



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:46 AM UTC

PDB ID : 2XAV / pdb_00002xav
Title : Ribonucleotide reductase Y731NO2Y and Y730F modified R1 subunit of E. coli
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on : 2010-03-31
Resolution : 2.80 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:

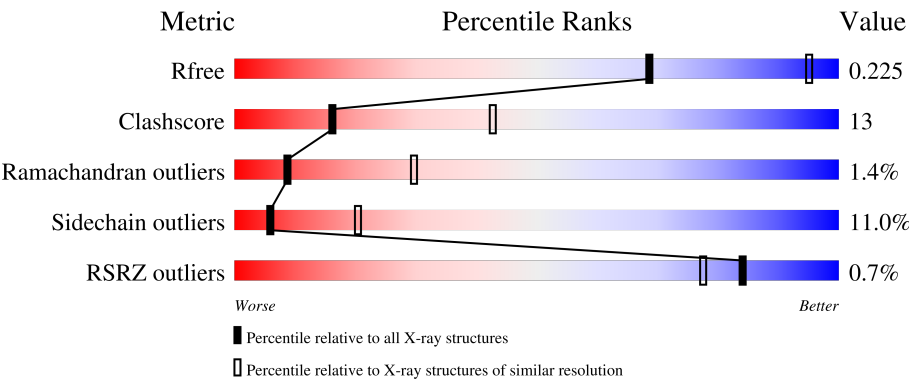
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	10% 68%23%...
1	B	761	64%27%...5%
1	C	761	68%24%...5%
2	D	20	40%25%15%20%
2	E	20	10%55%20%5%20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	20	 60% 15% 5% 20%
2	P	20	 10% 5% 85%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18459 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	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1098	24			
1	B	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1098	24			
1	C	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1098	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 RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA.

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	176	Total	O	0	0
			176	176		

Continued on next page...

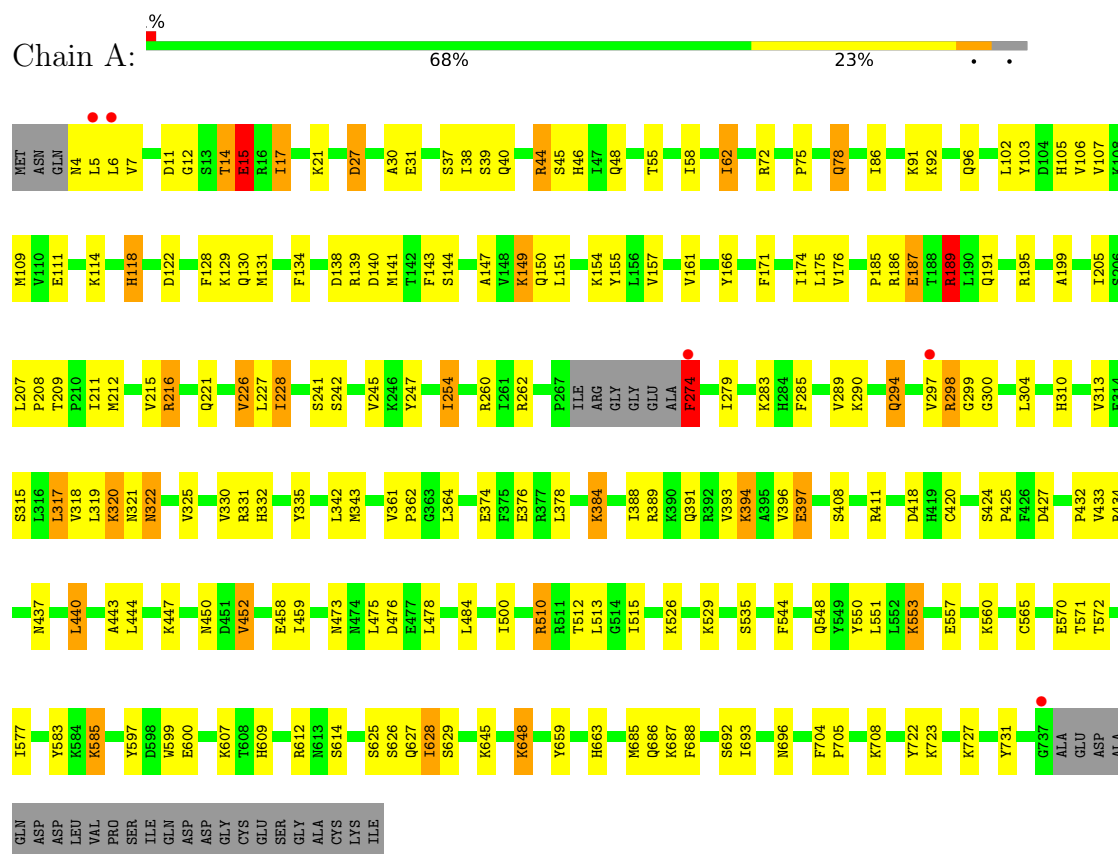
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	183	Total 183	O 183	0	0
3	C	259	Total 259	O 259	0	0
3	D	2	Total 2	O 2	0	0
3	F	3	Total 3	O 3	0	0
3	P	4	Total 4	O 4	0	0

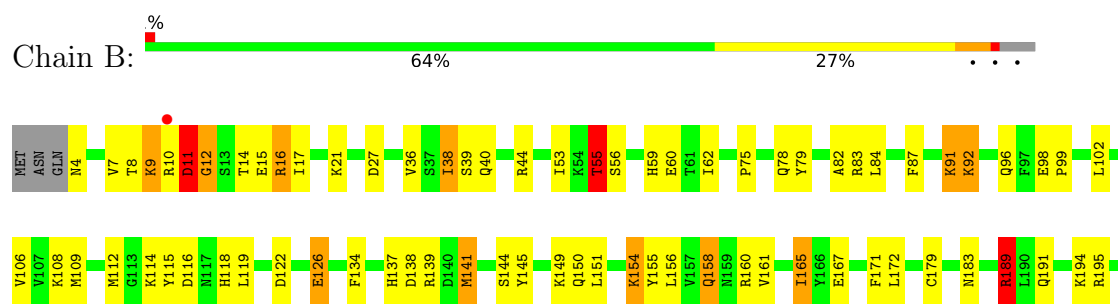
3 Residue-property plots [i](#)

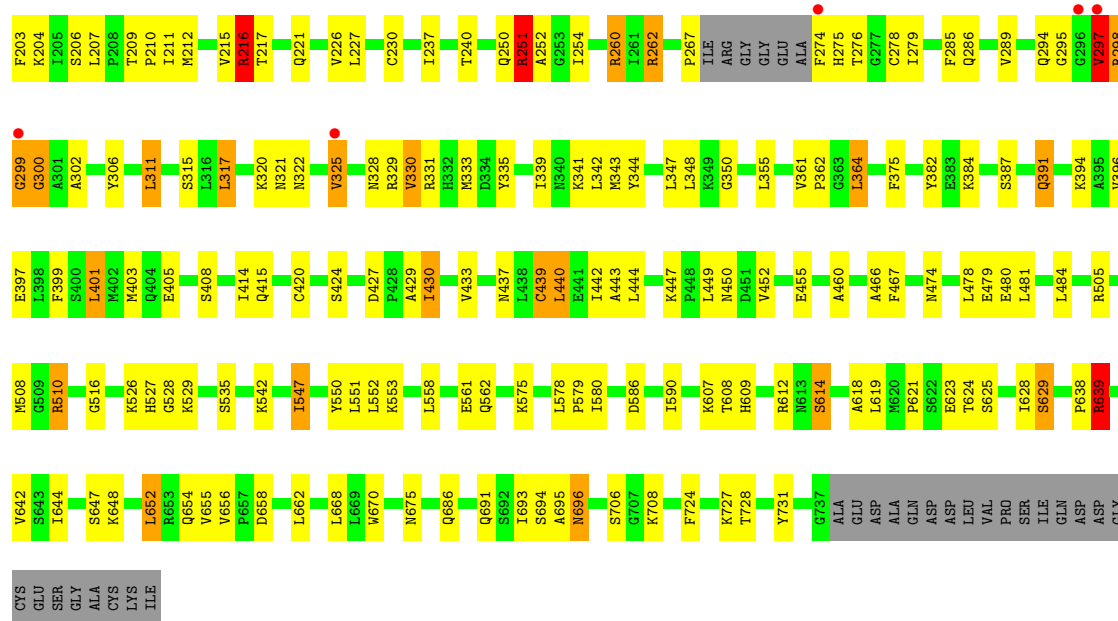
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



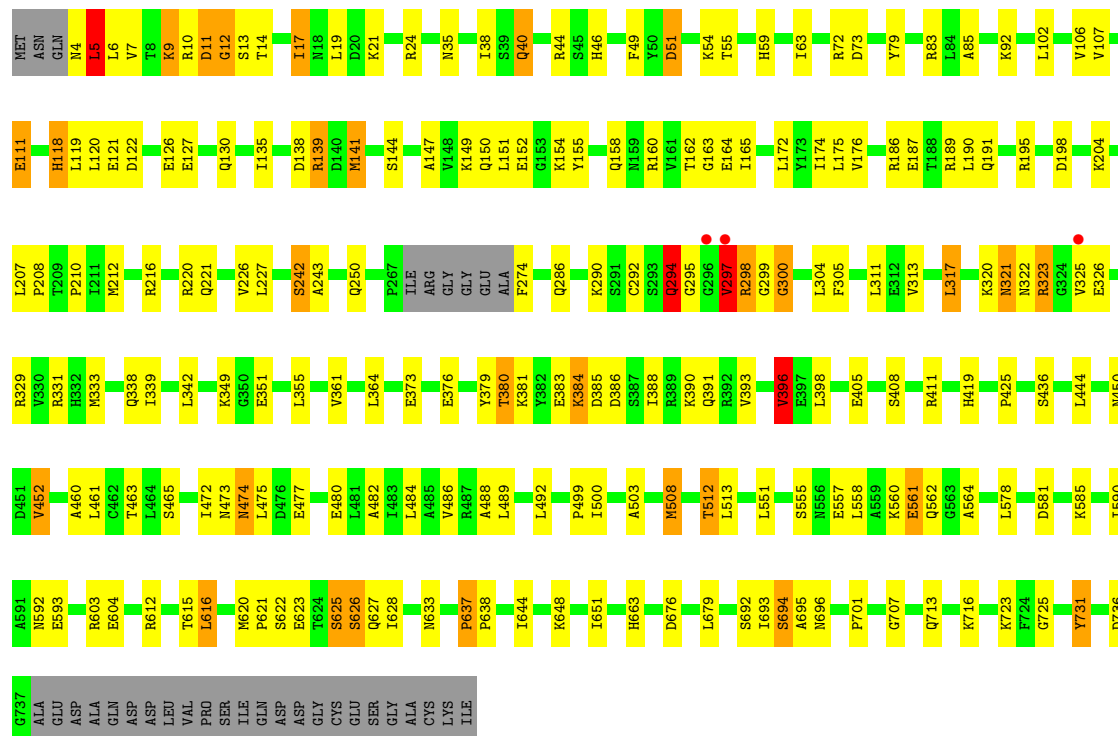
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA





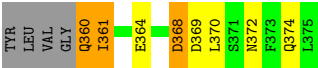
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C: 68% 24%

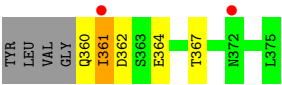


• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

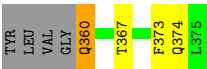
Chain D: 40% 25% 15% 20%



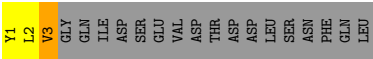
● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



● 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	224.66Å 224.66Å 336.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.80 168.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (169.03-2.80) 93.6 (168.42-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.169 , 0.247 (Not available) , 0.225	Depositor DCC
R_{free} test set	3787 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18459	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.84	2/5916 (0.0%)	1.03	5/8010 (0.1%)
1	B	0.87	5/5916 (0.1%)	1.05	15/8010 (0.2%)
1	C	0.98	4/5916 (0.1%)	1.10	12/8010 (0.1%)
2	D	0.69	0/129	1.02	1/173 (0.6%)
2	E	0.76	0/129	1.02	0/173
2	F	0.75	0/129	0.94	0/173
2	P	0.81	0/27	0.81	0/36
All	All	0.89	11/18162 (0.1%)	1.06	33/24585 (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	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	VAL	CA-CB	6.59	1.63	1.54
1	A	318	VAL	CA-CB	6.44	1.61	1.54
1	B	36	VAL	CA-CB	5.96	1.61	1.54
1	C	297	VAL	CA-CB	5.79	1.61	1.54
1	B	217	THR	CA-CB	5.41	1.60	1.53
1	C	488	ALA	CA-CB	-5.31	1.44	1.53
1	C	154	LYS	CA-C	5.25	1.57	1.52
1	B	299	GLY	N-CA	5.19	1.50	1.45
1	C	651	ILE	CA-CB	5.19	1.60	1.54
1	A	500	ILE	CA-CB	5.14	1.58	1.54
1	B	279	ILE	CA-CB	5.10	1.57	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	GLU	N-CA-C	-7.77	102.89	111.36
1	B	298	ARG	N-CA-C	7.23	122.34	107.37
1	B	211	ILE	N-CA-C	-6.75	105.17	111.45
1	A	247	TYR	N-CA-C	6.67	118.55	111.28
1	C	590	ILE	N-CA-C	6.50	118.41	112.43
1	B	656	VAL	CA-C-N	6.27	126.30	119.90
1	B	656	VAL	C-N-CA	6.27	126.30	119.90
1	A	427	ASP	CA-C-N	6.20	126.32	119.87
1	A	427	ASP	C-N-CA	6.20	126.32	119.87
1	B	430	ILE	N-CA-C	6.09	116.73	110.82
1	C	396	VAL	CB-CA-C	-5.89	104.34	111.88
1	B	278	CYS	N-CA-C	5.88	117.36	111.07
1	B	442	ILE	CB-CA-C	-5.81	103.71	110.91
1	B	639	ARG	N-CA-C	-5.74	105.10	111.36
1	B	439	CYS	N-CA-C	5.72	120.25	113.16
2	D	361	ILE	N-CA-C	5.67	116.64	108.48
1	C	551	LEU	N-CA-C	-5.63	105.06	111.14
1	C	637	PRO	CA-C-N	5.62	125.55	119.76
1	C	637	PRO	C-N-CA	5.62	125.55	119.76
1	B	325	VAL	N-CA-C	5.40	116.53	108.54
1	B	675	ASN	N-CA-C	5.39	119.86	113.28
1	C	676	ASP	N-CA-C	5.39	117.59	111.02
1	B	252	ALA	N-CA-C	5.39	117.67	110.35
1	A	176	VAL	N-CA-C	-5.37	105.14	110.62
1	C	626	SER	N-CA-C	5.31	119.60	113.18
1	B	299	GLY	CA-C-O	-5.30	118.64	122.45
1	C	620	MET	CA-C-N	-5.28	115.13	120.31
1	C	620	MET	C-N-CA	-5.28	115.13	120.31
1	A	279	ILE	O-C-N	5.24	123.78	120.42
1	B	306	TYR	N-CA-C	5.14	114.21	108.25
1	B	590	ILE	N-CA-C	5.12	117.11	112.29
1	C	59	HIS	N-CA-C	5.07	116.50	111.07
1	C	512	THR	N-CA-C	5.02	117.74	109.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	PHE	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	5806	0	5725	143	0
1	B	5806	0	5726	160	0
1	C	5806	0	5725	152	0
2	D	129	0	111	5	0
2	E	129	0	111	2	0
2	F	129	0	111	1	0
2	P	27	0	31	4	0
3	A	176	0	0	42	0
3	B	183	0	0	52	1
3	C	259	0	0	50	1
3	D	2	0	0	1	0
3	F	3	0	0	0	0
3	P	4	0	0	3	0
All	All	18459	0	17540	464	1

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 13.

All (464) 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:299:GLY:HA3	3:A:2073:HOH:O	1.51	1.11
1:C:480:GLU:HB3	3:C:2070:HOH:O	1.59	1.03
1:A:294:GLN:HB2	1:A:298:ARG:HH11	1.23	1.02
1:B:204:LYS:HB3	3:B:2057:HOH:O	1.59	1.01
1:A:450:ASN:HB2	3:A:2120:HOH:O	1.60	1.00
1:B:275:HIS:HB2	3:B:2030:HOH:O	1.61	1.00
1:A:118:HIS:HB3	3:A:2034:HOH:O	1.61	0.99
1:B:552:LEU:HB2	3:B:2141:HOH:O	1.66	0.94
1:A:14:THR:O	1:A:15:GLU:HB3	1.69	0.93
1:C:473:ASN:HB3	3:C:2167:HOH:O	1.68	0.92
1:B:387:SER:HB2	3:B:2105:HOH:O	1.68	0.92
1:C:118:HIS:CE1	3:C:2044:HOH:O	2.23	0.91
1:B:474:ASN:HB2	3:B:2122:HOH:O	1.70	0.89
1:C:508:MET:HE2	1:C:508:MET:HA	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:HD3	1:C:10:ARG:H	1.37	0.88
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.57	0.87
1:A:384:LYS:HE3	1:A:384:LYS:HA	1.56	0.86
1:C:141:MET:CG	3:C:2015:HOH:O	2.24	0.84
1:B:230:CYS:O	1:B:260:ARG:HD2	1.78	0.84
1:A:260:ARG:HH21	1:A:434:ARG:HH22	1.26	0.83
1:B:450:ASN:HB2	3:B:2116:HOH:O	1.78	0.83
1:C:561:GLU:HG2	1:C:562:GLN:HG3	1.60	0.83
1:A:262:ARG:HG2	1:A:274:PHE:HB2	1.62	0.82
1:B:118:HIS:HB3	3:B:2032:HOH:O	1.79	0.82
1:A:30:ALA:HB3	3:A:2008:HOH:O	1.79	0.81
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.62	0.81
1:B:480:GLU:HB3	3:B:2051:HOH:O	1.80	0.81
1:C:160:ARG:HB2	3:C:2058:HOH:O	1.80	0.81
1:C:122:ASP:O	1:C:189:ARG:NH2	2.15	0.79
1:C:141:MET:HG2	3:C:2015:HOH:O	1.81	0.79
1:A:141:MET:HG2	3:A:2009:HOH:O	1.84	0.77
1:C:14:THR:HG23	3:C:2010:HOH:O	1.83	0.77
1:B:274:PHE:HD1	3:B:2073:HOH:O	1.66	0.76
1:B:75:PRO:O	1:B:78:GLN:HB2	1.85	0.76
1:A:109:MET:HE2	1:A:114:LYS:HB2	1.66	0.76
1:B:92:LYS:HD3	3:B:2044:HOH:O	1.85	0.76
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.67	0.76
1:C:450:ASN:HB2	3:C:2157:HOH:O	1.83	0.76
1:C:163:GLY:HA3	3:C:2060:HOH:O	1.85	0.75
1:C:195:ARG:HD3	3:C:2071:HOH:O	1.86	0.75
1:A:548:GLN:OE1	1:A:548:GLN:HA	1.85	0.75
1:C:72:ARG:HD2	3:C:2029:HOH:O	1.87	0.74
1:A:150:GLN:NE2	1:A:627:GLN:OE1	2.21	0.74
1:A:46:HIS:HB3	3:A:2020:HOH:O	1.87	0.74
1:C:73:ASP:HA	3:C:2028:HOH:O	1.87	0.73
1:B:10:ARG:HG2	3:B:2003:HOH:O	1.88	0.73
1:C:11:ASP:HB3	3:C:2009:HOH:O	1.87	0.73
1:B:387:SER:CB	3:B:2105:HOH:O	2.30	0.73
1:A:139:ARG:HD3	3:A:2044:HOH:O	1.89	0.72
1:C:111:GLU:HG2	3:C:2041:HOH:O	1.89	0.72
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.70	0.72
1:A:207:LEU:HD12	1:A:212:MET:CE	2.20	0.72
1:C:450:ASN:CB	3:C:2157:HOH:O	2.37	0.72
1:A:260:ARG:HH21	1:A:434:ARG:NH2	1.88	0.71
1:B:561:GLU:HG2	1:B:562:GLN:HG3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:O	1:A:189:ARG:NH2	2.24	0.70
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.73	0.70
1:A:384:LYS:HD2	3:A:2104:HOH:O	1.91	0.70
1:C:294:GLN:HB2	1:C:298:ARG:HB2	1.71	0.70
1:B:11:ASP:CG	1:B:12:GLY:H	1.99	0.70
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.26	0.70
1:A:221:GLN:HG2	3:A:2071:HOH:O	1.90	0.69
1:B:527:HIS:HE1	3:B:2132:HOH:O	1.74	0.69
1:B:443:ALA:O	1:B:444:LEU:HD23	1.93	0.69
1:C:4:ASN:N	3:C:2002:HOH:O	2.26	0.69
1:B:91:LYS:HD2	3:B:2029:HOH:O	1.91	0.69
1:A:600:GLU:HG2	3:A:2153:HOH:O	1.92	0.68
1:A:114:LYS:HE2	1:A:166:TYR:HE2	1.56	0.68
1:A:103:TYR:O	1:A:107:VAL:HG23	1.94	0.68
1:B:527:HIS:CE1	3:B:2132:HOH:O	2.45	0.68
1:C:40:GLN:HE21	1:C:44:ARG:HD2	1.58	0.68
1:A:109:MET:HE3	1:A:109:MET:HA	1.74	0.68
1:C:79:TYR:O	1:C:83:ARG:HG3	1.94	0.68
1:A:195:ARG:CD	3:A:2057:HOH:O	2.42	0.67
1:C:139:ARG:HD3	3:C:2051:HOH:O	1.94	0.67
1:B:415:GLN:HG3	1:B:728:THR:HG22	1.77	0.67
1:B:481:LEU:HD13	3:B:2057:HOH:O	1.95	0.67
1:A:139:ARG:CD	3:A:2044:HOH:O	2.43	0.67
1:B:300:GLY:HA2	3:B:2082:HOH:O	1.95	0.67
1:B:481:LEU:CD1	3:B:2057:HOH:O	2.43	0.67
1:B:15:GLU:HG3	3:B:2006:HOH:O	1.95	0.66
1:B:91:LYS:HE3	3:B:2002:HOH:O	1.95	0.66
1:B:108:LYS:O	1:B:112:MET:HG3	1.95	0.66
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.10	0.66
1:A:290:LYS:HE3	1:A:332:HIS:HB3	1.78	0.65
1:A:609:HIS:HE1	3:A:2154:HOH:O	1.78	0.65
1:C:72:ARG:CD	3:C:2029:HOH:O	2.43	0.65
1:A:212:MET:O	1:A:216:ARG:NH2	2.26	0.65
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.30	0.65
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.77	0.65
1:A:242:SER:HB2	1:A:452:VAL:HG13	1.79	0.64
1:A:294:GLN:HB2	1:A:298:ARG:NH1	2.06	0.64
1:A:199:ALA:HB1	1:A:205:ILE:HD12	1.79	0.64
1:A:195:ARG:HD3	3:A:2057:HOH:O	1.98	0.64
1:C:139:ARG:NH2	1:C:198:ASP:OD1	2.31	0.64
1:C:274:PHE:HD1	3:C:2100:HOH:O	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:CA	3:A:2073:HOH:O	2.25	0.63
1:A:215:VAL:O	1:A:216:ARG:HB3	1.99	0.63
1:C:17:ILE:CD1	1:C:19:LEU:HD23	2.28	0.63
1:C:40:GLN:NE2	1:C:44:ARG:HD2	2.14	0.63
1:B:250:GLN:O	1:B:251:ARG:HB2	1.97	0.63
1:C:592:ASN:O	1:C:593:GLU:C	2.39	0.62
1:B:311:LEU:HD12	1:B:311:LEU:O	2.00	0.62
1:B:275:HIS:HB3	3:B:2076:HOH:O	2.00	0.62
1:B:56:SER:O	1:B:60:GLU:HG2	1.99	0.62
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.81	0.62
1:C:46:HIS:CE1	3:C:2020:HOH:O	2.52	0.61
1:A:27:ASP:HA	3:A:2008:HOH:O	2.01	0.61
1:B:122:ASP:O	1:B:189:ARG:NH2	2.33	0.61
1:C:242:SER:HB3	1:C:452:VAL:HG13	1.81	0.61
1:B:207:LEU:HD22	1:B:212:MET:HE3	1.82	0.61
1:B:505:ARG:HD3	3:B:2117:HOH:O	2.01	0.61
1:C:9:LYS:NZ	1:C:10:ARG:HG3	2.16	0.61
2:P:3:VAL:HG23	3:P:2004:HOH:O	2.00	0.61
1:A:44:ARG:O	1:A:48:GLN:NE2	2.34	0.60
1:A:396:VAL:HG23	3:A:2095:HOH:O	2.00	0.60
1:B:275:HIS:CB	3:B:2030:HOH:O	2.33	0.60
1:C:46:HIS:HE1	3:C:2020:HOH:O	1.85	0.60
1:B:642:VAL:HG22	1:B:655:VAL:HG22	1.83	0.60
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.36	0.60
1:B:215:VAL:O	1:B:216:ARG:HB3	1.99	0.60
1:C:411:ARG:NH1	1:C:731:NIY:HE2	2.17	0.60
1:A:583:TYR:CE2	1:A:687:LYS:HE3	2.37	0.60
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.84	0.59
1:C:274:PHE:HA	3:C:2100:HOH:O	2.01	0.59
1:B:212:MET:O	1:B:216:ARG:NH2	2.36	0.59
1:A:432:PRO:HG3	3:A:2113:HOH:O	2.02	0.59
1:B:138:ASP:O	1:B:141:MET:HB2	2.02	0.59
1:A:140:ASP:HA	1:A:143:PHE:CE2	2.38	0.59
1:A:130:GLN:HG2	3:A:2040:HOH:O	2.02	0.59
1:A:75:PRO:O	1:A:78:GLN:HB2	2.03	0.59
2:D:360:GLN:HB2	3:D:2001:HOH:O	2.04	0.58
1:C:158:GLN:HB2	1:C:164:GLU:O	2.03	0.58
2:P:3:VAL:HA	3:P:2002:HOH:O	2.04	0.58
1:B:317:LEU:HD23	1:B:401:LEU:HD23	1.84	0.58
1:C:17:ILE:CD1	1:C:19:LEU:CD2	2.82	0.58
1:C:701:PRO:O	1:C:707:GLY:HA2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:ND2	1:A:322:ASN:H	2.01	0.58
1:B:7:VAL:HG12	1:B:8:THR:N	2.19	0.58
1:B:297:VAL:HG12	3:B:2080:HOH:O	2.03	0.58
1:A:7:VAL:HG21	1:A:17:ILE:HG12	1.87	0.57
1:B:11:ASP:CG	1:B:12:GLY:N	2.61	0.57
1:B:59:HIS:HE1	1:B:91:LYS:HE2	1.68	0.57
1:B:299:GLY:HA3	3:B:2081:HOH:O	2.04	0.57
1:C:17:ILE:HD12	1:C:19:LEU:CD2	2.35	0.57
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.86	0.57
1:B:696:ASN:N	1:B:696:ASN:HD22	2.02	0.57
1:C:150:GLN:NE2	1:C:627:GLN:OE1	2.33	0.56
1:C:508:MET:HA	1:C:508:MET:CE	2.33	0.56
1:A:553:LYS:O	1:A:557:GLU:HG2	2.05	0.56
1:A:141:MET:CG	3:A:2009:HOH:O	2.48	0.56
1:B:116:ASP:CG	1:B:118:HIS:CD2	2.83	0.56
1:B:275:HIS:HE1	3:B:2074:HOH:O	1.89	0.56
1:B:621:PRO:HD3	1:B:694:SER:CB	2.35	0.56
1:C:12:GLY:HA2	3:C:2008:HOH:O	2.05	0.56
1:A:374:GLU:HG3	1:A:378:LEU:HD12	1.87	0.56
1:B:322:ASN:HA	3:B:2086:HOH:O	2.06	0.55
1:B:695:ALA:C	1:B:696:ASN:HD22	2.14	0.55
1:A:174:ILE:HG23	1:A:175:LEU:HG	1.88	0.55
1:C:17:ILE:HD12	1:C:19:LEU:HD21	1.87	0.55
1:C:242:SER:HB3	1:C:452:VAL:CG1	2.36	0.55
1:C:9:LYS:HZ3	1:C:10:ARG:CG	2.20	0.55
1:B:9:LYS:HG2	3:B:2005:HOH:O	2.06	0.55
1:A:320:LYS:HA	1:A:331:ARG:HG2	1.89	0.54
1:C:557:GLU:HA	1:C:560:LYS:HD2	1.89	0.54
1:C:663:HIS:HD2	3:C:2226:HOH:O	1.89	0.54
1:A:144:SER:O	1:A:147:ALA:HB3	2.07	0.54
1:B:639:ARG:HE	1:B:670:TRP:HE1	1.56	0.54
1:A:40:GLN:HE21	1:A:44:ARG:HD2	1.73	0.53
1:C:107:VAL:HG12	3:C:2040:HOH:O	2.07	0.53
1:C:321:ASN:O	1:C:329:ARG:HD2	2.08	0.53
1:B:299:GLY:CA	3:B:2081:HOH:O	2.57	0.53
1:C:292:CYS:HB3	3:C:2107:HOH:O	2.08	0.53
1:C:625:SER:OG	3:C:2219:HOH:O	2.18	0.53
1:C:736:ASP:HA	3:C:2259:HOH:O	2.09	0.53
1:C:696:ASN:N	1:C:696:ASN:HD22	2.05	0.53
1:A:171:PHE:O	1:A:175:LEU:HD12	2.08	0.53
1:C:138:ASP:O	1:C:141:MET:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASN:O	1:C:323:ARG:HB2	2.09	0.53
1:A:447:LYS:HE3	3:A:2119:HOH:O	2.09	0.52
1:B:466:ALA:HA	1:B:516:GLY:O	2.08	0.52
1:C:604:GLU:HG2	3:C:2212:HOH:O	2.09	0.52
1:B:195:ARG:HD3	3:B:2053:HOH:O	2.08	0.52
1:B:116:ASP:CG	1:B:118:HIS:HD2	2.18	0.52
1:C:5:LEU:HA	1:C:51:ASP:OD1	2.10	0.52
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.39	0.52
1:A:114:LYS:HE2	1:A:166:TYR:CE2	2.42	0.52
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.91	0.52
1:C:463:THR:HG21	1:C:492:LEU:HD23	1.91	0.52
1:B:260:ARG:HG3	3:B:2069:HOH:O	2.09	0.52
1:C:118:HIS:HB3	3:C:2043:HOH:O	2.09	0.52
1:C:713:GLN:HA	3:C:2252:HOH:O	2.08	0.52
1:C:294:GLN:CB	1:C:298:ARG:HB2	2.40	0.52
1:A:304:LEU:O	1:A:335:TYR:HA	2.09	0.52
1:C:9:LYS:NZ	1:C:10:ARG:CG	2.73	0.52
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.92	0.52
1:A:241:SER:O	1:A:245:VAL:HG23	2.09	0.51
1:A:663:HIS:HB2	3:A:2162:HOH:O	2.09	0.51
1:C:384:LYS:HD2	3:C:2143:HOH:O	2.09	0.51
1:B:439:CYS:O	1:B:440:LEU:HB2	2.10	0.51
1:A:394:LYS:HB2	1:A:397:GLU:HG3	1.92	0.51
1:A:585:LYS:HE3	3:A:2150:HOH:O	2.10	0.51
1:A:560:LYS:HE2	1:A:609:HIS:CD2	2.45	0.51
1:B:708:LYS:HB3	2:E:362:ASP:HB2	1.93	0.51
1:C:342:LEU:HD12	1:C:376:GLU:HG3	1.93	0.51
1:A:450:ASN:CB	3:A:2120:HOH:O	2.34	0.51
1:B:285:PHE:O	1:B:289:VAL:HG23	2.09	0.51
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.92	0.51
1:A:14:THR:O	1:A:15:GLU:CB	2.52	0.51
1:A:140:ASP:HA	1:A:143:PHE:CD2	2.45	0.51
1:B:7:VAL:HG12	1:B:8:THR:H	1.75	0.51
1:B:508:MET:HA	1:B:508:MET:HE2	1.93	0.51
1:A:191:GLN:HB2	3:A:2054:HOH:O	2.10	0.51
1:B:203:PHE:HB3	1:B:629:SER:HB3	1.93	0.50
1:B:478:LEU:CD1	1:B:547:ILE:HG13	2.41	0.50
1:C:331:ARG:HD2	3:C:2120:HOH:O	2.11	0.50
1:A:285:PHE:O	1:A:289:VAL:HG23	2.11	0.50
1:A:648:LYS:HA	3:A:2165:HOH:O	2.11	0.50
1:C:163:GLY:CA	3:C:2060:HOH:O	2.53	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.93	0.50
1:B:119:LEU:HD21	1:B:179:CYS:SG	2.52	0.50
1:B:619:LEU:HB2	1:B:693:ILE:HG23	1.93	0.50
1:A:723:LYS:NZ	2:D:374:GLN:O	2.39	0.50
1:A:150:GLN:OE1	1:A:154:LYS:HD2	2.12	0.50
1:C:141:MET:HG3	3:C:2015:HOH:O	2.03	0.50
1:C:736:ASP:CA	3:C:2259:HOH:O	2.59	0.50
1:C:663:HIS:CD2	3:C:2226:HOH:O	2.63	0.49
1:B:109:MET:HB2	1:B:115:TYR:CD2	2.47	0.49
1:B:167:GLU:OE2	1:B:216:ARG:NH1	2.45	0.49
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.93	0.49
1:A:548:GLN:HB2	1:A:688:PHE:HB3	1.94	0.49
1:B:206:SER:OG	1:B:625:SER:HB2	2.11	0.49
1:B:399:PHE:O	1:B:403:MET:HG2	2.13	0.49
2:E:361:ILE:HD13	2:E:361:ILE:H	1.77	0.49
1:A:157:VAL:HG23	1:A:216:ARG:HH11	1.77	0.49
1:A:226:VAL:HG22	1:A:254:ILE:HG23	1.94	0.49
1:A:331:ARG:HD3	3:A:2093:HOH:O	2.13	0.49
1:B:437:ASN:HB2	3:B:2113:HOH:O	2.13	0.49
1:C:172:LEU:O	1:C:176:VAL:HG23	2.13	0.49
1:A:560:LYS:HE2	1:A:609:HIS:CG	2.47	0.49
1:A:609:HIS:CE1	3:A:2154:HOH:O	2.59	0.49
1:B:7:VAL:HG11	1:B:55:THR:HG23	1.94	0.49
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.38	0.49
1:C:46:HIS:HD2	1:C:49:PHE:CE2	2.30	0.49
1:A:458:GLU:OE2	1:A:510:ARG:NH1	2.45	0.49
1:B:79:TYR:O	1:B:83:ARG:HG3	2.12	0.49
1:B:126:GLU:CG	3:B:2035:HOH:O	2.59	0.49
1:B:150:GLN:HB2	1:B:628:ILE:HD11	1.93	0.49
1:A:105:HIS:CD2	1:A:171:PHE:CD2	3.01	0.49
1:B:114:LYS:HE3	3:B:2045:HOH:O	2.12	0.49
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.95	0.49
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.94	0.49
1:B:9:LYS:HD3	1:B:10:ARG:H	1.77	0.48
1:B:391:GLN:HG3	3:B:2106:HOH:O	2.12	0.48
1:C:221:GLN:CD	1:C:250:GLN:HG2	2.38	0.48
1:C:349:LYS:O	1:C:351:GLU:HG3	2.14	0.48
1:C:581:ASP:HA	3:C:2200:HOH:O	2.13	0.48
1:A:515:ILE:HD12	1:A:551:LEU:HD22	1.96	0.48
1:C:304:LEU:HD23	1:C:304:LEU:C	2.39	0.48
1:A:425:PRO:O	1:A:571:THR:HB	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLU:HG2	1:B:16:ARG:N	2.27	0.48
1:C:9:LYS:HD3	1:C:10:ARG:N	2.18	0.48
1:A:440:LEU:N	1:A:440:LEU:CD2	2.76	0.48
1:B:344:TYR:O	1:B:347:LEU:HB3	2.14	0.48
1:A:38:ILE:HD11	3:A:2008:HOH:O	2.13	0.47
1:A:310:HIS:O	1:A:313:VAL:HG12	2.14	0.47
1:A:58:ILE:O	1:A:62:ILE:HG23	2.15	0.47
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.95	0.47
1:A:274:PHE:N	1:A:274:PHE:CD2	2.82	0.47
1:B:325:VAL:HG13	1:B:328:ASN:HB2	1.94	0.47
1:B:474:ASN:HB3	3:B:2121:HOH:O	2.14	0.47
1:B:115:TYR:CE1	1:B:216:ARG:HG3	2.50	0.47
1:B:553:LYS:HG2	3:B:2142:HOH:O	2.14	0.47
1:C:46:HIS:CD2	1:C:49:PHE:CE2	3.02	0.47
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.96	0.47
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.39	0.47
1:A:319:LEU:HD22	1:A:330:VAL:HG23	1.95	0.47
1:A:663:HIS:CD2	3:A:2162:HOH:O	2.67	0.47
1:B:150:GLN:HB2	1:B:628:ILE:CD1	2.45	0.47
1:A:155:TYR:CE2	1:A:628:ILE:HD12	2.49	0.47
1:A:692:SER:OG	1:A:693:ILE:N	2.48	0.46
1:A:130:GLN:CG	3:A:2040:HOH:O	2.61	0.46
1:B:478:LEU:HD13	1:B:547:ILE:HG13	1.97	0.46
1:C:6:LEU:HD23	3:C:2011:HOH:O	2.15	0.46
1:A:195:ARG:HD2	3:A:2057:HOH:O	2.12	0.46
1:C:388:ILE:O	1:C:390:LYS:NZ	2.46	0.46
1:A:109:MET:CE	1:A:114:LYS:HB2	2.42	0.46
1:B:267:PRO:C	3:B:2075:HOH:O	2.57	0.46
1:C:9:LYS:HZ2	1:C:10:ARG:HG3	1.79	0.46
1:C:208:PRO:HB2	1:C:210:PRO:HD2	1.98	0.46
1:B:149:LYS:HG3	1:B:652:LEU:HD11	1.97	0.46
1:B:547:ILE:HG23	3:B:2140:HOH:O	2.16	0.46
1:C:149:LYS:HD2	1:C:149:LYS:HA	1.68	0.46
1:C:290:LYS:HD2	1:C:297:VAL:HA	1.97	0.46
1:C:473:ASN:HB2	1:C:477:GLU:OE2	2.15	0.46
1:B:156:LEU:O	1:B:158:GLN:HG2	2.15	0.46
1:C:150:GLN:O	1:C:151:LEU:C	2.59	0.46
1:C:195:ARG:CD	3:C:2071:HOH:O	2.53	0.46
1:C:294:GLN:HB3	3:C:2109:HOH:O	2.15	0.46
1:B:9:LYS:HE2	3:B:2005:HOH:O	2.15	0.46
1:B:275:HIS:CE1	3:B:2074:HOH:O	2.66	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:N	1:C:141:MET:HE2	2.31	0.45
1:B:27:ASP:HA	1:B:38:ILE:HD11	1.98	0.45
1:B:62:ILE:HD12	1:B:84:LEU:HD22	1.98	0.45
1:C:63:ILE:HD13	1:C:85:ALA:HA	1.98	0.45
1:C:313:VAL:HG22	1:C:317:LEU:CD2	2.46	0.45
1:C:207:LEU:HD23	1:C:465:SER:OG	2.16	0.45
1:A:376:GLU:HG2	3:A:2103:HOH:O	2.16	0.45
1:B:158:GLN:HB3	1:B:165:ILE:HG13	1.97	0.45
1:A:659:TYR:CE1	1:A:663:HIS:HB3	2.51	0.45
1:B:154:LYS:HD2	1:B:624:THR:HG21	1.98	0.45
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.99	0.45
1:B:467:PHE:HE2	3:B:2140:HOH:O	1.99	0.45
1:B:639:ARG:NE	1:B:670:TRP:HE1	2.14	0.45
1:B:608:THR:CG2	1:B:609:HIS:CE1	3.00	0.45
1:C:419:HIS:CD2	1:C:725:GLY:HA2	2.52	0.45
1:A:322:ASN:H	1:A:322:ASN:HD22	1.65	0.45
1:A:572:THR:HB	1:A:577:ILE:HB	1.98	0.45
1:A:138:ASP:O	1:A:141:MET:HB2	2.17	0.45
1:B:212:MET:HE2	1:B:212:MET:HA	1.98	0.45
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.52	0.45
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.99	0.44
1:B:362:PRO:O	1:B:382:TYR:OH	2.33	0.44
1:A:394:LYS:HB2	1:A:397:GLU:CG	2.48	0.44
1:B:92:LYS:HB3	3:B:2044:HOH:O	2.17	0.44
1:C:321:ASN:O	1:C:329:ARG:NE	2.50	0.44
1:B:150:GLN:O	1:B:151:LEU:C	2.60	0.44
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.76	0.44
1:C:555:SER:HB2	1:C:616:LEU:HD21	1.99	0.44
1:B:361:VAL:HG21	1:B:364:LEU:HD12	1.98	0.44
1:C:102:LEU:O	1:C:106:VAL:HG23	2.18	0.44
1:C:384:LYS:HE3	1:C:384:LYS:HA	1.99	0.44
1:C:461:LEU:HD11	1:C:503:ALA:HB1	1.98	0.44
1:A:207:LEU:CD1	1:A:212:MET:HE3	2.48	0.44
1:B:171:PHE:O	1:B:172:LEU:C	2.60	0.44
1:B:317:LEU:O	1:B:405:GLU:HG3	2.18	0.44
1:C:578:LEU:HD11	1:C:603:ARG:HB2	1.99	0.44
1:A:298:ARG:HA	3:A:2087:HOH:O	2.18	0.44
1:A:529:LYS:HD2	1:A:535:SER:O	2.17	0.44
1:C:135:ILE:HD11	1:C:174:ILE:HG21	2.00	0.44
1:C:127:GLU:HG2	1:C:190:LEU:HD11	1.99	0.43
1:C:482:ALA:O	1:C:486:VAL:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLY:HA3	3:C:2114:HOH:O	2.18	0.43
1:C:342:LEU:C	1:C:342:LEU:HD23	2.42	0.43
1:B:343:MET:HE2	1:B:343:MET:HA	2.00	0.43
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.54	0.43
1:B:618:ALA:HB2	1:B:691:GLN:HB2	1.99	0.43
1:A:686:GLN:CD	1:A:727:LYS:HE3	2.43	0.43
1:C:195:ARG:NE	3:C:2071:HOH:O	2.51	0.43
1:A:114:LYS:HE3	3:A:2049:HOH:O	2.19	0.43
1:A:131:MET:HA	1:A:134:PHE:CD2	2.54	0.43
1:A:475:LEU:O	1:A:478:LEU:HB2	2.18	0.43
1:C:622:SER:O	1:C:633:ASN:HB3	2.18	0.43
1:A:420:CYS:O	1:A:424:SER:HB2	2.19	0.43
1:B:420:CYS:O	1:B:424:SER:HB2	2.19	0.43
1:A:476:ASP:OD1	1:A:550:TYR:OH	2.25	0.43
1:B:230:CYS:HB2	1:B:240:THR:HG21	2.00	0.43
1:C:338:GLN:C	1:C:339:ILE:HG13	2.43	0.43
1:B:321:ASN:O	1:B:329:ARG:NE	2.51	0.43
1:B:639:ARG:CD	3:B:2157:HOH:O	2.66	0.43
1:C:499:PRO:O	1:C:500:ILE:HG12	2.18	0.43
1:A:186:ARG:HG2	3:A:2052:HOH:O	2.17	0.43
1:A:704:PHE:HA	1:A:705:PRO:HD2	1.78	0.43
1:B:621:PRO:HD3	1:B:694:SER:OG	2.19	0.43
1:C:118:HIS:HE1	3:C:2044:HOH:O	1.78	0.43
1:C:294:GLN:HB3	1:C:295:GLY:H	1.75	0.43
1:A:648:LYS:CA	3:A:2165:HOH:O	2.66	0.43
1:C:317:LEU:O	1:C:405:GLU:HG3	2.18	0.43
1:C:716:LYS:HE3	3:C:2253:HOH:O	2.19	0.43
2:P:3:VAL:C	3:P:2003:HOH:O	2.62	0.42
1:A:4:ASN:N	3:A:2001:HOH:O	2.52	0.42
1:A:149:LYS:HE3	3:A:2046:HOH:O	2.19	0.42
1:B:53:ILE:HG23	1:B:53:ILE:O	2.19	0.42
1:B:330:VAL:HB	1:B:335:TYR:OH	2.19	0.42
1:C:144:SER:O	1:C:147:ALA:HB3	2.19	0.42
1:A:260:ARG:NH2	1:A:434:ARG:HH22	2.06	0.42
1:B:286:GLN:HB2	1:B:333:MET:HE2	2.01	0.42
1:C:243:ALA:HA	1:C:500:ILE:CD1	2.50	0.42
1:A:86:ILE:HD12	1:A:140:ASP:HB3	2.02	0.42
1:A:475:LEU:HA	1:A:475:LEU:HD23	1.66	0.42
1:A:696:ASN:N	1:A:696:ASN:HD22	2.17	0.42
1:B:529:LYS:HD2	1:B:535:SER:O	2.19	0.42
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:LEU:HD12	1:B:449:LEU:N	2.34	0.42
1:A:11:ASP:OD1	1:A:12:GLY:N	2.43	0.42
1:C:696:ASN:N	1:C:696:ASN:ND2	2.68	0.42
1:A:185:PRO:HB2	1:A:187:GLU:OE2	2.20	0.42
1:B:427:ASP:OD1	1:B:429:ALA:N	2.48	0.42
1:B:578:LEU:HB3	1:B:579:PRO:HD2	2.02	0.42
1:A:418:ASP:OD2	1:A:722:TYR:OH	2.37	0.42
1:B:262:ARG:HD3	1:B:274:PHE:HB3	2.01	0.42
1:C:118:HIS:HD2	1:C:220:ARG:HH22	1.68	0.42
1:B:126:GLU:HG2	3:B:2035:HOH:O	2.19	0.42
1:C:450:ASN:HB2	3:C:2161:HOH:O	2.20	0.42
1:C:465:SER:HB2	1:C:489:LEU:HD11	2.01	0.42
1:A:565:CYS:HB3	1:A:612:ARG:O	2.20	0.41
1:B:286:GLN:OE1	1:B:330:VAL:HG12	2.20	0.41
1:B:551:LEU:HG	3:B:2140:HOH:O	2.18	0.41
1:B:608:THR:HG21	1:B:609:HIS:CE1	2.55	0.41
1:C:321:ASN:O	1:C:329:ARG:CD	2.67	0.41
1:B:172:LEU:C	1:B:172:LEU:HD23	2.45	0.41
1:B:528:GLY:HA2	3:B:2168:HOH:O	2.20	0.41
1:B:642:VAL:HA	1:B:654:GLN:O	2.20	0.41
1:C:385:ASP:OD1	1:C:386:ASP:N	2.53	0.41
1:C:695:ALA:C	1:C:696:ASN:HD22	2.27	0.41
1:B:364:LEU:HD22	1:B:375:PHE:CE1	2.55	0.41
1:C:38:ILE:HG21	1:C:38:ILE:HD13	1.70	0.41
1:C:72:ARG:H	1:C:72:ARG:HG2	1.67	0.41
1:C:300:GLY:CA	3:C:2113:HOH:O	2.67	0.41
1:C:396:VAL:CG2	3:C:2128:HOH:O	2.68	0.41
1:B:87:PHE:CD2	1:B:87:PHE:C	2.98	0.41
1:B:134:PHE:CD1	1:B:194:LYS:HG3	2.56	0.41
1:C:46:HIS:HA	1:C:49:PHE:CD2	2.55	0.41
1:C:298:ARG:HG3	3:C:2109:HOH:O	2.20	0.41
1:C:475:LEU:HD23	1:C:475:LEU:HA	1.78	0.41
2:D:368:ASP:OD1	2:D:368:ASP:N	2.51	0.41
1:C:162:THR:OG1	1:C:164:GLU:OE1	2.29	0.41
1:C:512:THR:C	1:C:513:LEU:HD23	2.45	0.41
1:A:37:SER:HB3	1:A:40:GLN:HB2	2.01	0.41
1:A:102:LEU:O	1:A:106:VAL:HG23	2.21	0.41
1:A:228:ILE:HG23	1:A:459:ILE:HG12	2.01	0.41
1:B:209:THR:N	1:B:210:PRO:HD2	2.34	0.41
1:A:298:ARG:HB2	3:A:2083:HOH:O	2.21	0.41
1:A:215:VAL:O	1:A:216:ARG:CB	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:PHE:CZ	1:A:685:MET:HE2	2.56	0.41
1:C:379:TYR:O	1:C:383:GLU:HG3	2.21	0.41
1:C:385:ASP:OD1	1:C:385:ASP:C	2.64	0.41
1:C:473:ASN:O	1:C:474:ASN:HB3	2.21	0.41
2:D:370:LEU:O	2:D:372:ASN:N	2.54	0.41
1:A:128:PHE:CD1	1:A:131:MET:HE3	2.56	0.41
1:A:283:LYS:HG2	1:A:330:VAL:HG22	2.03	0.41
1:A:389:ARG:HD3	3:A:2108:HOH:O	2.20	0.41
1:B:9:LYS:CG	3:B:2005:HOH:O	2.68	0.41
1:B:179:CYS:SG	1:B:216:ARG:HA	2.61	0.41
1:B:254:ILE:O	1:B:302:ALA:HA	2.21	0.41
1:B:341:LYS:HE2	3:B:2096:HOH:O	2.20	0.41
1:C:155:TYR:CZ	1:C:212:MET:HG3	2.56	0.41
1:C:286:GLN:HB2	1:C:333:MET:HE2	2.02	0.41
1:C:396:VAL:HG23	3:C:2128:HOH:O	2.21	0.41
1:C:637:PRO:HA	1:C:638:PRO:HD3	1.96	0.41
2:F:360:GLN:N	2:F:360:GLN:OE1	2.54	0.41
1:A:510:ARG:HB3	1:A:614:SER:OG	2.20	0.41
1:A:663:HIS:HD2	3:A:2162:HOH:O	2.02	0.41
1:B:396:VAL:HG23	3:B:2098:HOH:O	2.20	0.41
1:B:510:ARG:O	1:B:614:SER:OG	2.39	0.41
1:B:82:ALA:HB2	1:B:145:TYR:N	2.36	0.40
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.97	0.40
1:B:78:GLN:HG2	1:B:144:SER:HB2	2.01	0.40
1:B:109:MET:CB	1:B:115:TYR:CD2	3.03	0.40
1:B:138:ASP:HB2	3:B:2038:HOH:O	2.21	0.40
1:B:348:LEU:C	1:B:350:GLY:H	2.29	0.40
1:B:427:ASP:OD1	1:B:427:ASP:C	2.63	0.40
1:C:692:SER:C	1:C:693:ILE:HG13	2.45	0.40
1:B:638:PRO:HG2	1:B:668:LEU:HD23	2.03	0.40
1:B:658:ASP:HB3	1:B:662:LEU:HD12	2.03	0.40
1:C:380:THR:O	1:C:381:LYS:C	2.65	0.40
1:A:313:VAL:HG22	1:A:317:LEU:HD22	2.04	0.40
1:A:597:TYR:O	1:A:599:TRP:HD1	2.05	0.40
1:C:119:LEU:HD13	1:C:175:LEU:HD22	2.04	0.40
1:C:621:PRO:HD3	1:C:694:SER:OG	2.21	0.40
1:A:512:THR:O	1:A:513:LEU:HD23	2.22	0.40
1:B:102:LEU:O	1:B:106:VAL:HG23	2.22	0.40
1:B:724:PHE:O	3:B:2178:HOH:O	2.22	0.40
2:D:370:LEU:C	2:D:372:ASN:H	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2011:HOH:O	3:C:2016:HOH:O[15_554]	2.06	0.14

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	723/761 (95%)	669 (92%)	44 (6%)	10 (1%)	9	30
1	B	723/761 (95%)	673 (93%)	39 (5%)	11 (2%)	8	28
1	C	723/761 (95%)	680 (94%)	34 (5%)	9 (1%)	10	34
2	D	14/20 (70%)	12 (86%)	2 (14%)	0	100	100
2	E	14/20 (70%)	10 (71%)	4 (29%)	0	100	100
2	F	14/20 (70%)	11 (79%)	2 (14%)	1 (7%)	1	2
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2212/2363 (94%)	2056 (93%)	125 (6%)	31 (1%)	9	30

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	294	GLN
1	B	294	GLN
1	B	300	GLY
1	C	294	GLN
1	C	323	ARG
1	A	189	ARG
1	A	216	ARG
1	A	297	VAL
1	A	300	GLY
1	B	11	ASP
1	B	154	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	216	ARG
1	C	216	ARG
1	A	14	THR
1	A	31	GLU
1	B	12	GLY
1	B	55	THR
1	C	11	ASP
1	C	564	ALA
1	C	694	SER
2	F	373	PHE
1	A	362	PRO
1	B	189	ARG
1	B	297	VAL
1	C	300	GLY
1	C	5	LEU
1	C	12	GLY
1	B	251	ARG
1	B	295	GLY
1	A	161	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	625/650 (96%)	563 (90%)	62 (10%)	7	24
1	B	625/650 (96%)	549 (88%)	76 (12%)	5	16
1	C	625/650 (96%)	566 (91%)	59 (9%)	8	27
2	D	16/19 (84%)	11 (69%)	5 (31%)	0	1
2	E	16/19 (84%)	12 (75%)	4 (25%)	0	2
2	F	16/19 (84%)	13 (81%)	3 (19%)	1	5
2	P	3/19 (16%)	1 (33%)	2 (67%)	0	0
All	All	1926/2026 (95%)	1715 (89%)	211 (11%)	6	20

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	15	GLU
1	A	17	ILE
1	A	21	LYS
1	A	27	ASP
1	A	39	SER
1	A	44	ARG
1	A	45	SER
1	A	55	THR
1	A	62	ILE
1	A	72	ARG
1	A	78	GLN
1	A	91	LYS
1	A	92	LYS
1	A	96	GLN
1	A	111	GLU
1	A	118	HIS
1	A	129	LYS
1	A	149	LYS
1	A	187	GLU
1	A	189	ARG
1	A	209	THR
1	A	226	VAL
1	A	228	ILE
1	A	254	ILE
1	A	274	PHE
1	A	298	ARG
1	A	315	SER
1	A	317	LEU
1	A	320	LYS
1	A	321	ASN
1	A	322	ASN
1	A	325	VAL
1	A	342	LEU
1	A	343	MET
1	A	361	VAL
1	A	364	LEU
1	A	384	LYS
1	A	388	ILE
1	A	391	GLN
1	A	393	VAL
1	A	394	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	397	GLU
1	A	408	SER
1	A	411	ARG
1	A	440	LEU
1	A	452	VAL
1	A	473	ASN
1	A	484	LEU
1	A	510	ARG
1	A	526	LYS
1	A	553	LYS
1	A	585	LYS
1	A	607	LYS
1	A	625	SER
1	A	626	SER
1	A	628	ILE
1	A	629	SER
1	A	645	LYS
1	A	648	LYS
1	A	708	LYS
1	B	4	ASN
1	B	9	LYS
1	B	11	ASP
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	38	ILE
1	B	39	SER
1	B	40	GLN
1	B	44	ARG
1	B	55	THR
1	B	91	LYS
1	B	92	LYS
1	B	96	GLN
1	B	98	GLU
1	B	126	GLU
1	B	139	ARG
1	B	141	MET
1	B	158	GLN
1	B	160	ARG
1	B	161	VAL
1	B	165	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	183	ASN
1	B	189	ARG
1	B	191	GLN
1	B	216	ARG
1	B	221	GLN
1	B	226	VAL
1	B	237	ILE
1	B	251	ARG
1	B	260	ARG
1	B	262	ARG
1	B	276	THR
1	B	297	VAL
1	B	298	ARG
1	B	311	LEU
1	B	315	SER
1	B	317	LEU
1	B	320	LYS
1	B	330	VAL
1	B	331	ARG
1	B	339	ILE
1	B	342	LEU
1	B	364	LEU
1	B	384	LYS
1	B	391	GLN
1	B	394	LYS
1	B	397	GLU
1	B	401	LEU
1	B	408	SER
1	B	414	ILE
1	B	430	ILE
1	B	440	LEU
1	B	447	LYS
1	B	452	VAL
1	B	455	GLU
1	B	484	LEU
1	B	510	ARG
1	B	526	LYS
1	B	542	LYS
1	B	547	ILE
1	B	575	LYS
1	B	580	ILE
1	B	586	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	607	LYS
1	B	614	SER
1	B	623	GLU
1	B	629	SER
1	B	639	ARG
1	B	644	ILE
1	B	647	SER
1	B	648	LYS
1	B	652	LEU
1	B	696	ASN
1	B	706	SER
1	C	5	LEU
1	C	7	VAL
1	C	9	LYS
1	C	13	SER
1	C	17	ILE
1	C	21	LYS
1	C	24	ARG
1	C	35	ASN
1	C	40	GLN
1	C	51	ASP
1	C	54	LYS
1	C	55	THR
1	C	92	LYS
1	C	111	GLU
1	C	118	HIS
1	C	121	GLU
1	C	130	GLN
1	C	139	ARG
1	C	141	MET
1	C	152	GLU
1	C	165	ILE
1	C	186	ARG
1	C	187	GLU
1	C	191	GLN
1	C	204	LYS
1	C	226	VAL
1	C	242	SER
1	C	294	GLN
1	C	297	VAL
1	C	298	ARG
1	C	317	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	320	LYS
1	C	321	ASN
1	C	325	VAL
1	C	326	GLU
1	C	361	VAL
1	C	364	LEU
1	C	373	GLU
1	C	380	THR
1	C	384	LYS
1	C	391	GLN
1	C	393	VAL
1	C	396	VAL
1	C	408	SER
1	C	452	VAL
1	C	472	ILE
1	C	474	ASN
1	C	484	LEU
1	C	508	MET
1	C	561	GLU
1	C	585	LYS
1	C	616	LEU
1	C	623	GLU
1	C	625	SER
1	C	626	SER
1	C	628	ILE
1	C	644	ILE
1	C	648	LYS
1	C	723	LYS
2	D	360	GLN
2	D	361	ILE
2	D	364	GLU
2	D	368	ASP
2	D	369	ASP
2	E	360	GLN
2	E	361	ILE
2	E	364	GLU
2	E	367	THR
2	F	360	GLN
2	F	367	THR
2	F	374	GLN
2	P	2	LEU
2	P	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	183	ASN
1	A	238	ASN
1	A	321	ASN
1	A	322	ASN
1	A	328	ASN
1	A	404	GLN
1	A	450	ASN
1	A	609	HIS
1	A	663	HIS
1	A	713	GLN
1	B	4	ASN
1	B	35	ASN
1	B	59	HIS
1	B	117	ASN
1	B	130	GLN
1	B	150	GLN
1	B	183	ASN
1	B	250	GLN
1	B	328	ASN
1	B	416	ASN
1	B	435	GLN
1	B	456	ASN
1	B	527	HIS
1	B	596	HIS
1	B	696	ASN
1	B	713	GLN
1	B	733	ASN
1	C	40	GLN
1	C	46	HIS
1	C	59	HIS
1	C	137	HIS
1	C	183	ASN
1	C	191	GLN
1	C	250	GLN
1	C	321	ASN
1	C	328	ASN
1	C	453	ASN
1	C	569	ASN
1	C	630	ASN
1	C	661	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	663	HIS
1	C	696	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	B	731	1	14,15,16	1.22	1 (7%)	11,20,22	0.70	0
1	NIY	A	731	1	14,15,16	1.03	1 (7%)	11,20,22	0.89	0
1	NIY	C	731	1	14,15,16	1.21	1 (7%)	11,20,22	1.43	2 (18%)

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	B	731	1	-	2/7/10/12	0/1/1/1
1	NIY	A	731	1	-	2/7/10/12	0/1/1/1
1	NIY	C	731	1	-	2/7/10/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	731	NIY	CE1-NN	-3.57	1.39	1.45
1	C	731	NIY	CE1-NN	-3.07	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	731	NIY	CE1-NN	-2.07	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	731	NIY	CB-CG-CD1	-3.35	114.67	120.43
1	C	731	NIY	CD2-CG-CD1	2.08	121.42	118.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	731	NIY	CD1-CE1-NN-O2
1	A	731	NIY	CZ-CE1-NN-O2
1	B	731	NIY	CA-CB-CG-CD2
1	C	731	NIY	CA-CB-CG-CD1
1	C	731	NIY	CA-CB-CG-CD2
1	B	731	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	C	731	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 ⓘ

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	727/761 (95%)	-0.49	5 (0%) 84 77	27, 42, 68, 89	0
1	B	727/761 (95%)	-0.45	6 (0%) 82 75	25, 41, 66, 89	0
1	C	727/761 (95%)	-0.73	3 (0%) 88 84	17, 30, 55, 79	0
2	D	16/20 (80%)	0.63	0 100 100	78, 90, 92, 94	0
2	E	16/20 (80%)	0.88	2 (12%) 8 6	69, 82, 93, 93	0
2	F	16/20 (80%)	0.39	0 100 100	64, 78, 84, 85	0
2	P	3/20 (15%)	-0.22	0 100 100	33, 33, 36, 42	0
All	All	2232/2363 (94%)	-0.53	16 (0%) 84 77	17, 38, 69, 94	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	361	ILE	3.3
1	B	299	GLY	3.0
1	B	297	VAL	2.9
1	C	297	VAL	2.9
1	B	274	PHE	2.8
1	A	297	VAL	2.8
1	A	274	PHE	2.6
2	E	372	ASN	2.6
1	A	737	GLY	2.5
1	B	325	VAL	2.3
1	B	296	GLY	2.3
1	A	5	LEU	2.1
1	B	10	ARG	2.0
1	C	296	GLY	2.0
1	C	325	VAL	2.0
1	A	6	LEU	2.0

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	731	15/16	0.93	0.14	36,41,51,52	0
1	NIY	B	731	15/16	0.94	0.11	32,37,45,46	0
1	NIY	C	731	15/16	0.96	0.08	22,27,39,42	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.