B:633:ASN:ND2	2.62	0.47
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.97	0.47
1:A:18:ASN:ND2	1:A:21:LYS:HB2	2.29	0.47
1:B:264:LEU:O	1:B:389:ARG:NH2	2.47	0.47
1:A:373:GLU:HA	1:A:376:GLU:HB3	1.95	0.47
1:B:465:SER:O	1:B:515:ILE:HA	2.14	0.47
1:B:150:GLN:HB2	1:B:628:ILE:HD13	1.97	0.47
1:B:160:ARG:NE	1:B:160:ARG:CA	2.57	0.47
1:B:442:ILE:HG13	1:B:462:CYS:SG	2.54	0.47
1:B:701:PRO:C	1:B:703:ARG:H	2.22	0.47
1:A:644:ILE:HG23	1:A:651:ILE:HG23	1.97	0.47
1:C:219:THR:O	1:C:220:ARG:NH1	2.44	0.47
1:C:227:LEU:N	1:C:227:LEU:HD12	2.30	0.47
1:C:418:ASP:O	1:C:422:THR:HG23	2.15	0.47
1:A:244:ILE:O	1:A:248:VAL:HG22	2.14	0.47
1:A:339:ILE:O	1:A:416:ASN:HA	2.15	0.47
1:A:435:GLN:HG2	3:A:2060:HOH:O	2.15	0.47
1:B:7:VAL:HG22	1:B:17:ILE:HG12	1.96	0.47
1:C:572:THR:HB	1:C:577:ILE:HB	1.96	0.47
1:A:83:ARG:HD2	1:A:141:MET:HG3	1.96	0.47
1:A:542:LYS:HG3	1:A:596:HIS:CD2	2.50	0.47
1:B:8:THR:HB	1:B:54:LYS:HA	1.97	0.47
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:PRO:HB3	1:B:573:TYR:CE2	2.50	0.47
1:B:711:MET:HE3	3:B:2105:HOH:O	2.15	0.47
1:B:9:LYS:NZ	1:B:10:ARG:HD3	2.30	0.47
1:B:633:ASN:O	1:B:634:GLY:C	2.58	0.47
1:C:207:LEU:HD23	1:C:465:SER:OG	2.15	0.47
1:C:248:VAL:HG11	1:C:289:VAL:HA	1.97	0.47
1:C:294:GLN:HB2	1:C:298:ARG:O	2.15	0.47
1:C:531:TYR:CE2	1:C:637:PRO:HD3	2.50	0.47
1:A:437:ASN:ND2	1:A:439:CYS:H	2.13	0.46
1:B:307:PRO:HA	1:B:338:GLN:HB2	1.95	0.46
1:C:225:CYS:CB	3:C:2128:HOH:O	2.62	0.46
1:A:134:PHE:CD1	1:A:194:LYS:HD2	2.51	0.46
1:A:623:GLU:O	1:A:627:GLN:HB2	2.15	0.46
1:B:458:GLU:OE1	1:B:510:ARG:NH1	2.48	0.46
1:B:226:VAL:HG12	1:B:461:LEU:HD23	1.97	0.46
1:B:711:MET:HA	1:B:714:LEU:HD12	1.96	0.46
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.96	0.46
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.97	0.46
1:C:109:MET:HG3	1:C:115:TYR:CE2	2.51	0.46
1:C:552:LEU:HD21	1:C:573:TYR:CZ	2.50	0.46
1:A:424:SER:HB2	1:A:425:PRO:HD2	1.96	0.46
1:B:134:PHE:CD2	1:B:194:LYS:HB2	2.50	0.46
1:C:389:ARG:HA	3:C:2116:HOH:O	2.16	0.46
1:A:379:TYR:O	1:A:383:GLU:HG2	2.15	0.46
1:A:548:GLN:OE1	1:A:548:GLN:HA	2.15	0.46
1:C:508:MET:HE2	1:C:508:MET:HA	1.97	0.46
1:A:325:VAL:HG13	1:A:328:ASN:HD21	1.79	0.46
1:A:385:ASP:OD1	1:A:385:ASP:C	2.59	0.46
1:B:226:VAL:HG11	1:B:247:TYR:CD2	2.51	0.46
1:A:307:PRO:HA	1:A:338:GLN:HB2	1.97	0.46
1:C:364:LEU:CD2	1:C:375:PHE:CE1	2.99	0.46
1:B:418:ASP:N	1:B:418:ASP:OD1	2.46	0.45
1:A:122:ASP:O	1:A:189:ARG:NH2	2.50	0.45
1:A:159:ASN:OD1	1:A:162:THR:N	2.47	0.45
1:B:102:LEU:HD11	1:B:175:LEU:HD21	1.99	0.45
1:C:44:ARG:NH1	3:C:2022:HOH:O	2.50	0.45
1:C:134:PHE:CD2	1:C:194:LYS:HB2	2.51	0.45
1:A:91:LYS:HE2	3:A:2028:HOH:O	2.17	0.45
1:A:371:ASP:CG	1:A:374:GLU:HB3	2.42	0.45
1:A:76:ASP:C	1:A:78:GLN:N	2.71	0.45
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:THR:OG1	1:A:732:GLN:HG3	2.17	0.45
1:B:670:TRP:CE2	1:B:735:ARG:HG3	2.51	0.45
1:C:47:ILE:HG13	1:C:47:ILE:O	2.17	0.45
1:C:307:PRO:HD3	3:C:2098:HOH:O	2.16	0.45
1:C:386:ASP:HA	1:C:390:LYS:NZ	2.30	0.45
1:B:171:PHE:HA	1:B:174:ILE:HG22	1.98	0.45
1:B:279:ILE:HD11	1:B:315:SER:HB3	1.99	0.45
1:B:436:SER:OG	1:B:442:ILE:O	2.30	0.45
1:B:10:ARG:NH1	1:B:55:THR:HG21	2.32	0.45
1:C:297:VAL:HG22	3:C:2086:HOH:O	2.17	0.45
1:A:149:LYS:HE2	1:A:152:GLU:OE1	2.17	0.45
1:A:294:GLN:CG	1:A:295:GLY:N	2.80	0.45
1:A:5:LEU:HB3	1:A:17:ILE:CG2	2.47	0.44
1:B:85:ALA:O	1:B:89:LEU:HG	2.18	0.44
1:C:229:GLU:O	1:C:448:PRO:HA	2.18	0.44
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.99	0.44
1:B:568:PHE:CE2	1:B:574:ALA:HB2	2.51	0.44
1:B:662:LEU:O	1:B:665:ALA:HB3	2.17	0.44
1:A:227:LEU:HB2	1:A:460:ALA:HB3	2.00	0.44
1:A:338:GLN:NE2	1:A:434:ARG:O	2.50	0.44
1:B:154:LYS:HD2	1:B:624:THR:HG21	1.99	0.44
1:A:736:ASP:OD2	1:A:736:ASP:N	2.43	0.44
1:B:568:PHE:CD2	1:B:574:ALA:HB2	2.53	0.44
1:C:420:CYS:HA	1:C:727:LYS:HE2	1.99	0.44
1:A:232:ASP:HB2	1:A:260:ARG:O	2.18	0.44
1:A:276:THR:HG21	1:B:292:CYS:O	2.18	0.44
1:A:286:GLN:HG3	1:A:333:MET:HG3	2.00	0.44
1:C:392:ARG:HB3	1:C:392:ARG:HH11	1.83	0.44
1:A:332:HIS:CD2	3:A:2075:HOH:O	2.71	0.44
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.51	0.44
1:B:619:LEU:HB2	1:B:693:ILE:HG23	2.00	0.43
1:C:27:ASP:HA	1:C:38:ILE:HD11	2.00	0.43
1:C:442:ILE:HD11	1:C:464:LEU:HD21	1.98	0.43
1:B:91:LYS:HE3	3:B:2007:HOH:O	2.18	0.43
1:B:191:GLN:HE21	1:B:191:GLN:HB2	1.51	0.43
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.18	0.43
1:B:421:ASN:HB3	1:B:428:PRO:HB3	2.00	0.43
1:C:37:SER:CB	1:C:40:GLN:HB2	2.48	0.43
1:C:586:ASP:OD1	1:C:586:ASP:N	2.49	0.43
1:B:167:GLU:OE2	1:B:216:ARG:NH1	2.51	0.43
1:C:221:GLN:HG2	3:C:2072:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:HB3	1:B:40:GLN:HB2	2.01	0.43
1:B:331:ARG:HH11	1:B:331:ARG:H	1.65	0.43
1:B:587:LEU:CD1	1:B:687:LYS:HB2	2.48	0.43
1:C:46:HIS:HA	1:C:49:PHE:CD2	2.54	0.43
1:C:215:VAL:O	1:C:216:ARG:CB	2.65	0.43
1:C:283:LYS:NZ	1:C:327:GLY:HA2	2.34	0.43
1:C:701:PRO:C	1:C:703:ARG:H	2.25	0.43
1:B:386:ASP:C	1:B:388:ILE:H	2.26	0.43
1:B:729:LEU:HA	1:B:729:LEU:HD23	1.71	0.43
1:A:296:GLY:CA	3:A:2072:HOH:O	2.61	0.43
1:A:383:GLU:HA	1:A:390:LYS:HE2	1.99	0.43
1:A:642:VAL:HG22	1:A:655:VAL:HG22	2.00	0.43
1:B:371:ASP:CG	1:B:374:GLU:HB3	2.44	0.43
1:C:37:SER:HB3	1:C:40:GLN:HB2	2.00	0.43
1:A:701:PRO:HB3	1:A:707:GLY:O	2.19	0.43
1:B:110:VAL:HG11	1:B:117:ASN:HB3	2.00	0.43
1:B:227:LEU:HD11	1:B:437:ASN:HB3	2.00	0.43
1:A:24:ARG:HD2	3:A:2009:HOH:O	2.18	0.43
1:C:561:GLU:HB3	1:C:562:GLN:HG3	2.01	0.43
1:A:207:LEU:HB2	1:A:212:MET:HE3	2.01	0.42
1:C:432:PRO:HG2	1:C:434:ARG:HD3	2.00	0.42
1:A:294:GLN:HG3	1:A:295:GLY:N	2.25	0.42
1:A:436:SER:OG	1:A:440:LEU:HA	2.19	0.42
1:A:529:LYS:HD2	1:A:535:SER:O	2.19	0.42
1:C:37:SER:OG	1:C:40:GLN:HB2	2.19	0.42
1:C:109:MET:HE3	1:C:114:LYS:HB2	2.00	0.42
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.49	0.42
1:C:639:ARG:HH11	1:C:639:ARG:H	1.66	0.42
1:A:475:LEU:HD21	1:A:543:THR:HG23	2.01	0.42
1:A:639:ARG:NH1	3:A:2134:HOH:O	2.48	0.42
1:B:663:HIS:CD2	3:B:2155:HOH:O	2.72	0.42
1:C:685:MET:O	1:C:686:GLN:C	2.61	0.42
1:A:10:ARG:HB3	3:A:2003:HOH:O	2.19	0.42
1:A:322:ASN:O	1:A:323:ARG:CB	2.63	0.42
1:B:9:LYS:NZ	3:B:2006:HOH:O	2.51	0.42
1:C:116:ASP:OD2	1:C:220:ARG:NH2	2.44	0.42
1:B:72:ARG:H	1:B:72:ARG:HG2	1.34	0.42
1:B:207:LEU:CD2	1:B:465:SER:OG	2.67	0.42
1:B:322:ASN:HA	3:B:2082:HOH:O	2.19	0.42
1:A:352:ASP:OD2	1:A:394:LYS:HD3	2.18	0.42
1:A:572:THR:HB	1:A:577:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ILE:HD11	1:B:174:ILE:HG21	2.01	0.42
1:B:218:PRO:O	1:B:220:ARG:NH1	2.52	0.42
1:B:264:LEU:HD12	1:B:276:THR:C	2.45	0.42
1:B:325:VAL:HG12	3:B:2079:HOH:O	2.19	0.42
1:B:343:MET:HE2	1:B:343:MET:HA	2.01	0.42
1:B:518:ILE:O	1:B:518:ILE:HG13	2.19	0.42
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.68	0.42
1:C:309:TRP:O	1:C:355:LEU:HA	2.20	0.42
1:C:322:ASN:HD22	1:C:322:ASN:HA	1.64	0.42
1:C:557:GLU:H	1:C:557:GLU:HG2	1.72	0.42
1:A:131:MET:HA	1:A:134:PHE:CD2	2.55	0.42
1:A:385:ASP:OD1	1:A:386:ASP:N	2.52	0.42
1:B:385:ASP:OD1	1:B:386:ASP:N	2.53	0.42
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.19	0.42
1:C:96:GLN:HE21	1:C:98:GLU:HB3	1.85	0.41
1:C:208:PRO:HB2	3:C:2062:HOH:O	2.19	0.41
1:C:349:LYS:O	1:C:351:GLU:HG3	2.20	0.41
1:A:244:ILE:HG12	1:A:254:ILE:HG21	2.01	0.41
1:A:297:VAL:HG23	3:A:2074:HOH:O	2.19	0.41
1:A:538:ASN:HB3	1:A:593:GLU:OE1	2.20	0.41
1:B:463:THR:HG22	1:B:489:LEU:HD22	2.03	0.41
1:B:545:GLU:HG3	1:B:595:LEU:HD23	2.02	0.41
1:B:701:PRO:O	1:B:707:GLY:HA2	2.20	0.41
1:A:457:GLY:C	1:A:502:ALA:HB1	2.46	0.41
1:B:86:ILE:HD11	1:B:148:VAL:HG22	2.02	0.41
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.82	0.41
1:B:568:PHE:HE1	1:B:611:LEU:HB2	1.85	0.41
1:C:31:GLU:OE1	1:C:31:GLU:HA	2.21	0.41
1:A:151:LEU:HA	1:A:155:TYR:HB2	2.02	0.41
1:A:331:ARG:HD3	3:A:2079:HOH:O	2.20	0.41
1:B:149:LYS:HA	1:B:149:LYS:HD2	1.41	0.41
1:B:262:ARG:HD3	1:B:266:SER:HB2	2.01	0.41
1:C:374:GLU:HG3	1:C:378:LEU:HD12	2.03	0.41
1:C:403:MET:HE2	1:C:718:LEU:HB2	2.02	0.41
1:C:639:ARG:H	1:C:639:ARG:NH1	2.17	0.41
1:A:294:GLN:NE2	1:A:294:GLN:CA	2.56	0.41
1:A:390:LYS:HD2	1:A:392:ARG:NH2	2.35	0.41
1:B:730:NIY:CG	1:B:731:PHE:H	2.33	0.41
1:C:10:ARG:HB2	3:C:2009:HOH:O	2.19	0.41
1:A:7:VAL:HG23	1:A:17:ILE:HB	2.03	0.41
2:E:372:ASN:ND2	2:E:372:ASN:N	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:O	1:A:23:HIS:C	2.63	0.41
1:A:262:ARG:HE	1:A:262:ARG:HB3	1.62	0.41
1:B:244:ILE:HG12	1:B:254:ILE:HG21	2.01	0.41
1:B:586:ASP:OD1	1:B:586:ASP:N	2.53	0.41
1:C:394:LYS:HD3	3:C:2103:HOH:O	2.21	0.41
1:A:55:THR:O	1:A:56:SER:C	2.64	0.41
1:A:107:VAL:O	1:A:111:GLU:HB2	2.21	0.41
1:B:174:ILE:O	1:B:177:ALA:HB3	2.21	0.41
1:C:45:SER:HA	1:C:48:GLN:HE21	1.86	0.41
1:C:292:CYS:HB3	3:C:2084:HOH:O	2.20	0.41
1:C:323:ARG:HG3	1:C:323:ARG:O	2.20	0.41
1:C:548:GLN:CB	1:C:688:PHE:HB3	2.50	0.41
1:B:711:MET:HB3	2:E:365:VAL:HG22	2.03	0.41
1:B:143:PHE:CE1	1:B:203:PHE:HE1	2.38	0.40
1:B:568:PHE:CE1	1:B:611:LEU:HB2	2.56	0.40
1:A:701:PRO:O	1:A:707:GLY:HA2	2.21	0.40
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.92	0.40
1:C:370:ALA:HA	1:C:428:PRO:HB2	2.02	0.40
1:A:400:SER:O	1:A:404:GLN:HB2	2.21	0.40
1:A:639:ARG:NH2	3:A:2134:HOH:O	2.48	0.40
1:C:297:VAL:CG2	3:C:2086:HOH:O	2.69	0.40
1:A:159:ASN:HB3	1:A:164:GLU:H	1.87	0.40
1:A:294:GLN:HB3	1:A:297:VAL:H	1.87	0.40
1:A:489:LEU:O	1:A:492:LEU:HB3	2.22	0.40
1:A:592:ASN:OD1	1:A:592:ASN:C	2.65	0.40
1:B:9:LYS:HZ2	1:B:10:ARG:HD3	1.87	0.40
1:B:518:ILE:O	1:B:519:ASN:CB	2.69	0.40
1:C:217:THR:HB	1:C:218:PRO:CD	2.51	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	B	407/761 (54%)	371 (91%)	33 (8%)	3 (1%)	18	49
1	C	722/761 (95%)	665 (92%)	52 (7%)	5 (1%)	18	49
2	D	9/20 (45%)	5 (56%)	3 (33%)	1 (11%)	0	2
2	E	9/20 (45%)	7 (78%)	1 (11%)	1 (11%)	0	2
2	F	10/20 (50%)	9 (90%)	1 (10%)	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	1158/1602 (72%)	1058 (91%)	90 (8%)	10 (1%)	14	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	VAL
1	C	216	ARG
1	C	10	ARG
1	C	300	GLY
2	D	371	SER
2	E	371	SER
1	B	519	ASN
1	B	691	GLN
1	C	5	LEU
1	B	452	VAL

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	624/650 (96%)	547 (88%)	77 (12%)	4	20
1	B	624/650 (96%)	544 (87%)	80 (13%)	4	18
1	C	624/650 (96%)	551 (88%)	73 (12%)	5	22
2	D	11/19 (58%)	7 (64%)	4 (36%)	0	0
2	E	11/19 (58%)	9 (82%)	2 (18%)	2	8
2	F	12/19 (63%)	9 (75%)	3 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	3/19 (16%)	2 (67%)	1 (33%)	0 0
All	All	1909/2026 (94%)	1669 (87%)	240 (13%)	4 19

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	11	ASP
1	A	14	THR
1	A	15	GLU
1	A	17	ILE
1	A	20	ASP
1	A	21	LYS
1	A	27	ASP
1	A	35	ASN
1	A	44	ARG
1	A	53	ILE
1	A	58	ILE
1	A	60	GLU
1	A	62	ILE
1	A	72	ARG
1	A	83	ARG
1	A	92	LYS
1	A	96	GLN
1	A	118	HIS
1	A	129	LYS
1	A	130	GLN
1	A	139	ARG
1	A	149	LYS
1	A	158	GLN
1	A	165	ILE
1	A	183	ASN
1	A	187	GLU
1	A	189	ARG
1	A	190	LEU
1	A	204	LYS
1	A	206	SER
1	A	216	ARG
1	A	225	CYS
1	A	260	ARG
1	A	276	THR

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Mol	Chain	Res	Type
1	A	283	LYS
1	A	294	GLN
1	A	297	VAL
1	A	298	ARG
1	A	314	GLU
1	A	315	SER
1	A	317	LEU
1	A	321	ASN
1	A	325	VAL
1	A	326	GLU
1	A	329	ARG
1	A	331	ARG
1	A	341	LYS
1	A	343	MET
1	A	364	LEU
1	A	376	GLU
1	A	381	LYS
1	A	396	VAL
1	A	411	ARG
1	A	430	ILE
1	A	434	ARG
1	A	440	LEU
1	A	452	VAL
1	A	465	SER
1	A	474	ASN
1	A	562	GLN
1	A	570	GLU
1	A	581	ASP
1	A	585	LYS
1	A	616	LEU
1	A	624	THR
1	A	625	SER
1	A	629	SER
1	A	645	LYS
1	A	647	SER
1	A	648	LYS
1	A	653	ARG
1	A	698	ASN
1	A	713	GLN
1	A	733	ASN
1	A	734	THR
1	B	5	LEU

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Mol	Chain	Res	Type
1	B	7	VAL
1	B	9	LYS
1	B	10	ARG
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	24	ARG
1	B	60	GLU
1	B	72	ARG
1	B	73	ASP
1	B	80	LEU
1	B	91	LYS
1	B	92	LYS
1	B	96	GLN
1	B	122	ASP
1	B	125	GLU
1	B	126	GLU
1	B	129	LYS
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	152	GLU
1	B	160	ARG
1	B	161	VAL
1	B	183	ASN
1	B	186	ARG
1	B	191	GLN
1	B	194	LYS
1	B	206	SER
1	B	207	LEU
1	B	216	ARG
1	B	221	GLN
1	B	225	CYS
1	B	260	ARG
1	B	266	SER
1	B	276	THR
1	B	278	CYS
1	B	313	VAL
1	B	317	LEU
1	B	325	VAL
1	B	331	ARG
1	B	341	LYS

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Mol	Chain	Res	Type
1	B	364	LEU
1	B	373	GLU
1	B	380	THR
1	B	391	GLN
1	B	394	LYS
1	B	411	ARG
1	B	414	ILE
1	B	418	ASP
1	B	430	ILE
1	B	434	ARG
1	B	436	SER
1	B	440	LEU
1	B	447	LYS
1	B	451	ASP
1	B	452	VAL
1	B	465	SER
1	B	484	LEU
1	B	557	GLU
1	B	569	ASN
1	B	570	GLU
1	B	575	LYS
1	B	577	ILE
1	B	585	LYS
1	B	603	ARG
1	B	604	GLU
1	B	609	HIS
1	B	616	LEU
1	B	623	GLU
1	B	625	SER
1	B	629	SER
1	B	633	ASN
1	B	636	GLU
1	B	651	ILE
1	B	664	ASP
1	B	681	LEU
1	B	706	SER
1	B	736	ASP
1	C	5	LEU
1	C	9	LYS
1	C	13	SER
1	C	14	THR
1	C	15	GLU

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Mol	Chain	Res	Type
1	C	16	ARG
1	C	17	ILE
1	C	21	LYS
1	C	35	ASN
1	C	38	ILE
1	C	40	GLN
1	C	44	ARG
1	C	55	THR
1	C	58	ILE
1	C	60	GLU
1	C	62	ILE
1	C	92	LYS
1	C	98	GLU
1	C	111	GLU
1	C	126	GLU
1	C	129	LYS
1	C	130	GLN
1	C	139	ARG
1	C	141	MET
1	C	152	GLU
1	C	165	ILE
1	C	183	ASN
1	C	187	GLU
1	C	204	LYS
1	C	216	ARG
1	C	260	ARG
1	C	276	THR
1	C	294	GLN
1	C	298	ARG
1	C	317	LEU
1	C	325	VAL
1	C	326	GLU
1	C	343	MET
1	C	345	THR
1	C	364	LEU
1	C	380	THR
1	C	392	ARG
1	C	396	VAL
1	C	403	MET
1	C	411	ARG
1	C	434	ARG
1	C	439	CYS

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Mol	Chain	Res	Type
1	C	440	LEU
1	C	447	LYS
1	C	451	ASP
1	C	452	VAL
1	C	461	LEU
1	C	465	SER
1	C	484	LEU
1	C	510	ARG
1	C	530	ARG
1	C	553	LYS
1	C	557	GLU
1	C	561	GLU
1	C	566	PRO
1	C	570	GLU
1	C	575	LYS
1	C	586	ASP
1	C	607	LYS
1	C	616	LEU
1	C	625	SER
1	C	626	SER
1	C	629	SER
1	C	639	ARG
1	C	645	LYS
1	C	648	LYS
1	C	676	ASP
1	C	708	LYS
2	D	365	VAL
2	D	367	THR
2	D	368	ASP
2	D	375	LEU
2	E	367	THR
2	E	372	ASN
2	F	364	GLU
2	F	368	ASP
2	F	374	GLN
2	P	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	88	HIS

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Mol	Chain	Res	Type
1	A	117	ASN
1	A	158	GLN
1	A	294	GLN
1	A	453	ASN
1	A	609	HIS
1	A	627	GLN
1	A	686	GLN
1	A	696	ASN
1	A	732	GLN
1	A	733	ASN
1	B	18	ASN
1	B	46	HIS
1	B	88	HIS
1	B	130	GLN
1	B	150	GLN
1	B	191	GLN
1	B	250	GLN
1	B	275	HIS
1	B	328	ASN
1	B	453	ASN
1	B	556	ASN
1	B	613	ASN
1	B	633	ASN
1	B	663	HIS
1	B	696	ASN
1	B	732	GLN
1	B	733	ASN
1	C	18	ASN
1	C	46	HIS
1	C	48	GLN
1	C	59	HIS
1	C	88	HIS
1	C	117	ASN
1	C	275	HIS
1	C	322	ASN
1	C	328	ASN
1	C	332	HIS
1	C	391	GLN
1	C	456	ASN
1	C	596	HIS
1	C	609	HIS
1	C	613	ASN

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Mol	Chain	Res	Type
1	C	661	HIS
1	C	663	HIS
1	C	732	GLN
2	E	372	ASN
2	F	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	NIY	C	730	1	14,15,16	0.99	1 (7%)	11,20,22	1.21	1 (9%)
1	NIY	A	730	1	14,15,16	0.96	1 (7%)	11,20,22	1.36	2 (18%)
1	NIY	B	730	1	14,15,16	1.02	1 (7%)	11,20,22	1.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NIY	C	730	1	-	3/7/10/12	0/1/1/1
1	NIY	A	730	1	-	3/7/10/12	0/1/1/1
1	NIY	B	730	1	-	3/7/10/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	730	NIY	CE1-NN	-2.74	1.40	1.45
1	C	730	NIY	CE1-NN	-2.64	1.40	1.45
1	A	730	NIY	CE1-NN	-2.63	1.40	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	730	NIY	CB-CG-CD1	-2.65	115.88	120.43
1	A	730	NIY	CD2-CG-CD1	2.28	121.69	118.55
1	C	730	NIY	CB-CG-CD1	-2.09	116.83	120.43

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	730	NIY	O-C-CA-CB
1	B	730	NIY	O-C-CA-CB
1	C	730	NIY	O-C-CA-CB
1	B	730	NIY	CA-CB-CG-CD2
1	B	730	NIY	CA-CB-CG-CD1
1	C	730	NIY	CA-CB-CG-CD2
1	C	730	NIY	CA-CB-CG-CD1
1	A	730	NIY	CA-CB-CG-CD2
1	A	730	NIY	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	730	NIY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/761 (95%)	-0.63	1 (0%) 92 86	26, 44, 66, 93	0
1	B	726/761 (95%)	-0.54	2 (0%) 90 80	32, 46, 64, 89	0
1	C	726/761 (95%)	-0.78	2 (0%) 90 80	20, 34, 54, 82	0
2	D	11/20 (55%)	0.07	0 100 100	74, 84, 90, 91	0
2	E	11/20 (55%)	0.49	1 (9%) 15 8	77, 82, 88, 89	0
2	F	12/20 (60%)	0.32	0 100 100	71, 80, 88, 88	0
2	P	3/20 (15%)	0.15	0 100 100	43, 43, 46, 47	0
All	All	2215/2363 (93%)	-0.63	6 (0%) 90 80	20, 41, 67, 93	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	VAL	3.6
1	C	737	GLY	3.4
1	A	737	GLY	2.9
1	B	737	GLY	2.3
2	E	365	VAL	2.3
1	C	297	VAL	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	NIY	A	730	15/16	0.95	0.08	40,42,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	NIY	B	730	15/16	0.97	0.07	37,40,43,45	0
1	NIY	C	730	15/16	0.97	0.06	30,34,39,40	0

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.