



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:44 AM UTC

PDB ID : 1TT5 / pdb_00001tt5
Title : Structure of APPBP1-UBA3-Ubc12N26: a unique E1-E2 interaction required for optimal conjugation of the ubiquitin-like protein NEDD8
Authors : Huang, D.T.; Miller, D.W.; Mathew, R.; Cassell, R.; Holton, J.M.; Roussel, M.F.; Schulman, B.A.
Deposited on : 2004-06-21
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

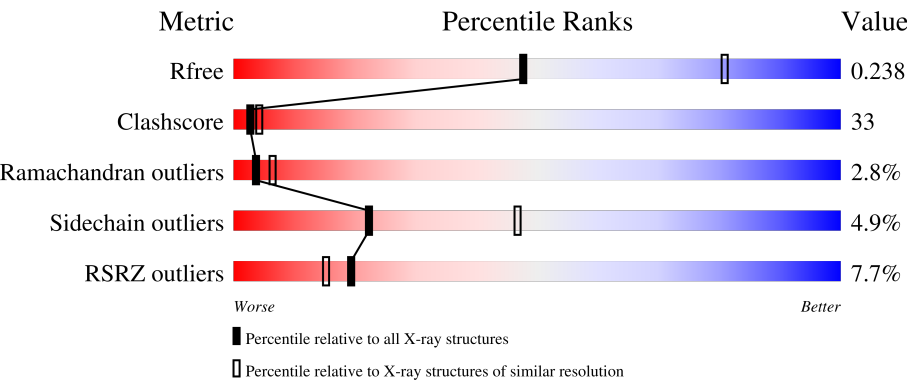
1 Overall quality at a glance i

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))
R_{free}	180053	4008 (2.60-2.60)
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	531	4% 53%39%5%..
1	C	531	6% 49%40%5%..
2	B	434	4% 56%34%6%5%
2	D	434	16% 44%40%6%.9%
3	E	26	42%8%50%

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Mol	Chain	Length	Quality of chain
3	F	26	12%19%19%62%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14637 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 amyloid protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	4	0	0
			4108	2600	701	792	15			
1	C	512	Total	C	N	O	S	4	0	0
			4020	2546	684	775	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	GB 4502169
A	0	SER	-	cloning artifact	GB 4502169
A	?	-	ASN	deletion	GB 4502169
A	?	-	GLU	deletion	GB 4502169
A	?	-	ASN	deletion	GB 4502169
A	?	-	GLY	deletion	GB 4502169
A	?	-	ALA	deletion	GB 4502169
C	-1	GLY	-	cloning artifact	GB 4502169
C	0	SER	-	cloning artifact	GB 4502169
C	?	-	ASN	deletion	GB 4502169
C	?	-	GLU	deletion	GB 4502169
C	?	-	ASN	deletion	GB 4502169
C	?	-	GLY	deletion	GB 4502169
C	?	-	ALA	deletion	GB 4502169

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	0	0
			3152	2010	540	584	18			
2	D	395	Total	C	N	O	S	12	0	0
			2866	1806	503	540	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	-	cloning artifact	GB 38045942
B	10	LYS	-	cloning artifact	GB 38045942
B	11	LEU	-	cloning artifact	GB 38045942
D	9	MET	-	cloning artifact	GB 38045942
D	10	LYS	-	cloning artifact	GB 38045942
D	11	LEU	-	cloning artifact	GB 38045942

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	S	2	0	0
			108	72	19	16	1			
3	F	10	Total	C	N	O		9	0	0
			83	55	15	13				

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

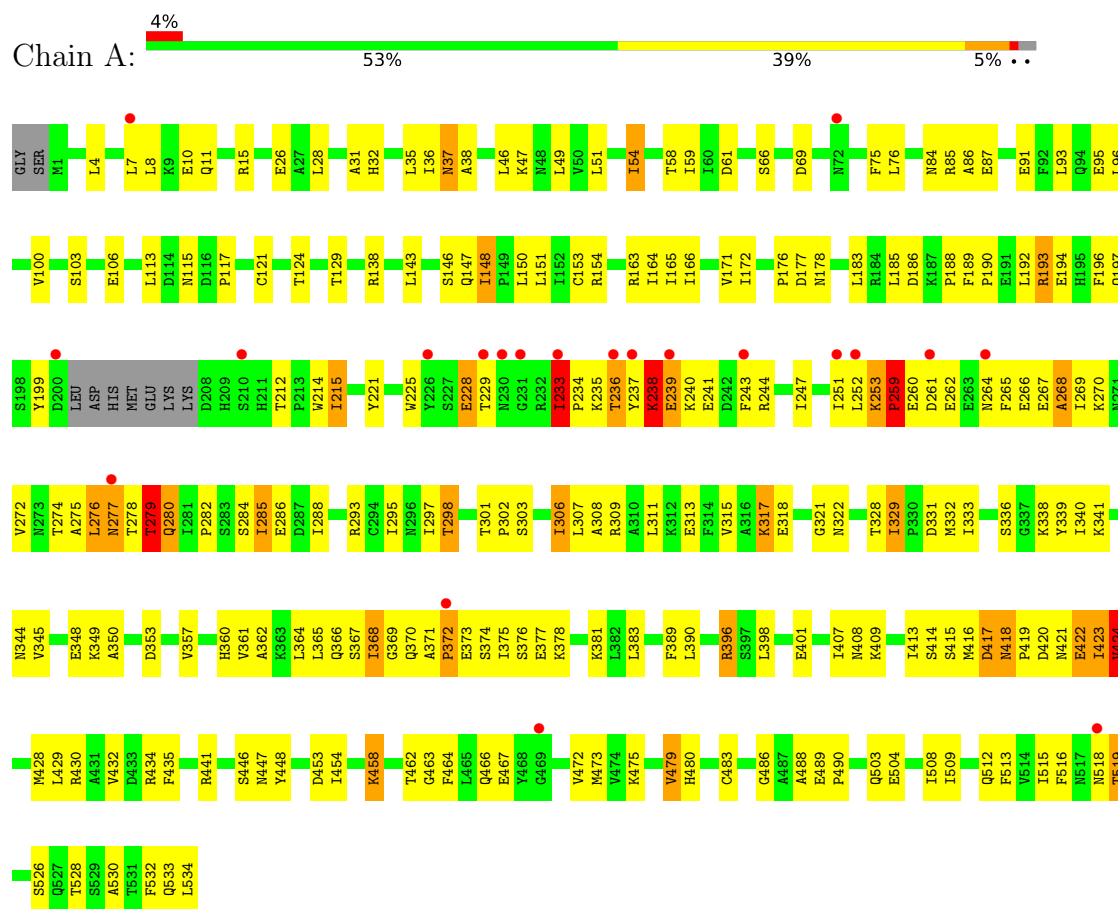
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	114	Total	O	0	0
			114	114		
5	C	45	Total	O	0	0
			45	45		
5	D	29	Total	O	0	0
			29	29		
5	E	5	Total	O	0	0
			5	5		

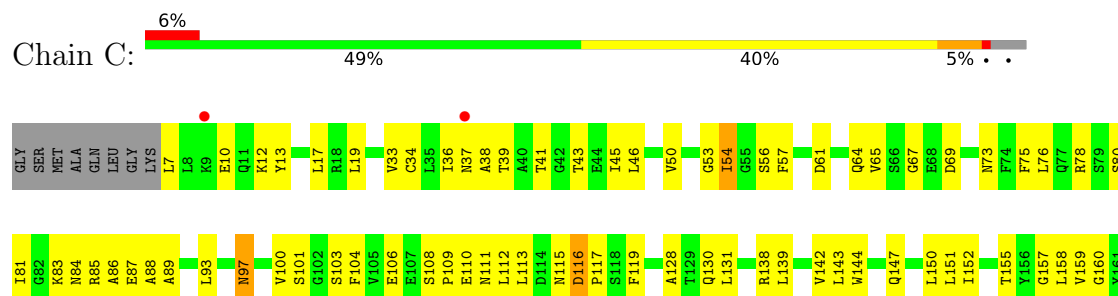
3 Residue-property plots

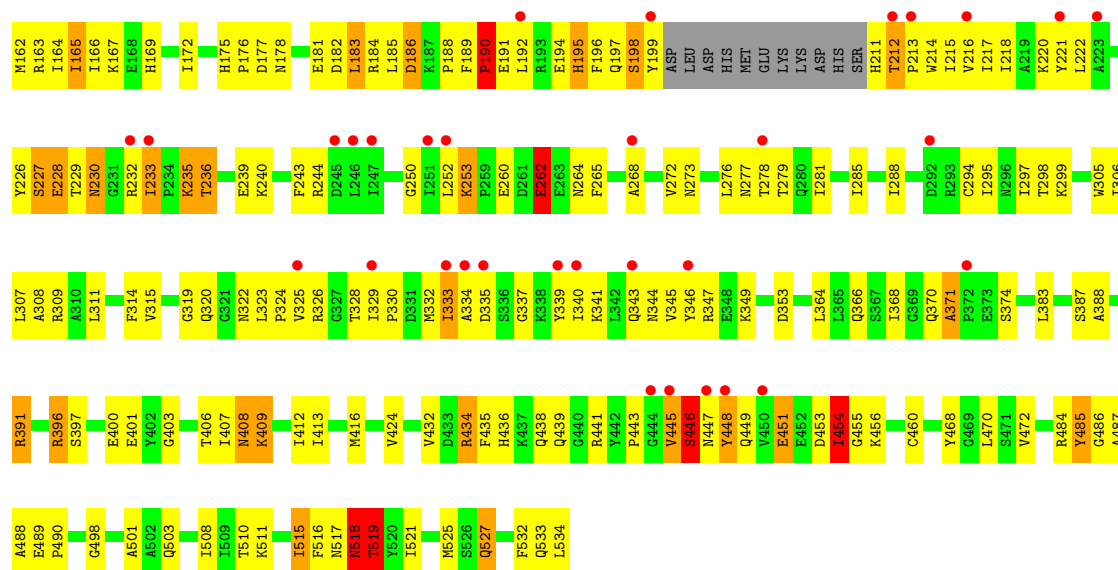
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

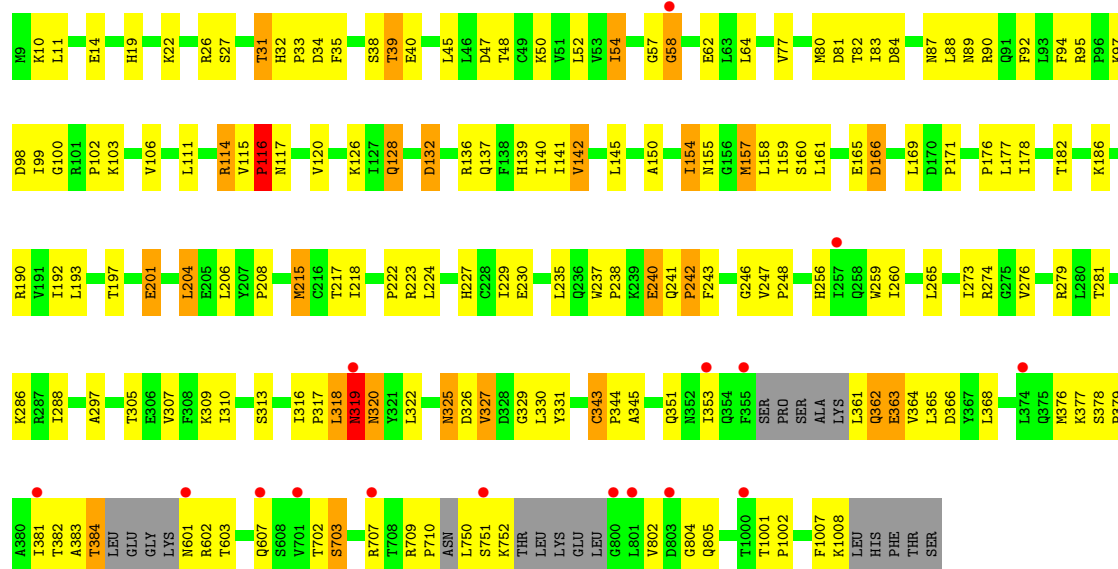


• Molecule 1: amyloid protein-binding protein 1

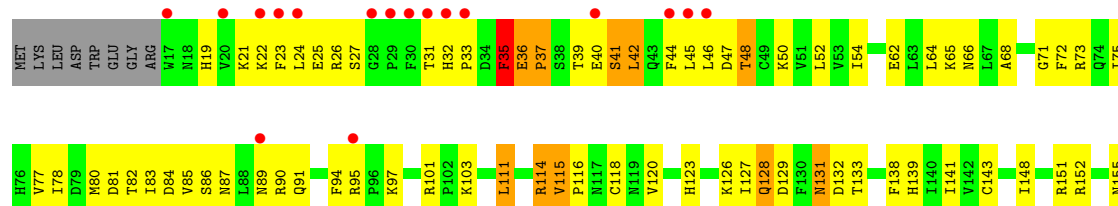
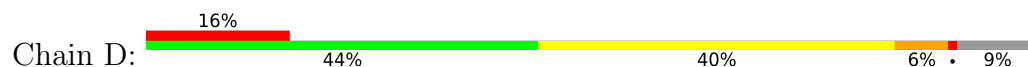


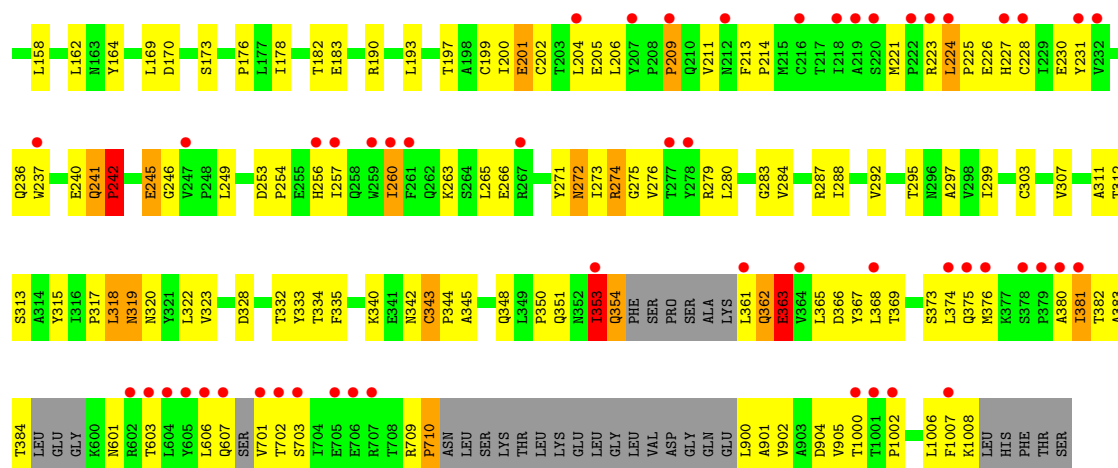


• Molecule 2: ubiquitin-activating enzyme E1C isoform 1

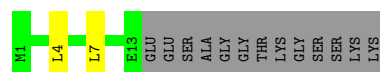


• Molecule 2: ubiquitin-activating enzyme E1C isoform 1

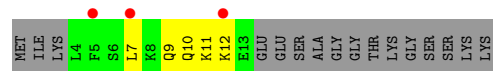




● Molecule 3: Ubiquitin-conjugating enzyme E2 M



● Molecule 3: Ubiquitin-conjugating enzyme E2 M



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.41Å 122.77Å 195.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.60 18.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (18.00-2.60) 98.5 (18.00-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.279 0.238 , 0.238	Depositor DCC
R_{free} test set	3377 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 45.2	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	0.93	EDS
Total number of atoms	14637	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.55	0/4187	1.05	20/5664 (0.4%)
1	C	0.42	0/4099	0.95	14/5547 (0.3%)
2	B	0.54	1/3219 (0.0%)	1.09	28/4380 (0.6%)
2	D	0.50	0/2923	1.14	29/3962 (0.7%)
3	E	0.43	0/108	0.64	0/139
3	F	0.82	0/83	1.09	1/107 (0.9%)
All	All	0.51	1/14619 (0.0%)	1.05	92/19799 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	157	MET	SD-CE	-5.17	1.66	1.79

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	GLU	N-CA-C	-15.11	94.63	113.97
1	A	233	ILE	N-CA-C	11.43	133.57	108.88
2	D	702	THR	N-CA-C	-11.19	98.85	111.71
1	A	279	THR	N-CA-C	-11.11	91.94	109.72
1	A	519	THR	N-CA-C	10.65	125.89	110.24
2	D	36	GLU	CA-C-N	9.81	132.10	119.84
2	D	36	GLU	C-N-CA	9.81	132.10	119.84
2	D	41	SER	N-CA-C	-9.64	100.27	112.90
2	D	363	GLU	N-CA-C	-9.61	101.69	113.50
2	B	115	VAL	CA-C-N	9.56	131.80	119.84
2	B	115	VAL	C-N-CA	9.56	131.80	119.84
1	A	238	LYS	N-CA-C	9.22	125.27	112.45
1	A	260	GLU	N-CA-C	-9.06	94.98	109.39
1	A	276	LEU	N-CA-C	-8.78	101.67	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	LEU	N-CA-C	-8.32	99.60	110.33
2	D	211	VAL	N-CA-C	-8.12	98.17	108.89
2	D	42	LEU	N-CA-C	-8.06	101.77	111.69
1	A	259	PRO	CA-C-N	-7.89	110.08	122.23
1	A	259	PRO	C-N-CA	-7.89	110.08	122.23
1	A	424	VAL	CB-CA-C	-7.66	101.80	112.14
2	D	213	PHE	N-CA-C	7.62	121.37	110.24
2	B	327	VAL	N-CA-C	7.61	117.58	110.42
1	C	409	LYS	N-CA-C	7.53	120.14	111.11
2	D	710	PRO	N-CA-CB	7.41	111.15	103.00
2	B	241	GLN	CA-C-N	7.15	128.78	119.84
2	B	241	GLN	C-N-CA	7.15	128.78	119.84
2	B	240	GLU	N-CA-C	-7.08	101.18	110.53
2	D	318	LEU	N-CA-C	-7.00	100.38	110.24
2	D	1002	PRO	N-CA-CB	6.94	109.91	103.46
2	D	209	PRO	N-CA-C	-6.85	101.14	111.41
2	D	343	CYS	CA-C-N	6.79	128.33	119.84
2	D	343	CYS	C-N-CA	6.79	128.33	119.84
2	B	39	THR	N-CA-C	-6.78	104.91	112.57
2	D	48	THR	N-CA-C	6.75	121.38	112.13
2	D	288	ILE	N-CA-C	6.73	118.01	108.93
2	B	702	THR	N-CA-C	-6.69	104.38	112.54
2	B	316	ILE	N-CA-C	-6.48	103.00	109.02
2	B	1002	PRO	N-CA-CB	6.43	109.31	103.20
2	B	319	ASN	N-CA-C	-6.39	97.18	110.80
2	B	710	PRO	N-CA-CB	6.35	109.99	103.00
1	A	148	ILE	N-CA-C	6.25	114.08	107.76
2	D	115	VAL	CA-C-N	6.18	126.54	119.93
2	D	115	VAL	C-N-CA	6.18	126.54	119.93
1	C	396	ARG	N-CA-C	-6.16	102.36	110.43
2	B	363	GLU	N-CA-C	-6.14	105.92	113.41
2	D	353	ILE	N-CA-C	6.14	122.11	109.34
1	C	177	ASP	N-CA-C	-6.01	99.47	109.46
1	C	178	ASN	N-CA-C	6.01	119.53	111.24
2	D	47	ASP	N-CA-C	5.95	121.59	113.97
1	A	260	GLU	CB-CA-C	5.91	121.52	112.00
2	B	48	THR	N-CA-C	5.85	121.99	114.56
2	B	88	LEU	N-CA-C	5.85	123.26	110.80
2	B	343	CYS	CA-C-N	5.85	125.71	119.28
2	B	343	CYS	C-N-CA	5.85	125.71	119.28
2	B	47	ASP	N-CA-C	5.84	121.07	113.88
2	D	37	PRO	N-CA-C	5.77	124.35	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	35	PHE	N-CA-C	5.75	117.71	110.24
2	B	126	LYS	N-CA-C	-5.68	101.34	110.14
1	C	306	ILE	N-CA-C	-5.67	105.20	110.53
2	B	27	SER	N-CA-C	-5.66	103.23	110.53
2	B	329	GLY	N-CA-C	-5.63	101.55	112.02
2	D	381	ILE	N-CA-C	5.61	116.66	108.58
1	C	212	THR	CA-C-N	5.60	125.53	119.76
1	C	212	THR	C-N-CA	5.60	125.53	119.76
1	A	268	ALA	N-CA-C	-5.60	105.26	111.36
2	B	703	SER	N-CA-C	-5.53	105.65	112.90
2	B	319	ASN	CA-C-N	-5.51	111.02	121.54
2	B	319	ASN	C-N-CA	-5.51	111.02	121.54
1	A	259	PRO	CA-N-CD	-5.46	104.36	112.00
1	C	159	VAL	N-CA-C	5.46	116.34	108.48
2	D	81	ASP	N-CA-C	5.45	118.59	110.14
1	C	519	THR	N-CA-C	5.44	122.38	110.80
1	C	116	ASP	CA-C-N	5.41	124.59	118.97
1	C	116	ASP	C-N-CA	5.41	124.59	118.97
2	D	118	CYS	N-CA-C	-5.39	100.91	109.59
1	C	165	ILE	N-CA-C	5.38	115.27	106.72
1	A	479	VAL	N-CA-C	-5.35	105.32	110.72
1	C	230	ASN	N-CA-C	-5.35	106.75	113.28
1	A	193	ARG	N-CA-C	-5.35	105.37	111.14
1	A	417	ASP	N-CA-C	-5.30	104.91	111.33
1	A	259	PRO	N-CA-C	5.28	123.35	112.47
2	D	138	PHE	N-CA-C	5.18	118.15	110.48
2	D	224	LEU	CA-C-N	5.17	124.62	119.24
2	D	224	LEU	C-N-CA	5.17	124.62	119.24
2	B	1002	PRO	N-CA-C	-5.13	107.34	114.27
3	F	12	LYS	N-CA-C	-5.11	102.12	110.20
2	B	320	ASN	N-CA-C	5.08	121.61	110.80
2	B	1001	THR	N-CA-C	5.02	114.07	108.25
2	D	111	LEU	N-CA-C	5.01	116.82	111.36
1	A	396	ARG	N-CA-C	-5.01	104.25	110.41
2	B	318	LEU	N-CA-C	-5.01	103.11	110.42
1	A	306	ILE	N-CA-C	-5.00	105.52	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4108	0	4038	305	0
1	C	4020	0	3937	276	0
2	B	3152	0	2998	173	0
2	D	2866	0	2608	227	0
3	E	108	0	128	3	0
3	F	83	0	92	6	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	105	0	0	12	0
5	B	114	0	0	9	0
5	C	45	0	0	4	0
5	D	29	0	0	3	0
5	E	5	0	0	0	0
All	All	14637	0	13801	933	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 33.

All (933) 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:518:ASN:ND2	1:A:534:LEU:H	1.07	1.41
1:A:518:ASN:ND2	1:A:534:LEU:N	1.76	1.31
1:A:225:TRP:NE1	1:A:233:ILE:HD11	1.58	1.19
1:A:282:PRO:HB2	1:A:285:ILE:HD13	1.19	1.18
1:A:235:LYS:HB2	1:A:239:GLU:HG3	1.22	1.17
2:D:353:ILE:HG12	2:D:1008:LYS:HA	1.38	1.06
2:B:111:LEU:HD23	2:B:120:VAL:HG21	1.36	1.05
2:D:249:LEU:HD11	2:D:256:HIS:HB3	1.40	1.03
1:C:215:ILE:HG13	1:C:332:MET:HE1	1.40	1.02
1:A:259:PRO:HB3	1:A:261:ASP:CG	1.84	1.02
1:A:434:ARG:HH12	1:A:463:GLY:HA3	1.21	1.02
1:C:214:TRP:HA	1:C:217:ILE:HD13	1.38	1.02
1:A:396:ARG:NH1	1:A:408:ASN:HD21	1.57	1.01
1:A:489:GLU:H	2:B:19:HIS:CD2	1.79	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ASN:HD21	1:A:534:LEU:N	1.48	0.99
2:D:155:ASN:HB2	2:D:200:ILE:HD12	1.42	0.99
1:A:236:THR:O	1:A:240:LYS:HB2	1.60	0.99
2:D:83:ILE:HD13	2:D:103:LYS:HG2	1.44	0.98
1:A:396:ARG:HH12	1:A:408:ASN:HD21	0.98	0.98
1:A:396:ARG:HH12	1:A:408:ASN:ND2	1.61	0.97
2:B:128:GLN:HE21	2:B:128:GLN:H	0.97	0.97
2:B:64:LEU:HB3	2:B:111:LEU:HD22	1.45	0.96
1:A:278:THR:HG22	1:A:279:THR:O	1.67	0.95
1:A:172:ILE:HD13	1:A:390:LEU:HD22	1.46	0.94
1:A:447:ASN:HD22	2:B:26:ARG:HH21	1.13	0.94
1:C:244:ARG:HH21	1:C:273:ASN:HB2	1.31	0.94
1:C:143:LEU:HD12	1:C:150:LEU:HD22	1.48	0.94
1:A:233:ILE:HG23	1:A:239:GLU:HB2	1.48	0.94
1:C:489:GLU:H	2:D:19:HIS:CD2	1.85	0.94
2:D:249:LEU:HD11	2:D:256:HIS:CB	1.99	0.93
2:D:353:ILE:CG1	2:D:1008:LYS:HA	1.97	0.93
1:A:235:LYS:CB	1:A:239:GLU:HG3	1.98	0.92
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.51	0.92
2:D:253:ASP:CG	2:D:256:HIS:HB2	1.93	0.92
1:A:244:ARG:HG2	1:A:272:VAL:HG11	1.52	0.92
1:A:489:GLU:H	2:B:19:HIS:HD2	0.94	0.91
2:D:27:SER:HA	2:D:35:PHE:HZ	1.35	0.90
1:A:251:ILE:CG2	1:A:259:PRO:HB2	2.00	0.90
2:D:95:ARG:HD2	2:D:97:LYS:HE2	1.54	0.90
1:A:251:ILE:O	1:A:259:PRO:HG2	1.72	0.90
1:C:489:GLU:H	2:D:19:HIS:HD2	1.18	0.90
1:A:46:LEU:CD2	1:A:59:ILE:HD11	2.00	0.90
2:D:31:THR:HG21	2:D:35:PHE:CG	2.08	0.89
2:D:50:LYS:H	2:D:139:HIS:HD2	1.17	0.89
2:D:249:LEU:CD1	2:D:256:HIS:HB3	2.02	0.89
1:A:225:TRP:HE1	1:A:233:ILE:HD11	1.35	0.88
2:B:84:ASP:H	2:B:87:ASN:ND2	1.69	0.88
1:A:243:PHE:O	1:A:247:ILE:HD13	1.73	0.88
1:A:518:ASN:HD22	1:A:534:LEU:N	1.57	0.88
1:A:251:ILE:O	1:A:259:PRO:HD2	1.73	0.87
1:A:35:LEU:HD23	1:A:59:ILE:HD12	1.55	0.87
1:A:447:ASN:ND2	2:B:26:ARG:HH21	1.72	0.87
2:B:223:ARG:H	2:B:227:HIS:HD2	1.23	0.87
2:D:295:THR:O	2:D:299:ILE:HD12	1.75	0.87
1:A:518:ASN:HD22	1:A:533:GLN:CA	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HG22	1:A:233:ILE:O	1.73	0.86
1:A:236:THR:CA	1:A:240:LYS:HD2	2.04	0.86
1:C:311:LEU:HD21	1:C:387:SER:HB2	1.55	0.85
2:B:128:GLN:H	2:B:128:GLN:NE2	1.72	0.85
1:C:213:PRO:HB3	1:C:332:MET:HE2	1.56	0.85
1:C:41:THR:O	1:C:45:ILE:HD13	1.75	0.85
1:C:307:LEU:HD22	1:C:383:LEU:HD22	1.57	0.85
2:D:368:LEU:O	2:D:376:MET:HG2	1.75	0.85
2:D:83:ILE:CD1	2:D:103:LYS:HG2	2.07	0.85
1:C:515:ILE:HD13	1:C:515:ILE:H	1.40	0.84
1:A:434:ARG:NH1	1:A:463:GLY:HA3	1.92	0.84
1:A:518:ASN:HD22	1:A:533:GLN:HA	1.41	0.84
1:C:130:GLN:HE22	1:C:155:THR:H	1.24	0.84
2:D:353:ILE:HG12	2:D:1008:LYS:CA	2.08	0.84
1:A:183:LEU:HD13	1:A:215:ILE:HD11	1.60	0.84
1:A:266:GLU:OE1	1:A:269:ILE:HD12	1.78	0.84
2:D:353:ILE:HG22	2:D:354:GLN:H	1.42	0.83
1:A:518:ASN:HD21	1:A:534:LEU:H	0.84	0.83
2:D:27:SER:HA	2:D:35:PHE:CZ	2.13	0.83
2:B:128:GLN:HE21	2:B:128:GLN:N	1.77	0.83
1:A:228:GLU:HG2	1:A:229:THR:H	1.43	0.83
2:D:84:ASP:OD2	2:D:86:SER:OG	1.96	0.82
1:A:454:ILE:HD12	1:A:480:HIS:HA	1.60	0.82
1:C:438:GLN:HG2	1:C:439:GLN:HE22	1.45	0.82
2:D:83:ILE:HD11	2:D:103:LYS:HA	1.61	0.81
1:C:484:ARG:HA	2:D:26:ARG:NH1	1.96	0.81
1:C:438:GLN:HG2	1:C:439:GLN:NE2	1.96	0.81
2:D:353:ILE:HD12	2:D:353:ILE:H	1.45	0.81
1:A:252:LEU:C	1:A:259:PRO:HD2	2.06	0.81
1:C:489:GLU:N	2:D:19:HIS:HD2	1.79	0.80
1:A:225:TRP:CE2	1:A:233:ILE:HD11	2.17	0.80
2:D:32:HIS:O	2:D:35:PHE:HB3	1.80	0.80
1:C:449:GLN:HB3	1:C:453:ASP:OD2	1.81	0.80
1:A:251:ILE:O	1:A:259:PRO:CG	2.30	0.80
2:B:32:HIS:HD2	2:B:34:ASP:H	1.30	0.80
2:D:31:THR:HG21	2:D:35:PHE:CD2	2.17	0.80
1:A:518:ASN:HD22	1:A:533:GLN:C	1.89	0.79
1:A:274:THR:O	1:A:277:ASN:ND2	2.15	0.79
1:A:454:ILE:CD1	1:A:480:HIS:HA	2.12	0.79
1:A:251:ILE:HG22	1:A:259:PRO:HB2	1.63	0.78
1:C:484:ARG:HA	2:D:26:ARG:HH11	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:O	1:A:259:PRO:CD	2.31	0.78
2:D:253:ASP:OD2	2:D:256:HIS:CD2	2.36	0.78
2:D:46:LEU:HA	2:D:71:GLY:O	1.83	0.78
1:A:518:ASN:CG	1:A:519:THR:H	1.90	0.78
2:D:31:THR:HG22	2:D:32:HIS:N	1.99	0.77
1:A:396:ARG:HH11	1:A:396:ARG:HG3	1.49	0.77
1:A:241:GLU:HA	1:A:244:ARG:HH11	1.50	0.77
1:A:447:ASN:HD22	2:B:26:ARG:NH2	1.82	0.77
2:B:318:LEU:O	2:B:319:ASN:O	2.01	0.77
2:D:249:LEU:CD2	2:D:260:ILE:HD11	2.15	0.77
1:A:251:ILE:HG23	1:A:259:PRO:HB2	1.67	0.77
2:B:31:THR:HG23	2:B:35:PHE:HB3	1.67	0.77
2:B:703:SER:O	2:B:707:ARG:N	2.18	0.76
1:A:454:ILE:HD13	1:A:483:CYS:SG	2.26	0.76
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.66	0.76
1:A:113:LEU:O	1:A:117:PRO:HG3	1.85	0.75
1:A:237:TYR:O	1:A:241:GLU:HB3	1.86	0.75
2:D:260:ILE:HD13	2:D:260:ILE:N	2.01	0.75
1:A:233:ILE:HD13	1:A:233:ILE:N	2.02	0.75
1:C:215:ILE:CG1	1:C:332:MET:HE1	2.16	0.75
2:D:42:LEU:HG	2:D:46:LEU:HD11	1.67	0.75
2:B:243:PHE:O	2:B:247:VAL:HG21	1.88	0.74
2:D:362:GLN:O	2:D:366:ASP:HB2	1.85	0.74
2:D:363:GLU:O	2:D:367:TYR:HB3	1.86	0.74
1:A:240:LYS:O	1:A:244:ARG:HG3	1.87	0.74
1:A:518:ASN:HD22	1:A:534:LEU:H	1.18	0.74
1:C:298:THR:HG22	1:C:299:LYS:H	1.51	0.74
1:C:454:ILE:HG23	1:C:455:GLY:H	1.51	0.74
1:A:4:LEU:O	1:A:8:LEU:HB2	1.88	0.74
1:A:423:ILE:HD13	1:A:423:ILE:O	1.87	0.74
1:A:518:ASN:HB3	1:A:532:PHE:O	1.86	0.74
1:C:45:ILE:HD12	1:C:498:GLY:HA2	1.69	0.73
2:D:170:ASP:O	2:D:173:SER:HB3	1.87	0.73
1:A:409:LYS:O	1:A:413:ILE:HG12	1.88	0.73
2:B:64:LEU:HB3	2:B:111:LEU:CD2	2.18	0.73
2:B:58:GLY:N	5:B:1015:HOH:O	2.22	0.73
1:A:172:ILE:HD13	1:A:390:LEU:CD2	2.19	0.72
2:D:295:THR:HG22	2:D:299:ILE:HD11	1.72	0.72
1:A:163:ARG:NH1	1:A:401:GLU:OE2	2.22	0.72
1:A:282:PRO:HB2	1:A:285:ILE:CD1	2.11	0.72
1:C:339:TYR:HE2	2:D:224:LEU:HD21	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:380:ALA:O	2:D:902:VAL:HA	1.89	0.72
1:A:84:ASN:ND2	1:A:87:GLU:H	1.87	0.72
1:A:489:GLU:N	2:B:19:HIS:HD2	1.80	0.72
1:A:253:LYS:N	1:A:259:PRO:CD	2.53	0.71
1:C:412:ILE:HD11	1:C:534:LEU:HD22	1.70	0.71
1:C:515:ILE:HD13	1:C:515:ILE:N	2.06	0.71
1:C:328:THR:C	1:C:329:ILE:HD12	2.15	0.71
1:A:235:LYS:HG2	1:A:239:GLU:OE2	1.90	0.71
1:A:236:THR:O	1:A:240:LYS:CB	2.35	0.71
1:A:306:ILE:HD11	1:A:370:GLN:HE22	1.55	0.70
5:A:573:HOH:O	2:B:186:LYS:HE3	1.91	0.70
1:C:434:ARG:HG2	1:C:434:ARG:HH11	1.56	0.70
2:B:318:LEU:O	2:B:319:ASN:C	2.34	0.70
2:D:295:THR:HG22	2:D:299:ILE:CD1	2.21	0.70
1:C:37:ASN:C	1:C:39:THR:H	1.99	0.70
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.74	0.69
1:A:518:ASN:HD21	1:A:534:LEU:CA	2.05	0.69
1:C:281:ILE:HD12	1:C:323:LEU:HG	1.73	0.69
1:A:340:ILE:HD11	2:B:273:ILE:CD1	2.22	0.69
1:C:262:GLU:HB2	1:C:264:ASN:OD1	1.92	0.69
2:B:32:HIS:CD2	2:B:34:ASP:H	2.11	0.69
1:C:222:LEU:HG	1:C:226:TYR:CE2	2.27	0.69
1:C:232:ARG:C	1:C:233:ILE:HD13	2.18	0.69
1:A:253:LYS:N	1:A:259:PRO:HD2	2.08	0.69
2:B:57:GLY:C	5:B:1015:HOH:O	2.35	0.69
2:D:78:ILE:HD13	2:D:123:HIS:HB2	1.75	0.68
1:C:217:ILE:H	1:C:217:ILE:HD12	1.56	0.68
1:A:285:ILE:N	1:A:285:ILE:HD12	2.08	0.68
1:A:233:ILE:HG23	1:A:239:GLU:CB	2.21	0.68
1:C:518:ASN:O	1:C:532:PHE:O	2.11	0.68
1:C:46:LEU:HD23	1:C:93:LEU:HD13	1.76	0.68
2:B:237:TRP:O	2:B:240:GLU:O	2.11	0.68
1:A:189:PHE:CE1	1:A:192:LEU:HB2	2.29	0.68
2:D:65:LYS:HE3	2:D:66:ASN:OD1	1.93	0.68
1:A:228:GLU:HG2	1:A:229:THR:N	2.08	0.67
2:D:353:ILE:HG13	2:D:1007:PHE:O	1.94	0.67
1:A:344:ASN:O	1:A:348:GLU:HG2	1.94	0.67
1:C:213:PRO:CB	1:C:332:MET:HE2	2.24	0.67
1:C:253:LYS:HE3	1:C:260:GLU:OE2	1.94	0.67
2:D:201:GLU:HG2	2:D:345:ALA:HB2	1.75	0.67
2:D:237:TRP:CH2	2:D:249:LEU:HD13	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:HB2	5:A:605:HOH:O	1.94	0.67
1:A:297:ILE:HG22	1:A:298:THR:N	2.10	0.67
1:A:279:THR:HG22	1:A:322:ASN:ND2	2.09	0.67
1:C:10:GLU:HG3	2:D:279:ARG:HH12	1.60	0.67
1:C:13:TYR:O	1:C:17:LEU:HG	1.93	0.67
1:A:462:THR:O	1:A:466:GLN:HG3	1.95	0.66
2:B:256:HIS:O	2:B:260:ILE:HG12	1.95	0.66
2:D:64:LEU:HD21	2:D:77:VAL:HG22	1.77	0.66
2:D:83:ILE:HD12	2:D:94:PHE:CE1	2.30	0.66
1:A:46:LEU:HD22	1:A:59:ILE:HD11	1.77	0.66
2:D:201:GLU:O	2:D:204:LEU:HG	1.96	0.66
2:D:353:ILE:HG22	2:D:354:GLN:N	2.10	0.66
2:D:50:LYS:H	2:D:139:HIS:CD2	2.08	0.66
1:A:7:LEU:O	1:A:11:GLN:HG3	1.96	0.66
1:A:236:THR:C	1:A:240:LYS:HB2	2.20	0.66
1:C:244:ARG:NH2	1:C:273:ASN:HB2	2.06	0.66
1:C:164:ILE:HD11	1:C:508:ILE:HD11	1.76	0.66
1:A:240:LYS:HG2	1:A:276:LEU:HD12	1.78	0.65
2:B:62:GLU:HG2	2:B:297:ALA:HA	1.78	0.65
2:D:45:LEU:HD11	2:D:72:PHE:CZ	2.30	0.65
1:C:515:ILE:H	1:C:515:ILE:CD1	2.08	0.65
2:D:201:GLU:HA	2:D:204:LEU:CD2	2.26	0.65
1:C:297:ILE:HD12	1:C:297:ILE:O	1.97	0.65
1:C:400:GLU:O	1:C:406:THR:HG23	1.97	0.65
1:C:486:GLY:HA3	2:D:22:LYS:NZ	2.11	0.65
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.78	0.65
1:A:46:LEU:HD23	1:A:93:LEU:HD13	1.79	0.65
1:A:269:ILE:O	1:A:272:VAL:HG12	1.96	0.65
2:D:226:GLU:CD	2:D:226:GLU:H	2.05	0.65
2:D:318:LEU:O	2:D:319:ASN:C	2.39	0.65
1:A:518:ASN:OD1	1:A:519:THR:N	2.30	0.65
1:C:341:LYS:O	1:C:345:VAL:HG23	1.97	0.65
2:D:201:GLU:HA	2:D:204:LEU:HD21	1.77	0.65
1:A:267:GLU:HA	1:A:270:LYS:HE2	1.79	0.64
2:B:361:LEU:C	2:B:363:GLU:H	2.06	0.64
2:B:141:ILE:HD12	2:B:158:LEU:HD21	1.78	0.64
1:A:235:LYS:CG	1:A:239:GLU:OE2	2.45	0.64
1:C:297:ILE:HD13	1:C:368:ILE:HD11	1.79	0.64
1:A:259:PRO:C	1:A:261:ASP:N	2.55	0.64
2:D:249:LEU:HD22	2:D:260:ILE:HD11	1.79	0.64
1:A:278:THR:HG22	1:A:279:THR:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:HD3	1:A:238:LYS:O	1.98	0.64
1:A:447:ASN:ND2	2:B:26:ARG:HE	1.95	0.64
2:D:31:THR:CG2	2:D:35:PHE:CG	2.78	0.64
1:C:281:ILE:CD1	1:C:323:LEU:HG	2.28	0.64
2:D:42:LEU:O	2:D:46:LEU:HG	1.98	0.64
1:A:251:ILE:HG23	1:A:261:ASP:HB2	1.80	0.63
2:D:381:ILE:HA	2:D:901:ALA:O	1.98	0.63
1:A:228:GLU:CG	1:A:229:THR:N	2.61	0.63
1:C:7:LEU:HD23	5:C:560:HOH:O	1.97	0.63
1:C:347:ARG:NH1	2:D:274:ARG:HG3	2.13	0.63
1:C:184:ARG:CZ	1:C:325:VAL:HG12	2.28	0.63
2:D:46:LEU:O	2:D:73:ARG:HB2	1.98	0.63
1:C:163:ARG:NH1	1:C:401:GLU:OE2	2.32	0.63
3:F:10:GLN:HG2	3:F:11:LYS:H	1.64	0.63
2:B:54:ILE:N	2:B:54:ILE:HD12	2.13	0.63
1:C:236:THR:HG22	1:C:239:GLU:H	1.64	0.63
1:A:49:LEU:HB3	1:A:54:ILE:HD12	1.78	0.63
1:C:138:ARG:O	1:C:142:VAL:HG23	1.98	0.63
1:A:259:PRO:HB3	1:A:261:ASP:OD2	1.99	0.62
2:B:155:ASN:O	2:B:159:ILE:HG12	1.99	0.62
2:D:42:LEU:HG	2:D:46:LEU:CD1	2.30	0.62
2:D:182:THR:OG1	2:D:299:ILE:HD13	1.98	0.62
2:B:32:HIS:HD2	2:B:34:ASP:N	1.98	0.62
2:D:318:LEU:HD11	2:D:334:THR:HG23	1.81	0.62
2:D:353:ILE:HG12	2:D:1008:LYS:CB	2.29	0.62
1:A:357:VAL:O	1:A:361:VAL:HG23	2.00	0.61
1:C:525:MET:HG3	2:D:315:TYR:CE2	2.34	0.61
1:A:46:LEU:HD21	1:A:59:ILE:HD11	1.79	0.61
1:A:121:CYS:HA	1:A:148:ILE:HD11	1.81	0.61
1:A:284:SER:O	1:A:288:ILE:HG12	1.98	0.61
2:B:132:ASP:HA	2:B:157:MET:HE1	1.82	0.61
2:B:242:PRO:HG3	2:B:259:TRP:CZ2	2.35	0.61
1:C:294:CYS:O	1:C:309:ARG:HD2	1.99	0.61
2:D:253:ASP:OD2	2:D:256:HIS:HB2	2.00	0.61
1:A:235:LYS:CG	1:A:239:GLU:HG3	2.29	0.61
1:A:336:SER:O	1:A:340:ILE:HG12	1.99	0.61
2:B:274:ARG:HG3	5:B:1104:HOH:O	2.00	0.61
1:C:215:ILE:H	1:C:332:MET:HE1	1.65	0.61
1:A:193:ARG:O	1:A:197:GLN:HG3	2.00	0.61
1:A:366:GLN:C	1:A:368:ILE:H	2.08	0.61
2:B:223:ARG:O	2:B:273:ILE:HD12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LYS:O	1:A:458:LYS:HD3	2.01	0.61
2:B:39:THR:HG23	2:B:39:THR:O	1.99	0.61
1:A:84:ASN:HD21	1:A:86:ALA:HB3	1.66	0.61
1:A:516:PHE:CD1	1:A:518:ASN:O	2.53	0.61
1:C:340:ILE:O	1:C:344:ASN:ND2	2.34	0.61
1:C:451:GLU:HG3	1:C:451:GLU:O	2.00	0.61
1:C:213:PRO:HB2	1:C:216:VAL:HG23	1.83	0.60
1:C:199:TYR:HB2	1:C:220:LYS:HE2	1.83	0.60
1:A:418:ASN:ND2	1:A:420:ASP:H	2.00	0.60
1:C:37:ASN:HB3	1:C:39:THR:HG23	1.84	0.60
1:A:259:PRO:HB3	1:A:261:ASP:CB	2.31	0.60
1:C:78:ARG:HD2	1:C:81:ILE:HD11	1.82	0.60
1:C:525:MET:HG3	2:D:315:TYR:CD2	2.35	0.60
2:B:206:LEU:C	2:B:208:PRO:HD3	2.27	0.60
1:C:54:ILE:HD12	1:C:54:ILE:O	2.02	0.60
2:D:350:PRO:HB3	2:D:1006:LEU:O	2.02	0.60
1:A:259:PRO:O	1:A:261:ASP:N	2.34	0.60
1:C:347:ARG:HH12	2:D:274:ARG:HG3	1.67	0.60
1:A:333:ILE:HD13	2:B:223:ARG:NH2	2.16	0.60
1:A:416:MET:HE1	1:A:424:VAL:HG13	1.84	0.60
2:B:215:MET:HA	2:B:215:MET:HE2	1.84	0.60
2:D:237:TRP:CZ2	2:D:249:LEU:HB2	2.37	0.60
1:C:186:ASP:OD2	1:C:279:THR:HB	2.01	0.60
1:C:226:TYR:CE1	1:C:233:ILE:HG23	2.36	0.60
1:C:298:THR:HG22	1:C:299:LYS:N	2.14	0.60
2:D:182:THR:CG2	2:D:183:GLU:N	2.65	0.60
2:D:85:VAL:HG23	5:D:1028:HOH:O	2.02	0.59
2:D:318:LEU:O	2:D:319:ASN:O	2.19	0.59
2:D:362:GLN:HE22	2:D:365:LEU:HD23	1.67	0.59
1:C:371:ALA:HB3	1:C:374:SER:OG	2.02	0.59
1:A:516:PHE:CE1	1:A:518:ASN:O	2.55	0.59
2:B:246:GLY:O	2:B:248:PRO:HD3	2.02	0.59
1:A:272:VAL:O	1:A:276:LEU:HG	2.02	0.59
2:B:361:LEU:HB3	2:B:750:LEU:HA	1.84	0.59
1:C:409:LYS:O	1:C:413:ILE:HG12	2.01	0.59
1:C:162:MET:O	1:C:519:THR:HA	2.03	0.59
1:C:211:HIS:HA	1:C:335:ASP:CG	2.28	0.59
2:D:260:ILE:HD13	2:D:260:ILE:H	1.66	0.59
1:A:214:TRP:HB2	1:A:268:ALA:HA	1.84	0.59
1:A:235:LYS:HB2	1:A:239:GLU:CG	2.15	0.59
1:A:303:SER:HA	1:A:306:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ARG:NH1	1:A:408:ASN:ND2	2.34	0.59
1:A:434:ARG:HH12	1:A:463:GLY:CA	2.06	0.59
2:B:82:THR:HG23	2:B:100:GLY:C	2.28	0.59
1:C:186:ASP:C	1:C:188:PRO:HD3	2.27	0.59
1:A:396:ARG:NH1	1:A:396:ARG:HG3	2.13	0.59
1:A:421:ASN:O	1:A:424:VAL:HG22	2.02	0.59
2:D:249:LEU:HD11	2:D:256:HIS:HB2	1.84	0.59
2:B:111:LEU:HD23	2:B:120:VAL:CG2	2.23	0.58
1:C:518:ASN:ND2	1:C:534:LEU:H	2.00	0.58
2:D:127:ILE:HG12	2:D:128:GLN:OE1	2.03	0.58
2:D:271:TYR:O	2:D:272:ASN:HB2	2.03	0.58
1:A:233:ILE:HD13	1:A:233:ILE:H	1.65	0.58
1:A:518:ASN:HD21	1:A:534:LEU:CB	2.16	0.58
2:D:369:THR:HA	2:D:376:MET:O	2.04	0.58
1:C:84:ASN:HB3	1:C:87:GLU:HG2	1.85	0.58
2:D:190:ARG:HB2	2:D:320:ASN:O	2.04	0.58
1:A:279:THR:O	1:A:280:GLN:HB2	2.04	0.58
1:A:441:ARG:NH2	1:A:453:ASP:OD2	2.36	0.58
2:B:139:HIS:CB	2:B:140:ILE:HD12	2.34	0.58
2:D:381:ILE:N	2:D:381:ILE:HD12	2.19	0.58
1:A:237:TYR:O	1:A:241:GLU:CB	2.51	0.58
1:C:222:LEU:HA	1:C:243:PHE:HE1	1.68	0.58
1:C:486:GLY:HA3	2:D:22:LYS:HZ3	1.69	0.58
2:D:44:PHE:CD2	3:F:9:GLN:HG2	2.38	0.58
2:D:44:PHE:CE1	3:F:9:GLN:HA	2.39	0.58
2:D:162:LEU:HA	2:D:173:SER:OG	2.03	0.58
1:A:333:ILE:HD13	2:B:223:ARG:HH22	1.69	0.57
2:D:253:ASP:OD2	2:D:256:HIS:HD2	1.86	0.57
2:B:381:ILE:HD12	2:B:381:ILE:N	2.19	0.57
1:C:213:PRO:HG3	1:C:334:ALA:HB2	1.85	0.57
1:C:445:VAL:HG12	1:C:446:SER:N	2.19	0.57
2:B:132:ASP:HA	2:B:157:MET:CE	2.34	0.57
1:C:110:GLU:CD	1:C:110:GLU:H	2.13	0.57
1:C:115:ASN:O	1:C:117:PRO:HD3	2.03	0.57
1:C:295:ILE:O	1:C:309:ARG:NH1	2.37	0.57
1:C:297:ILE:HD13	1:C:368:ILE:CD1	2.34	0.57
2:D:131:ASN:C	2:D:131:ASN:HD22	2.12	0.57
1:A:233:ILE:HD12	1:A:239:GLU:HB3	1.86	0.57
1:A:259:PRO:C	1:A:261:ASP:H	2.11	0.57
2:B:142:VAL:HG13	2:B:178:ILE:HB	1.85	0.57
2:B:201:GLU:HG2	2:B:345:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:VAL:HG21	1:C:349:LYS:HG2	1.85	0.57
1:C:329:ILE:HD11	1:C:346:TYR:CD1	2.38	0.57
1:C:337:GLY:O	1:C:341:LYS:HG3	2.05	0.57
1:A:143:LEU:HD12	1:A:150:LEU:HD22	1.86	0.57
1:A:371:ALA:HB3	1:A:374:SER:HB3	1.86	0.57
2:B:154:ILE:O	2:B:154:ILE:HD13	2.04	0.57
1:C:56:SER:HB3	1:C:101:SER:HB2	1.87	0.57
1:C:152:ILE:HD12	1:C:152:ILE:N	2.20	0.57
1:C:297:ILE:HD13	1:C:368:ILE:CG1	2.35	0.57
2:B:222:PRO:HB3	5:B:1041:HOH:O	2.05	0.57
1:C:163:ARG:NH2	1:C:396:ARG:O	2.37	0.57
1:C:158:LEU:HG	2:D:23:PHE:CE2	2.40	0.56
2:D:31:THR:HG21	2:D:35:PHE:CD1	2.40	0.56
1:A:407:ILE:HD12	5:A:592:HOH:O	2.05	0.56
2:B:83:ILE:HG22	2:B:99:ILE:HD13	1.88	0.56
2:D:284:VAL:O	2:D:287:ARG:HG2	2.05	0.56
1:A:285:ILE:CD1	1:A:285:ILE:N	2.68	0.56
2:B:265:LEU:HD23	2:B:276:VAL:HB	1.87	0.56
1:C:297:ILE:HD12	1:C:297:ILE:C	2.29	0.56
1:C:333:ILE:HD13	2:D:223:ARG:NH2	2.20	0.56
2:D:265:LEU:HD23	2:D:276:VAL:HB	1.87	0.56
1:A:276:LEU:O	1:A:277:ASN:C	2.48	0.56
1:C:307:LEU:HB3	1:C:383:LEU:HD22	1.87	0.56
1:C:340:ILE:HG22	1:C:344:ASN:HD21	1.70	0.56
1:A:295:ILE:HA	5:A:595:HOH:O	2.05	0.56
1:C:279:THR:HG22	1:C:322:ASN:ND2	2.20	0.56
1:C:439:GLN:HB3	1:C:441:ARG:HG2	1.87	0.56
2:D:253:ASP:CG	2:D:256:HIS:CD2	2.84	0.56
1:A:35:LEU:HB3	1:A:59:ILE:CD1	2.35	0.56
2:B:31:THR:CG2	2:B:35:PHE:HB3	2.33	0.56
1:C:232:ARG:O	1:C:233:ILE:HD13	2.05	0.56
1:C:438:GLN:HE21	1:C:439:GLN:HE22	1.52	0.56
2:B:80:MET:HG3	2:B:80:MET:O	2.05	0.56
1:C:45:ILE:CD1	1:C:498:GLY:HA2	2.36	0.56
1:C:112:LEU:HD13	1:C:119:PHE:HD2	1.71	0.56
2:D:241:GLN:HE21	2:D:245:GLU:C	2.14	0.56
2:D:42:LEU:HD11	2:D:46:LEU:HD21	1.88	0.56
2:B:136:ARG:HG3	2:B:161:LEU:HD22	1.86	0.56
1:C:115:ASN:C	1:C:117:PRO:HD3	2.31	0.56
1:C:329:ILE:HD11	1:C:346:TYR:CG	2.40	0.56
2:D:114:ARG:O	2:D:116:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ASN:ND2	1:C:86:ALA:HB3	2.21	0.56
2:B:54:ILE:CG2	2:B:145:LEU:HD11	2.36	0.55
1:A:214:TRP:CD1	1:A:267:GLU:HG2	2.40	0.55
1:A:84:ASN:HD22	1:A:87:GLU:H	1.54	0.55
2:B:141:ILE:CD1	2:B:158:LEU:HD21	2.36	0.55
2:D:303:CYS:O	2:D:307:VAL:HG23	2.06	0.55
1:C:143:LEU:CD1	1:C:150:LEU:HD22	2.28	0.55
1:A:447:ASN:ND2	2:B:26:ARG:NH2	2.47	0.55
2:D:164:TYR:CE2	2:D:169:LEU:HD13	2.41	0.55
1:C:403:GLY:HA3	1:C:406:THR:HG22	1.89	0.55
1:C:416:MET:HE2	1:C:472:VAL:CG1	2.37	0.55
2:B:169:LEU:O	2:B:171:PRO:HD3	2.06	0.55
2:D:31:THR:CG2	2:D:32:HIS:N	2.67	0.55
2:D:83:ILE:HD12	2:D:94:PHE:CD1	2.41	0.55
2:B:286:LYS:HB2	2:B:288:ILE:HG13	1.88	0.54
2:B:317:PRO:O	2:B:318:LEU:C	2.49	0.54
1:C:50:VAL:HG13	1:C:100:VAL:HG21	1.87	0.54
1:C:162:MET:HE3	1:C:516:PHE:CE2	2.42	0.54
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.90	0.54
1:A:415:SER:HB3	1:A:421:ASN:ND2	2.22	0.54
1:C:213:PRO:O	1:C:217:ILE:HD12	2.07	0.54
2:D:35:PHE:CD2	2:D:35:PHE:C	2.86	0.54
2:D:182:THR:HB	5:D:1035:HOH:O	2.06	0.54
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.37	0.54
1:C:112:LEU:HD13	1:C:119:PHE:CD2	2.42	0.54
1:C:527:GLN:HE21	1:C:527:GLN:HA	1.70	0.54
2:D:382:THR:O	2:D:900:LEU:HA	2.08	0.54
1:A:503:GLN:HA	1:A:503:GLN:HE21	1.72	0.54
2:B:190:ARG:HG3	2:B:192:ILE:CD1	2.37	0.54
1:A:84:ASN:ND2	1:A:106:GLU:HG2	2.23	0.54
1:A:329:ILE:N	1:A:329:ILE:HD13	2.22	0.54
2:D:21:LYS:HD3	2:D:25:GLU:CD	2.33	0.54
1:C:184:ARG:NE	1:C:325:VAL:HG12	2.23	0.54
1:C:213:PRO:HG3	1:C:334:ALA:CB	2.38	0.54
2:B:362:GLN:HG2	2:B:366:ASP:OD1	2.08	0.54
1:C:37:ASN:O	1:C:39:THR:N	2.33	0.54
1:C:130:GLN:HE22	1:C:155:THR:N	2.01	0.54
2:D:381:ILE:O	2:D:603:THR:HA	2.07	0.54
1:A:503:GLN:HA	1:A:503:GLN:NE2	2.23	0.54
2:B:136:ARG:CG	2:B:161:LEU:HD22	2.38	0.54
1:C:370:GLN:O	1:C:371:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:HD12	1:A:297:ILE:N	2.23	0.53
1:C:488:ALA:C	1:C:490:PRO:HD3	2.32	0.53
2:D:362:GLN:NE2	2:D:365:LEU:HB3	2.23	0.53
2:D:606:LEU:O	2:D:607:GLN:C	2.51	0.53
1:A:36:ILE:O	1:A:37:ASN:HB2	2.08	0.53
1:A:434:ARG:NH1	1:A:463:GLY:CA	2.67	0.53
2:D:209:PRO:HG3	2:D:375:GLN:OE1	2.08	0.53
2:B:54:ILE:HD11	2:B:141:ILE:HG23	1.89	0.53
1:C:43:THR:HG21	1:C:73:ASN:HD21	1.72	0.53
1:C:76:LEU:HD21	1:C:89:ALA:HB2	1.91	0.53
1:C:87:GLU:HG3	1:C:88:ALA:N	2.22	0.53
1:C:157:GLY:HA3	1:C:485:TYR:CG	2.43	0.53
1:C:297:ILE:HD13	1:C:368:ILE:HG12	1.90	0.53
2:D:68:ALA:HB1	2:D:115:VAL:HG11	1.90	0.53
1:C:181:GLU:CD	1:C:330:PRO:HG3	2.34	0.53
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.91	0.53
1:A:331:ASP:OD1	2:B:223:ARG:HD2	2.07	0.53
2:B:224:LEU:H	2:B:227:HIS:CD2	2.26	0.53
1:A:371:ALA:HB1	1:A:372:PRO:HD2	1.91	0.53
2:D:283:GLY:O	2:D:287:ARG:HA	2.09	0.53
2:D:182:THR:HG22	2:D:183:GLU:N	2.22	0.53
1:A:340:ILE:HD11	2:B:273:ILE:HD13	1.90	0.53
2:B:709:ARG:O	2:B:750:LEU:N	2.42	0.53
1:C:36:ILE:HG21	1:C:131:LEU:HD21	1.91	0.53
1:C:218:ILE:HD11	1:C:268:ALA:O	2.08	0.53
1:C:240:LYS:O	1:C:244:ARG:HG3	2.09	0.53
1:A:372:PRO:HG2	1:A:373:GLU:H	1.74	0.52
1:C:84:ASN:ND2	1:C:106:GLU:HG2	2.23	0.52
1:A:151:LEU:HD13	1:A:164:ILE:HD13	1.92	0.52
2:B:325:ASN:ND2	2:B:327:VAL:H	2.06	0.52
2:D:249:LEU:HD21	2:D:260:ILE:HD11	1.88	0.52
1:C:175:HIS:N	1:C:176:PRO:HD3	2.24	0.52
2:D:224:LEU:H	2:D:227:HIS:HD2	1.57	0.52
1:A:235:LYS:O	1:A:240:LYS:HG3	2.09	0.52
1:A:329:ILE:HD13	5:A:559:HOH:O	2.09	0.52
2:D:201:GLU:HB3	2:D:343:CYS:SG	2.50	0.52
2:D:253:ASP:CG	2:D:256:HIS:CB	2.77	0.52
2:B:117:ASN:ND2	5:B:1058:HOH:O	2.41	0.52
2:D:178:ILE:N	2:D:178:ILE:HD12	2.25	0.52
2:D:260:ILE:H	2:D:260:ILE:CD1	2.22	0.52
1:A:297:ILE:CG2	1:A:298:THR:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:LEU:H	2:D:197:THR:HG1	1.55	0.52
1:C:10:GLU:CG	2:D:279:ARG:HH12	2.23	0.52
1:C:460:CYS:HA	5:C:573:HOH:O	2.09	0.52
1:A:51:LEU:HB3	2:B:89:ASN:O	2.10	0.52
1:A:243:PHE:HD2	1:A:272:VAL:HG21	1.75	0.52
1:A:467:GLU:HB2	5:A:584:HOH:O	2.10	0.52
1:C:396:ARG:NH2	1:C:406:THR:O	2.38	0.52
2:D:24:LEU:HD21	2:D:312:THR:HG21	1.92	0.52
2:D:199:CYS:H	2:D:202:CYS:HB2	1.75	0.52
1:A:31:ALA:CB	1:A:509:ILE:HD12	2.40	0.51
1:A:265:PHE:O	1:A:268:ALA:HB3	2.10	0.51
2:B:376:MET:HB3	2:B:379:PRO:HG3	1.92	0.51
1:C:447:ASN:O	1:C:448:TYR:C	2.53	0.51
1:A:87:GLU:O	1:A:91:GLU:HG3	2.10	0.51
1:A:339:TYR:CD2	2:B:223:ARG:HB3	2.44	0.51
2:B:218:ILE:HD12	2:B:230:GLU:HB3	1.92	0.51
1:C:484:ARG:O	1:C:486:GLY:N	2.43	0.51
2:D:21:LYS:HD3	2:D:25:GLU:OE1	2.10	0.51
1:A:54:ILE:O	1:A:100:VAL:HG22	2.09	0.51
1:A:95:GLU:HB3	2:B:95:ARG:CZ	2.41	0.51
2:B:351:GLN:HB3	2:B:1007:PHE:CB	2.40	0.51
2:D:237:TRP:CE2	2:D:249:LEU:HB2	2.46	0.51
1:A:370:GLN:O	1:A:371:ALA:HB2	2.11	0.51
1:C:252:LEU:HD23	1:C:252:LEU:H	1.74	0.51
2:B:165:GLU:O	2:B:166:ASP:HB2	2.10	0.51
2:B:274:ARG:HD2	5:B:1107:HOH:O	2.10	0.51
2:D:225:PRO:HG3	2:D:274:ARG:O	2.11	0.51
2:B:751:SER:O	2:B:752:LYS:C	2.53	0.51
2:D:52:LEU:HD11	2:D:78:ILE:HG12	1.92	0.51
2:D:380:ALA:O	2:D:901:ALA:O	2.29	0.51
1:A:95:GLU:HB3	2:B:95:ARG:NH2	2.26	0.51
2:B:305:THR:HG22	2:B:309:LYS:HE3	1.92	0.51
1:C:41:THR:O	1:C:45:ILE:CD1	2.54	0.51
1:C:189:PHE:CE1	1:C:191:GLU:HB2	2.46	0.51
2:B:378:SER:N	2:B:379:PRO:HD3	2.25	0.51
2:D:249:LEU:CD1	2:D:256:HIS:CB	2.74	0.51
1:A:284:SER:OG	1:A:285:ILE:HD12	2.12	0.50
2:D:44:PHE:CD1	2:D:48:THR:HB	2.47	0.50
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.46	0.50
1:A:333:ILE:CD1	2:B:223:ARG:HH22	2.24	0.50
2:B:325:ASN:HD22	2:B:327:VAL:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:PHE:CE2	3:F:9:GLN:HG2	2.46	0.50
2:D:164:TYR:CE2	2:D:348:GLN:NE2	2.79	0.50
1:C:227:SER:O	1:C:229:THR:N	2.44	0.50
1:C:485:TYR:C	1:C:487:ALA:H	2.19	0.50
1:C:272:VAL:O	1:C:276:LEU:HG	2.11	0.50
1:A:377:GLU:O	1:A:381:LYS:HG3	2.12	0.50
1:C:172:ILE:N	1:C:172:ILE:HD12	2.26	0.50
1:C:408:ASN:O	1:C:412:ILE:HD13	2.12	0.50
2:D:132:ASP:OD1	2:D:133:THR:N	2.45	0.50
1:A:199:TYR:OH	1:A:338:LYS:HD3	2.11	0.50
1:A:251:ILE:O	1:A:252:LEU:HB2	2.11	0.50
1:A:317:LYS:HD2	1:A:360:HIS:CE1	2.46	0.50
1:A:518:ASN:HD21	1:A:534:LEU:HB2	1.77	0.50
1:C:213:PRO:O	1:C:217:ILE:CD1	2.59	0.50
1:C:335:ASP:O	2:D:221:MET:HB3	2.11	0.50
1:C:470:LEU:C	1:C:472:VAL:H	2.20	0.50
2:D:249:LEU:CD2	2:D:260:ILE:CD1	2.89	0.50
1:A:66:SER:O	1:A:69:ASP:HB2	2.11	0.50
1:A:278:THR:HG22	1:A:279:THR:H	1.76	0.50
1:C:439:GLN:O	1:C:441:ARG:HG2	2.11	0.50
2:D:21:LYS:HE2	2:D:42:LEU:HD22	1.92	0.50
2:D:383:ALA:O	2:D:384:THR:C	2.55	0.50
1:A:192:LEU:HG	1:A:196:PHE:CE1	2.47	0.49
1:A:374:SER:O	1:A:375:ILE:HD13	2.12	0.49
2:B:322:LEU:C	2:B:322:LEU:HD23	2.37	0.49
2:D:257:ILE:C	2:D:260:ILE:HG12	2.37	0.49
2:D:257:ILE:O	2:D:260:ILE:HG12	2.12	0.49
1:A:329:ILE:HD13	1:A:329:ILE:H	1.77	0.49
1:C:215:ILE:H	1:C:332:MET:CE	2.25	0.49
1:A:243:PHE:HD2	1:A:272:VAL:CG2	2.25	0.49
1:A:275:ALA:C	1:A:277:ASN:N	2.68	0.49
1:A:473:MET:HE1	1:A:475:LYS:HG2	1.93	0.49
2:B:54:ILE:CD1	2:B:141:ILE:HG23	2.42	0.49
1:A:317:LYS:HD2	1:A:360:HIS:HE1	1.77	0.49
1:A:252:LEU:HB2	1:A:259:PRO:HD2	1.94	0.49
2:D:365:LEU:O	2:D:369:THR:HB	2.13	0.49
1:A:35:LEU:HD23	1:A:59:ILE:CD1	2.35	0.49
2:D:263:LYS:O	2:D:266:GLU:HB3	2.12	0.49
1:A:430:ARG:NH1	1:A:464:PHE:HE1	2.11	0.49
1:C:217:ILE:HD12	1:C:217:ILE:N	2.26	0.49
2:D:253:ASP:CG	2:D:256:HIS:HD2	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:LYS:HB2	5:B:1095:HOH:O	2.13	0.49
1:C:196:PHE:O	1:C:198:SER:N	2.44	0.49
1:C:325:VAL:CG2	1:C:349:LYS:HG2	2.43	0.49
1:C:485:TYR:O	1:C:487:ALA:N	2.39	0.49
1:A:235:LYS:O	1:A:240:LYS:N	2.45	0.49
2:B:81:ASP:HB2	2:B:103:LYS:HD2	1.94	0.48
2:B:139:HIS:HB3	2:B:140:ILE:HD12	1.95	0.48
1:C:215:ILE:HG13	1:C:332:MET:CE	2.28	0.48
2:D:204:LEU:C	2:D:206:LEU:H	2.21	0.48
1:A:488:ALA:C	1:A:490:PRO:HD3	2.38	0.48
1:A:518:ASN:CG	1:A:519:THR:N	2.60	0.48
2:B:128:GLN:NE2	2:B:128:GLN:N	2.47	0.48
2:D:139:HIS:O	2:D:176:PRO:HD2	2.13	0.48
1:C:314:PHE:HZ	1:C:353:ASP:OD2	1.96	0.48
1:C:435:PHE:CG	1:C:443:PRO:HG3	2.47	0.48
2:D:709:ARG:O	2:D:710:PRO:CB	2.60	0.48
1:C:416:MET:SD	1:C:424:VAL:HG22	2.54	0.48
1:C:222:LEU:HA	1:C:243:PHE:CE1	2.48	0.48
1:A:84:ASN:CG	1:A:106:GLU:HG2	2.38	0.48
1:A:238:LYS:O	1:A:238:LYS:CD	2.62	0.48
1:A:241:GLU:OE1	1:A:244:ARG:HD2	2.14	0.48
2:B:361:LEU:HB3	2:B:750:LEU:CA	2.43	0.48
1:C:36:ILE:O	1:C:37:ASN:HB2	2.14	0.48
1:C:309:ARG:HB3	1:C:364:LEU:HD21	1.96	0.48
2:D:318:LEU:HD11	2:D:334:THR:CG2	2.43	0.48
1:C:446:SER:HB3	1:C:448:TYR:CE2	2.49	0.48
2:D:62:GLU:HG3	5:D:1020:HOH:O	2.14	0.48
1:C:214:TRP:HB2	1:C:268:ALA:HA	1.96	0.48
1:C:343:GLN:HE22	2:D:224:LEU:CD2	2.27	0.48
1:A:189:PHE:CD1	1:A:192:LEU:HB2	2.49	0.48
2:B:378:SER:O	2:B:378:SER:OG	2.28	0.48
2:D:90:ARG:NH1	2:D:91:GLN:HE21	2.11	0.48
1:A:486:GLY:HA3	2:B:22:LYS:HZ3	1.79	0.48
2:B:38:SER:OG	2:B:40:GLU:HG3	2.14	0.47
2:D:148:ILE:O	2:D:152:ARG:HG3	2.14	0.47
1:C:235:LYS:O	1:C:240:LYS:HE2	2.14	0.47
1:C:391:ARG:NH2	2:D:328:ASP:OD1	2.47	0.47
2:D:317:PRO:O	2:D:318:LEU:C	2.57	0.47
2:B:83:ILE:HD11	2:B:106:VAL:HG21	1.96	0.47
2:B:140:ILE:HD11	3:E:7:LEU:HD22	1.95	0.47
1:C:281:ILE:HD11	1:C:322:ASN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:ARG:HG2	1:C:434:ARG:NH1	2.23	0.47
1:C:447:ASN:O	1:C:449:GLN:N	2.47	0.47
2:B:229:ILE:HD13	2:B:281:THR:HA	1.97	0.47
1:C:189:PHE:CD2	1:C:349:LYS:HD3	2.50	0.47
1:C:218:ILE:HD12	1:C:272:VAL:HG22	1.95	0.47
2:D:276:VAL:HA	2:D:280:LEU:HD23	1.95	0.47
1:A:306:ILE:CD1	1:A:370:GLN:HE22	2.24	0.47
1:A:518:ASN:ND2	1:A:533:GLN:HA	2.19	0.47
2:B:94:PHE:CZ	2:B:103:LYS:HB3	2.49	0.47
2:D:241:GLN:O	2:D:242:PRO:C	2.56	0.47
3:F:10:GLN:HG2	3:F:11:LYS:N	2.29	0.47
2:B:365:LEU:C	2:B:365:LEU:HD23	2.40	0.47
1:C:150:LEU:HG	1:C:152:ILE:HD11	1.97	0.47
1:C:182:ASP:C	1:C:183:LEU:O	2.53	0.47
1:C:236:THR:HB	1:C:239:GLU:HG3	1.96	0.47
2:D:253:ASP:O	2:D:257:ILE:N	2.48	0.47
2:B:52:LEU:HG	2:B:54:ILE:CD1	2.45	0.47
2:B:158:LEU:HD12	2:B:177:LEU:HB2	1.97	0.47
2:B:383:ALA:O	2:B:601:ASN:N	2.48	0.47
1:A:376:SER:OG	1:A:378:LYS:HG2	2.15	0.47
1:A:434:ARG:NH2	5:A:584:HOH:O	2.48	0.47
1:C:115:ASN:HB2	5:C:576:HOH:O	2.15	0.47
1:C:332:MET:C	2:D:223:ARG:NH1	2.73	0.47
1:C:113:LEU:O	1:C:117:PRO:HG3	2.14	0.47
2:D:26:ARG:O	2:D:35:PHE:CZ	2.68	0.47
1:C:236:THR:HB	1:C:239:GLU:OE1	2.15	0.46
2:D:230:GLU:O	2:D:231:TYR:C	2.58	0.46
2:D:240:GLU:C	2:D:242:PRO:HD3	2.40	0.46
1:C:33:VAL:HG22	1:C:34:CYS:N	2.30	0.46
1:C:109:PRO:HB2	1:C:110:GLU:OE2	2.15	0.46
1:C:311:LEU:O	1:C:315:VAL:HG23	2.16	0.46
1:A:349:LYS:HE3	1:A:353:ASP:OD2	2.15	0.46
1:A:362:ALA:O	1:A:366:GLN:HG3	2.15	0.46
1:C:152:ILE:HD12	1:C:152:ILE:H	1.80	0.46
2:D:343:CYS:HA	2:D:344:PRO:HD3	1.75	0.46
1:A:115:ASN:C	1:A:117:PRO:HD3	2.40	0.46
1:A:215:ILE:HG13	1:A:332:MET:HE1	1.98	0.46
1:A:238:LYS:HD3	1:A:238:LYS:HA	1.35	0.46
1:A:293:ARG:HG3	5:A:611:HOH:O	2.15	0.46
1:A:428:MET:HE2	1:A:479:VAL:HA	1.96	0.46
2:B:52:LEU:HG	2:B:54:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.97	0.46
2:B:361:LEU:C	2:B:363:GLU:N	2.72	0.46
1:C:36:ILE:N	1:C:36:ILE:HD12	2.31	0.46
1:C:307:LEU:HB3	1:C:383:LEU:CD2	2.46	0.46
1:C:339:TYR:CE2	2:D:224:LEU:HD21	2.42	0.46
1:C:510:THR:O	1:C:511:LYS:HB2	2.14	0.46
2:D:353:ILE:CG2	2:D:354:GLN:H	2.20	0.46
2:D:900:LEU:N	2:D:1008:LYS:O	2.49	0.46
1:A:75:PHE:CE2	1:A:96:LEU:HD11	2.50	0.46
1:C:329:ILE:HG22	1:C:330:PRO:N	2.31	0.46
2:D:353:ILE:H	2:D:353:ILE:CD1	2.06	0.46
1:A:422:GLU:CD	1:A:422:GLU:H	2.24	0.46
1:C:190:PRO:O	1:C:194:GLU:HG2	2.15	0.46
1:A:235:LYS:HB3	1:A:238:LYS:HB3	1.98	0.46
1:A:430:ARG:NH1	1:A:464:PHE:CE1	2.84	0.46
2:B:376:MET:CB	2:B:379:PRO:HG3	2.45	0.46
2:B:382:THR:HG23	2:B:603:THR:HA	1.97	0.46
1:C:347:ARG:HH12	2:D:274:ARG:CG	2.29	0.46
1:C:407:ILE:HG23	1:C:409:LYS:HG3	1.98	0.46
2:D:224:LEU:N	2:D:227:HIS:HD2	2.14	0.46
2:D:283:GLY:O	2:D:287:ARG:CA	2.63	0.46
2:D:362:GLN:HE22	2:D:365:LEU:HB3	1.80	0.46
1:A:58:THR:HA	1:A:103:SER:O	2.16	0.46
2:B:319:ASN:O	2:B:320:ASN:HB3	2.16	0.46
1:C:162:MET:HG2	1:C:516:PHE:CZ	2.51	0.46
1:C:184:ARG:O	1:C:185:LEU:C	2.58	0.46
1:C:319:GLY:O	1:C:320:GLN:HB2	2.16	0.46
2:D:271:TYR:O	2:D:272:ASN:CB	2.64	0.46
1:A:236:THR:O	1:A:240:LYS:CA	2.64	0.46
2:B:223:ARG:H	2:B:227:HIS:CD2	2.16	0.46
1:C:12:LYS:NZ	1:C:97:ASN:HD21	2.14	0.46
1:C:19:LEU:HD12	2:D:292:VAL:HG13	1.98	0.46
1:C:189:PHE:HE1	1:C:191:GLU:HB2	1.81	0.46
1:C:396:ARG:NH1	1:C:534:LEU:OXT	2.49	0.46
1:C:486:GLY:CA	2:D:22:LYS:HZ2	2.29	0.46
1:A:28:LEU:HA	1:A:509:ILE:HG21	1.98	0.45
1:A:313:GLU:HB3	1:A:360:HIS:CE1	2.51	0.45
1:A:422:GLU:HG2	1:A:530:ALA:HB3	1.98	0.45
2:B:62:GLU:HG3	5:B:1016:HOH:O	2.16	0.45
1:C:218:ILE:O	1:C:222:LEU:HB2	2.16	0.45
1:C:221:TYR:OH	1:C:250:GLY:HA3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ILE:HD12	1:C:329:ILE:N	2.30	0.45
1:A:124:THR:HG21	1:A:509:ILE:CD1	2.47	0.45
1:A:297:ILE:HG22	1:A:298:THR:H	1.79	0.45
2:B:54:ILE:N	2:B:54:ILE:CD1	2.79	0.45
2:B:193:LEU:HB2	2:B:197:THR:HG23	1.98	0.45
1:C:144:TRP:CH2	1:C:167:LYS:HG3	2.52	0.45
1:C:194:GLU:O	1:C:195:HIS:C	2.58	0.45
1:A:8:LEU:HD23	1:A:8:LEU:O	2.17	0.45
1:A:113:LEU:HD13	1:A:138:ARG:HG2	1.99	0.45
1:A:318:GLU:CD	1:A:318:GLU:H	2.24	0.45
2:B:325:ASN:HD22	2:B:325:ASN:C	2.23	0.45
2:B:353:ILE:N	2:B:1008:LYS:O	2.49	0.45
1:C:67:GLY:HA2	1:C:78:ARG:HH12	1.82	0.45
1:C:75:PHE:O	1:C:76:LEU:HD23	2.16	0.45
1:C:169:HIS:CD2	1:C:515:ILE:HD12	2.51	0.45
2:B:90:ARG:HH11	2:B:90:ARG:HG2	1.80	0.45
2:B:237:TRP:CE3	2:B:260:ILE:HD11	2.51	0.45
2:B:361:LEU:O	2:B:364:VAL:HG22	2.17	0.45
2:B:804:GLY:O	2:B:805:GLN:C	2.60	0.45
1:A:286:GLU:OE1	1:A:286:GLU:HA	2.16	0.45
1:A:373:GLU:C	1:A:375:ILE:H	2.23	0.45
1:A:418:ASN:C	1:A:418:ASN:HD22	2.23	0.45
2:B:242:PRO:HB2	2:B:243:PHE:HD1	1.81	0.45
2:B:343:CYS:HA	2:B:344:PRO:HD3	1.77	0.45
1:C:144:TRP:CZ2	1:C:167:LYS:HE2	2.51	0.45
1:C:229:THR:HG22	1:C:230:ASN:N	2.32	0.45
1:A:265:PHE:O	1:A:269:ILE:HG13	2.16	0.45
1:A:315:VAL:HG13	1:A:321:GLY:C	2.41	0.45
2:B:102:PRO:O	2:B:106:VAL:HG23	2.16	0.45
1:C:333:ILE:HD13	2:D:223:ARG:HH22	1.81	0.45
2:D:39:THR:C	2:D:41:SER:H	2.25	0.45
1:A:454:ILE:HD11	1:A:480:HIS:HA	1.95	0.45
1:A:512:GLN:O	1:A:513:PHE:HB2	2.16	0.45
1:C:151:LEU:HD13	1:C:164:ILE:HD13	1.98	0.45
2:D:126:LYS:NZ	2:D:128:GLN:HG2	2.32	0.45
2:D:241:GLN:NE2	2:D:245:GLU:C	2.74	0.45
2:D:904:ASP:C	2:D:1000:THR:H	2.25	0.45
1:A:235:LYS:O	1:A:236:THR:O	2.35	0.45
1:A:313:GLU:HB3	1:A:360:HIS:ND1	2.32	0.45
1:A:435:PHE:C	1:A:435:PHE:CD2	2.95	0.45
2:B:32:HIS:HB3	2:B:313:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:OD2	1:A:85:ARG:HD2	2.17	0.44
1:C:407:ILE:HD12	1:C:468:TYR:CD2	2.53	0.44
1:C:445:VAL:N	1:C:449:GLN:OE1	2.49	0.44
2:D:202:CYS:O	2:D:340:LYS:HE3	2.17	0.44
1:A:146:SER:O	1:A:147:GLN:HB2	2.17	0.44
1:A:278:THR:CG2	1:A:279:THR:N	2.79	0.44
1:A:458:LYS:HD3	1:A:458:LYS:C	2.41	0.44
2:B:368:LEU:O	2:B:376:MET:HB2	2.17	0.44
2:D:209:PRO:CG	2:D:375:GLN:OE1	2.64	0.44
1:C:397:SER:OG	1:C:400:GLU:HG3	2.17	0.44
1:A:221:TYR:CD1	1:A:247:ILE:HG13	2.53	0.44
1:A:340:ILE:CD1	2:B:273:ILE:HD13	2.47	0.44
2:B:190:ARG:HG3	2:B:192:ILE:HD11	2.00	0.44
1:C:33:VAL:O	1:C:57:PHE:HA	2.18	0.44
1:C:139:LEU:O	1:C:143:LEU:HG	2.18	0.44
1:C:164:ILE:O	1:C:164:ILE:HG23	2.18	0.44
2:D:141:ILE:CD1	2:D:158:LEU:HD21	2.47	0.44
2:B:331:TYR:CD1	2:B:331:TYR:C	2.94	0.44
1:C:50:VAL:O	1:C:53:GLY:N	2.49	0.44
1:C:78:ARG:HA	1:C:81:ILE:CD1	2.48	0.44
1:C:113:LEU:HD22	1:C:142:VAL:HG21	1.98	0.44
1:C:166:ILE:HG21	1:C:169:HIS:HB2	1.99	0.44
2:D:83:ILE:CD1	2:D:94:PHE:CE1	3.00	0.44
1:A:317:LYS:HB2	1:A:318:GLU:OE2	2.18	0.44
2:D:83:ILE:CD1	2:D:103:LYS:HA	2.39	0.44
2:D:126:LYS:HZ3	2:D:128:GLN:HG2	1.83	0.44
2:D:369:THR:HG23	2:D:376:MET:O	2.18	0.44
1:A:297:ILE:O	1:A:298:THR:HG22	2.18	0.44
1:A:341:LYS:O	1:A:345:VAL:HG23	2.18	0.44
1:A:350:ALA:HB1	5:A:581:HOH:O	2.18	0.44
1:A:508:ILE:HD13	1:A:515:ILE:HG21	2.00	0.44
1:C:299:LYS:HA	1:C:368:ILE:CG2	2.47	0.44
1:C:326:ARG:HH21	1:C:388:ALA:HB3	1.83	0.44
1:A:518:ASN:CB	1:A:533:GLN:HA	2.47	0.44
2:B:190:ARG:NE	2:B:192:ILE:HD11	2.32	0.44
2:B:383:ALA:O	2:B:384:THR:C	2.60	0.44
1:A:486:GLY:O	2:B:22:LYS:NZ	2.51	0.43
1:C:236:THR:HB	1:C:239:GLU:CD	2.42	0.43
1:A:235:LYS:HG3	1:A:239:GLU:OE2	2.17	0.43
1:A:236:THR:CA	1:A:240:LYS:CD	2.88	0.43
2:B:54:ILE:HG22	2:B:145:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:GLU:OE1	2:B:204:LEU:HD11	2.18	0.43
1:C:12:LYS:O	2:D:89:ASN:HB3	2.18	0.43
1:C:305:TRP:HA	1:C:308:ALA:HB3	1.99	0.43
1:C:517:ASN:HD22	1:C:533:GLN:HG2	1.83	0.43
2:D:42:LEU:CG	2:D:46:LEU:HD11	2.43	0.43
2:D:701:VAL:C	2:D:703:SER:N	2.67	0.43
1:A:297:ILE:CG2	1:A:298:THR:H	2.31	0.43
2:B:54:ILE:HG22	2:B:145:LEU:CG	2.48	0.43
2:B:80:MET:HA	2:B:80:MET:HE3	2.00	0.43
1:C:194:GLU:O	1:C:196:PHE:N	2.51	0.43
2:D:26:ARG:O	2:D:35:PHE:HZ	2.01	0.43
1:A:35:LEU:HB3	1:A:59:ILE:HD13	2.00	0.43
1:A:446:SER:C	1:A:448:TYR:N	2.75	0.43
2:B:381:ILE:HD12	2:B:381:ILE:H	1.82	0.43
1:C:65:VAL:HB	1:C:81:ILE:HA	2.00	0.43
1:C:109:PRO:O	1:C:113:LEU:HG	2.18	0.43
2:D:204:LEU:CD1	2:D:373:SER:C	2.91	0.43
1:A:165:ILE:C	1:A:166:ILE:HG13	2.43	0.43
1:A:504:GLU:O	1:A:508:ILE:HG12	2.18	0.43
2:D:333:TYR:CE2	2:D:335:PHE:HB3	2.54	0.43
1:A:309:ARG:HG3	1:A:364:LEU:HD11	2.01	0.43
1:C:181:GLU:HG3	1:C:330:PRO:HG2	1.99	0.43
2:D:31:THR:HG22	2:D:32:HIS:H	1.82	0.43
2:D:227:HIS:O	2:D:228:CYS:C	2.62	0.43
2:D:607:GLN:O	2:D:701:VAL:CB	2.67	0.43
1:A:308:ALA:O	1:A:311:LEU:HB2	2.19	0.43
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.92	0.43
2:B:11:LEU:HD22	2:B:117:ASN:OD1	2.19	0.43
1:C:152:ILE:HD11	1:C:165:ILE:HD12	2.00	0.43
1:C:396:ARG:HD3	1:C:534:LEU:O	2.19	0.43
1:C:436:HIS:HA	1:C:441:ARG:O	2.19	0.43
1:A:176:PRO:HG3	1:A:389:PHE:CD1	2.54	0.43
1:A:212:THR:H	1:A:264:ASN:HD21	1.66	0.43
1:A:378:LYS:HA	1:A:381:LYS:NZ	2.34	0.43
1:A:259:PRO:CB	1:A:261:ASP:OD2	2.67	0.43
1:A:274:THR:C	1:A:277:ASN:ND2	2.75	0.43
1:A:353:ASP:O	1:A:357:VAL:HG23	2.18	0.43
1:A:365:LEU:O	1:A:369:GLY:N	2.51	0.43
1:A:414:SER:O	1:A:417:ASP:HB2	2.18	0.43
2:B:217:THR:OG1	2:B:223:ARG:NH2	2.49	0.43
1:C:454:ILE:HG13	1:C:455:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:TYR:C	1:C:487:ALA:N	2.77	0.43
2:D:82:THR:HA	2:D:101:ARG:O	2.19	0.43
1:A:75:PHE:O	1:A:76:LEU:HD23	2.18	0.42
2:B:235:LEU:C	2:B:238:PRO:HD2	2.44	0.42
1:C:65:VAL:HG13	1:C:69:ASP:CB	2.49	0.42
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.49	0.42
1:C:128:ALA:HB1	1:C:131:LEU:CD1	2.50	0.42
1:A:341:LYS:HB2	5:A:587:HOH:O	2.18	0.42
1:A:518:ASN:ND2	1:A:533:GLN:CA	2.70	0.42
2:B:58:GLY:HA3	5:B:1063:HOH:O	2.18	0.42
2:B:139:HIS:C	2:B:140:ILE:HD12	2.44	0.42
2:B:259:TRP:HE3	2:B:260:ILE:HD13	1.85	0.42
1:C:186:ASP:OD2	1:C:279:THR:CB	2.68	0.42
1:C:407:ILE:HG12	1:C:408:ASN:N	2.34	0.42
1:A:129:THR:HA	1:A:153:CYS:O	2.20	0.42
1:A:186:ASP:C	1:A:188:PRO:HD3	2.45	0.42
1:A:225:TRP:CE2	1:A:233:ILE:CD1	2.98	0.42
1:A:434:ARG:NH1	1:A:463:GLY:C	2.77	0.42
2:B:218:ILE:HD13	2:B:218:ILE:HA	1.89	0.42
1:C:69:ASP:OD2	1:C:85:ARG:NE	2.52	0.42
1:A:176:PRO:HG3	1:A:389:PHE:CG	2.54	0.42
1:A:398:LEU:HD12	1:A:398:LEU:HA	1.90	0.42
2:B:10:LYS:CD	2:B:11:LEU:H	2.33	0.42
2:B:31:THR:HG21	2:B:35:PHE:HD2	1.84	0.42
1:C:344:ASN:HA	1:C:347:ARG:HD2	2.00	0.42
2:D:201:GLU:HA	2:D:204:LEU:HD23	1.99	0.42
1:A:185:LEU:HD11	1:A:215:ILE:CD1	2.49	0.42
2:B:145:LEU:CD1	2:B:150:ALA:HB1	2.50	0.42
1:C:435:PHE:CD1	1:C:443:PRO:HG3	2.55	0.42
2:D:253:ASP:O	2:D:254:PRO:C	2.62	0.42
1:A:10:GLU:OE2	2:B:279:ARG:NH2	2.33	0.42
1:A:165:ILE:HG21	5:A:544:HOH:O	2.20	0.42
1:A:328:THR:HA	5:A:559:HOH:O	2.20	0.42
1:C:212:THR:HA	1:C:213:PRO:HD3	1.87	0.42
1:C:448:TYR:CD2	1:C:448:TYR:N	2.88	0.42
2:D:201:GLU:OE1	2:D:204:LEU:HD21	2.19	0.42
2:D:201:GLU:OE1	2:D:204:LEU:CD2	2.68	0.42
2:D:284:VAL:HG12	2:D:287:ARG:HH12	1.85	0.42
1:A:190:PRO:O	1:A:194:GLU:HG3	2.20	0.42
1:A:236:THR:O	1:A:240:LYS:N	2.52	0.42
1:A:261:ASP:O	1:A:264:ASN:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ASN:ND2	1:A:418:ASN:C	2.76	0.42
2:B:81:ASP:O	2:B:103:LYS:HG3	2.19	0.42
2:B:190:ARG:HB2	2:B:320:ASN:O	2.20	0.42
1:C:87:GLU:HB3	1:C:104:PHE:CD1	2.54	0.42
2:D:45:LEU:HD12	2:D:45:LEU:HA	1.79	0.42
1:A:276:LEU:O	1:A:277:ASN:O	2.37	0.42
1:A:366:GLN:C	1:A:368:ILE:N	2.75	0.42
2:D:228:CYS:SG	2:D:273:ILE:HD12	2.60	0.42
2:D:365:LEU:O	2:D:369:THR:CB	2.67	0.42
1:A:526:SER:O	1:A:528:THR:HG23	2.20	0.42
1:C:285:ILE:HA	1:C:288:ILE:HD12	2.01	0.42
2:D:36:GLU:HA	2:D:37:PRO:HD3	1.66	0.42
2:D:85:VAL:C	2:D:87:ASN:H	2.28	0.42
2:D:361:LEU:HG	2:D:710:PRO:C	2.44	0.42
2:B:33:PRO:HD2	3:E:4:LEU:HD21	2.02	0.41
2:B:165:GLU:O	2:B:166:ASP:CB	2.67	0.41
1:C:12:LYS:HZ3	1:C:97:ASN:HD21	1.67	0.41
1:C:45:ILE:HG13	1:C:501:ALA:HB3	2.02	0.41
1:C:64:GLN:HA	1:C:83:LYS:O	2.19	0.41
1:C:486:GLY:HA3	2:D:22:LYS:HZ2	1.81	0.41
2:D:151:ARG:HB3	2:D:200:ILE:HD13	2.01	0.41
2:D:322:LEU:HD23	2:D:322:LEU:C	2.45	0.41
2:B:83:ILE:CD1	2:B:106:VAL:HG21	2.50	0.41
2:B:382:THR:HG23	2:B:602:ARG:C	2.45	0.41
1:C:150:LEU:HD12	1:C:151:LEU:H	1.84	0.41
1:C:453:ASP:HA	1:C:456:LYS:HB3	2.02	0.41
1:A:26:GLU:OE2	1:A:26:GLU:HA	2.20	0.41
1:A:177:ASP:O	1:A:178:ASN:C	2.63	0.41
2:B:50:LYS:HD3	2:B:137:GLN:HE21	1.86	0.41
2:B:141:ILE:HD12	2:B:158:LEU:CD2	2.49	0.41
2:D:80:MET:HG3	2:D:80:MET:O	2.20	0.41
1:A:301:THR:HA	1:A:302:PRO:HD3	1.92	0.41
2:B:176:PRO:HG2	2:B:310:ILE:HG21	2.03	0.41
2:B:325:ASN:HD22	2:B:326:ASP:N	2.18	0.41
2:D:253:ASP:OD2	2:D:256:HIS:CG	2.71	0.41
2:D:311:ALA:HA	3:F:7:LEU:HD23	2.03	0.41
1:A:297:ILE:HD12	1:A:297:ILE:H	1.85	0.41
1:A:297:ILE:C	1:A:298:THR:CG2	2.94	0.41
2:B:140:ILE:HD11	3:E:7:LEU:CD2	2.50	0.41
1:A:473:MET:C	1:A:473:MET:SD	3.04	0.41
1:C:160:GLY:O	1:C:521:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ASN:ND2	1:C:265:PHE:HD1	2.19	0.41
2:D:206:LEU:HD12	2:D:206:LEU:HA	1.82	0.41
2:D:323:VAL:O	2:D:332:THR:HA	2.20	0.41
1:C:43:THR:CG2	1:C:73:ASN:HD21	2.32	0.41
1:C:150:LEU:HD12	1:C:151:LEU:N	2.36	0.41
1:C:488:ALA:O	1:C:490:PRO:HD3	2.20	0.41
1:C:503:GLN:HA	1:C:503:GLN:OE1	2.20	0.41
2:D:284:VAL:HG12	2:D:287:ARG:NH1	2.35	0.41
2:B:223:ARG:C	2:B:273:ILE:HD12	2.46	0.41
1:C:75:PHE:CD1	1:C:75:PHE:N	2.89	0.41
1:C:101:SER:HB3	5:C:567:HOH:O	2.21	0.41
1:C:150:LEU:HG	1:C:152:ILE:CD1	2.51	0.41
1:C:366:GLN:C	1:C:368:ILE:N	2.78	0.41
2:D:126:LYS:HG2	2:D:129:ASP:CG	2.45	0.41
1:A:31:ALA:HB1	1:A:509:ILE:HD12	2.03	0.41
1:A:421:ASN:HD22	1:A:423:ILE:HG22	1.86	0.41
1:A:486:GLY:HA3	2:B:22:LYS:NZ	2.35	0.41
2:B:178:ILE:HG13	2:B:307:VAL:HG22	2.03	0.41
2:B:242:PRO:HG3	2:B:259:TRP:CH2	2.56	0.41
1:C:65:VAL:HG13	1:C:69:ASP:HB3	2.03	0.41
1:C:217:ILE:H	1:C:217:ILE:CD1	2.28	0.41
1:C:412:ILE:HD12	1:C:412:ILE:N	2.36	0.41
2:D:54:ILE:HB	2:D:143:CYS:HA	2.02	0.41
2:D:199:CYS:O	2:D:202:CYS:HB2	2.19	0.41
2:D:236:GLN:O	2:D:240:GLU:HG3	2.21	0.41
1:A:413:ILE:HD13	1:A:472:VAL:CG1	2.51	0.41
1:A:418:ASN:HD22	1:A:419:PRO:N	2.19	0.41
2:B:330:LEU:HD23	2:B:330:LEU:N	2.35	0.41
1:A:189:PHE:HE1	1:A:345:VAL:HG12	1.86	0.40
1:A:332:MET:O	1:A:333:ILE:C	2.64	0.40
2:B:139:HIS:HB2	2:B:140:ILE:HD12	2.03	0.40
2:B:140:ILE:HG21	2:B:307:VAL:HG13	2.03	0.40
1:C:37:ASN:C	1:C:39:THR:N	2.68	0.40
1:C:119:PHE:O	1:C:119:PHE:CG	2.73	0.40
1:C:189:PHE:O	1:C:190:PRO:C	2.64	0.40
1:C:189:PHE:CZ	1:C:192:LEU:HB2	2.56	0.40
1:C:277:ASN:HD22	1:C:278:THR:N	2.19	0.40
1:C:314:PHE:CE2	1:C:324:PRO:HG3	2.56	0.40
1:C:416:MET:HG3	1:C:472:VAL:HG11	2.03	0.40
1:C:432:VAL:HG22	1:C:443:PRO:HG2	2.03	0.40
1:A:84:ASN:HD22	1:A:87:GLU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:OE2	1:A:318:GLU:N	2.52	0.40
1:A:416:MET:CE	1:A:424:VAL:HG13	2.50	0.40
2:B:82:THR:HG23	2:B:100:GLY:O	2.21	0.40
2:D:126:LYS:HZ3	2:D:128:GLN:CG	2.35	0.40
2:D:204:LEU:O	2:D:206:LEU:N	2.42	0.40
1:A:285:ILE:CD1	1:A:285:ILE:H	2.34	0.40
2:B:361:LEU:O	2:B:363:GLU:N	2.51	0.40
2:D:75:ILE:O	2:D:120:VAL:HA	2.21	0.40
2:B:31:THR:HG23	2:B:35:PHE:CB	2.46	0.40
2:B:97:LYS:HG3	2:B:98:ASP:N	2.37	0.40
2:D:342:ASN:O	2:D:343:CYS:C	2.64	0.40
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.79	0.40
2:B:114:ARG:O	2:B:116:PRO:HD3	2.22	0.40
1:C:80:SER:O	1:C:81:ILE:C	2.65	0.40
1:C:108:SER:HB3	1:C:111:ASN:ND2	2.36	0.40
1:C:112:LEU:O	1:C:116:ASP:C	2.65	0.40
1:C:236:THR:HB	1:C:239:GLU:CG	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/531 (98%)	477 (92%)	30 (6%)	11 (2%)	5	11
1	C	508/531 (96%)	435 (86%)	56 (11%)	17 (3%)	3	5
2	B	404/434 (93%)	362 (90%)	33 (8%)	9 (2%)	5	10
2	D	385/434 (89%)	330 (86%)	41 (11%)	14 (4%)	2	4
3	E	11/26 (42%)	11 (100%)	0	0	100	100
3	F	8/26 (31%)	7 (88%)	1 (12%)	0	100	100
All	All	1834/1982 (92%)	1622 (88%)	161 (9%)	51 (3%)	4	6

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	THR
2	B	384	THR
1	C	38	ALA
1	C	227	SER
1	C	228	GLU
1	C	333	ILE
2	D	242	PRO
2	D	275	GLY
2	D	374	LEU
2	D	601	ASN
1	A	38	ALA
1	A	277	ASN
2	B	58	GLY
2	B	92	PHE
2	B	319	ASN
2	B	607	GLN
2	B	802	VAL
1	C	262	GLU
1	C	445	VAL
1	C	446	SER
1	C	448	TYR
1	C	485	TYR
1	C	519	THR
2	D	905	VAL
1	A	317	LYS
2	B	362	GLN
1	C	195	HIS
1	C	197	GLN
2	D	319	ASN
1	A	253	LYS
2	B	116	PRO
1	C	518	ASN
2	D	40	GLU
2	D	205	GLU
1	A	37	ASN
1	A	262	GLU
1	A	280	GLN
1	A	367	SER
1	C	454	ILE
2	D	33	PRO
2	D	241	GLN
2	D	272	ASN

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Mol	Chain	Res	Type
2	D	274	ARG
2	D	351	GLN
1	C	190	PRO
1	C	198	SER
2	B	242	PRO
1	C	371	ALA
2	D	246	GLY
1	A	368	ILE
1	A	372	PRO

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	445/462 (96%)	424 (95%)	21 (5%)	23	48
1	C	435/462 (94%)	414 (95%)	21 (5%)	23	47
2	B	325/383 (85%)	307 (94%)	18 (6%)	19	41
2	D	278/383 (73%)	264 (95%)	14 (5%)	22	46
3	E	12/22 (54%)	12 (100%)	0	100	100
3	F	9/22 (41%)	9 (100%)	0	100	100
All	All	1504/1734 (87%)	1430 (95%)	74 (5%)	22	47

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	47	LYS
1	A	54	ILE
1	A	154	ARG
1	A	171	VAL
1	A	215	ILE
1	A	228	GLU
1	A	233	ILE
1	A	234	PRO

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Mol	Chain	Res	Type
1	A	238	LYS
1	A	259	PRO
1	A	279	THR
1	A	285	ILE
1	A	298	THR
1	A	329	ILE
1	A	418	ASN
1	A	422	GLU
1	A	423	ILE
1	A	424	VAL
1	A	432	VAL
1	A	458	LYS
2	B	14	GLU
2	B	31	THR
2	B	45	LEU
2	B	54	ILE
2	B	77	VAL
2	B	114	ARG
2	B	116	PRO
2	B	128	GLN
2	B	132	ASP
2	B	142	VAL
2	B	154	ILE
2	B	160	SER
2	B	166	ASP
2	B	182	THR
2	B	201	GLU
2	B	204	LEU
2	B	215	MET
2	B	325	ASN
1	C	54	ILE
1	C	97	ASN
1	C	103	SER
1	C	147	GLN
1	C	186	ASP
1	C	190	PRO
1	C	228	GLU
1	C	233	ILE
1	C	235	LYS
1	C	236	THR
1	C	253	LYS
1	C	262	GLU

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Mol	Chain	Res	Type
1	C	391	ARG
1	C	408	ASN
1	C	434	ARG
1	C	446	SER
1	C	451	GLU
1	C	454	ILE
1	C	515	ILE
1	C	518	ASN
1	C	527	GLN
2	D	35	PHE
2	D	114	ARG
2	D	128	GLN
2	D	131	ASN
2	D	201	GLU
2	D	214	PRO
2	D	242	PRO
2	D	245	GLU
2	D	260	ILE
2	D	313	SER
2	D	353	ILE
2	D	354	GLN
2	D	362	GLN
2	D	363	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	48	ASN
1	A	77	GLN
1	A	84	ASN
1	A	111	ASN
1	A	115	ASN
1	A	195	HIS
1	A	264	ASN
1	A	271	ASN
1	A	273	ASN
1	A	277	ASN
1	A	322	ASN
1	A	344	ASN
1	A	359	ASN
1	A	366	GLN

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	408	ASN
1	A	418	ASN
1	A	421	ASN
1	A	436	HIS
1	A	447	ASN
1	A	503	GLN
1	A	518	ASN
2	B	19	HIS
2	B	32	HIS
2	B	87	ASN
2	B	128	GLN
2	B	137	GLN
2	B	227	HIS
2	B	236	GLN
2	B	241	GLN
2	B	325	ASN
2	B	348	GLN
2	B	351	GLN
2	B	375	GLN
1	C	77	GLN
1	C	84	ASN
1	C	97	ASN
1	C	111	ASN
1	C	130	GLN
1	C	145	ASN
1	C	147	GLN
1	C	169	HIS
1	C	195	HIS
1	C	273	ASN
1	C	277	ASN
1	C	322	ASN
1	C	343	GLN
1	C	344	ASN
1	C	360	HIS
1	C	439	GLN
1	C	517	ASN
1	C	518	ASN
1	C	527	GLN
2	D	19	HIS
2	D	32	HIS
2	D	131	ASN

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Mol	Chain	Res	Type
2	D	137	GLN
2	D	139	HIS
2	D	188	ASN
2	D	227	HIS
2	D	241	GLN
2	D	256	HIS
2	D	272	ASN
2	D	282	GLN
2	D	319	ASN
2	D	348	GLN
2	D	362	GLN
3	F	9	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	608:SER	C	701:VAL	N	6.15

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	521/531 (98%)	-0.05	21 (4%)	42	37	24, 52, 111, 130	0
1	C	511/531 (96%)	0.43	34 (6%)	24	19	38, 74, 122, 143	0
2	B	414/434 (95%)	-0.06	16 (3%)	43	38	25, 44, 107, 125	0
2	D	392/434 (90%)	0.79	69 (17%)	4	3	34, 82, 141, 160	0
3	E	13/26 (50%)	0.23	0	100	100	53, 69, 83, 88	1 (7%)
3	F	10/26 (38%)	1.63	3 (30%)	1	1	68, 105, 110, 112	3 (30%)
All	All	1861/1982 (93%)	0.27	143 (7%)	19	15	24, 61, 126, 160	4 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	33	PRO	6.3
2	D	259	TRP	5.9
1	A	236	THR	5.5
2	D	31	THR	5.1
2	D	703	SER	4.8
1	C	334	ALA	4.8
2	D	46	LEU	4.4
1	C	37	ASN	4.3
1	A	233	ILE	4.2
1	A	229	THR	4.1
2	D	361	LEU	3.9
2	D	207	TYR	3.9
2	D	247	VAL	3.9
2	D	24	LEU	3.8
2	D	603	THR	3.8
2	D	606	LEU	3.8
2	D	257	ILE	3.8
2	D	702	THR	3.7
2	D	1002	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	247	ILE	3.6
1	A	243	PHE	3.6
1	C	447	ASN	3.6
1	A	518	ASN	3.6
1	C	192	LEU	3.5
2	B	800	GLY	3.5
2	D	707	ARG	3.5
2	D	705	GLU	3.4
2	D	604	LEU	3.4
2	D	376	MET	3.4
1	C	445	VAL	3.4
1	C	450	VAL	3.4
2	D	706	GLU	3.4
2	D	379	PRO	3.3
2	D	22	LYS	3.3
2	D	364	VAL	3.3
2	D	20	VAL	3.2
2	B	381	ILE	3.2
2	D	23	PHE	3.2
2	B	803	ASP	3.1
2	D	28	GLY	3.1
2	D	32	HIS	3.1
2	D	219	ALA	3.1
1	C	340	ILE	3.1
2	D	381	ILE	3.1
1	A	230	ASN	3.0
2	D	223	ARG	3.0
1	C	333	ILE	3.0
1	C	252	LEU	2.9
2	D	368	LEU	2.9
1	A	277	ASN	2.9
1	C	246	LEU	2.9
1	C	292	ASP	2.9
1	C	9	LYS	2.9
2	D	374	LEU	2.9
1	A	261	ASP	2.8
2	D	278	TYR	2.8
3	F	7	LEU	2.8
2	D	261	PHE	2.8
1	C	232	ARG	2.8
1	C	213	PRO	2.8
1	A	210	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	607	GLN	2.7
2	B	1000	THR	2.7
1	C	329	ILE	2.7
2	D	212	ASN	2.7
1	C	325	VAL	2.7
1	C	221	TYR	2.6
2	D	45	LEU	2.6
2	D	44	PHE	2.6
2	D	232	VAL	2.6
2	D	260	ILE	2.6
1	C	212	THR	2.6
1	C	233	ILE	2.6
2	B	751	SER	2.5
2	D	227	HIS	2.5
1	C	372	PRO	2.5
2	B	374	LEU	2.5
2	D	605	TYR	2.5
1	C	335	ASP	2.5
2	D	204	LEU	2.5
1	A	239	GLU	2.5
1	C	339	TYR	2.5
1	C	278	THR	2.5
2	D	228	CYS	2.5
1	C	444	GLY	2.5
2	D	222	PRO	2.4
2	B	319	ASN	2.4
1	C	343	GLN	2.4
2	D	375	GLN	2.4
2	D	231	TYR	2.4
2	D	1007	PHE	2.4
3	F	5	PHE	2.4
2	B	801	LEU	2.3
2	D	224	LEU	2.3
2	D	1001	THR	2.3
2	D	353	ILE	2.3
2	D	277	THR	2.3
1	C	245	ASP	2.3
2	D	378	SER	2.3
2	B	58	GLY	2.3
2	B	707	ARG	2.3
2	D	29	PRO	2.3
1	C	216	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	701	VAL	2.3
2	D	602	ARG	2.2
1	A	200	ASP	2.2
2	D	30	PHE	2.2
2	D	40	GLU	2.2
1	A	231	GLY	2.2
1	A	251	ILE	2.2
1	C	251	ILE	2.2
2	B	355	PHE	2.2
2	D	218	ILE	2.2
2	D	216	CYS	2.2
2	D	1000	THR	2.2
2	D	267	ARG	2.2
2	D	89	ASN	2.2
2	D	209	PRO	2.2
2	B	353	ILE	2.2
1	A	72	ASN	2.2
1	A	226	TYR	2.2
1	C	448	TYR	2.2
2	B	601	ASN	2.2
2	D	220	SER	2.2
1	C	268	ALA	2.1
2	B	607	GLN	2.1
1	A	7	LEU	2.1
1	C	223	ALA	2.1
2	D	237	TRP	2.1
1	C	346	TYR	2.1
2	B	257	ILE	2.1
2	D	17	TRP	2.1
2	D	256	HIS	2.1
2	D	380	ALA	2.1
3	F	12	LYS	2.1
1	A	237	TYR	2.1
2	D	701	VAL	2.1
1	A	252	LEU	2.0
1	A	264	ASN	2.0
1	A	469	GLY	2.0
2	D	95	ARG	2.0
1	A	372	PRO	2.0
1	C	199	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	B	1014	1/1	0.99	0.02	49,49,49,49	0
4	ZN	D	1014	1/1	0.99	0.03	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.