



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:46 AM UTC

PDB ID : 1H6K / pdb_00001h6k
Title : nuclear Cap Binding Complex
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Deposited on : 2001-06-18
Resolution : 2.00 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

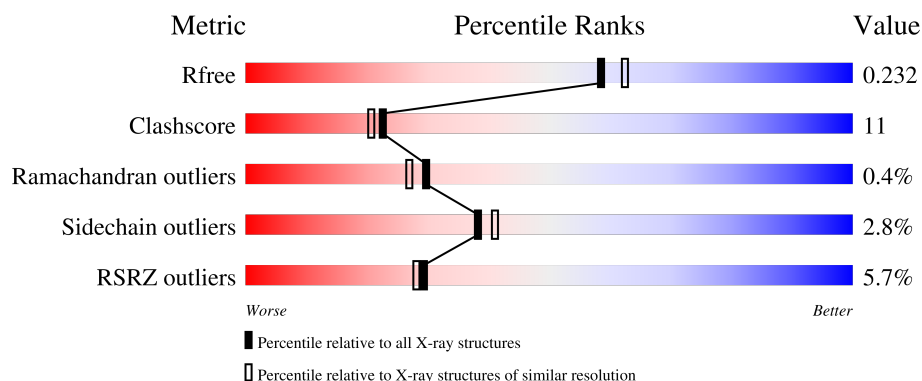
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	757	5% 78% 16% • •
1	B	757	6% 79% 16% • •
1	C	757	6% 78% 16% • •
2	X	98	4% 64% 13% • 21%
2	Y	98	5% 64% 13% 22%

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Mol	Chain	Length	Quality of chain
2	Z	98	5% 68% 10% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21515 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 CBP80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5959	3842	1004	1075	38			
1	B	729	Total	C	N	O	S	0	0	0
			5968	3846	1004	1080	38			
1	C	733	Total	C	N	O	S	0	0	0
			5998	3866	1009	1085	38			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	479	SER	ALA	engineered mutation	UNP Q09161
B	479	SER	ALA	engineered mutation	UNP Q09161
C	479	SER	ALA	engineered mutation	UNP Q09161

- Molecule 2 is a protein called 20 KDA NUCLEAR CAP BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	77	Total	C	N	O	S	0	0	0
			625	396	102	121	6			
2	Y	76	Total	C	N	O	S	0	0	0
			621	394	101	120	6			
2	Z	78	Total	C	N	O	S	0	0	0
			634	402	104	122	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	527	Total	O	0	0
			527	527		
3	B	535	Total	O	0	0
			535	535		

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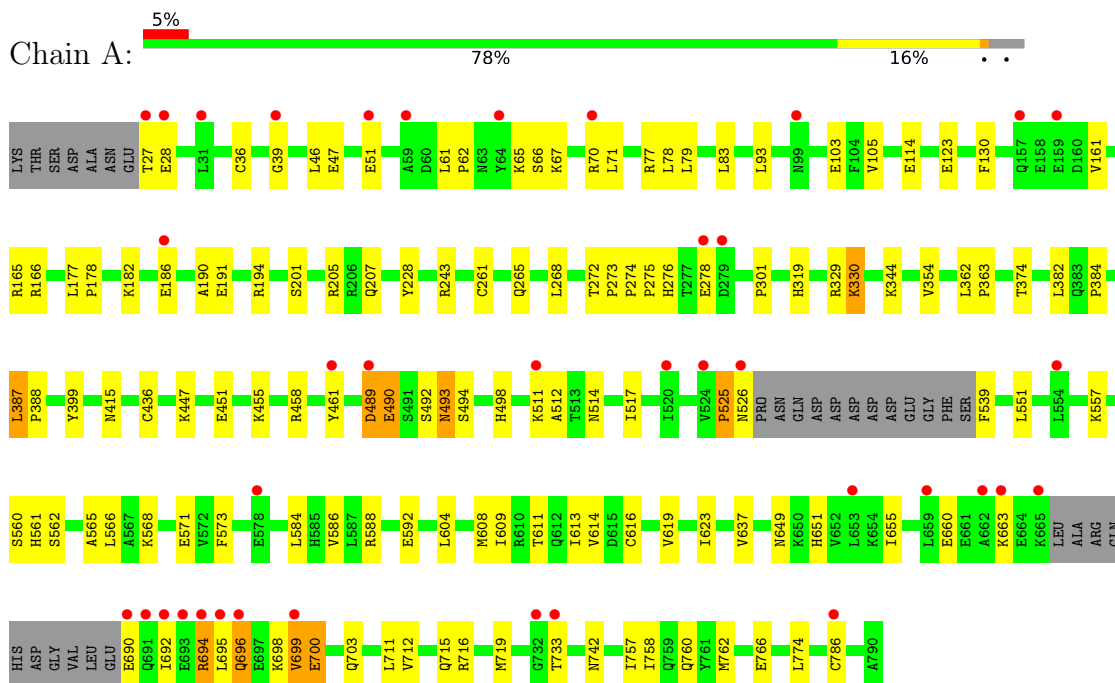
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	435	Total 435	O 435	0	0
3	X	79	Total 79	O 79	0	0
3	Y	63	Total 63	O 63	0	0
3	Z	71	Total 71	O 71	0	0

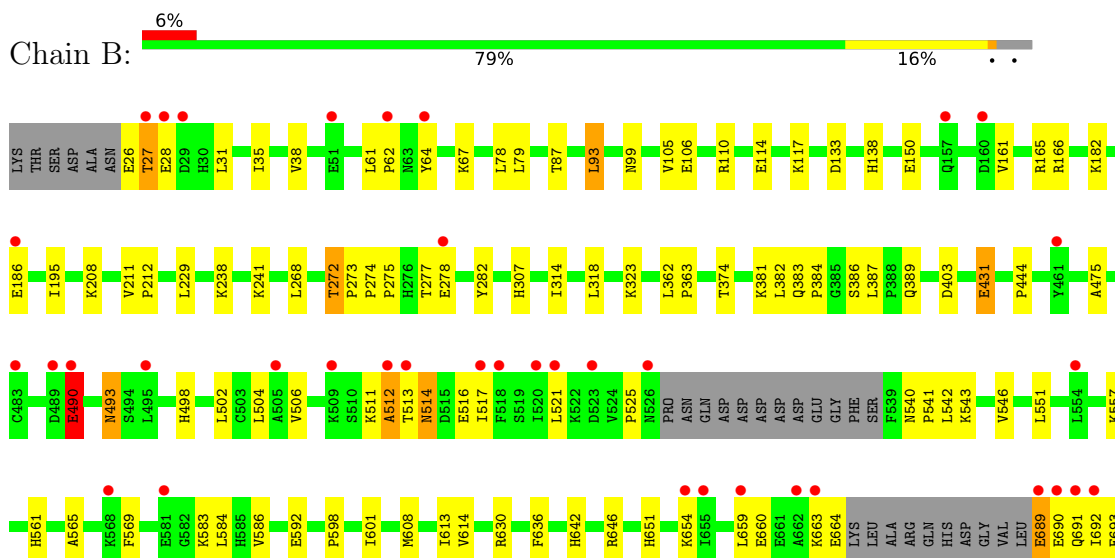
3 Residue-property plots

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: CBP80

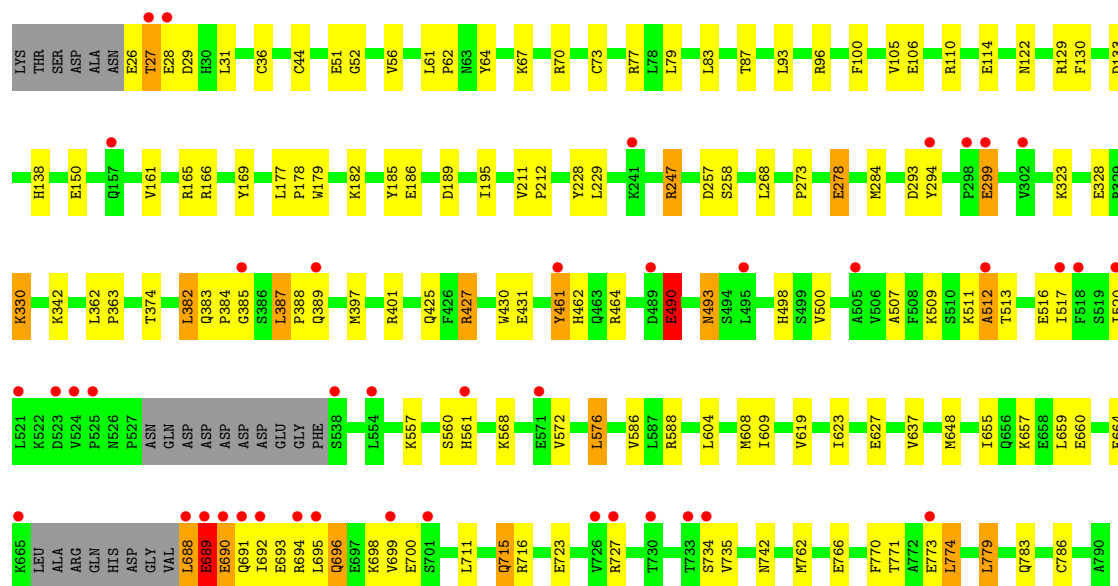
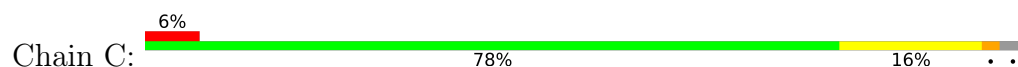


• Molecule 1: CBP80





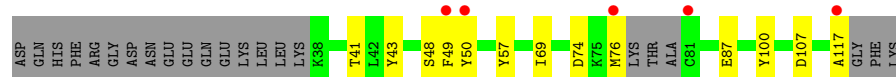
• Molecule 1: CBP80



• Molecule 2: 20 KDA NUCLEAR CAP BINDING PROTEIN



• Molecule 2: 20 KDA NUCLEAR CAP BINDING PROTEIN



• Molecule 2: 20 KDA NUCLEAR CAP BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.53Å 161.48Å 303.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	83.0 (20.00-2.00) 82.9 (20.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.203 , 0.234 0.201 , 0.232	Depositor DCC
R_{free} test set	2291 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21515	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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](#)

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	0.52	0/6111	0.82	1/8291 (0.0%)
1	B	0.51	0/6120	0.81	0/8304
1	C	0.50	0/6151	0.82	2/8346 (0.0%)
2	X	0.55	0/635	0.89	0/850
2	Y	0.54	0/631	0.89	1/845 (0.1%)
2	Z	0.54	0/644	0.94	1/861 (0.1%)
All	All	0.52	0/20292	0.82	5/27497 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	462	HIS	N-CA-C	6.15	118.49	111.11
2	Y	43	TYR	N-CA-C	-5.44	101.60	110.20
1	C	228	TYR	N-CA-C	5.29	117.05	111.28
2	Z	43	TYR	N-CA-C	-5.23	101.94	110.20
1	A	228	TYR	N-CA-C	5.13	116.88	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5959	0	5944	130	0
1	B	5968	0	5943	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5998	0	5979	139	0
2	X	625	0	602	12	0
2	Y	621	0	599	10	0
2	Z	634	0	615	8	0
3	A	527	0	0	44	0
3	B	535	0	0	36	0
3	C	435	0	0	46	0
3	X	79	0	0	5	0
3	Y	63	0	0	4	0
3	Z	71	0	0	1	0
All	All	21515	0	19682	416	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 11.

All (416) 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:C:36:CYS:HB3	3:C:2002:HOH:O	1.31	1.25
1:B:689:GLU:HB3	3:B:2475:HOH:O	1.30	1.23
1:C:186:GLU:HB3	3:C:2102:HOH:O	1.43	1.19
1:C:773:GLU:HB2	3:C:2421:HOH:O	1.46	1.16
1:A:526:ASN:HA	3:A:2404:HOH:O	1.47	1.13
1:A:62:PRO:HG2	3:A:2014:HOH:O	1.50	1.09
1:B:186:GLU:HG2	3:B:2125:HOH:O	1.51	1.09
1:C:568:LYS:HE2	3:C:2328:HOH:O	1.52	1.08
1:C:294:TYR:HA	3:C:2175:HOH:O	1.54	1.08
1:A:649:ASN:HB3	3:A:2467:HOH:O	1.50	1.07
1:C:284:MET:HE1	1:C:363:PRO:HG2	1.39	1.03
1:B:278:GLU:HA	3:B:2218:HOH:O	1.60	1.00
1:A:207:GLN:HG2	3:A:2128:HOH:O	1.60	1.00
1:A:186:GLU:HG2	3:A:2103:HOH:O	1.62	0.98
1:A:278:GLU:HG3	3:A:2193:HOH:O	1.64	0.97
1:C:742:ASN:HB2	3:C:2405:HOH:O	1.66	0.96
1:B:106:GLU:HG2	1:B:110:ARG:HH12	1.31	0.95
1:A:742:ASN:HB2	3:A:2495:HOH:O	1.69	0.93
1:A:592:GLU:HG2	3:A:2425:HOH:O	1.65	0.93
2:Y:76:MET:HG3	3:Y:2035:HOH:O	1.69	0.92
1:B:99:ASN:HB3	3:B:2035:HOH:O	1.66	0.92
1:A:511:LYS:CE	3:A:2400:HOH:O	2.19	0.90
1:A:51:GLU:HG2	3:A:2013:HOH:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLU:HG2	3:C:2179:HOH:O	1.70	0.89
1:A:207:GLN:CD	3:A:2128:HOH:O	2.17	0.87
1:B:490:GLU:HB2	3:B:2415:HOH:O	1.74	0.86
1:C:299:GLU:CG	3:C:2179:HOH:O	2.21	0.86
1:C:490:GLU:HB3	3:C:2312:HOH:O	1.76	0.86
1:B:241:LYS:HD3	3:B:2187:HOH:O	1.76	0.86
1:A:36:CYS:HB3	3:A:2003:HOH:O	1.74	0.85
1:B:182:LYS:O	1:B:186:GLU:HG3	1.77	0.85
1:C:723:GLU:HG2	3:C:2397:HOH:O	1.75	0.85
1:A:586:VAL:CG1	1:A:608:MET:HE1	2.08	0.83
1:C:374:THR:HG21	2:Z:100:TYR:O	1.78	0.82
1:A:191:GLU:HG2	3:A:2116:HOH:O	1.80	0.81
1:C:727:ARG:CZ	3:C:2397:HOH:O	2.29	0.80
1:C:28:GLU:HB3	1:C:67:LYS:HE2	1.63	0.80
1:A:511:LYS:HE2	3:A:2400:HOH:O	1.80	0.79
1:A:786:CYS:SG	3:A:2213:HOH:O	2.40	0.79
1:C:105:VAL:CG1	1:C:268:LEU:HD23	2.12	0.79
1:A:511:LYS:HE3	3:A:2400:HOH:O	1.82	0.77
1:B:431:GLU:H	1:B:431:GLU:CD	1.93	0.77
1:C:61:LEU:N	1:C:62:PRO:HD2	2.00	0.77
1:A:207:GLN:CG	3:A:2128:HOH:O	2.20	0.77
1:A:61:LEU:N	1:A:62:PRO:HD2	2.00	0.76
1:C:105:VAL:CG1	1:C:268:LEU:CD2	2.64	0.75
1:A:561:HIS:CE1	3:A:2416:HOH:O	2.39	0.75
1:A:586:VAL:HG12	1:A:608:MET:HE1	1.68	0.74
1:C:513:THR:HG22	1:C:516:GLU:HG3	1.70	0.74
1:A:757:ILE:HD11	3:A:2467:HOH:O	1.88	0.73
1:C:734:SER:HB2	3:C:2401:HOH:O	1.88	0.73
1:B:586:VAL:CG1	1:B:608:MET:HE1	2.19	0.73
1:A:588:ARG:HD2	3:A:2449:HOH:O	1.89	0.73
1:C:110:ARG:HD2	3:C:2044:HOH:O	1.89	0.72
1:A:561:HIS:CE1	3:A:2413:HOH:O	2.42	0.72
1:A:568:LYS:NZ	3:A:2419:HOH:O	2.21	0.72
1:B:61:LEU:N	1:B:62:PRO:HD2	2.04	0.72
1:A:766:GLU:CD	3:A:2509:HOH:O	2.32	0.72
1:B:278:GLU:CA	3:B:2218:HOH:O	2.25	0.72
1:A:696:GLN:O	1:A:700:GLU:HG2	1.90	0.71
1:B:651:HIS:HA	1:B:654:LYS:HE3	1.73	0.71
1:A:51:GLU:CG	3:A:2013:HOH:O	2.36	0.71
1:B:186:GLU:HB3	3:B:2129:HOH:O	1.89	0.71
1:C:278:GLU:HG3	3:C:2161:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:81:CYS:N	3:Z:2045:HOH:O	2.22	0.70
2:Y:117:ALA:C	3:Y:2063:HOH:O	2.35	0.69
1:A:586:VAL:HG11	1:A:608:MET:HE1	1.75	0.69
1:C:105:VAL:HG11	1:C:268:LEU:HD23	1.75	0.69
1:B:741:LYS:NZ	3:B:2501:HOH:O	2.25	0.69
1:A:655:ILE:HG22	1:A:699:VAL:HG12	1.74	0.69
1:C:689:GLU:HA	1:C:692:ILE:HG22	1.75	0.69
1:A:557:LYS:HD3	1:A:561:HIS:CD2	2.28	0.68
1:B:208:LYS:NZ	3:B:2148:HOH:O	2.20	0.68
1:A:586:VAL:HG11	1:A:608:MET:CE	2.24	0.68
1:C:427:ARG:HG3	1:C:427:ARG:HH11	1.58	0.68
1:B:692:ILE:HD13	3:B:2473:HOH:O	1.94	0.68
1:C:26:GLU:HG3	1:C:27:THR:H	1.58	0.68
1:C:385:GLY:O	1:C:389:GLN:NE2	2.27	0.68
1:A:243:ARG:NE	3:A:2163:HOH:O	2.27	0.67
1:B:138:HIS:NE2	3:B:2074:HOH:O	2.26	0.67
1:B:278:GLU:N	3:B:2218:HOH:O	2.26	0.67
1:A:243:ARG:CZ	3:A:2163:HOH:O	2.42	0.67
1:C:427:ARG:HH11	1:C:427:ARG:CG	2.07	0.67
1:B:764:THR:HG23	1:B:768:LEU:HD12	1.76	0.67
1:B:106:GLU:HG2	1:B:110:ARG:NH1	2.05	0.67
1:C:93:LEU:HD23	1:C:100:PHE:CE2	2.29	0.66
1:B:708:ASN:HD22	1:B:711:LEU:HD22	1.62	0.65
1:C:786:CYS:SG	3:C:2418:HOH:O	2.29	0.65
1:C:105:VAL:HG13	1:C:268:LEU:CD2	2.26	0.65
1:B:78:LEU:C	1:B:79:LEU:HD12	2.21	0.65
1:C:604:LEU:O	1:C:608:MET:HG3	1.97	0.65
1:B:161:VAL:HG23	1:B:166:ARG:HE	1.62	0.64
1:B:586:VAL:HG11	1:B:608:MET:HE1	1.79	0.64
1:A:105:VAL:HG11	1:A:268:LEU:HD23	1.80	0.63
1:B:166:ARG:CZ	3:B:2105:HOH:O	2.46	0.63
1:C:431:GLU:CD	1:C:431:GLU:H	2.06	0.63
1:C:511:LYS:O	1:C:512:ALA:HB2	1.99	0.62
2:Y:57:TYR:CD2	2:Y:69:ILE:HD12	2.33	0.62
1:B:278:GLU:HG3	3:B:2219:HOH:O	1.99	0.62
1:A:261:CYS:HB3	3:A:2184:HOH:O	1.97	0.62
1:C:689:GLU:C	1:C:691:GLN:H	2.07	0.62
1:B:186:GLU:CG	3:B:2125:HOH:O	2.20	0.62
1:A:330:LYS:HD2	3:X:2032:HOH:O	1.99	0.61
1:B:663:LYS:HE2	1:B:692:ILE:HD11	1.82	0.61
1:B:105:VAL:HG13	1:B:268:LEU:CD2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ILE:O	1:A:760:GLN:HG2	2.00	0.61
1:B:381:LYS:HE2	3:B:2324:HOH:O	1.98	0.61
1:C:138:HIS:HB2	3:C:2064:HOH:O	2.00	0.61
1:A:28:GLU:HG2	1:A:67:LYS:HG2	1.83	0.61
1:B:660:GLU:O	1:B:664:GLU:HG3	2.00	0.60
1:C:700:GLU:CG	3:C:2384:HOH:O	2.50	0.60
1:C:166:ARG:NE	3:C:2086:HOH:O	2.35	0.59
1:A:551:LEU:HD11	1:A:565:ALA:HB1	1.84	0.59
1:B:374:THR:HG21	2:Y:100:TYR:O	2.01	0.59
1:A:105:VAL:CG1	1:A:268:LEU:CD2	2.80	0.59
1:C:660:GLU:O	1:C:664:GLU:HG3	2.01	0.59
1:B:105:VAL:CG1	1:B:268:LEU:HD23	2.33	0.59
1:C:161:VAL:HG23	1:C:166:ARG:HE	1.67	0.59
1:A:525:PRO:O	1:A:526:ASN:HB2	2.03	0.59
1:B:583:LYS:NZ	3:B:2425:HOH:O	2.35	0.59
1:A:78:LEU:C	1:A:79:LEU:HD12	2.27	0.59
1:B:161:VAL:CG2	1:B:166:ARG:HE	2.16	0.59
1:A:330:LYS:HD3	1:A:330:LYS:H	1.68	0.58
1:A:699:VAL:HG23	1:A:703:GLN:NE2	2.17	0.58
1:B:592:GLU:HG2	3:B:2428:HOH:O	2.03	0.58
1:A:655:ILE:HD13	1:A:698:LYS:HE2	1.84	0.58
1:B:586:VAL:HG12	1:B:608:MET:HE1	1.85	0.58
1:B:386:SER:HA	1:B:389:GLN:HE22	1.67	0.58
1:B:150:GLU:HG3	1:B:195:ILE:HD11	1.84	0.58
1:A:660:GLU:O	1:A:663:LYS:HB3	2.04	0.57
1:B:138:HIS:HB2	3:B:2073:HOH:O	2.04	0.57
1:C:464:ARG:HD3	3:C:2299:HOH:O	2.04	0.57
1:B:166:ARG:NH1	3:B:2105:HOH:O	2.38	0.57
1:C:330:LYS:NZ	3:C:2205:HOH:O	2.38	0.57
1:C:659:LEU:HD12	1:C:692:ILE:HD12	1.86	0.57
1:C:105:VAL:HG13	1:C:268:LEU:HD21	1.85	0.57
1:B:646:ARG:HD3	3:B:2466:HOH:O	2.05	0.56
1:B:383:GLN:OE1	3:B:2327:HOH:O	2.18	0.56
2:X:50:TYR:N	2:X:50:TYR:CD2	2.73	0.56
1:A:374:THR:HG21	2:X:100:TYR:O	2.05	0.56
2:X:81:CYS:N	3:X:2050:HOH:O	2.38	0.56
1:C:73:CYS:O	1:C:77:ARG:HG2	2.05	0.56
1:C:689:GLU:C	1:C:691:GLN:N	2.62	0.56
2:Z:50:TYR:CD2	2:Z:50:TYR:N	2.72	0.56
1:C:770:PHE:HA	1:C:774:LEU:HD12	1.87	0.56
1:A:651:HIS:CE1	1:A:655:ILE:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:GLU:CD	3:C:2384:HOH:O	2.48	0.55
2:Z:57:TYR:CD2	2:Z:69:ILE:HD12	2.42	0.55
1:C:211:VAL:HB	1:C:212:PRO:HD3	1.88	0.55
1:A:382:LEU:C	1:A:384:PRO:HD3	2.31	0.55
1:C:689:GLU:O	1:C:691:GLN:N	2.40	0.55
1:A:611:THR:HG21	3:A:2440:HOH:O	2.07	0.54
1:A:265:GLN:NE2	3:A:2187:HOH:O	2.40	0.54
1:A:539:PHE:N	3:A:2405:HOH:O	2.41	0.54
1:B:557:LYS:HB3	1:B:561:HIS:CD2	2.42	0.54
1:B:362:LEU:HA	1:B:363:PRO:C	2.32	0.54
1:C:182:LYS:O	1:C:186:GLU:HG3	2.05	0.54
2:X:81:CYS:HA	3:X:2050:HOH:O	2.07	0.54
2:X:81:CYS:CA	3:X:2050:HOH:O	2.55	0.54
2:Y:74:ASP:O	3:Y:2034:HOH:O	2.18	0.54
1:A:182:LYS:O	1:A:186:GLU:HG3	2.08	0.54
1:A:712:VAL:O	1:A:716:ARG:HG2	2.07	0.54
1:A:609:ILE:HD11	1:A:619:VAL:HG21	1.90	0.54
1:B:27:THR:HG21	1:B:64:TYR:OH	2.07	0.54
1:A:243:ARG:HD3	3:A:2163:HOH:O	2.07	0.54
1:A:616:CYS:HB3	3:A:2462:HOH:O	2.07	0.54
1:B:165:ARG:HD2	1:B:282:TYR:OH	2.08	0.54
1:C:284:MET:HE1	1:C:363:PRO:CG	2.26	0.54
1:B:708:ASN:O	1:B:712:VAL:HG23	2.07	0.54
1:B:659:LEU:HD13	1:B:695:LEU:HB3	1.90	0.54
1:C:727:ARG:NH2	3:C:2397:HOH:O	2.39	0.54
1:C:328:GLU:HB3	3:C:2205:HOH:O	2.08	0.53
1:B:490:GLU:HG2	1:B:490:GLU:O	2.07	0.53
1:C:61:LEU:N	1:C:62:PRO:CD	2.71	0.53
1:A:786:CYS:CB	3:A:2213:HOH:O	2.56	0.53
2:Y:117:ALA:O	3:Y:2063:HOH:O	2.18	0.53
1:C:110:ARG:HG3	3:C:2043:HOH:O	2.09	0.53
1:C:328:GLU:HG2	3:C:2202:HOH:O	2.08	0.53
1:A:715:GLN:NE2	3:A:2485:HOH:O	2.42	0.53
1:B:557:LYS:HD3	1:B:561:HIS:NE2	2.24	0.53
1:A:514:ASN:N	1:A:514:ASN:HD22	2.06	0.53
1:C:27:THR:HG21	1:C:64:TYR:OH	2.08	0.52
1:C:430:TRP:NE1	3:C:2275:HOH:O	2.24	0.52
1:A:161:VAL:CG2	1:A:166:ARG:HE	2.21	0.52
1:A:514:ASN:OD1	1:A:571:GLU:HB2	2.10	0.52
1:B:773:GLU:HB2	3:B:2521:HOH:O	2.07	0.52
1:A:61:LEU:O	1:A:65:LYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:TYR:O	1:C:189:ASP:HB3	2.09	0.52
1:C:762:MET:O	1:C:766:GLU:HG3	2.10	0.52
1:B:663:LYS:HA	3:B:2473:HOH:O	2.09	0.52
1:A:716:ARG:HH12	1:A:719:MET:CE	2.23	0.52
1:C:382:LEU:C	1:C:384:PRO:HD3	2.35	0.52
1:A:105:VAL:CG1	1:A:268:LEU:HD23	2.39	0.52
1:A:105:VAL:HG13	1:A:268:LEU:CD2	2.39	0.52
1:A:568:LYS:CE	3:A:2419:HOH:O	2.58	0.52
1:C:493:ASN:HA	1:C:498:HIS:CG	2.45	0.52
1:A:161:VAL:HG23	1:A:166:ARG:HE	1.73	0.51
1:B:314:ILE:O	1:B:318:LEU:HG	2.11	0.51
1:C:67:LYS:HD2	1:C:70:ARG:NH1	2.26	0.51
1:B:642:HIS:CE1	1:B:750:ILE:HD13	2.45	0.51
1:B:586:VAL:HG11	1:B:608:MET:CE	2.41	0.51
1:B:598:PRO:HA	1:B:601:ILE:HD12	1.91	0.51
1:B:381:LYS:HG3	3:B:2322:HOH:O	2.09	0.51
2:Z:50:TYR:H	2:Z:50:TYR:HD2	1.56	0.51
1:A:243:ARG:CD	3:A:2163:HOH:O	2.58	0.51
1:A:301:PRO:HG3	1:A:344:LYS:HG2	1.92	0.51
1:B:511:LYS:O	1:B:512:ALA:HB2	2.11	0.51
1:A:651:HIS:NE2	1:A:655:ILE:HD11	2.26	0.51
1:B:608:MET:HE3	1:B:613:ILE:HG21	1.93	0.51
1:B:764:THR:CG2	1:B:768:LEU:HD12	2.41	0.51
1:C:427:ARG:CG	1:C:427:ARG:NH1	2.71	0.51
1:C:387:LEU:HB3	1:C:388:PRO:HD3	1.92	0.50
1:A:489:ASP:O	1:A:490:GLU:HB2	2.12	0.50
1:B:78:LEU:O	1:B:79:LEU:HD12	2.12	0.50
1:A:758:ILE:HG22	1:A:762:MET:HE3	1.93	0.50
1:B:513:THR:HG23	1:B:516:GLU:H	1.75	0.50
1:B:659:LEU:HD22	1:B:699:VAL:HG21	1.92	0.50
1:A:47:GLU:H	1:A:47:GLU:CD	2.19	0.50
1:C:257:ASP:CB	3:C:2150:HOH:O	2.59	0.50
2:X:91:ARG:O	2:X:95:GLU:HG3	2.12	0.50
1:A:191:GLU:CG	3:A:2116:HOH:O	2.50	0.50
1:A:762:MET:HA	1:A:762:MET:HE2	1.94	0.50
1:B:701:SER:O	1:B:705:GLU:HG3	2.11	0.50
1:A:79:LEU:HD12	1:A:79:LEU:N	2.27	0.49
1:B:513:THR:HG22	1:B:516:GLU:HG3	1.93	0.49
1:B:770:PHE:HA	1:B:774:LEU:HD12	1.94	0.49
1:C:609:ILE:HD11	1:C:619:VAL:HG21	1.93	0.49
1:B:161:VAL:HG22	1:B:166:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:CZ	3:C:2086:HOH:O	2.59	0.49
1:A:699:VAL:HG23	1:A:703:GLN:HE21	1.76	0.49
1:A:557:LYS:HD3	1:A:561:HIS:HD2	1.76	0.49
1:B:87:THR:HG21	1:B:133:ASP:HB3	1.94	0.49
1:C:122:ASN:ND2	3:C:2048:HOH:O	2.46	0.49
1:A:490:GLU:HB3	3:A:2399:HOH:O	2.13	0.49
1:C:735:VAL:N	3:C:2401:HOH:O	2.45	0.49
1:B:28:GLU:HB3	1:B:67:LYS:HG2	1.94	0.49
1:B:150:GLU:CG	1:B:195:ILE:HD11	2.43	0.49
1:B:517:ILE:HD13	1:B:569:PHE:HE2	1.78	0.48
1:A:493:ASN:C	1:A:493:ASN:HD22	2.20	0.48
1:A:592:GLU:OE2	3:A:2428:HOH:O	2.19	0.48
1:A:103:GLU:OE1	3:A:2034:HOH:O	2.19	0.48
1:C:572:VAL:O	1:C:576:LEU:HB2	2.13	0.48
1:A:562:SER:O	1:A:566:LEU:HG	2.13	0.48
1:B:382:LEU:C	1:B:384:PRO:HD3	2.38	0.48
2:X:57:TYR:CD2	2:X:69:ILE:HD12	2.48	0.48
1:A:592:GLU:CD	3:A:2428:HOH:O	2.57	0.48
1:C:387:LEU:N	1:C:388:PRO:CD	2.77	0.48
1:A:461:TYR:HH	2:X:50:TYR:HD1	1.62	0.47
1:C:588:ARG:HD3	1:C:627:GLU:OE2	2.15	0.47
1:C:87:THR:HG21	1:C:133:ASP:HB3	1.96	0.47
1:B:659:LEU:HA	1:B:695:LEU:HD13	1.96	0.47
1:B:755:HIS:O	1:B:759:GLN:HG3	2.15	0.47
1:C:52:GLY:O	1:C:56:VAL:HG23	2.14	0.47
1:C:727:ARG:NH1	3:C:2398:HOH:O	2.46	0.47
1:B:323:LYS:NZ	3:B:2277:HOH:O	2.39	0.47
1:C:51:GLU:OE2	1:C:96:ARG:NH2	2.41	0.47
1:A:66:SER:HB3	3:A:2018:HOH:O	2.14	0.47
1:B:514:ASN:N	1:B:514:ASN:HD22	2.12	0.47
1:B:659:LEU:HD11	1:B:696:GLN:HG3	1.96	0.47
1:B:786:CYS:SG	3:B:2518:HOH:O	2.61	0.47
1:C:293:ASP:OD2	1:C:293:ASP:C	2.57	0.47
1:B:161:VAL:H	1:B:166:ARG:HH21	1.63	0.47
1:C:586:VAL:HG12	1:C:608:MET:HE1	1.97	0.47
1:C:655:ILE:HD13	1:C:698:LYS:HG2	1.96	0.47
1:A:329:ARG:HG2	1:A:330:LYS:HD3	1.97	0.47
1:B:663:LYS:HG2	3:B:2473:HOH:O	2.15	0.47
1:C:509:LYS:C	1:C:511:LYS:H	2.23	0.47
1:B:26:GLU:HG3	1:B:27:THR:H	1.80	0.46
1:B:105:VAL:CG1	1:B:268:LEU:CD2	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:LEU:O	1:C:688:LEU:HD12	2.14	0.46
1:C:70:ARG:HD2	3:C:2017:HOH:O	2.14	0.46
1:C:323:LYS:HD3	3:C:2055:HOH:O	2.15	0.46
1:C:660:GLU:HG2	1:C:664:GLU:OE1	2.15	0.46
1:A:319:HIS:CE1	1:A:354:VAL:HG13	2.50	0.46
1:B:551:LEU:HD11	1:B:565:ALA:HB1	1.98	0.46
1:C:557:LYS:HD3	1:C:561:HIS:CD2	2.50	0.46
1:C:690:GLU:O	1:C:694:ARG:HG3	2.16	0.46
2:Y:49:PHE:HD2	2:Y:50:TYR:CD1	2.34	0.46
1:B:608:MET:HE2	1:B:614:VAL:HG13	1.98	0.46
1:C:461:TYR:CD2	1:C:464:ARG:HB2	2.50	0.46
1:C:490:GLU:O	1:C:490:GLU:HG2	2.15	0.46
1:A:83:LEU:HD11	1:A:130:PHE:HA	1.98	0.46
1:A:207:GLN:OE1	3:A:2128:HOH:O	2.20	0.46
1:C:362:LEU:HA	1:C:363:PRO:C	2.40	0.46
1:C:727:ARG:NH2	3:C:2399:HOH:O	2.48	0.46
1:B:504:LEU:HD11	1:B:521:LEU:HD21	1.97	0.46
1:C:397:MET:HE3	1:C:401:ARG:NH2	2.30	0.46
1:C:517:ILE:HD12	1:C:517:ILE:H	1.81	0.46
1:A:694:ARG:CZ	1:A:694:ARG:HB3	2.46	0.45
1:B:403:ASP:HA	1:B:444:PRO:HG2	1.99	0.45
1:C:659:LEU:HD11	1:C:696:GLN:HG3	1.97	0.45
1:C:513:THR:HG23	1:C:516:GLU:H	1.81	0.45
1:A:623:ILE:HD12	1:A:637:VAL:HG13	1.98	0.45
1:B:381:LYS:CE	3:B:2324:HOH:O	2.61	0.45
1:B:493:ASN:HA	1:B:498:HIS:CG	2.52	0.45
1:C:500:VAL:HG13	1:C:520:ILE:HG22	1.99	0.45
1:B:502:LEU:O	1:B:506:VAL:HG23	2.15	0.45
1:C:27:THR:HG21	1:C:64:TYR:CZ	2.52	0.45
1:C:161:VAL:HB	1:C:165:ARG:HD3	1.98	0.45
1:C:299:GLU:HG3	3:C:2179:HOH:O	1.99	0.45
1:A:61:LEU:N	1:A:62:PRO:CD	2.73	0.45
1:C:383:GLN:N	1:C:384:PRO:HD3	2.31	0.45
1:C:648:MET:HE3	1:C:648:MET:HA	1.98	0.45
1:A:716:ARG:HH12	1:A:719:MET:HE2	1.82	0.45
1:C:83:LEU:HD11	1:C:130:PHE:HA	1.99	0.45
1:C:493:ASN:N	1:C:493:ASN:HD22	2.15	0.45
1:B:493:ASN:N	1:B:493:ASN:HD22	2.13	0.45
1:C:716:ARG:HA	1:C:716:ARG:HH11	1.82	0.45
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.75	0.44
1:C:169:TYR:CE1	1:C:273:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:VAL:HG11	1:A:608:MET:HE3	1.98	0.44
1:B:431:GLU:CD	1:B:431:GLU:N	2.70	0.44
1:B:630:ARG:HH11	1:B:630:ARG:HG2	1.83	0.44
1:C:257:ASP:HB3	3:C:2150:HOH:O	2.17	0.44
1:A:415:ASN:OD1	1:A:455:LYS:HE3	2.18	0.44
1:A:690:GLU:O	1:A:690:GLU:HG2	2.17	0.44
1:C:715:GLN:HE21	1:C:715:GLN:HB3	1.60	0.44
1:B:61:LEU:N	1:B:62:PRO:CD	2.77	0.44
1:B:630:ARG:NH1	3:B:2457:HOH:O	2.51	0.44
1:C:694:ARG:HG3	1:C:694:ARG:HH11	1.82	0.44
1:A:330:LYS:HD3	1:A:330:LYS:N	2.31	0.44
1:B:779:LEU:HD22	1:B:779:LEU:HA	1.65	0.44
1:A:77:ARG:HD2	1:A:123:GLU:OE1	2.17	0.44
1:A:490:GLU:O	1:A:490:GLU:HG2	2.17	0.44
1:A:177:LEU:N	1:A:178:PRO:CD	2.81	0.43
1:C:106:GLU:HG2	1:C:110:ARG:NH1	2.33	0.43
2:X:102:ASN:HB2	2:X:113:THR:OG1	2.18	0.43
1:A:733:THR:HG22	3:A:2492:HOH:O	2.17	0.43
1:B:642:HIS:HE1	1:B:750:ILE:HD13	1.83	0.43
1:C:490:GLU:CB	3:C:2312:HOH:O	2.51	0.43
2:Z:44:VAL:O	2:Z:83:PHE:HA	2.17	0.43
1:B:26:GLU:HG3	1:B:27:THR:N	2.34	0.43
1:A:362:LEU:HA	1:A:363:PRO:C	2.43	0.43
1:B:773:GLU:CB	3:B:2521:HOH:O	2.66	0.43
1:C:129:ARG:HD3	1:C:179:TRP:CZ3	2.54	0.43
1:C:773:GLU:CD	3:C:2423:HOH:O	2.62	0.43
1:A:608:MET:HE2	1:A:614:VAL:HG13	2.01	0.43
1:B:105:VAL:HG11	1:B:268:LEU:HD23	1.99	0.43
1:C:294:TYR:CA	3:C:2175:HOH:O	2.35	0.43
1:C:511:LYS:O	1:C:512:ALA:CB	2.64	0.43
1:A:182:LYS:O	1:A:186:GLU:CG	2.67	0.43
1:B:475:ALA:HB3	3:B:2405:HOH:O	2.19	0.43
1:A:201:SER:O	1:A:205:ARG:HG2	2.19	0.43
1:A:447:LYS:NZ	1:A:451:GLU:OE2	2.52	0.43
1:A:715:GLN:NE2	1:A:716:ARG:HD2	2.34	0.43
1:C:507:ALA:O	1:C:511:LYS:O	2.37	0.43
1:A:458:ARG:HD3	2:X:58:GLU:OE1	2.19	0.42
1:A:493:ASN:HA	1:A:498:HIS:CG	2.54	0.42
1:C:342:LYS:NZ	3:C:2215:HOH:O	2.51	0.42
1:C:657:LYS:HD2	3:C:2376:HOH:O	2.18	0.42
1:B:117:LYS:HE3	3:B:2049:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ASN:ND2	1:B:543:LYS:HG3	2.34	0.42
1:A:651:HIS:CE1	1:A:655:ILE:CD1	3.02	0.42
1:C:688:LEU:HA	3:C:2381:HOH:O	2.20	0.42
1:C:734:SER:CB	3:C:2401:HOH:O	2.55	0.42
1:A:274:PRO:HA	1:A:275:PRO:HD3	1.90	0.42
1:B:386:SER:HA	1:B:389:GLN:NE2	2.33	0.42
1:C:93:LEU:HD12	1:C:93:LEU:HA	1.91	0.42
1:C:106:GLU:HG2	3:C:2043:HOH:O	2.18	0.42
1:A:330:LYS:H	1:A:330:LYS:CD	2.31	0.42
2:X:44:VAL:O	2:X:83:PHE:HA	2.20	0.42
2:Y:41:THR:OG1	2:Y:87:GLU:HG3	2.20	0.42
1:A:190:ALA:O	1:A:194:ARG:HG3	2.20	0.42
1:A:387:LEU:N	1:A:388:PRO:CD	2.83	0.42
1:B:238:LYS:HD3	1:B:307:HIS:O	2.20	0.42
2:Z:50:TYR:CE1	2:Z:107:ASP:OD2	2.73	0.42
1:A:39:GLY:HA2	1:A:46:LEU:HD13	2.02	0.42
1:B:663:LYS:HG2	1:B:692:ILE:HD13	2.01	0.42
1:C:247:ARG:O	1:C:342:LYS:HB3	2.20	0.42
1:A:165:ARG:HD2	1:A:276:HIS:HB2	2.01	0.41
1:C:229:LEU:HD23	1:C:229:LEU:HA	1.91	0.41
1:B:664:GLU:O	3:B:2474:HOH:O	2.22	0.41
1:C:67:LYS:CD	1:C:70:ARG:NH1	2.83	0.41
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.88	0.41
1:B:540:ASN:HA	1:B:541:PRO:HD2	1.85	0.41
1:C:397:MET:CE	1:C:401:ARG:NH2	2.83	0.41
1:C:516:GLU:O	1:C:520:ILE:HG13	2.20	0.41
1:C:696:GLN:HE21	1:C:696:GLN:HB2	1.59	0.41
2:X:68:LYS:CD	3:X:2038:HOH:O	2.68	0.41
1:A:272:THR:HA	1:A:273:PRO:HD2	1.86	0.41
1:B:229:LEU:HD23	1:B:229:LEU:HA	1.82	0.41
1:C:557:LYS:HD3	1:C:561:HIS:NE2	2.35	0.41
2:Z:102:ASN:HB2	2:Z:113:THR:OG1	2.20	0.41
1:A:698:LYS:HE2	1:A:698:LYS:HB3	1.83	0.41
1:B:542:LEU:O	1:B:546:VAL:HG22	2.19	0.41
1:B:716:ARG:HH11	1:B:716:ARG:HA	1.85	0.41
1:C:330:LYS:NZ	1:C:330:LYS:H	2.19	0.41
1:C:695:LEU:O	1:C:699:VAL:HG23	2.21	0.41
1:B:272:THR:HA	1:B:273:PRO:HD2	1.87	0.41
1:A:715:GLN:HE22	1:A:716:ARG:HD2	1.85	0.41
1:B:35:ILE:O	1:B:38:VAL:HG12	2.21	0.41
1:B:598:PRO:HB3	1:B:636:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:GLU:O	1:B:691:GLN:C	2.64	0.41
1:C:150:GLU:HG3	1:C:195:ILE:HD11	2.03	0.41
1:C:425:GLN:CD	3:C:2268:HOH:O	2.64	0.41
1:C:779:LEU:HD12	1:C:783:GLN:NE2	2.35	0.41
1:B:211:VAL:HB	1:B:212:PRO:HD3	2.03	0.41
1:B:274:PRO:HA	1:B:275:PRO:HD3	1.87	0.41
1:B:277:THR:C	3:B:2218:HOH:O	2.62	0.41
2:Y:49:PHE:HD2	2:Y:50:TYR:CE1	2.39	0.41
1:A:399:TYR:OH	1:A:436:CYS:HB3	2.21	0.40
1:A:492:SER:C	1:A:494:SER:H	2.28	0.40
1:A:573:PHE:HB3	1:A:613:ILE:HG23	2.03	0.40
1:A:695:LEU:O	1:A:699:VAL:HG13	2.20	0.40
1:B:493:ASN:N	1:B:493:ASN:ND2	2.67	0.40
1:B:774:LEU:HB3	1:B:779:LEU:HD23	2.03	0.40
1:C:771:THR:O	1:C:774:LEU:HB2	2.22	0.40
1:A:694:ARG:HH11	1:A:694:ARG:HG3	1.85	0.40
1:C:690:GLU:O	1:C:690:GLU:HG2	2.21	0.40
1:A:604:LEU:HD23	1:A:604:LEU:HA	1.86	0.40
1:C:734:SER:CA	3:C:2401:HOH:O	2.69	0.40
1:A:512:ALA:HB3	1:A:517:ILE:HD11	2.04	0.40
1:C:67:LYS:CD	1:C:70:ARG:HH12	2.35	0.40
1:C:177:LEU:N	1:C:178:PRO:CD	2.85	0.40
1:C:623:ILE:HD12	1:C:637:VAL:HG13	2.04	0.40
2:Y:48:SER:OG	2:Y:107:ASP:OD2	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	722/757 (95%)	704 (98%)	15 (2%)	3 (0%)	30 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	723/757 (96%)	702 (97%)	18 (2%)	3 (0%)	30	27
1	C	727/757 (96%)	709 (98%)	14 (2%)	4 (1%)	21	17
2	X	73/98 (74%)	72 (99%)	1 (1%)	0	100	100
2	Y	72/98 (74%)	72 (100%)	0	0	100	100
2	Z	74/98 (76%)	74 (100%)	0	0	100	100
All	All	2391/2565 (93%)	2333 (98%)	48 (2%)	10 (0%)	30	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	GLU
1	B	490	GLU
1	B	525	PRO
1	C	490	GLU
1	C	512	ALA
1	C	690	GLU
1	A	525	PRO
1	B	512	ALA
1	C	689	GLU
1	A	489	ASP

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	669/694 (96%)	653 (98%)	16 (2%)	43	47
1	B	670/694 (96%)	655 (98%)	15 (2%)	45	50
1	C	674/694 (97%)	647 (96%)	27 (4%)	28	27
2	X	67/86 (78%)	65 (97%)	2 (3%)	36	38
2	Y	67/86 (78%)	67 (100%)	0	100	100
2	Z	68/86 (79%)	67 (98%)	1 (2%)	57	64
All	All	2215/2340 (95%)	2154 (97%)	61 (3%)	38	41

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	70	ARG
1	A	93	LEU
1	A	114	GLU
1	A	330	LYS
1	A	387	LEU
1	A	493	ASN
1	A	560	SER
1	A	584	LEU
1	A	692	ILE
1	A	694	ARG
1	A	696	GLN
1	A	699	VAL
1	A	700	GLU
1	A	711	LEU
1	A	774	LEU
1	B	27	THR
1	B	31	LEU
1	B	93	LEU
1	B	114	GLU
1	B	272	THR
1	B	387	LEU
1	B	431	GLU
1	B	490	GLU
1	B	493	ASN
1	B	514	ASN
1	B	584	LEU
1	B	689	GLU
1	B	693	GLU
1	B	774	LEU
1	B	779	LEU
1	C	27	THR
1	C	29	ASP
1	C	31	LEU
1	C	44	CYS
1	C	79	LEU
1	C	114	GLU
1	C	247	ARG
1	C	258	SER
1	C	278	GLU
1	C	299	GLU
1	C	330	LYS

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Mol	Chain	Res	Type
1	C	382	LEU
1	C	387	LEU
1	C	427	ARG
1	C	461	TYR
1	C	490	GLU
1	C	493	ASN
1	C	560	SER
1	C	576	LEU
1	C	688	LEU
1	C	689	GLU
1	C	693	GLU
1	C	696	GLN
1	C	711	LEU
1	C	715	GLN
1	C	774	LEU
1	C	779	LEU
2	X	38	LYS
2	X	50	TYR
2	Z	50	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	215	GLN
1	A	439	GLN
1	A	493	ASN
1	A	498	HIS
1	A	553	HIS
1	A	561	HIS
1	A	596	ASN
1	A	649	ASN
1	A	656	GLN
1	A	696	GLN
1	A	706	GLN
1	A	708	ASN
1	A	715	GLN
1	A	753	GLN
1	A	756	GLN
1	A	759	GLN
1	B	30	HIS
1	B	49	ASN

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Mol	Chain	Res	Type
1	B	63	ASN
1	B	198	ASN
1	B	215	GLN
1	B	267	ASN
1	B	493	ASN
1	B	498	HIS
1	B	540	ASN
1	B	553	HIS
1	B	561	HIS
1	B	649	ASN
1	B	656	GLN
1	B	691	GLN
1	B	696	GLN
1	B	706	GLN
1	B	708	ASN
1	B	715	GLN
1	B	753	GLN
1	B	756	GLN
1	B	789	GLN
1	C	63	ASN
1	C	111	GLN
1	C	136	ASN
1	C	198	ASN
1	C	223	HIS
1	C	245	GLN
1	C	343	ASN
1	C	493	ASN
1	C	540	ASN
1	C	553	HIS
1	C	649	ASN
1	C	656	GLN
1	C	696	GLN
1	C	703	GLN
1	C	706	GLN
1	C	708	ASN
1	C	715	GLN
1	C	753	GLN
1	C	756	GLN
1	C	760	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	728/757 (96%)	0.14	38 (5%)	33	31	22, 35, 67, 81	0
1	B	729/757 (96%)	0.21	43 (5%)	28	27	22, 36, 70, 82	0
1	C	733/757 (96%)	0.44	42 (5%)	29	28	24, 39, 69, 81	0
2	X	77/98 (78%)	0.04	4 (5%)	33	31	27, 34, 47, 54	0
2	Y	76/98 (77%)	0.12	5 (6%)	24	23	28, 35, 51, 61	0
2	Z	78/98 (79%)	0.18	5 (6%)	25	24	27, 35, 52, 66	0
All	All	2421/2565 (94%)	0.25	137 (5%)	29	28	22, 37, 67, 82	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	ILE	5.8
2	Y	117	ALA	5.2
1	C	692	ILE	5.1
1	C	385	GLY	4.6
1	B	27	THR	4.5
2	X	50	TYR	4.4
1	A	27	THR	4.2
2	Y	76	MET	4.0
1	C	688	LEU	3.9
1	A	695	LEU	3.9
1	B	655	ILE	3.7
1	C	294	TYR	3.6
1	C	554	LEU	3.4
1	A	489	ASP	3.4
1	C	689	GLU	3.4
1	B	581	GLU	3.4
2	Z	50	TYR	3.3
1	B	28	GLU	3.3
1	C	157	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
2	Z	49	PHE	3.3
1	B	689	GLU	3.3
1	A	59	ALA	3.3
1	C	690	GLU	3.3
1	A	51	GLU	3.2
2	X	49	PHE	3.2
1	C	695	LEU	3.1
1	A	693	GLU	3.1
1	C	461	TYR	3.1
1	B	517	ILE	3.1
1	A	699	VAL	3.0
1	B	694	ARG	3.0
2	X	118	GLY	3.0
1	B	700	GLU	2.9
1	C	734	SER	2.9
1	B	520	ILE	2.9
1	C	27	THR	2.9
1	C	489	ASP	2.9
1	A	694	ARG	2.9
1	A	461	TYR	2.9
1	B	512	ALA	2.9
1	B	513	THR	2.9
1	A	28	GLU	2.9
1	B	523	ASP	2.8
1	C	520	ILE	2.8
1	A	690	GLU	2.8
1	C	665	LYS	2.8
1	B	160	ASP	2.8
1	A	691	GLN	2.8
1	B	461	TYR	2.8
1	B	186	GLU	2.8
1	B	554	LEU	2.8
1	C	701	SER	2.8
1	C	727	ARG	2.8
2	Z	76	MET	2.8
1	B	278	GLU	2.8
1	A	31	LEU	2.8
1	B	29	ASP	2.7
1	C	733	THR	2.7
1	B	64	TYR	2.7
1	C	538	SER	2.7
1	B	690	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	726	VAL	2.7
1	C	299	GLU	2.6
1	A	733	THR	2.6
1	C	521	LEU	2.6
1	A	70	ARG	2.6
1	C	512	ALA	2.6
1	B	692	ILE	2.6
1	A	662	ALA	2.6
1	C	730	THR	2.6
1	A	665	LYS	2.5
1	A	186	GLU	2.5
1	B	662	ALA	2.5
1	B	691	GLN	2.5
1	C	28	GLU	2.5
1	B	659	LEU	2.5
1	A	663	LYS	2.5
2	Z	118	GLY	2.5
1	C	524	VAL	2.5
1	A	64	TYR	2.5
1	B	495	LEU	2.5
1	C	523	ASP	2.4
1	C	773	GLU	2.4
1	B	62	PRO	2.4
1	A	659	LEU	2.4
1	C	495	LEU	2.4
1	A	732	GLY	2.4
1	A	279	ASP	2.4
2	X	76	MET	2.4
1	A	520	ILE	2.4
2	Z	77	LYS	2.4
1	B	157	GLN	2.3
1	C	525	PRO	2.3
1	A	157	GLN	2.3
1	A	696	GLN	2.3
2	Y	50	TYR	2.3
1	C	694	ARG	2.3
1	A	99	ASN	2.3
1	A	39	GLY	2.3
1	B	654	LYS	2.3
1	C	561	HIS	2.2
1	C	518	PHE	2.2
1	B	509	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	2.2
1	B	526	ASN	2.2
1	B	51	GLU	2.2
1	C	505	ALA	2.2
1	C	302	VAL	2.2
1	C	571	GLU	2.2
1	A	526	ASN	2.2
1	B	490	GLU	2.1
1	A	524	VAL	2.1
1	B	695	LEU	2.1
1	B	568	LYS	2.1
1	A	278	GLU	2.1
1	B	518	PHE	2.1
1	C	517	ILE	2.1
1	C	241	LYS	2.1
1	C	691	GLN	2.1
1	B	699	VAL	2.1
1	C	699	VAL	2.1
1	B	772	ALA	2.1
1	A	554	LEU	2.1
1	A	578	GLU	2.1
1	A	786	CYS	2.1
1	B	483	CYS	2.1
2	Y	49	PHE	2.1
1	B	505	ALA	2.1
1	B	489	ASP	2.0
1	B	663	LYS	2.0
1	A	159	GLU	2.0
1	A	653	LEU	2.0
1	B	759	GLN	2.0
1	C	389	GLN	2.0
2	Y	81	CYS	2.0
1	A	511	LYS	2.0
1	C	298	PRO	2.0

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

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.