



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 PM UTC

PDB ID : 1O9K / pdb_00001o9k
Title : Crystal structure of the retinoblastoma tumour suppressor protein bound to E2F peptide
Authors : Xiao, B.; Spencer, J.; Clements, A.; Ali-Khan, N.; Mittnacht, S.; Broceno, C.; Burghammer, M.; Perrakis, A.; Marmorstein, R.; Gamblin, S.J.
Deposited on : 2002-12-16
Resolution : 2.60 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

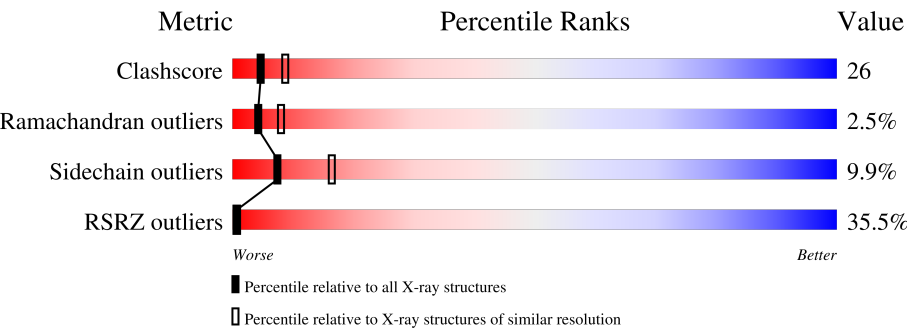
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	218	7% 54% 28% 6% 11%
1	C	218	9% 57% 24% 7% 11%
1	E	218	20% 50% 32% 6% 11%
1	G	218	36% 52% 29% 7% 11%
2	B	152	19% 59% 30% 6% 5%
2	D	152	16% 59% 32% 5% 5%
2	F	152	73% 56% 33% • 5%

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Mol	Chain	Length	Quality of chain
2	H	152	93% 43% 45% 6% 5%
3	P	18	33% 72% 22% 6%
3	Q	18	28% 50% 39% 11%
3	R	18	78% 39% 44% 11% 6%
3	S	18	100% 39% 50% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11974 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 RETINOBLASTOMA-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	C	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	E	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			
1	G	194	Total	C	N	O	S	0	0	0
			1569	1003	263	290	13			

- Molecule 2 is a protein called RETINOBLASTOMA-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	D	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	F	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			
2	H	144	Total	C	N	O	S	0	0	0
			1213	789	205	211	8			

- Molecule 3 is a protein called TRANSCRIPTION FACTOR E2F1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	Q	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	R	18	Total	C	N	O	0	0	0
			149	96	23	30			
3	S	18	Total	C	N	O	0	0	0
			149	96	23	30			

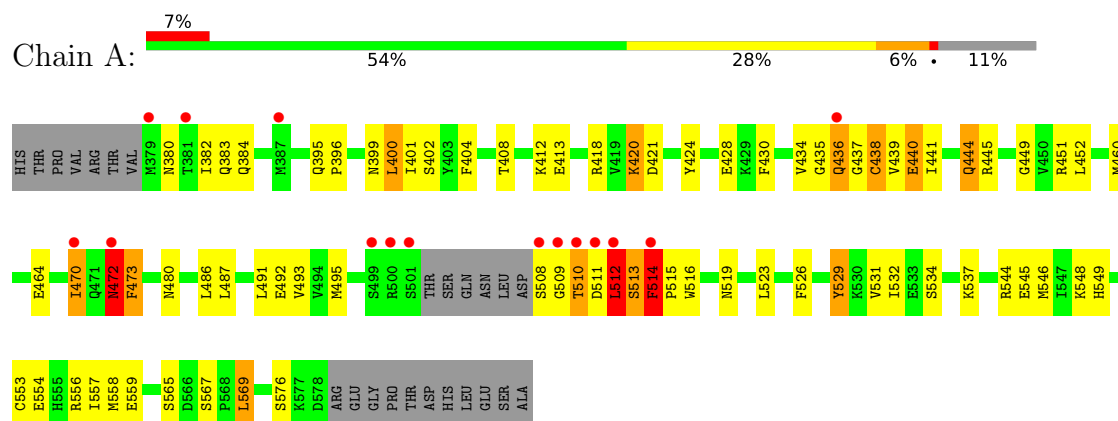
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	39	Total O 39 39	0	0
4	B	18	Total O 18 18	0	0
4	C	47	Total O 47 47	0	0
4	D	24	Total O 24 24	0	0
4	E	38	Total O 38 38	0	0
4	F	16	Total O 16 16	0	0
4	G	39	Total O 39 39	0	0
4	H	15	Total O 15 15	0	0
4	P	1	Total O 1 1	0	0
4	Q	4	Total O 4 4	0	0
4	R	4	Total O 4 4	0	0
4	S	5	Total O 5 5	0	0

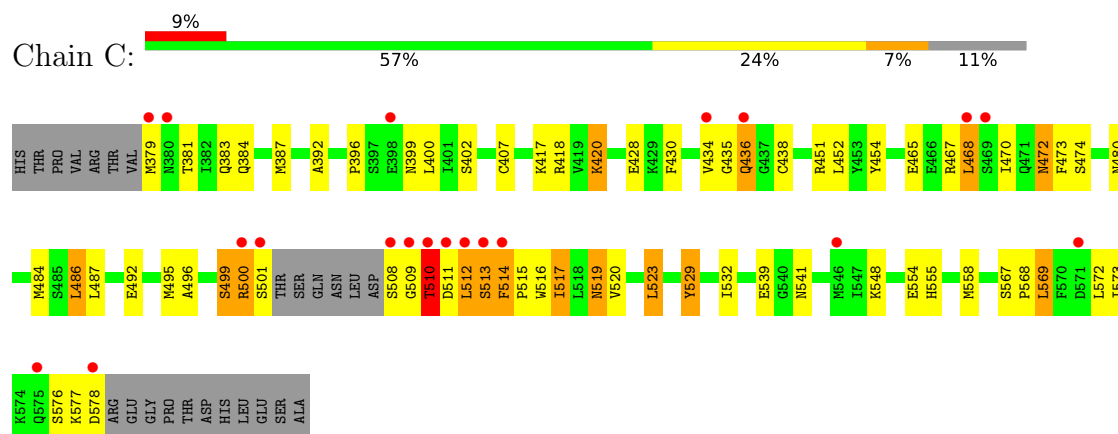
3 Residue-property plots

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.

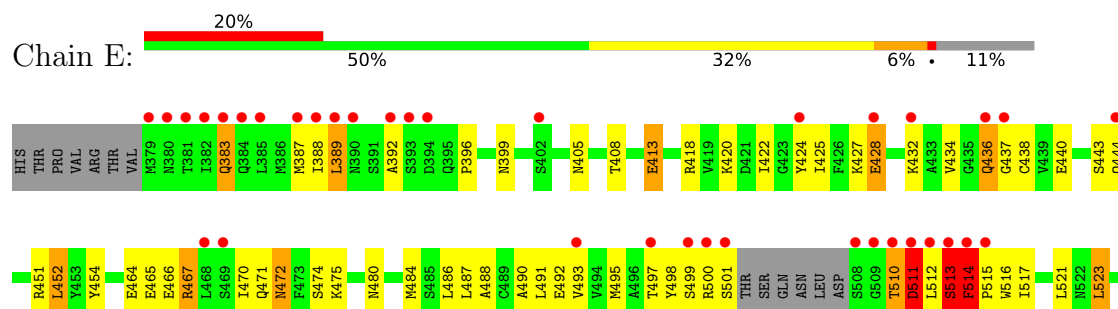
• Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN



• Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN

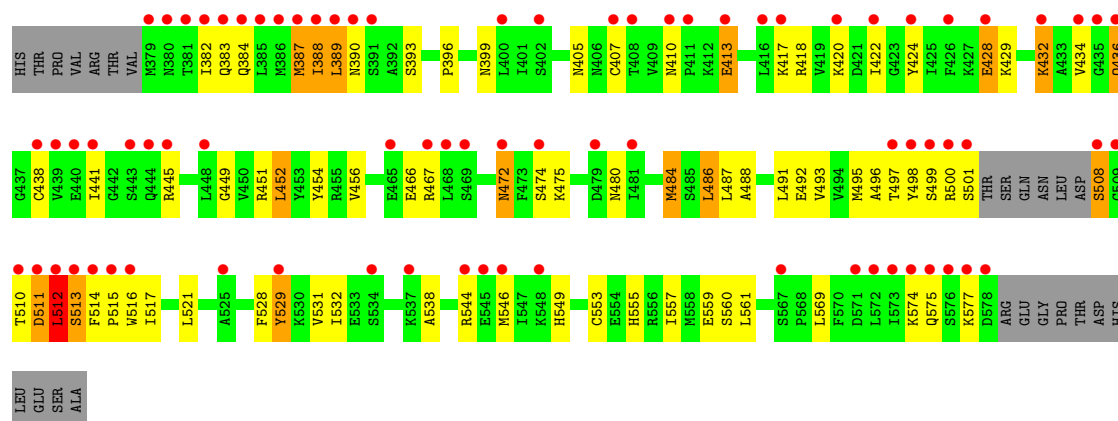


• Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN

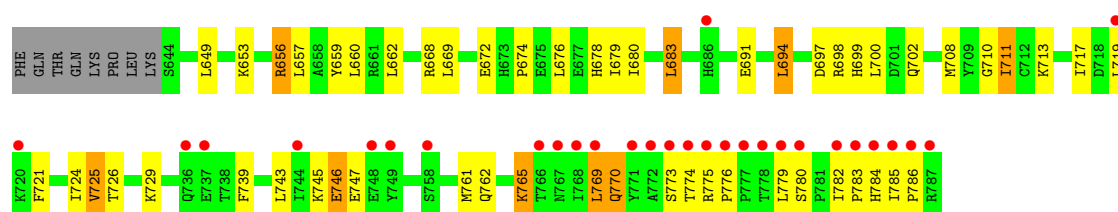




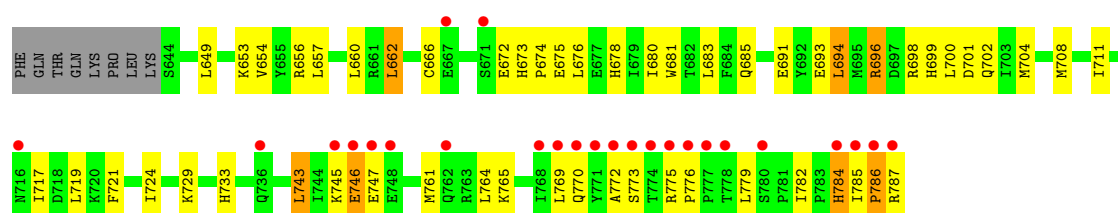
• Molecule 1: RETINOBLASTOMA-ASSOCIATED PROTEIN



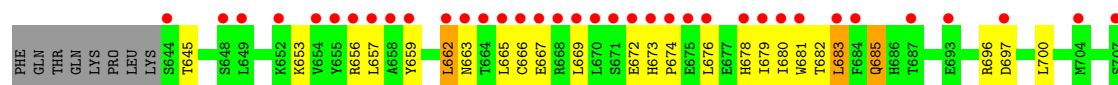
• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

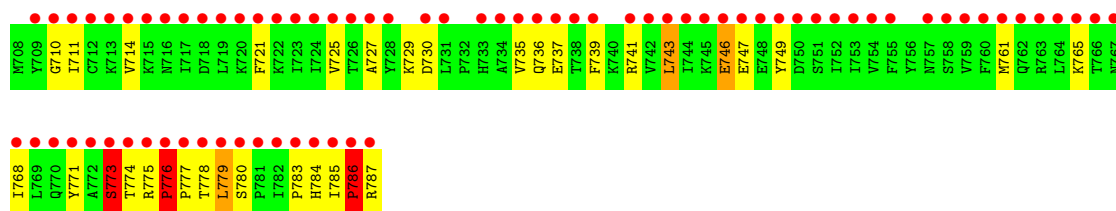


• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

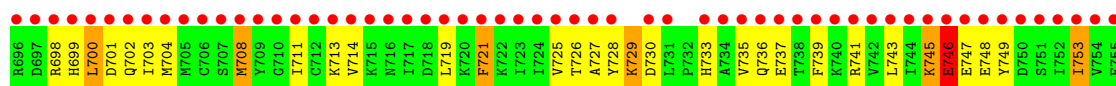
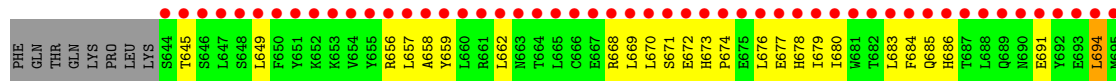


• Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN

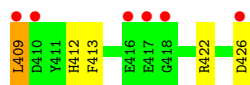




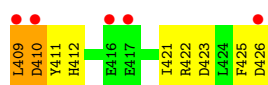
● Molecule 2: RETINOBLASTOMA-ASSOCIATED PROTEIN



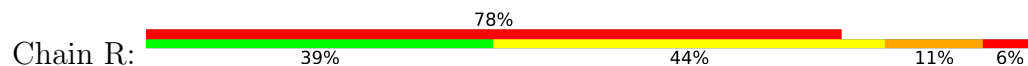
● Molecule 3: TRANSCRIPTION FACTOR E2F1



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● Molecule 3: TRANSCRIPTION FACTOR E2F1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.00Å 158.55Å 110.62Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.00-2.60) 87.9 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.229 , 0.285 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	1/1595 (0.1%)	1.07	9/2141 (0.4%)
1	C	0.67	0/1595	1.04	3/2141 (0.1%)
1	E	0.66	0/1595	1.02	4/2141 (0.2%)
1	G	0.67	0/1595	1.01	5/2141 (0.2%)
2	B	0.60	0/1242	0.93	0/1680
2	D	0.55	0/1242	0.93	0/1680
2	F	0.52	0/1242	0.94	2/1680 (0.1%)
2	H	0.58	1/1242 (0.1%)	0.94	0/1680
3	P	0.52	0/152	0.80	0/203
3	Q	0.45	0/152	0.77	0/203
3	R	0.55	0/152	0.98	0/203
3	S	0.51	0/152	0.88	0/203
All	All	0.63	2/11956 (0.0%)	0.99	23/16096 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	THR	CA-C	-6.67	1.44	1.52
2	H	708	MET	SD-CE	5.73	1.93	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	468	LEU	N-CA-C	-10.51	93.24	109.85
1	E	513	SER	N-CA-C	-10.34	95.61	110.59
1	A	509	GLY	N-CA-C	-9.77	90.02	113.18
1	G	513	SER	N-CA-C	-9.70	96.96	110.35
1	C	513	SER	N-CA-C	-7.92	100.70	110.61
1	E	532	ILE	N-CA-C	7.74	117.81	110.30
1	A	512	LEU	N-CA-C	7.33	126.41	110.80
1	G	532	ILE	N-CA-C	7.23	117.31	110.30
1	A	437	GLY	N-CA-C	7.17	120.27	111.45
1	A	567	SER	N-CA-C	6.38	117.70	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ILE	N-CA-C	6.30	116.41	110.30
2	F	778	THR	N-CA-C	-6.12	103.14	112.99
1	E	514	PHE	N-CA-C	-5.87	104.82	113.16
1	G	432	LYS	N-CA-C	-5.80	105.69	112.89
1	G	413	GLU	N-CA-C	5.70	117.49	111.28
2	F	776	PRO	N-CA-C	5.66	117.61	110.70
1	A	383	GLN	N-CA-C	5.47	117.25	111.28
1	E	557	ILE	N-CA-C	-5.44	105.07	111.00
1	A	514	PHE	N-CA-C	5.31	121.55	109.81
1	A	509	GLY	CA-C-N	-5.28	112.51	121.85
1	A	509	GLY	C-N-CA	-5.28	112.51	121.85
1	G	538	ALA	N-CA-C	5.15	117.80	111.82
1	C	532	ILE	N-CA-C	5.10	115.32	110.42

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	1569	0	1592	87	0
1	C	1569	0	1592	79	0
1	E	1569	0	1592	110	0
1	G	1569	0	1592	116	0
2	B	1213	0	1246	48	0
2	D	1213	0	1246	43	0
2	F	1213	0	1246	56	0
2	H	1213	0	1246	69	0
3	P	149	0	129	5	0
3	Q	149	0	129	11	0
3	R	149	0	129	17	0
3	S	149	0	129	10	0
4	A	39	0	0	9	0
4	B	18	0	0	3	0
4	C	47	0	0	14	0
4	D	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	38	0	0	9	0
4	F	16	0	0	3	0
4	G	39	0	0	9	0
4	H	15	0	0	8	0
4	P	1	0	0	0	0
4	Q	4	0	0	1	0
4	R	4	0	0	1	0
4	S	5	0	0	3	0
All	All	11974	0	11868	610	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 26.

All (610) 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:512:LEU:HD22	1:A:512:LEU:O	1.28	1.27
1:C:513:SER:O	1:C:515:PRO:HD2	1.35	1.23
2:H:737:GLU:HB2	4:H:2008:HOH:O	1.36	1.21
1:C:509:GLY:HA2	4:C:2028:HOH:O	1.50	1.10
1:A:512:LEU:O	1:A:512:LEU:CD2	2.05	1.04
1:G:511:ASP:HB2	4:G:2025:HOH:O	1.55	1.04
1:G:514:PHE:HB2	1:G:553:CYS:SG	2.00	1.02
1:A:511:ASP:CG	1:A:512:LEU:H	1.61	0.98
1:G:428:GLU:HG3	1:G:432:LYS:NZ	1.81	0.96
1:G:495:MET:HG3	1:G:512:LEU:HG	1.50	0.94
1:E:493:VAL:O	1:E:497:THR:HG23	1.69	0.93
1:A:438:CYS:HG	1:G:438:CYS:HG	1.08	0.93
1:A:554:GLU:HG2	1:A:558:MET:HE2	1.48	0.92
1:G:512:LEU:O	1:G:512:LEU:HD13	1.69	0.91
1:G:428:GLU:HG3	1:G:432:LYS:HZ2	1.35	0.91
1:G:493:VAL:O	1:G:497:THR:HG23	1.71	0.90
2:H:691:GLU:HB3	2:H:694:LEU:HD23	1.52	0.90
1:C:418:ARG:HH11	1:C:480:ASN:HD22	1.15	0.89
1:A:438:CYS:CB	1:G:438:CYS:HG	1.87	0.87
2:H:763:ARG:HD2	4:H:2013:HOH:O	1.74	0.87
2:F:761:MET:HG2	2:F:765:LYS:HE2	1.56	0.87
1:E:512:LEU:HD13	1:E:512:LEU:C	2.00	0.86
2:F:776:PRO:HB2	2:F:777:PRO:HD3	1.56	0.86
2:H:670:LEU:HD21	2:H:719:LEU:HD22	1.58	0.86
1:G:555:HIS:O	1:G:559:GLU:HG2	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:O	1:A:513:SER:C	2.19	0.85
3:Q:410:ASP:HB3	4:Q:2001:HOH:O	1.76	0.84
1:C:509:GLY:CA	4:C:2028:HOH:O	2.17	0.83
2:F:741:ARG:NH2	4:F:2013:HOH:O	2.10	0.83
1:E:514:PHE:N	1:E:515:PRO:CD	2.41	0.83
1:A:512:LEU:HD13	1:A:512:LEU:C	2.04	0.83
1:E:513:SER:HB2	1:E:515:PRO:HD2	1.58	0.82
1:C:492:GLU:OE1	1:C:512:LEU:HD11	1.80	0.82
2:F:714:VAL:HG21	2:F:768:ILE:CG2	2.09	0.82
1:A:511:ASP:CG	1:A:512:LEU:N	2.37	0.81
1:A:513:SER:O	1:A:515:PRO:HD2	1.81	0.81
2:H:679:ILE:HG22	2:H:711:ILE:HD13	1.61	0.81
2:F:680:ILE:HA	2:F:711:ILE:HD12	1.61	0.80
2:H:680:ILE:HA	2:H:711:ILE:HD12	1.62	0.80
1:C:519:ASN:HB3	4:C:2031:HOH:O	1.80	0.79
1:C:492:GLU:CD	1:C:512:LEU:HD11	2.08	0.79
1:G:513:SER:C	1:G:515:PRO:HD2	2.08	0.79
2:H:764:LEU:O	2:H:768:ILE:HG13	1.82	0.79
1:E:418:ARG:HH11	1:E:480:ASN:HD22	1.30	0.78
2:B:776:PRO:HG2	4:B:2018:HOH:O	1.84	0.78
1:E:537:LYS:HG2	3:R:413:PHE:HE2	1.46	0.78
1:E:512:LEU:HD13	1:E:512:LEU:O	1.84	0.78
1:E:428:GLU:HB3	1:E:432:LYS:NZ	1.99	0.78
1:A:472:ASN:O	1:A:473:PHE:HB2	1.84	0.77
2:D:765:LYS:O	2:D:769:LEU:HD23	1.83	0.76
1:A:519:ASN:HB3	4:A:2023:HOH:O	1.86	0.76
1:C:554:GLU:HG2	1:C:558:MET:HE2	1.66	0.76
2:F:785:ILE:HG22	2:F:787:ARG:HH11	1.50	0.76
2:H:765:LYS:O	2:H:769:LEU:HD23	1.85	0.76
1:A:512:LEU:HD22	1:A:512:LEU:C	2.10	0.76
1:E:513:SER:CB	1:E:515:PRO:HD2	2.16	0.76
1:A:451:ARG:HH22	1:G:508:SER:HB2	1.50	0.75
1:E:470:ILE:HG22	1:E:472:ASN:H	1.50	0.75
2:H:714:VAL:HG11	2:H:768:ILE:HG22	1.68	0.75
1:C:512:LEU:HA	1:C:516:TRP:HB3	1.68	0.75
1:E:436:GLN:HG3	4:E:2019:HOH:O	1.86	0.75
1:G:512:LEU:HD13	1:G:512:LEU:C	2.12	0.74
1:E:514:PHE:CD2	1:E:514:PHE:C	2.66	0.73
2:F:771:TYR:HA	2:F:776:PRO:HB3	1.70	0.73
3:Q:409:LEU:C	3:Q:411:TYR:H	1.95	0.73
2:F:714:VAL:HG21	2:F:768:ILE:HG22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:787:ARG:HG3	2:H:787:ARG:HH11	1.54	0.73
3:Q:422:ARG:O	3:Q:426:ASP:HB2	1.87	0.72
1:C:501:SER:HA	4:C:2027:HOH:O	1.89	0.72
1:A:428:GLU:HG3	1:E:424:TYR:HE2	1.54	0.71
1:E:513:SER:C	1:E:515:PRO:HD2	2.15	0.71
2:H:784:HIS:O	2:H:786:PRO:HD3	1.90	0.71
2:F:776:PRO:HD2	2:F:777:PRO:HD2	1.73	0.71
1:G:512:LEU:HD22	1:G:513:SER:O	1.91	0.71
2:F:737:GLU:HB2	4:F:2011:HOH:O	1.91	0.70
3:S:416:GLU:HB2	3:S:419:GLU:HG3	1.72	0.70
1:A:382:ILE:HD12	4:A:2037:HOH:O	1.91	0.70
2:D:746:GLU:CD	2:D:746:GLU:H	1.99	0.70
1:E:472:ASN:HD22	1:E:472:ASN:C	1.99	0.70
2:H:746:GLU:HG2	2:H:747:GLU:H	1.56	0.70
1:E:514:PHE:N	1:E:515:PRO:HD2	2.06	0.70
2:B:660:LEU:HD11	2:B:785:ILE:HD11	1.72	0.70
1:A:556:ARG:HA	1:A:559:GLU:HG2	1.74	0.70
2:H:703:ILE:HD12	2:H:703:ILE:N	2.07	0.70
1:A:445:ARG:NE	4:A:2010:HOH:O	2.18	0.69
2:D:678:HIS:ND1	2:D:779:LEU:HD13	2.08	0.69
1:G:512:LEU:O	1:G:512:LEU:CD1	2.39	0.69
1:E:436:GLN:NE2	4:E:2018:HOH:O	2.25	0.69
1:A:556:ARG:CZ	4:A:2032:HOH:O	2.39	0.69
1:C:383:GLN:HG2	1:C:387:MET:HE2	1.74	0.69
1:G:512:LEU:HD22	1:G:516:TRP:HB3	1.75	0.69
2:F:680:ILE:HA	2:F:711:ILE:CD1	2.23	0.69
1:G:514:PHE:N	1:G:515:PRO:CD	2.56	0.69
1:G:512:LEU:CD2	1:G:516:TRP:HB3	2.23	0.68
1:G:428:GLU:CG	1:G:432:LYS:NZ	2.55	0.68
2:H:678:HIS:HE1	2:H:780:SER:O	1.76	0.68
2:F:735:VAL:HG12	2:F:737:GLU:H	1.58	0.68
1:G:508:SER:N	1:G:513:SER:HG	1.92	0.68
2:B:668:ARG:HB3	1:C:500:ARG:HG3	1.74	0.68
1:G:495:MET:HB2	1:G:512:LEU:HD12	1.76	0.68
1:E:514:PHE:HB2	1:E:553:CYS:SG	2.34	0.67
2:B:668:ARG:HD3	1:C:500:ARG:NH1	2.09	0.67
1:C:435:GLY:H	1:C:508:SER:HA	1.58	0.67
1:C:436:GLN:HE21	1:C:436:GLN:N	1.92	0.67
1:E:511:ASP:OD1	1:E:512:LEU:N	2.26	0.67
1:G:384:GLN:HA	1:G:387:MET:HE3	1.75	0.67
1:C:407:CYS:HA	1:C:472:ASN:ND2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:510:THR:C	1:G:512:LEU:H	2.02	0.67
1:C:492:GLU:OE2	1:C:512:LEU:HD11	1.95	0.67
1:C:428:GLU:CD	4:C:2018:HOH:O	2.38	0.67
1:C:548:LYS:HD2	4:C:2040:HOH:O	1.94	0.67
1:E:492:GLU:OE2	1:E:512:LEU:HD11	1.94	0.67
1:A:495:MET:CE	1:A:512:LEU:HB2	2.26	0.66
1:E:565:SER:OG	2:F:697:ASP:OD2	2.13	0.66
2:H:763:ARG:CD	4:H:2013:HOH:O	2.38	0.66
2:B:668:ARG:O	1:C:500:ARG:HB2	1.95	0.66
3:Q:409:LEU:O	3:Q:411:TYR:N	2.28	0.66
2:B:656:ARG:NH1	3:P:412:HIS:HB2	2.09	0.66
2:D:746:GLU:CD	2:D:746:GLU:N	2.54	0.66
1:E:514:PHE:CD2	1:E:514:PHE:O	2.48	0.66
2:H:698:ARG:HG2	4:H:2010:HOH:O	1.94	0.66
1:C:418:ARG:HH11	1:C:480:ASN:ND2	1.91	0.65
2:D:672:GLU:C	2:D:674:PRO:HD3	2.22	0.65
2:F:656:ARG:NH2	4:F:2001:HOH:O	2.29	0.65
2:B:676:LEU:HD11	2:B:717:ILE:HG13	1.77	0.65
1:G:510:THR:O	1:G:512:LEU:N	2.30	0.65
1:G:577:LYS:O	4:G:2039:HOH:O	2.14	0.65
2:D:745:LYS:HB2	2:D:746:GLU:OE2	1.97	0.65
2:D:775:ARG:HB2	2:D:776:PRO:HD2	1.79	0.64
1:E:418:ARG:NH1	1:E:480:ASN:HD22	1.93	0.64
2:F:710:GLY:O	2:F:714:VAL:HG23	1.96	0.64
1:C:472:ASN:ND2	1:C:472:ASN:C	2.54	0.64
1:C:418:ARG:NH1	1:C:480:ASN:HD22	1.93	0.64
2:F:784:HIS:CD2	2:F:786:PRO:HG2	2.31	0.64
1:G:472:ASN:C	1:G:472:ASN:HD22	2.05	0.64
2:F:776:PRO:CB	2:F:777:PRO:HD3	2.27	0.64
2:D:785:ILE:HG22	2:D:785:ILE:O	1.98	0.64
1:G:513:SER:CB	1:G:515:PRO:HD2	2.26	0.64
1:A:440:GLU:HG2	1:G:434:VAL:HG11	1.78	0.64
1:A:492:GLU:OE1	1:A:512:LEU:HD21	1.98	0.64
1:C:465:GLU:O	1:C:468:LEU:O	2.16	0.63
1:G:418:ARG:HH11	1:G:480:ASN:HD22	1.45	0.63
1:E:495:MET:HB3	1:E:512:LEU:CB	2.28	0.63
2:B:785:ILE:O	2:B:785:ILE:HG23	1.99	0.63
1:A:472:ASN:O	1:A:473:PHE:CB	2.47	0.62
2:F:659:TYR:HB2	2:F:783:PRO:HG2	1.81	0.62
1:A:438:CYS:HB2	1:G:438:CYS:HG	1.64	0.62
2:B:775:ARG:NH1	4:B:2017:HOH:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:LEU:C	1:E:512:LEU:CD1	2.70	0.62
2:B:746:GLU:N	2:B:746:GLU:CD	2.57	0.62
1:E:510:THR:O	1:E:511:ASP:C	2.41	0.62
1:G:512:LEU:HD23	1:G:516:TRP:HE3	1.63	0.62
3:R:410:ASP:CG	3:R:410:ASP:O	2.41	0.62
1:A:438:CYS:HB2	1:G:438:CYS:SG	2.40	0.62
1:E:420:LYS:C	1:E:420:LYS:HD3	2.25	0.62
1:A:556:ARG:NE	4:A:2032:HOH:O	2.32	0.61
1:E:498:TYR:C	1:E:500:ARG:H	2.06	0.61
2:B:761:MET:HG2	2:B:762:GLN:NE2	2.14	0.61
1:C:512:LEU:HD13	1:C:512:LEU:C	2.25	0.61
1:E:383:GLN:O	1:E:387:MET:HG2	2.00	0.61
2:F:725:VAL:O	2:F:729:LYS:HG3	1.99	0.61
1:G:495:MET:HB3	1:G:512:LEU:HB3	1.82	0.61
1:A:408:THR:H	1:A:472:ASN:HD21	1.49	0.61
3:S:409:LEU:O	3:S:410:ASP:HB3	2.00	0.61
1:G:472:ASN:HD21	1:G:474:SER:HB2	1.66	0.61
2:D:662:LEU:HD22	2:D:666:CYS:SG	2.40	0.61
1:G:510:THR:C	1:G:512:LEU:N	2.56	0.61
2:F:776:PRO:HB2	2:F:777:PRO:CD	2.28	0.61
1:A:512:LEU:O	1:A:512:LEU:CG	2.48	0.60
1:G:420:LYS:HD3	4:G:2014:HOH:O	2.01	0.60
2:D:773:SER:OG	2:D:775:ARG:HG2	2.01	0.60
1:G:500:ARG:HA	1:G:500:ARG:NE	2.15	0.60
1:C:514:PHE:O	1:C:515:PRO:C	2.43	0.60
1:A:399:ASN:O	1:A:402:SER:HB3	2.01	0.60
1:C:430:PHE:HE2	1:C:495:MET:HE3	1.67	0.60
1:G:500:ARG:N	1:G:500:ARG:HE	1.98	0.60
2:H:691:GLU:HB3	2:H:694:LEU:CD2	2.30	0.60
3:Q:421:ILE:HD11	3:Q:425:PHE:HE1	1.67	0.60
1:G:383:GLN:O	1:G:387:MET:HG3	2.02	0.60
1:A:418:ARG:HH11	1:A:480:ASN:HD22	1.50	0.60
3:R:409:LEU:HD12	3:R:410:ASP:CB	2.31	0.60
1:E:512:LEU:O	1:E:512:LEU:CD1	2.49	0.60
1:E:427:LYS:HE2	1:E:443:SER:HA	1.83	0.59
1:E:475:LYS:NZ	3:R:426:ASP:HA	2.17	0.59
1:G:396:PRO:HD3	1:G:454:TYR:CZ	2.37	0.59
2:F:673:HIS:N	2:F:674:PRO:HD3	2.18	0.59
2:B:773:SER:OG	2:B:775:ARG:HG2	2.02	0.59
1:G:499:SER:HB3	4:G:2025:HOH:O	2.03	0.59
1:A:424:TYR:OH	1:E:428:GLU:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:MET:HE1	1:A:512:LEU:HB2	1.84	0.59
2:D:656:ARG:HD2	3:Q:412:HIS:CD2	2.37	0.59
2:F:746:GLU:HG2	2:F:747:GLU:N	2.17	0.59
1:G:432:LYS:CG	4:G:2015:HOH:O	2.51	0.59
1:G:500:ARG:HE	1:G:500:ARG:H	1.49	0.59
1:A:413:GLU:HA	1:A:413:GLU:OE1	2.02	0.59
1:A:546:MET:HE1	1:A:549:HIS:HD2	1.68	0.59
1:C:472:ASN:HD21	1:C:474:SER:HB2	1.68	0.59
1:E:569:LEU:HD22	1:E:569:LEU:O	2.03	0.59
1:E:422:ILE:HD11	1:E:484:MET:HE1	1.85	0.59
1:E:546:MET:HE1	1:E:549:HIS:HD2	1.68	0.58
2:F:676:LEU:O	2:F:680:ILE:HG13	2.03	0.58
2:H:745:LYS:NZ	2:H:746:GLU:OE2	2.35	0.58
2:D:746:GLU:HG2	2:D:747:GLU:H	1.68	0.58
2:B:678:HIS:HD2	2:B:779:LEU:HD13	1.68	0.58
1:C:472:ASN:C	1:C:472:ASN:HD22	2.11	0.58
2:D:691:GLU:HG3	2:D:764:LEU:HD21	1.85	0.58
2:H:770:GLN:HB3	2:H:777:PRO:HD3	1.85	0.58
1:E:413:GLU:CG	4:E:2010:HOH:O	2.50	0.58
2:F:678:HIS:CE1	2:F:779:LEU:HB3	2.38	0.58
1:G:546:MET:HE1	1:G:549:HIS:CD2	2.38	0.58
2:D:676:LEU:HD11	2:D:717:ILE:HG13	1.85	0.58
2:D:769:LEU:O	2:D:772:ALA:HB3	2.04	0.58
1:A:512:LEU:O	1:A:512:LEU:HD13	2.03	0.58
2:D:691:GLU:O	2:D:694:LEU:HD23	2.04	0.58
3:S:421:ILE:HD11	3:S:425:PHE:HE1	1.69	0.58
1:C:467:ARG:CZ	1:C:468:LEU:HD21	2.34	0.57
2:D:770:GLN:HG3	4:D:2023:HOH:O	2.03	0.57
2:F:746:GLU:HG2	2:F:747:GLU:H	1.69	0.57
1:A:440:GLU:HA	1:G:434:VAL:CG1	2.34	0.57
1:E:512:LEU:HD22	1:E:516:TRP:HB3	1.85	0.57
2:H:763:ARG:NH2	4:H:2011:HOH:O	2.36	0.57
1:A:512:LEU:CD2	1:A:512:LEU:C	2.74	0.57
1:E:472:ASN:C	1:E:472:ASN:ND2	2.62	0.57
2:B:773:SER:C	2:B:775:ARG:H	2.13	0.57
1:E:388:ILE:HG23	1:E:541:ASN:HD22	1.70	0.57
2:D:699:HIS:HB3	2:D:702:GLN:HG3	1.85	0.57
1:E:495:MET:HB3	1:E:512:LEU:HB3	1.87	0.57
1:G:388:ILE:O	1:G:388:ILE:HG22	2.02	0.57
3:Q:409:LEU:N	3:Q:409:LEU:HD23	2.20	0.57
1:E:418:ARG:HH11	1:E:480:ASN:ND2	1.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:VAL:O	1:A:435:GLY:C	2.47	0.56
1:G:500:ARG:NE	1:G:500:ARG:CA	2.68	0.56
1:G:528:PHE:O	1:G:531:VAL:HG12	2.05	0.56
3:R:409:LEU:HD12	3:R:410:ASP:N	2.20	0.56
1:A:464:GLU:OE1	1:A:464:GLU:HA	2.05	0.56
1:A:512:LEU:C	1:A:512:LEU:CD1	2.69	0.56
1:E:495:MET:HB2	1:E:512:LEU:HG	1.87	0.56
1:E:512:LEU:HD22	1:E:513:SER:O	2.05	0.56
3:R:409:LEU:HD12	3:R:409:LEU:C	2.30	0.56
2:H:645:THR:HG23	3:S:419:GLU:OE1	2.03	0.56
2:H:703:ILE:N	2:H:703:ILE:CD1	2.68	0.56
2:H:656:ARG:HH21	2:H:785:ILE:HA	1.70	0.56
1:A:440:GLU:HA	1:G:434:VAL:HG13	1.86	0.56
1:A:513:SER:O	1:A:515:PRO:CD	2.54	0.56
1:E:464:GLU:OE1	1:E:464:GLU:HA	2.06	0.56
1:A:428:GLU:HG3	1:E:424:TYR:CE2	2.38	0.56
1:G:492:GLU:OE1	1:G:512:LEU:HD11	2.05	0.56
2:H:694:LEU:HD21	2:H:763:ARG:HG2	1.87	0.56
1:C:516:TRP:O	1:C:520:VAL:HG23	2.06	0.55
1:E:392:ALA:O	1:E:451:ARG:HD2	2.06	0.55
2:D:701:ASP:OD2	2:D:733:HIS:HE1	1.88	0.55
2:H:783:PRO:O	2:H:785:ILE:HG13	2.06	0.55
2:D:673:HIS:N	2:D:674:PRO:HD3	2.21	0.55
2:H:699:HIS:HB3	2:H:702:GLN:HG3	1.88	0.55
1:A:545:GLU:N	1:A:545:GLU:CD	2.65	0.55
3:R:416:GLU:HB2	3:R:419:GLU:OE2	2.06	0.55
1:E:389:LEU:O	1:E:451:ARG:NH1	2.39	0.55
1:E:498:TYR:C	1:E:500:ARG:N	2.64	0.55
1:E:510:THR:O	1:E:511:ASP:O	2.24	0.55
2:F:662:LEU:HD22	2:F:666:CYS:SG	2.46	0.55
2:F:672:GLU:C	2:F:674:PRO:HD3	2.31	0.55
1:A:435:GLY:HA2	1:A:508:SER:N	2.21	0.55
1:A:438:CYS:CB	1:G:438:CYS:SG	2.92	0.55
1:A:401:ILE:HD12	1:A:412:LYS:HD2	1.88	0.55
1:A:430:PHE:CE1	1:A:434:VAL:HG21	2.41	0.55
1:G:514:PHE:O	1:G:514:PHE:CD2	2.59	0.55
1:G:480:ASN:HD21	1:G:484:MET:HE2	1.71	0.55
2:H:787:ARG:HG3	2:H:787:ARG:NH1	2.22	0.55
1:A:382:ILE:CD1	4:A:2037:HOH:O	2.51	0.54
1:A:508:SER:HA	4:A:2020:HOH:O	2.06	0.54
1:E:472:ASN:ND2	1:E:474:SER:H	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:428:GLU:CG	1:G:432:LYS:HZ1	2.19	0.54
3:S:409:LEU:O	3:S:410:ASP:CB	2.55	0.54
1:G:514:PHE:CD2	1:G:514:PHE:C	2.85	0.54
1:G:546:MET:HE1	1:G:549:HIS:HD2	1.71	0.54
2:H:673:HIS:N	2:H:674:PRO:HD3	2.22	0.54
2:B:678:HIS:HE1	2:B:780:SER:O	1.90	0.54
2:B:765:LYS:HB2	2:B:765:LYS:NZ	2.21	0.54
1:G:495:MET:CG	1:G:512:LEU:HG	2.32	0.54
1:G:514:PHE:CB	1:G:553:CYS:SG	2.86	0.54
3:Q:423:ASP:HA	3:Q:426:ASP:CB	2.37	0.54
2:B:678:HIS:CD2	2:B:779:LEU:HD13	2.41	0.54
2:B:725:VAL:HG13	2:B:739:PHE:CZ	2.42	0.54
1:C:558:MET:HB3	2:D:654:VAL:HG22	1.88	0.54
1:C:569:LEU:HD22	1:C:573:ILE:HG13	1.88	0.54
1:G:387:MET:O	1:G:389:LEU:N	2.40	0.54
1:G:514:PHE:N	1:G:515:PRO:HD2	2.20	0.54
1:C:379:MET:N	4:C:2001:HOH:O	2.40	0.54
2:F:663:ASN:O	2:F:667:GLU:HG3	2.08	0.54
1:C:509:GLY:C	4:C:2029:HOH:O	2.51	0.54
1:C:529:TYR:OH	2:D:649:LEU:HD12	2.08	0.54
1:A:435:GLY:O	1:A:436:GLN:HG3	2.08	0.54
2:B:745:LYS:HB3	2:B:746:GLU:OE1	2.09	0.53
1:A:513:SER:C	1:A:515:PRO:HD2	2.34	0.53
1:G:449:GLY:HA3	1:G:491:LEU:HD23	1.90	0.53
2:H:725:VAL:O	2:H:729:LYS:HG3	2.09	0.53
2:H:745:LYS:O	2:H:746:GLU:C	2.51	0.53
1:A:512:LEU:O	1:A:512:LEU:CD1	2.57	0.53
2:B:678:HIS:CE1	2:B:780:SER:O	2.61	0.53
1:C:430:PHE:O	1:C:434:VAL:HG23	2.09	0.53
1:E:388:ILE:HD12	1:E:541:ASN:HB3	1.90	0.53
1:G:475:LYS:HD3	4:S:2005:HOH:O	2.09	0.53
2:F:785:ILE:N	2:F:786:PRO:HD2	2.24	0.53
1:G:513:SER:C	1:G:515:PRO:CD	2.80	0.53
3:S:422:ARG:O	3:S:426:ASP:HB2	2.09	0.53
2:B:783:PRO:O	2:B:785:ILE:HG22	2.09	0.53
1:C:420:LYS:HE2	4:C:2015:HOH:O	2.08	0.52
1:E:488:ALA:HB2	1:E:521:LEU:HD12	1.90	0.52
3:Q:423:ASP:HA	3:Q:426:ASP:HB3	1.90	0.52
1:C:514:PHE:C	1:C:514:PHE:CD2	2.85	0.52
2:B:691:GLU:O	2:B:694:LEU:HB2	2.09	0.52
1:G:480:ASN:ND2	1:G:484:MET:HE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:GLU:HG2	4:E:2010:HOH:O	2.10	0.52
1:G:452:LEU:O	1:G:456:VAL:HG23	2.10	0.52
1:G:407:CYS:HA	1:G:472:ASN:ND2	2.25	0.52
1:G:418:ARG:NH1	1:G:480:ASN:HD22	2.08	0.52
1:A:435:GLY:HA2	4:A:2019:HOH:O	2.09	0.52
2:D:660:LEU:HD21	2:D:785:ILE:HD13	1.93	0.52
1:E:513:SER:C	1:E:515:PRO:CD	2.81	0.52
1:E:513:SER:O	1:E:514:PHE:C	2.52	0.52
1:G:432:LYS:HG2	4:G:2015:HOH:O	2.10	0.52
1:A:444:GLN:HE22	1:G:510:THR:HG22	1.75	0.51
1:A:514:PHE:C	1:A:514:PHE:CD2	2.84	0.51
2:B:680:ILE:HD13	2:B:708:MET:HA	1.92	0.51
1:E:475:LYS:HZ1	3:R:426:ASP:C	2.17	0.51
3:S:417:GLU:C	3:S:417:GLU:CD	2.79	0.51
1:A:544:ARG:CZ	1:A:545:GLU:OE2	2.59	0.51
2:B:769:LEU:O	2:B:770:GLN:C	2.54	0.51
1:C:511:ASP:O	1:C:512:LEU:C	2.53	0.51
3:P:422:ARG:O	3:P:426:ASP:HB2	2.09	0.51
1:E:383:GLN:HA	1:E:383:GLN:HE21	1.76	0.51
2:F:784:HIS:NE2	2:F:786:PRO:HG2	2.25	0.51
1:E:557:ILE:HA	1:E:561:LEU:HB2	1.91	0.51
1:E:428:GLU:HB3	1:E:432:LYS:HZ3	1.76	0.51
1:G:492:GLU:CD	1:G:512:LEU:HD11	2.36	0.51
2:H:686:HIS:NE2	2:H:767:ASN:ND2	2.58	0.51
1:G:436:GLN:HE21	1:G:436:GLN:N	2.09	0.51
1:G:511:ASP:HB3	4:G:2024:HOH:O	2.11	0.51
2:H:704:MET:O	2:H:708:MET:HG3	2.11	0.51
2:B:761:MET:HG2	2:B:762:GLN:HE21	1.74	0.51
1:E:405:ASN:ND2	4:E:2009:HOH:O	2.39	0.51
2:D:691:GLU:HB3	2:D:694:LEU:CD2	2.41	0.50
1:E:472:ASN:HD21	1:E:474:SER:HB2	1.74	0.50
1:A:400:LEU:HD22	1:A:404:PHE:CE1	2.46	0.50
2:D:676:LEU:O	2:D:680:ILE:HG13	2.11	0.50
1:C:436:GLN:N	1:C:436:GLN:NE2	2.57	0.50
2:B:725:VAL:HG12	2:B:726:THR:N	2.26	0.50
1:E:428:GLU:CB	1:E:432:LYS:NZ	2.73	0.50
2:H:745:LYS:NZ	2:H:745:LYS:HB3	2.26	0.50
1:A:545:GLU:CD	1:A:545:GLU:H	2.20	0.50
2:B:746:GLU:CD	2:B:746:GLU:H	2.20	0.50
2:H:669:LEU:HD11	2:H:727:ALA:CB	2.42	0.50
1:G:500:ARG:O	1:G:501:SER:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASP:HB3	1:E:425:ILE:CD1	2.42	0.50
1:E:511:ASP:OD1	1:E:511:ASP:C	2.55	0.50
1:G:475:LYS:HE3	4:S:2005:HOH:O	2.12	0.50
1:G:544:ARG:HH11	1:G:544:ARG:HG2	1.76	0.50
1:C:399:ASN:O	1:C:402:SER:HB3	2.12	0.49
2:D:704:MET:O	2:D:708:MET:HG3	2.13	0.49
1:G:491:LEU:O	1:G:495:MET:HG2	2.12	0.49
1:E:396:PRO:HD3	1:E:454:TYR:CZ	2.47	0.49
1:E:428:GLU:CG	1:E:432:LYS:HZ2	2.25	0.49
1:E:523:LEU:CD1	1:E:528:PHE:HB2	2.42	0.49
2:B:698:ARG:HG2	4:B:2010:HOH:O	2.12	0.49
1:E:452:LEU:HD11	1:E:535:PHE:HZ	1.75	0.49
1:E:452:LEU:HD12	1:E:490:ALA:HA	1.95	0.49
1:E:558:MET:SD	2:F:653:LYS:HB3	2.52	0.49
2:F:785:ILE:O	2:F:786:PRO:C	2.55	0.49
1:E:465:GLU:OE1	1:E:471:GLN:HG3	2.11	0.49
1:E:492:GLU:CD	1:E:512:LEU:HD11	2.37	0.49
1:E:544:ARG:HH11	1:E:544:ARG:HG2	1.78	0.49
2:D:691:GLU:O	2:D:694:LEU:CD2	2.61	0.49
2:F:774:THR:O	2:F:775:ARG:HB2	2.12	0.49
2:H:773:SER:C	2:H:775:ARG:H	2.21	0.49
1:A:430:PHE:HE2	1:A:495:MET:HE3	1.78	0.49
2:D:675:GLU:H	2:D:675:GLU:CD	2.20	0.49
2:H:787:ARG:HD2	2:H:787:ARG:N	2.27	0.49
3:R:410:ASP:OD2	3:R:410:ASP:C	2.56	0.49
2:F:679:ILE:HG22	2:F:711:ILE:HD13	1.94	0.49
2:F:776:PRO:CB	2:F:777:PRO:CD	2.87	0.49
2:H:736:GLN:HA	2:H:739:PHE:CE2	2.48	0.49
2:H:748:GLU:HA	2:H:748:GLU:OE1	2.13	0.49
2:B:679:ILE:HG22	2:B:711:ILE:HG12	1.95	0.49
1:C:513:SER:C	1:C:515:PRO:HD2	2.25	0.49
1:C:548:LYS:CD	4:C:2040:HOH:O	2.59	0.49
1:G:512:LEU:HD23	1:G:516:TRP:HB3	1.94	0.49
2:H:686:HIS:HE2	2:H:767:ASN:ND2	2.11	0.49
1:A:553:CYS:O	1:A:557:ILE:HG13	2.13	0.49
2:H:746:GLU:HG2	2:H:747:GLU:N	2.27	0.49
1:A:408:THR:O	2:F:696:ARG:NH2	2.44	0.48
1:G:557:ILE:HA	1:G:561:LEU:HB2	1.95	0.48
1:A:439:VAL:O	1:A:441:ILE:N	2.46	0.48
1:A:565:SER:OG	2:B:697:ASP:OD2	2.31	0.48
2:B:676:LEU:O	2:B:680:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:703:ILE:CD1	2:H:703:ILE:H	2.26	0.48
1:C:509:GLY:N	4:C:2029:HOH:O	2.47	0.48
1:G:434:VAL:HG12	1:G:434:VAL:O	2.12	0.48
1:A:546:MET:HE3	1:A:549:HIS:HB3	1.95	0.48
2:H:656:ARG:HE	2:H:785:ILE:HG12	1.78	0.48
2:H:656:ARG:HD2	3:S:412:HIS:CD2	2.48	0.48
1:A:435:GLY:N	1:A:508:SER:O	2.47	0.48
1:E:491:LEU:O	1:E:495:MET:HG2	2.13	0.48
1:C:513:SER:O	1:C:514:PHE:HB3	2.12	0.48
1:G:546:MET:HE3	1:G:549:HIS:HB3	1.95	0.48
2:H:745:LYS:HB3	2:H:745:LYS:HZ3	1.79	0.48
1:C:576:SER:C	1:C:578:ASP:N	2.71	0.48
1:E:388:ILE:HD12	1:E:541:ASN:CB	2.43	0.48
1:G:393:SER:O	1:G:451:ARG:HG2	2.13	0.48
2:F:785:ILE:N	2:F:786:PRO:CD	2.77	0.48
1:C:539:GLU:OE2	1:C:541:ASN:HB2	2.14	0.47
1:G:472:ASN:ND2	1:G:474:SER:H	2.11	0.47
1:G:467:ARG:NH2	3:S:423:ASP:OD2	2.47	0.47
2:F:743:LEU:HD23	2:F:749:TYR:CZ	2.49	0.47
2:H:701:ASP:OD2	2:H:733:HIS:HE1	1.97	0.47
1:E:436:GLN:C	1:E:438:CYS:H	2.21	0.47
1:G:428:GLU:CG	1:G:432:LYS:HZ2	2.15	0.47
1:E:512:LEU:HD13	1:E:513:SER:C	2.39	0.47
1:E:512:LEU:HD13	1:E:513:SER:O	2.14	0.47
1:A:449:GLY:HA3	1:A:491:LEU:HD23	1.96	0.47
2:B:784:HIS:O	2:B:785:ILE:HG22	2.13	0.47
1:G:480:ASN:HD21	1:G:484:MET:CE	2.27	0.47
1:C:434:VAL:O	1:C:435:GLY:C	2.57	0.47
1:E:444:GLN:HG3	4:E:2025:HOH:O	2.14	0.47
1:E:493:VAL:HG22	1:E:546:MET:HE2	1.97	0.47
1:E:495:MET:CB	1:E:512:LEU:HG	2.44	0.47
2:F:776:PRO:HD2	2:F:777:PRO:CD	2.42	0.47
2:H:756:TYR:CE2	2:H:761:MET:HE3	2.49	0.47
1:C:472:ASN:HD22	1:C:473:PHE:N	2.13	0.47
2:D:693:GLU:OE2	2:D:696:ARG:NH1	2.48	0.47
1:G:500:ARG:HB2	4:G:2021:HOH:O	2.15	0.47
1:G:500:ARG:HE	1:G:500:ARG:CA	2.28	0.47
2:H:684:PHE:HZ	2:H:700:LEU:HD22	1.80	0.47
1:A:512:LEU:HD13	1:A:513:SER:N	2.30	0.47
1:E:557:ILE:HG22	1:E:562:ALA:HB2	1.97	0.47
1:G:472:ASN:C	1:G:472:ASN:ND2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:488:ALA:HB2	1:G:521:LEU:HD12	1.96	0.46
1:A:420:LYS:HE2	1:A:420:LYS:O	2.14	0.46
2:B:678:HIS:CD2	2:B:779:LEU:HB3	2.50	0.46
1:E:464:GLU:OE1	1:E:467:ARG:NH1	2.48	0.46
1:E:408:THR:H	1:E:474:SER:HB2	1.80	0.46
2:H:669:LEU:HD11	2:H:727:ALA:HB2	1.97	0.46
2:F:773:SER:O	2:F:776:PRO:HG3	2.15	0.46
2:B:660:LEU:HD11	2:B:785:ILE:CD1	2.42	0.46
2:B:699:HIS:HB3	2:B:702:GLN:HG3	1.98	0.46
1:C:430:PHE:CE2	1:C:495:MET:HE3	2.48	0.46
1:E:452:LEU:CD1	1:E:535:PHE:HZ	2.27	0.46
1:G:511:ASP:O	1:G:512:LEU:HB2	2.16	0.46
2:H:728:TYR:C	2:H:730:ASP:H	2.23	0.46
1:C:514:PHE:HB3	1:C:515:PRO:CD	2.45	0.46
1:C:576:SER:C	1:C:578:ASP:H	2.24	0.46
2:D:675:GLU:OE1	2:D:675:GLU:N	2.35	0.46
3:R:419:GLU:HA	3:R:423:ASP:OD2	2.16	0.46
1:A:420:LYS:HE2	1:A:420:LYS:C	2.41	0.46
1:E:432:LYS:HE2	1:G:432:LYS:HD3	1.97	0.46
3:R:421:ILE:HD11	3:R:425:PHE:HE1	1.81	0.46
2:B:656:ARG:HG2	2:B:785:ILE:HD12	1.98	0.45
2:B:710:GLY:O	2:B:713:LYS:HB2	2.16	0.45
1:C:381:THR:O	1:C:384:GLN:HG2	2.16	0.45
1:C:435:GLY:O	1:C:436:GLN:HG3	2.16	0.45
1:G:472:ASN:HD22	1:G:474:SER:H	1.63	0.45
1:C:392:ALA:O	1:C:451:ARG:HD3	2.16	0.45
2:D:653:LYS:HD3	3:Q:412:HIS:CD2	2.52	0.45
1:E:436:GLN:CD	4:E:2018:HOH:O	2.60	0.45
2:H:658:ALA:HB1	2:H:684:PHE:CE2	2.51	0.45
2:H:672:GLU:C	2:H:674:PRO:HD3	2.41	0.45
2:H:714:VAL:HG13	4:H:2005:HOH:O	2.15	0.45
1:G:418:ARG:O	1:G:422:ILE:HG12	2.16	0.45
1:G:452:LEU:HD22	1:G:456:VAL:HG23	1.97	0.45
2:D:678:HIS:CE1	2:D:779:LEU:HB3	2.52	0.45
1:E:533:GLU:O	1:E:537:LYS:HG3	2.17	0.45
1:E:575:GLN:O	1:E:576:SER:C	2.60	0.45
2:F:784:HIS:C	2:F:786:PRO:HD2	2.42	0.45
1:G:384:GLN:CA	1:G:387:MET:HE3	2.45	0.45
1:A:413:GLU:HB3	4:A:2007:HOH:O	2.16	0.45
1:A:546:MET:HE1	1:A:549:HIS:CD2	2.48	0.45
2:B:746:GLU:HG2	2:B:747:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASN:ND2	1:C:474:SER:H	2.15	0.45
2:D:656:ARG:HG3	2:D:785:ILE:HD11	1.98	0.45
2:F:682:THR:HG23	2:F:780:SER:OG	2.17	0.45
2:B:719:LEU:HG	2:B:724:ILE:HD11	1.99	0.45
1:C:523:LEU:HD23	4:C:2035:HOH:O	2.17	0.45
1:C:576:SER:O	1:C:578:ASP:N	2.49	0.45
1:G:405:ASN:HD22	1:G:410:ASN:HD21	1.63	0.45
1:G:417:LYS:NZ	1:G:417:LYS:HB3	2.32	0.45
1:C:435:GLY:H	1:C:508:SER:CA	2.26	0.45
1:E:420:LYS:HD3	1:E:420:LYS:O	2.16	0.45
1:C:511:ASP:CG	1:C:512:LEU:H	2.25	0.44
1:E:472:ASN:HD22	1:E:474:SER:H	1.65	0.44
2:F:681:TRP:O	2:F:685:GLN:HB2	2.17	0.44
1:G:512:LEU:CD2	1:G:517:ILE:H	2.30	0.44
2:H:678:HIS:CE1	2:H:779:LEU:HB3	2.52	0.44
2:H:745:LYS:NZ	2:H:745:LYS:CB	2.79	0.44
1:C:512:LEU:HA	1:C:516:TRP:CB	2.44	0.44
1:G:389:LEU:HD12	1:G:389:LEU:HA	1.88	0.44
2:B:672:GLU:C	2:B:674:PRO:HD3	2.42	0.44
1:E:475:LYS:HZ2	3:R:426:ASP:HA	1.81	0.44
2:D:719:LEU:HD23	2:D:724:ILE:HD11	1.99	0.44
1:A:435:GLY:C	1:A:436:GLN:HG3	2.42	0.44
1:G:574:LYS:NZ	1:G:574:LYS:HB3	2.33	0.44
1:A:460:MET:HE2	1:A:534:SER:HB3	2.00	0.44
1:C:420:LYS:HE2	1:C:420:LYS:O	2.18	0.44
1:E:566:ASP:OD1	1:E:566:ASP:C	2.61	0.44
2:F:783:PRO:O	2:F:785:ILE:HD12	2.17	0.44
2:B:683:LEU:HD12	2:B:711:ILE:HD13	1.98	0.44
1:C:509:GLY:O	1:C:510:THR:C	2.60	0.44
2:F:775:ARG:N	2:F:776:PRO:HD3	2.33	0.44
2:B:694:LEU:HD12	2:B:694:LEU:HA	1.81	0.44
1:C:396:PRO:HG3	1:C:454:TYR:CE1	2.52	0.44
2:D:662:LEU:CD2	2:D:666:CYS:SG	3.06	0.44
2:D:681:TRP:CD1	2:D:782:ILE:HD13	2.53	0.44
2:F:761:MET:O	2:F:765:LYS:HB2	2.17	0.44
1:C:492:GLU:OE1	1:C:512:LEU:HD21	2.18	0.44
1:C:514:PHE:O	1:C:517:ILE:HG22	2.18	0.44
2:D:746:GLU:O	2:D:747:GLU:HG2	2.17	0.44
1:G:387:MET:O	1:G:390:ASN:ND2	2.51	0.43
1:G:513:SER:HB3	1:G:515:PRO:HD2	1.99	0.43
1:E:500:ARG:O	1:E:501:SER:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:SER:O	1:C:501:SER:N	2.51	0.43
2:D:698:ARG:NH1	2:D:743:LEU:O	2.52	0.43
2:F:785:ILE:N	2:F:785:ILE:HD12	2.34	0.43
1:C:417:LYS:HE2	4:C:2010:HOH:O	2.18	0.43
1:E:434:VAL:O	1:E:434:VAL:HG12	2.18	0.43
1:E:512:LEU:CD2	1:E:513:SER:O	2.66	0.43
1:G:432:LYS:HG3	4:G:2015:HOH:O	2.15	0.43
1:A:569:LEU:O	1:A:569:LEU:HD22	2.19	0.43
2:B:660:LEU:HD21	2:B:785:ILE:CD1	2.49	0.43
2:F:665:LEU:HD12	2:F:665:LEU:HA	1.84	0.43
1:G:512:LEU:C	1:G:512:LEU:CD1	2.82	0.43
2:H:668:ARG:C	2:H:669:LEU:HD12	2.43	0.43
3:Q:409:LEU:C	3:Q:411:TYR:N	2.64	0.43
3:R:409:LEU:C	3:R:409:LEU:CD1	2.92	0.43
2:D:711:ILE:HD13	2:D:711:ILE:HA	1.85	0.43
1:E:422:ILE:HD11	1:E:484:MET:CE	2.48	0.43
2:F:787:ARG:N	2:F:787:ARG:CD	2.81	0.43
1:A:512:LEU:HA	1:A:516:TRP:HB3	2.01	0.42
1:E:413:GLU:HG3	4:E:2010:HOH:O	2.16	0.42
2:H:784:HIS:C	2:H:786:PRO:HD3	2.44	0.42
1:A:440:GLU:HB3	1:G:511:ASP:OD2	2.20	0.42
2:B:783:PRO:O	2:B:784:HIS:C	2.63	0.42
2:D:761:MET:O	2:D:765:LYS:N	2.49	0.42
1:G:434:VAL:HG21	1:G:511:ASP:OD2	2.19	0.42
2:H:691:GLU:CB	2:H:694:LEU:HD23	2.36	0.42
2:H:782:ILE:HD13	2:H:782:ILE:HA	1.92	0.42
1:A:395:GLN:HE21	1:A:396:PRO:HD2	1.84	0.42
1:A:421:ASP:HB3	1:E:425:ILE:HD11	2.01	0.42
2:F:683:LEU:HB2	2:F:711:ILE:HD11	2.01	0.42
1:G:486:LEU:HD23	1:G:531:VAL:HG21	2.01	0.42
1:G:475:LYS:CE	4:S:2005:HOH:O	2.67	0.42
3:R:409:LEU:HD12	3:R:410:ASP:HB3	2.01	0.42
1:A:435:GLY:CA	1:A:508:SER:N	2.82	0.42
2:F:787:ARG:N	2:F:787:ARG:HD3	2.34	0.42
2:H:678:HIS:CD2	2:H:779:LEU:HD13	2.55	0.42
2:H:713:LYS:HA	4:H:2006:HOH:O	2.20	0.42
1:G:496:ALA:O	1:G:500:ARG:NH2	2.53	0.42
1:E:428:GLU:CB	1:E:432:LYS:HZ2	2.33	0.42
1:E:495:MET:CB	1:E:512:LEU:CB	2.98	0.42
1:G:382:ILE:HD12	1:G:498:TYR:CE1	2.55	0.42
1:G:529:TYR:OH	2:H:649:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:721:PHE:CB	2:H:753:ILE:HD11	2.50	0.42
3:R:416:GLU:HB2	3:R:419:GLU:HG3	2.01	0.42
2:B:659:TYR:CE1	2:B:782:ILE:HD12	2.54	0.42
1:C:514:PHE:CB	1:C:515:PRO:CD	2.98	0.42
1:C:555:HIS:HA	1:C:558:MET:HE3	2.02	0.42
1:E:499:SER:O	1:E:500:ARG:HB2	2.20	0.42
1:G:434:VAL:CG1	1:G:434:VAL:O	2.68	0.42
3:P:409:LEU:N	3:P:409:LEU:HD23	2.35	0.42
1:C:572:LEU:HD12	1:C:572:LEU:HA	1.86	0.41
1:E:548:LYS:HE2	3:R:409:LEU:N	2.35	0.41
2:H:773:SER:C	2:H:775:ARG:N	2.79	0.41
1:A:380:ASN:OD1	1:A:384:GLN:NE2	2.53	0.41
1:A:439:VAL:C	1:A:441:ILE:H	2.27	0.41
1:C:567:SER:HA	1:C:568:PRO:HD3	1.92	0.41
1:E:470:ILE:HD13	4:R:2003:HOH:O	2.21	0.41
1:G:428:GLU:HA	1:G:428:GLU:OE2	2.20	0.41
1:G:441:ILE:O	1:G:445:ARG:HG3	2.19	0.41
2:B:653:LYS:NZ	3:P:412:HIS:O	2.53	0.41
2:D:787:ARG:NH1	2:D:787:ARG:HB3	2.35	0.41
2:F:743:LEU:HD23	2:F:749:TYR:CE1	2.55	0.41
1:G:575:GLN:HA	1:G:575:GLN:OE1	2.20	0.41
1:C:435:GLY:N	1:C:508:SER:HA	2.31	0.41
2:H:714:VAL:CG1	4:H:2005:HOH:O	2.68	0.41
1:C:496:ALA:HA	1:C:499:SER:HB2	2.03	0.41
2:F:678:HIS:CG	2:F:779:LEU:HD13	2.55	0.41
1:C:512:LEU:HD13	1:C:514:PHE:H	1.86	0.41
1:A:470:ILE:HG23	1:A:472:ASN:H	1.85	0.41
1:A:526:PHE:O	1:A:529:TYR:HD2	2.03	0.41
2:D:786:PRO:HB2	2:D:787:ARG:H	1.62	0.41
2:F:645:THR:HG23	3:R:419:GLU:OE1	2.21	0.41
1:G:492:GLU:OE2	1:G:512:LEU:HD11	2.21	0.41
2:H:659:TYR:CE1	2:H:782:ILE:HD12	2.56	0.41
1:A:493:VAL:HG22	1:A:546:MET:HE2	2.03	0.41
1:C:486:LEU:HD23	1:C:486:LEU:HA	1.87	0.41
2:D:673:HIS:N	2:D:674:PRO:CD	2.83	0.41
1:E:437:GLY:HA2	4:E:2017:HOH:O	2.20	0.41
1:E:557:ILE:CG2	1:E:562:ALA:HB2	2.51	0.41
2:F:736:GLN:HA	2:F:739:PHE:CE2	2.55	0.41
2:H:741:ARG:HG2	2:H:749:TYR:CD2	2.55	0.41
2:H:774:THR:C	2:H:776:PRO:HD3	2.46	0.41
1:A:537:LYS:HE2	3:P:413:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:LYS:CE	4:C:2015:HOH:O	2.66	0.40
1:E:517:ILE:O	1:E:517:ILE:HG13	2.19	0.40
2:B:746:GLU:HG2	2:B:747:GLU:N	2.37	0.40
1:C:511:ASP:CG	1:C:512:LEU:N	2.78	0.40
2:H:769:LEU:N	2:H:769:LEU:CD2	2.84	0.40
1:E:526:PHE:O	1:E:529:TYR:HD2	2.05	0.40
2:F:727:ALA:O	2:F:730:ASP:HB2	2.21	0.40
2:B:784:HIS:C	2:B:785:ILE:HG22	2.47	0.40
1:E:515:PRO:O	1:E:516:TRP:C	2.64	0.40
2:H:676:LEU:O	2:H:677:GLU:C	2.65	0.40
3:S:421:ILE:CD1	3:S:425:PHE:HE1	2.35	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	190/218 (87%)	178 (94%)	6 (3%)	6 (3%)	3 5
1	C	190/218 (87%)	170 (90%)	14 (7%)	6 (3%)	3 5
1	E	190/218 (87%)	178 (94%)	10 (5%)	2 (1%)	11 25
1	G	190/218 (87%)	174 (92%)	10 (5%)	6 (3%)	3 5
2	B	142/152 (93%)	129 (91%)	11 (8%)	2 (1%)	9 19
2	D	142/152 (93%)	127 (89%)	13 (9%)	2 (1%)	9 19
2	F	142/152 (93%)	127 (89%)	11 (8%)	4 (3%)	4 6
2	H	142/152 (93%)	124 (87%)	15 (11%)	3 (2%)	5 11
3	P	16/18 (89%)	14 (88%)	2 (12%)	0	100 100
3	Q	16/18 (89%)	14 (88%)	1 (6%)	1 (6%)	1 1
3	R	16/18 (89%)	13 (81%)	1 (6%)	2 (12%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	16/18 (89%)	13 (81%)	2 (12%)	1 (6%)	1	1
All	All	1392/1552 (90%)	1261 (91%)	96 (7%)	35 (2%)	4	8

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PHE
1	C	514	PHE
2	D	784	HIS
2	D	786	PRO
2	F	779	LEU
1	G	389	LEU
1	G	512	LEU
2	H	746	GLU
3	Q	410	ASP
3	R	416	GLU
1	A	440	GLU
1	A	512	LEU
2	B	774	THR
2	B	786	PRO
1	C	499	SER
1	C	500	ARG
1	E	511	ASP
2	F	776	PRO
1	G	387	MET
1	G	511	ASP
2	H	784	HIS
3	R	417	GLU
1	A	472	ASN
1	A	473	PHE
1	C	510	THR
1	C	512	LEU
1	C	577	LYS
1	E	560	SER
2	F	786	PRO
1	G	388	ILE
1	A	513	SER
2	F	773	SER
3	S	410	ASP
1	G	560	SER
2	H	729	LYS

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	178/200 (89%)	160 (90%)	18 (10%)	7	15
1	C	178/200 (89%)	162 (91%)	16 (9%)	9	20
1	E	178/200 (89%)	158 (89%)	20 (11%)	6	12
1	G	178/200 (89%)	162 (91%)	16 (9%)	9	20
2	B	139/147 (95%)	122 (88%)	17 (12%)	5	10
2	D	139/147 (95%)	127 (91%)	12 (9%)	10	22
2	F	139/147 (95%)	128 (92%)	11 (8%)	11	26
2	H	139/147 (95%)	124 (89%)	15 (11%)	6	13
3	P	15/15 (100%)	14 (93%)	1 (7%)	15	33
3	Q	15/15 (100%)	14 (93%)	1 (7%)	15	33
3	R	15/15 (100%)	11 (73%)	4 (27%)	0	1
3	S	15/15 (100%)	14 (93%)	1 (7%)	15	33
All	All	1328/1448 (92%)	1196 (90%)	132 (10%)	7	16

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	LEU
1	A	420	LYS
1	A	436	GLN
1	A	438	CYS
1	A	444	GLN
1	A	452	LEU
1	A	470	ILE
1	A	472	ASN
1	A	486	LEU
1	A	487	LEU
1	A	510	THR
1	A	512	LEU
1	A	523	LEU
1	A	529	TYR

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Mol	Chain	Res	Type
1	A	531	VAL
1	A	548	LYS
1	A	569	LEU
1	A	576	SER
2	B	649	LEU
2	B	656	ARG
2	B	657	LEU
2	B	662	LEU
2	B	669	LEU
2	B	683	LEU
2	B	694	LEU
2	B	700	LEU
2	B	711	ILE
2	B	721	PHE
2	B	725	VAL
2	B	729	LYS
2	B	743	LEU
2	B	746	GLU
2	B	765	LYS
2	B	769	LEU
2	B	770	GLN
1	C	400	LEU
1	C	420	LYS
1	C	436	GLN
1	C	438	CYS
1	C	452	LEU
1	C	470	ILE
1	C	472	ASN
1	C	484	MET
1	C	486	LEU
1	C	487	LEU
1	C	510	THR
1	C	517	ILE
1	C	519	ASN
1	C	523	LEU
1	C	529	TYR
1	C	569	LEU
2	D	657	LEU
2	D	662	LEU
2	D	683	LEU
2	D	685	GLN
2	D	694	LEU

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Mol	Chain	Res	Type
2	D	696	ARG
2	D	700	LEU
2	D	721	PHE
2	D	729	LYS
2	D	743	LEU
2	D	746	GLU
2	D	784	HIS
1	E	383	GLN
1	E	389	LEU
1	E	399	ASN
1	E	413	GLU
1	E	428	GLU
1	E	436	GLN
1	E	440	GLU
1	E	452	LEU
1	E	466	GLU
1	E	467	ARG
1	E	472	ASN
1	E	486	LEU
1	E	487	LEU
1	E	510	THR
1	E	511	ASP
1	E	513	SER
1	E	514	PHE
1	E	523	LEU
1	E	529	TYR
1	E	569	LEU
2	F	657	LEU
2	F	662	LEU
2	F	669	LEU
2	F	683	LEU
2	F	685	GLN
2	F	700	LEU
2	F	721	PHE
2	F	743	LEU
2	F	746	GLU
2	F	773	SER
2	F	786	PRO
1	G	399	ASN
1	G	413	GLU
1	G	424	TYR
1	G	428	GLU

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Mol	Chain	Res	Type
1	G	429	LYS
1	G	436	GLN
1	G	452	LEU
1	G	466	GLU
1	G	472	ASN
1	G	484	MET
1	G	486	LEU
1	G	487	LEU
1	G	508	SER
1	G	512	LEU
1	G	529	TYR
1	G	569	LEU
2	H	657	LEU
2	H	662	LEU
2	H	671	SER
2	H	683	LEU
2	H	685	GLN
2	H	694	LEU
2	H	700	LEU
2	H	721	PHE
2	H	726	THR
2	H	735	VAL
2	H	743	LEU
2	H	745	LYS
2	H	746	GLU
2	H	753	ILE
2	H	787	ARG
3	P	409	LEU
3	Q	409	LEU
3	R	409	LEU
3	R	416	GLU
3	R	417	GLU
3	R	422	ARG
3	S	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	384	GLN
1	A	395	GLN
1	A	405	ASN

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Mol	Chain	Res	Type
1	A	436	GLN
1	A	444	GLN
1	A	472	ASN
1	A	480	ASN
1	A	555	HIS
2	B	678	HIS
2	B	685	GLN
2	B	686	HIS
2	B	689	GLN
2	B	690	ASN
2	B	733	HIS
2	B	767	ASN
2	B	770	GLN
1	C	383	GLN
1	C	384	GLN
1	C	395	GLN
1	C	405	ASN
1	C	436	GLN
1	C	472	ASN
1	C	480	ASN
1	C	541	ASN
1	C	555	HIS
2	D	689	GLN
2	D	733	HIS
2	D	736	GLN
1	E	383	GLN
1	E	395	GLN
1	E	399	ASN
1	E	405	ASN
1	E	472	ASN
1	E	480	ASN
1	E	541	ASN
2	F	673	HIS
2	F	685	GLN
2	F	689	GLN
2	F	690	ASN
2	F	767	ASN
2	F	770	GLN
1	G	390	ASN
1	G	405	ASN
1	G	436	GLN
1	G	444	GLN

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Mol	Chain	Res	Type
1	G	472	ASN
1	G	480	ASN
2	H	663	ASN
2	H	678	HIS
2	H	689	GLN
2	H	690	ASN
2	H	733	HIS
2	H	767	ASN
3	Q	412	HIS
3	R	412	HIS
3	S	412	HIS

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	194/218 (88%)	0.62	15 (7%) 19 15	20, 29, 56, 74	0
1	C	194/218 (88%)	0.72	20 (10%) 12 9	20, 29, 55, 69	0
1	E	194/218 (88%)	1.54	43 (22%) 2 2	21, 30, 56, 77	0
1	G	194/218 (88%)	2.02	78 (40%) 0 0	21, 29, 58, 75	0
2	B	144/152 (94%)	1.35	29 (20%) 3 2	21, 38, 71, 79	0
2	D	144/152 (94%)	1.12	25 (17%) 4 3	24, 39, 72, 80	0
2	F	144/152 (94%)	3.10	111 (77%) 0 0	27, 43, 73, 80	0
2	H	144/152 (94%)	4.84	142 (98%) 0 0	27, 40, 72, 83	0
3	P	18/18 (100%)	1.86	6 (33%) 1 1	41, 48, 61, 64	0
3	Q	18/18 (100%)	1.45	5 (27%) 1 1	40, 49, 58, 61	0
3	R	18/18 (100%)	3.15	14 (77%) 0 0	39, 52, 65, 68	0
3	S	18/18 (100%)	6.21	18 (100%) 0 0	41, 51, 62, 64	0
All	All	1424/1552 (91%)	1.88	506 (35%) 1 1	20, 36, 65, 83	0

All (506) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	774	THR	11.4
2	H	787	ARG	11.2
2	F	777	PRO	9.4
2	H	772	ALA	9.0
2	H	766	THR	9.0
3	S	414	GLY	8.9
3	S	417	GLU	8.7
3	S	409	LEU	8.4
2	H	785	ILE	8.4
3	S	418	GLY	8.3
1	G	388	ILE	7.9

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Mol	Chain	Res	Type	RSRZ
2	H	773	SER	7.9
2	H	749	TYR	7.8
2	H	715	LYS	7.8
3	S	422	ARG	7.7
2	H	775	ARG	7.5
2	H	779	LEU	7.5
2	H	778	THR	7.4
2	H	786	PRO	7.3
2	H	780	SER	7.2
2	H	782	ILE	7.2
2	H	744	ILE	7.0
3	S	424	LEU	6.8
1	G	379	MET	6.8
2	H	748	GLU	6.8
2	H	768	ILE	6.7
2	H	736	GLN	6.7
2	H	743	LEU	6.7
3	S	416	GLU	6.7
2	H	714	VAL	6.5
2	F	736	GLN	6.5
3	S	425	PHE	6.5
2	H	763	ARG	6.4
2	F	775	ARG	6.3
2	H	669	LEU	6.3
2	H	762	GLN	6.3
2	H	709	TYR	6.2
1	G	511	ASP	6.2
2	F	780	SER	6.1
2	H	733	HIS	6.1
2	H	649	LEU	6.0
3	S	412	HIS	6.0
2	H	692	TYR	5.9
2	H	758	SER	5.9
2	F	733	HIS	5.8
3	S	419	GLU	5.7
2	F	781	PRO	5.7
2	H	668	ARG	5.6
2	H	776	PRO	5.6
2	H	717	ILE	5.6
2	H	663	ASN	5.6
2	H	703	ILE	5.6
2	H	770	GLN	5.6

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Mol	Chain	Res	Type	RSRZ
2	H	681	TRP	5.6
2	H	784	HIS	5.5
2	H	764	LEU	5.5
2	F	742	VAL	5.5
2	H	754	VAL	5.5
2	B	776	PRO	5.5
2	H	707	SER	5.5
3	S	423	ASP	5.5
2	D	774	THR	5.5
2	H	777	PRO	5.4
2	H	755	PHE	5.4
1	G	575	GLN	5.4
2	H	711	ILE	5.4
2	H	722	LYS	5.4
2	H	741	ARG	5.4
2	H	735	VAL	5.4
2	H	750	ASP	5.4
2	H	676	LEU	5.4
2	H	756	TYR	5.3
2	H	660	LEU	5.3
3	S	415	LEU	5.3
2	H	678	HIS	5.2
2	H	667	GLU	5.2
1	E	500	ARG	5.2
3	S	413	PHE	5.2
2	H	742	VAL	5.2
1	E	578	ASP	5.1
2	H	771	TYR	5.1
3	S	411	TYR	5.1
2	H	696	ARG	5.1
2	H	718	ASP	5.1
2	H	683	LEU	5.1
2	F	785	ILE	5.1
3	R	411	TYR	5.1
1	E	513	SER	5.0
2	H	783	PRO	5.0
2	H	670	LEU	5.0
2	H	745	LYS	5.0
2	F	784	HIS	5.0
2	F	776	PRO	5.0
2	H	697	ASP	5.0
2	H	753	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	513	SER	4.9
2	H	781	PRO	4.9
3	R	418	GLY	4.9
2	H	751	SER	4.9
2	H	655	TYR	4.9
2	B	769	LEU	4.8
3	S	421	ILE	4.8
2	H	690	ASN	4.8
2	F	787	ARG	4.8
2	H	659	TYR	4.8
1	G	384	GLN	4.8
1	E	379	MET	4.7
2	H	708	MET	4.7
2	H	760	PHE	4.7
2	F	745	LYS	4.7
2	F	666	CYS	4.7
1	A	508	SER	4.7
3	S	426	ASP	4.7
2	F	719	LEU	4.7
2	H	664	THR	4.7
2	H	712	CYS	4.7
2	H	680	ILE	4.7
2	H	767	ASN	4.7
2	F	774	THR	4.6
1	C	501	SER	4.6
2	H	657	LEU	4.6
1	E	394	ASP	4.6
2	H	645	THR	4.6
2	H	769	LEU	4.5
3	R	426	ASP	4.5
2	H	759	VAL	4.5
2	F	772	ALA	4.5
2	H	673	HIS	4.5
2	D	776	PRO	4.5
1	E	508	SER	4.5
2	H	652	LYS	4.5
2	F	668	ARG	4.5
2	H	656	ARG	4.5
2	H	646	SER	4.4
2	F	769	LEU	4.4
2	H	662	LEU	4.4
1	G	508	SER	4.4

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Mol	Chain	Res	Type	RSRZ
3	R	409	LEU	4.4
1	E	437	GLY	4.4
2	H	713	LYS	4.4
2	D	785	ILE	4.4
2	F	767	ASN	4.4
2	F	773	SER	4.4
2	D	773	SER	4.4
2	H	688	LEU	4.4
2	H	685	GLN	4.4
3	R	416	GLU	4.4
2	H	654	VAL	4.4
2	F	754	VAL	4.3
2	H	723	ILE	4.3
2	B	774	THR	4.3
2	H	728	TYR	4.3
2	H	730	ASP	4.3
1	G	512	LEU	4.3
2	F	670	LEU	4.3
2	F	711	ILE	4.3
2	F	748	GLU	4.2
1	G	514	PHE	4.2
2	F	720	LYS	4.2
2	F	750	ASP	4.2
2	H	687	THR	4.2
2	H	765	LYS	4.2
1	G	468	LEU	4.2
2	F	749	TYR	4.2
2	H	658	ALA	4.2
1	C	512	LEU	4.2
1	E	381	THR	4.2
2	F	779	LEU	4.2
2	H	719	LEU	4.1
2	F	730	ASP	4.1
1	G	380	ASN	4.1
1	E	499	SER	4.1
2	H	684	PHE	4.1
2	H	694	LEU	4.1
2	H	734	ALA	4.1
2	F	663	ASN	4.1
2	B	787	ARG	4.1
1	G	499	SER	4.1
1	G	424	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	782	ILE	4.0
3	Q	426	ASP	4.0
2	H	666	CYS	4.0
1	G	544	ARG	4.0
2	H	727	ALA	4.0
2	B	785	ILE	4.0
2	F	753	ILE	4.0
2	F	714	VAL	4.0
2	F	758	SER	4.0
2	H	648	SER	4.0
1	G	444	GLN	4.0
2	H	650	PHE	4.0
2	D	777	PRO	4.0
2	B	775	ARG	4.0
3	P	409	LEU	4.0
2	H	686	HIS	3.9
1	G	500	ARG	3.9
2	B	779	LEU	3.9
2	F	752	ILE	3.9
2	F	722	LYS	3.9
2	H	739	PHE	3.9
2	B	786	PRO	3.9
2	F	771	TYR	3.9
2	H	651	TYR	3.9
2	D	787	ARG	3.9
2	H	689	GLN	3.9
2	H	705	MET	3.8
3	S	420	GLY	3.8
1	G	529	TYR	3.8
2	F	674	PRO	3.8
2	H	674	PRO	3.8
1	E	469	SER	3.8
2	H	700	LEU	3.8
3	R	420	GLY	3.8
2	F	735	VAL	3.8
1	G	578	ASP	3.8
1	C	513	SER	3.8
2	F	760	PHE	3.8
1	E	545	GLU	3.8
1	G	436	GLN	3.8
2	H	672	GLU	3.8
1	G	474	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	778	THR	3.7
2	H	724	ILE	3.7
2	B	773	SER	3.7
2	H	644	SER	3.7
2	H	698	ARG	3.7
2	F	762	GLN	3.7
1	G	567	SER	3.7
1	G	432	LYS	3.7
1	G	435	GLY	3.7
1	E	514	PHE	3.7
2	H	747	GLU	3.7
2	F	764	LEU	3.7
2	H	752	ILE	3.7
3	S	410	ASP	3.7
2	F	709	TYR	3.7
1	G	439	VAL	3.7
2	F	662	LEU	3.6
2	H	665	LEU	3.6
2	H	682	THR	3.6
1	G	434	VAL	3.6
2	H	737	GLU	3.6
1	A	512	LEU	3.6
2	H	731	LEU	3.6
3	R	412	HIS	3.6
2	B	778	THR	3.6
1	E	544	ARG	3.6
2	B	777	PRO	3.6
1	G	383	GLN	3.6
2	H	740	LYS	3.6
2	F	766	THR	3.6
2	B	767	ASN	3.6
1	E	428	GLU	3.6
2	F	763	ARG	3.5
2	H	761	MET	3.5
2	H	701	ASP	3.5
2	D	772	ALA	3.5
2	F	770	GLN	3.5
2	H	647	LEU	3.5
2	F	768	ILE	3.5
1	E	510	THR	3.5
1	G	571	ASP	3.5
3	R	410	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
3	R	414	GLY	3.5
1	G	576	SER	3.5
2	H	653	LYS	3.5
2	B	772	ALA	3.5
2	D	748	GLU	3.5
2	F	678	HIS	3.5
2	F	734	ALA	3.4
2	F	675	GLU	3.4
2	H	677	GLU	3.4
1	G	390	ASN	3.4
2	F	747	GLU	3.4
2	F	717	ILE	3.4
2	F	744	ILE	3.4
1	A	511	ASP	3.4
1	E	384	GLN	3.4
2	F	656	ARG	3.4
2	H	702	GLN	3.4
1	A	501	SER	3.4
2	H	671	SER	3.4
1	G	382	ILE	3.3
1	E	501	SER	3.3
2	D	769	LEU	3.3
3	P	418	GLY	3.3
2	H	757	ASN	3.3
2	F	731	LEU	3.3
2	F	658	ALA	3.3
2	D	778	THR	3.3
2	F	751	SER	3.3
2	B	784	HIS	3.3
1	E	575	GLN	3.3
2	H	710	GLY	3.3
2	H	721	PHE	3.3
1	G	385	LEU	3.2
2	H	675	GLU	3.2
2	H	693	GLU	3.2
2	H	704	MET	3.2
1	G	501	SER	3.2
2	B	780	SER	3.2
2	B	771	TYR	3.2
1	E	382	ILE	3.2
1	G	387	MET	3.2
2	F	652	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	444	GLN	3.2
2	F	723	ILE	3.2
2	F	716	ASN	3.2
2	F	757	ASN	3.2
3	P	426	ASP	3.2
1	G	386	MET	3.2
2	F	743	LEU	3.2
2	F	786	PRO	3.2
1	C	510	THR	3.2
2	F	671	SER	3.2
2	F	737	GLU	3.1
1	E	380	ASN	3.1
2	F	728	TYR	3.1
1	E	383	GLN	3.1
1	E	432	LYS	3.1
2	F	721	PHE	3.1
1	E	424	TYR	3.1
2	D	786	PRO	3.1
1	G	574	LYS	3.1
2	F	712	CYS	3.1
1	G	389	LEU	3.0
2	F	715	LYS	3.0
2	F	669	LEU	3.0
1	A	509	GLY	3.0
1	A	510	THR	3.0
1	E	388	ILE	3.0
2	H	738	THR	3.0
1	G	402	SER	3.0
2	F	765	LYS	3.0
2	F	759	VAL	3.0
1	E	387	MET	2.9
2	D	775	ARG	2.9
1	E	512	LEU	2.9
2	F	657	LEU	2.9
2	H	699	HIS	2.9
2	B	736	GLN	2.9
1	A	379	MET	2.9
1	E	468	LEU	2.9
2	F	673	HIS	2.9
2	H	720	LYS	2.9
3	R	417	GLU	2.9
1	G	515	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	573	ILE	2.9
2	D	768	ILE	2.9
1	G	381	THR	2.9
1	C	436	GLN	2.9
2	F	681	TRP	2.9
2	F	644	SER	2.9
2	F	679	ILE	2.9
1	E	392	ALA	2.9
2	F	665	LEU	2.9
2	D	746	GLU	2.8
1	C	508	SER	2.8
2	D	780	SER	2.8
2	B	744	ILE	2.8
3	Q	409	LEU	2.8
1	G	516	TRP	2.8
1	E	393	SER	2.8
1	G	548	LYS	2.8
3	Q	410	ASP	2.8
1	E	497	THR	2.8
1	G	498	TYR	2.8
2	B	766	THR	2.8
2	H	706	CYS	2.8
1	G	469	SER	2.8
1	G	537	LYS	2.8
2	F	755	PHE	2.8
2	B	720	LYS	2.8
1	E	509	GLY	2.8
2	F	676	LEU	2.8
2	D	784	HIS	2.8
2	F	727	ALA	2.8
2	F	739	PHE	2.8
3	P	416	GLU	2.8
1	E	436	GLN	2.7
2	F	724	ILE	2.7
1	G	472	ASN	2.7
3	R	424	LEU	2.7
1	C	511	ASP	2.7
2	B	748	GLU	2.7
2	F	655	TYR	2.7
1	C	468	LEU	2.7
1	E	385	LEU	2.7
1	G	391	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	761	MET	2.7
1	E	493	VAL	2.7
2	F	718	ASP	2.7
1	G	545	GLU	2.7
2	H	661	ARG	2.7
2	F	684	PHE	2.7
2	B	782	ILE	2.7
2	H	695	MET	2.7
1	G	440	GLU	2.7
2	F	654	VAL	2.7
2	D	770	GLN	2.6
2	H	679	ILE	2.6
3	R	421	ILE	2.6
1	C	546	MET	2.6
2	B	719	LEU	2.6
1	G	510	THR	2.6
1	C	379	MET	2.6
1	A	499	SER	2.6
2	F	659	TYR	2.6
1	E	390	ASN	2.6
1	G	534	SER	2.5
1	C	500	ARG	2.5
2	F	783	PRO	2.5
1	G	408	THR	2.5
1	C	469	SER	2.5
1	E	389	LEU	2.5
1	G	417	LYS	2.5
2	D	745	LYS	2.5
1	G	572	LEU	2.5
3	R	425	PHE	2.5
1	G	443	SER	2.5
1	G	467	ARG	2.5
3	P	410	ASP	2.5
1	G	413	GLU	2.5
1	A	387	MET	2.5
1	C	575	GLN	2.5
3	R	413	PHE	2.5
2	F	687	THR	2.4
2	H	716	ASN	2.4
1	G	400	LEU	2.4
1	G	407	CYS	2.4
2	F	648	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	747	GLU	2.4
2	F	672	GLU	2.4
1	G	497	THR	2.4
2	D	667	GLU	2.4
1	G	420	LYS	2.4
2	F	738	THR	2.4
2	H	726	THR	2.4
2	F	667	GLU	2.4
1	G	411	PRO	2.4
2	F	710	GLY	2.4
1	A	436	GLN	2.4
2	H	725	VAL	2.4
1	G	422	ILE	2.3
1	A	500	ARG	2.3
2	F	683	LEU	2.3
2	F	726	THR	2.3
1	C	398	GLU	2.3
1	G	428	GLU	2.3
2	H	691	GLU	2.3
2	F	707	SER	2.3
1	A	514	PHE	2.3
1	G	426	PHE	2.3
2	B	749	TYR	2.3
2	D	771	TYR	2.3
2	F	746	GLU	2.3
2	H	746	GLU	2.3
1	E	571	ASP	2.3
2	F	725	VAL	2.3
3	Q	416	GLU	2.3
2	D	716	ASN	2.3
1	C	571	ASP	2.3
1	C	578	ASP	2.3
1	A	470	ILE	2.2
1	G	481	ILE	2.2
2	F	680	ILE	2.2
1	G	465	GLU	2.2
2	B	783	PRO	2.2
1	E	402	SER	2.2
2	B	758	SER	2.2
1	C	509	GLY	2.2
2	F	649	LEU	2.2
1	G	546	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	441	ILE	2.2
2	B	686	HIS	2.2
1	G	525	ALA	2.1
2	F	693	GLU	2.1
3	Q	417	GLU	2.1
2	F	664	THR	2.1
1	E	515	PRO	2.1
1	E	574	LYS	2.1
1	C	434	VAL	2.1
1	G	479	ASP	2.1
3	P	417	GLU	2.1
1	G	445	ARG	2.1
2	F	741	ARG	2.1
1	A	381	THR	2.1
2	F	713	LYS	2.1
2	B	768	ILE	2.1
1	C	514	PHE	2.1
1	G	577	LYS	2.1
2	F	704	MET	2.1
1	G	416	LEU	2.1
1	G	448	LEU	2.1
1	C	380	ASN	2.1
1	G	410	ASN	2.1
1	G	438	CYS	2.1
1	E	511	ASP	2.1
2	F	697	ASP	2.1
2	B	737	GLU	2.1
2	D	736	GLN	2.1
2	D	762	GLN	2.1
1	A	472	ASN	2.1
1	G	509	GLY	2.0
2	D	671	SER	2.0
1	E	531	VAL	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 ⓘ

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.