



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:31 PM UTC

PDB ID : 2NUP / pdb_00002nup
Title : Crystal Structure of the human Sec23a/24a heterodimer, complexed with the SNARE protein Sec22b
Authors : Mancias, J.D.; Goldberg, J.
Deposited on : 2006-11-09
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

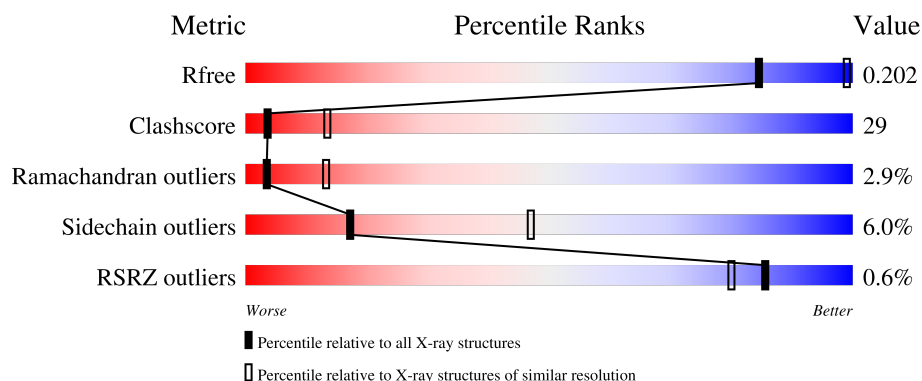
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	769	% 47% 37% 6% 9%
2	B	753	% 51% 38% 7% ...
3	C	196	33% 29% 8% • 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12641 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	699	5536	3527	953	1017	39	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP Q15436
A	-2	ALA	-	cloning artifact	UNP Q15436
A	-1	MET	-	cloning artifact	UNP Q15436
A	0	GLY	-	cloning artifact	UNP Q15436

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	731	5780	3690	983	1073	34	0	0	0

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	137	1103	708	182	205	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	cloning artifact	UNP O75396

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

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

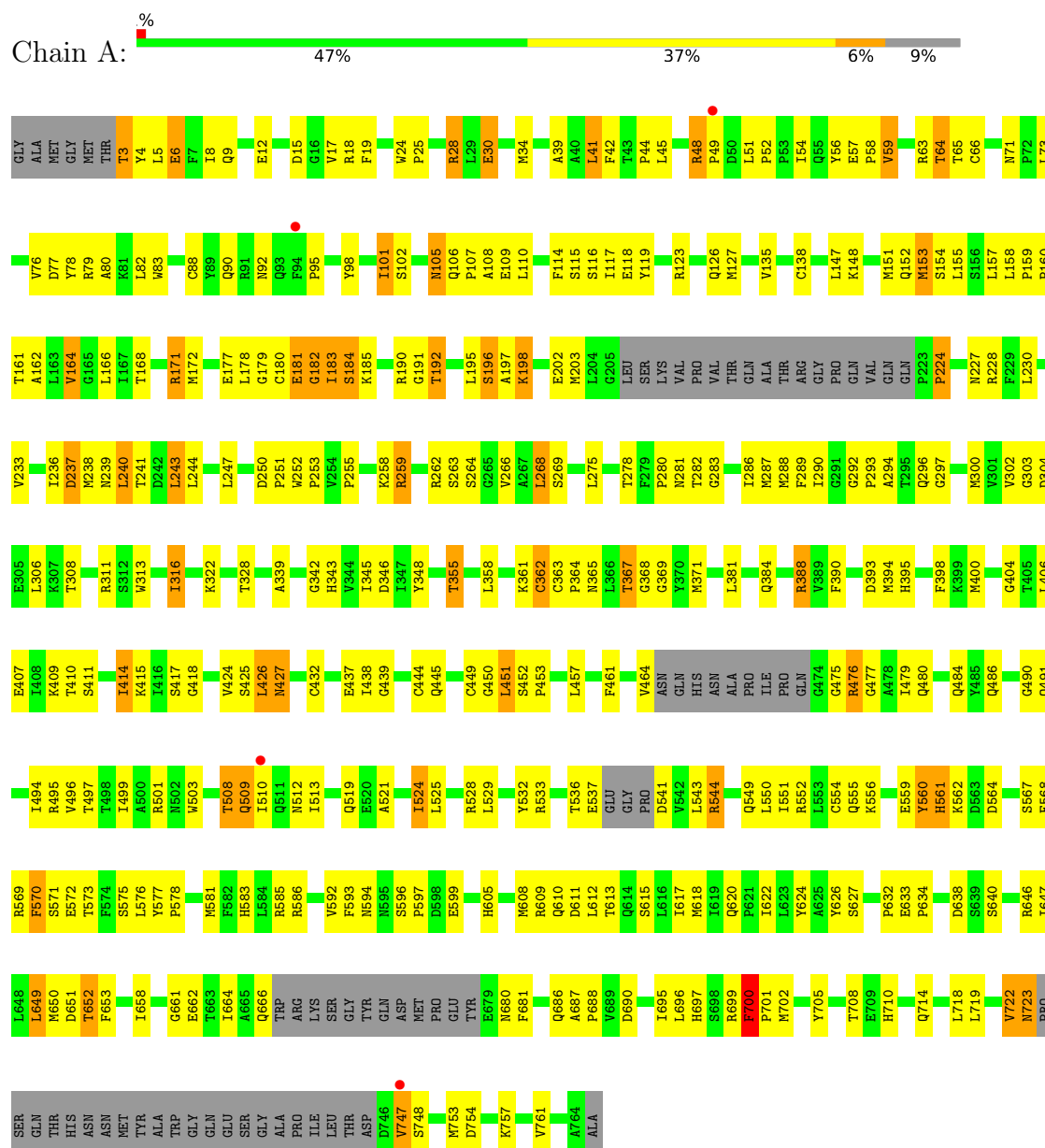
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total 92	O 92	0	0
5	B	118	Total 118	O 118	0	0
5	C	10	Total 10	O 10	0	0

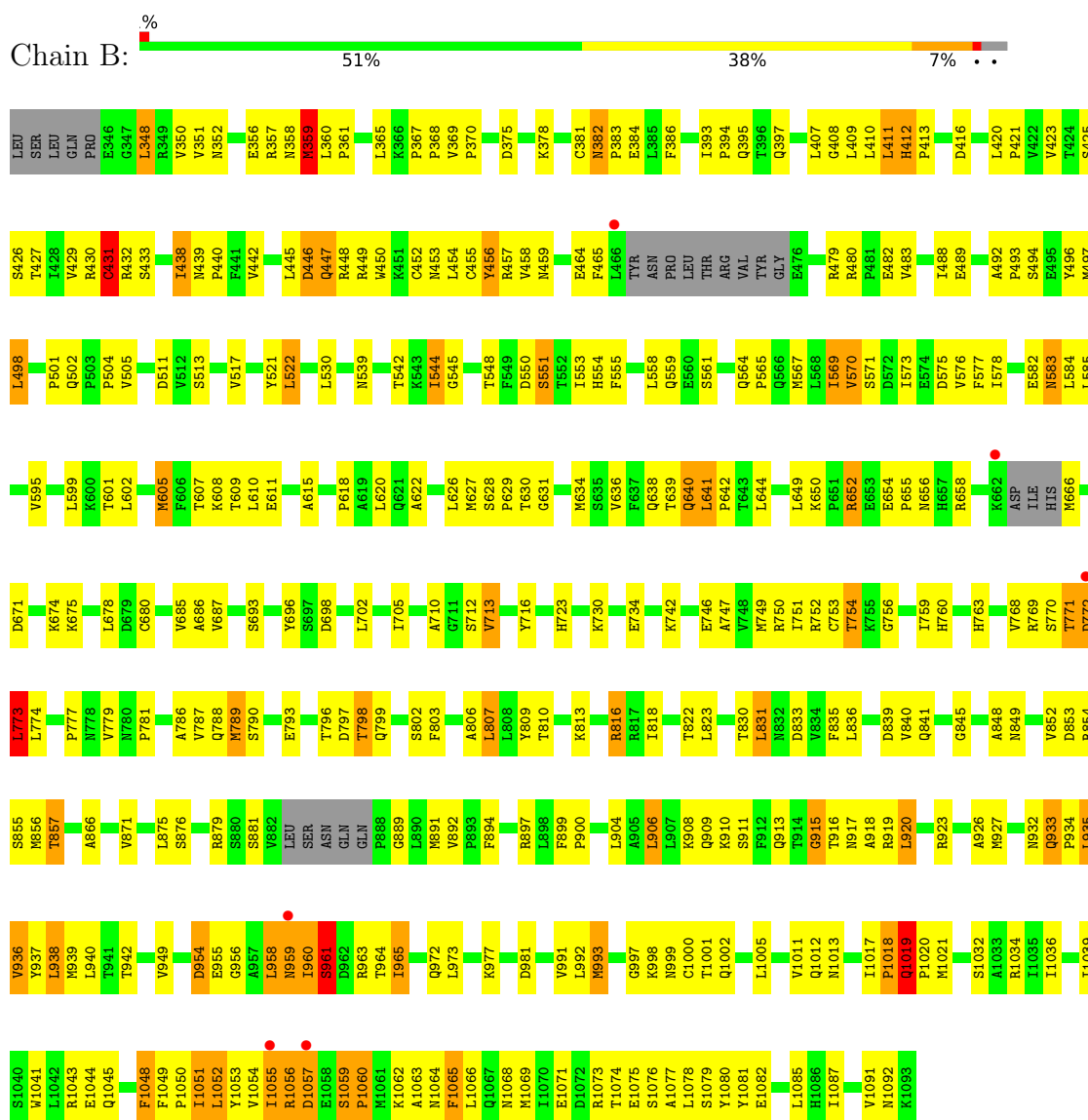
3 Residue-property plots

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: Protein transport protein Sec23A



• Molecule 2: Protein transport protein Sec24A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.20Å 97.40Å 129.62Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-2.80) 92.8 (20.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.275 0.205 , 0.202	Depositor DCC
R_{free} test set	2227 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12641	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.47	0/5663	1.04	34/7667 (0.4%)
2	B	0.47	0/5904	1.01	29/8024 (0.4%)
3	C	0.44	0/1122	0.95	3/1510 (0.2%)
All	All	0.47	0/12689	1.02	66/17201 (0.4%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-15.08	89.24	110.50
1	A	183	ILE	N-CA-C	10.67	120.54	111.90
1	A	135	VAL	N-CA-C	9.23	121.09	108.17
1	A	592	VAL	N-CA-C	8.93	119.74	110.72
1	A	426	LEU	N-CA-C	-8.77	102.72	112.72
2	B	1019	GLN	CA-C-N	-8.64	109.60	120.23
2	B	1019	GLN	C-N-CA	-8.64	109.60	120.23
1	A	652	THR	N-CA-C	-8.42	95.00	108.73
1	A	509	GLN	N-CA-C	8.11	124.67	111.37
1	A	367	THR	N-CA-C	-8.04	98.93	110.59
1	A	178	LEU	N-CA-C	7.92	121.71	110.23
1	A	198	LYS	N-CA-C	-7.81	102.09	111.69
1	A	322	LYS	N-CA-C	7.76	122.32	113.01
2	B	723	HIS	N-CA-C	7.61	119.21	111.07
2	B	1065	PHE	N-CA-C	-7.46	103.23	111.36
2	B	412	HIS	CA-C-N	7.33	129.00	119.84
2	B	412	HIS	C-N-CA	7.33	129.00	119.84
2	B	582	GLU	N-CA-C	7.27	122.59	113.43
2	B	348	LEU	N-CA-C	-7.15	102.53	112.25
2	B	583	ASN	N-CA-C	6.98	121.47	112.26
3	C	115	PHE	N-CA-C	-6.90	104.85	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	N-CA-C	-6.86	104.38	112.89
1	A	411	SER	N-CA-C	-6.76	101.60	110.53
3	C	10	VAL	N-CA-C	6.62	118.16	110.62
1	A	259	ARG	CA-C-N	-6.54	113.93	120.21
1	A	259	ARG	C-N-CA	-6.54	113.93	120.21
1	A	572	GLU	N-CA-C	-6.53	104.41	112.38
1	A	610	GLN	N-CA-C	6.47	118.67	110.33
1	A	237	ASP	N-CA-C	6.38	119.91	111.75
2	B	569	ILE	N-CA-C	6.37	117.75	108.58
3	C	3	LEU	N-CA-C	6.31	119.79	110.46
2	B	798	THR	N-CA-C	6.30	118.85	110.53
1	A	259	ARG	N-CA-C	-6.26	102.20	110.40
2	B	959	ASN	N-CA-C	-6.25	106.29	114.04
1	A	490	GLY	N-CA-C	-6.14	106.63	114.37
1	A	286	ILE	CB-CA-C	-6.01	105.83	112.68
2	B	933	GLN	N-CA-C	6.00	118.56	110.29
2	B	954	ASP	N-CA-C	5.98	121.31	113.30
2	B	936	VAL	N-CA-C	5.86	116.51	110.36
1	A	171	ARG	N-CA-C	-5.81	104.31	111.40
1	A	362	CYS	N-CA-C	5.80	118.35	111.33
2	B	938	LEU	N-CA-C	-5.78	104.89	111.07
1	A	550	LEU	N-CA-C	-5.70	104.98	111.14
2	B	973	LEU	N-CA-C	5.57	118.72	108.58
2	B	949	VAL	N-CA-C	5.56	120.91	109.34
1	A	6	GLU	N-CA-C	-5.38	104.83	111.33
2	B	426	SER	N-CA-C	-5.37	106.42	112.87
2	B	359	MET	N-CA-C	5.36	117.13	111.28
1	A	700	PHE	CA-C-N	-5.34	113.16	119.84
1	A	700	PHE	C-N-CA	-5.34	113.16	119.84
2	B	840	VAL	N-CA-C	5.33	115.54	110.42
2	B	716	TYR	CA-C-N	5.32	126.15	119.98
2	B	716	TYR	C-N-CA	5.32	126.15	119.98
1	A	182	GLY	N-CA-C	5.26	125.65	113.18
2	B	551	SER	N-CA-C	-5.23	106.90	113.28
1	A	41	LEU	N-CA-C	-5.22	98.05	107.75
1	A	224	PRO	N-CA-C	5.21	117.06	110.70
1	A	42	PHE	N-CA-C	5.18	117.68	109.24
2	B	1044	GLU	N-CA-C	-5.13	107.02	113.28
2	B	605	MET	N-CA-C	5.13	119.40	113.20
1	A	561	HIS	N-CA-C	-5.11	100.58	108.90
1	A	477	GLY	N-CA-C	-5.08	101.77	112.04
2	B	933	GLN	CA-C-N	5.08	124.84	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	933	GLN	C-N-CA	5.08	124.84	119.76
2	B	773	LEU	N-CA-C	-5.06	100.03	110.80
1	A	388	ARG	N-CA-C	-5.03	105.80	111.28

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	5536	0	5494	308	0
2	B	5780	0	5832	347	0
3	C	1103	0	1109	83	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	92	0	0	6	0
5	B	118	0	0	13	0
5	C	10	0	0	1	0
All	All	12641	0	12435	729	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 29.

All (729) 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:45:LEU:HA	1:A:495:ARG:HH12	1.07	1.09
3:C:2:VAL:HG12	3:C:3:LEU:H	1.19	1.08
1:A:48:ARG:HB2	1:A:49:PRO:CD	1.89	1.03
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.39	1.02
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.39	1.02
1:A:15:ASP:OD1	1:A:116:SER:HB2	1.62	1.00
1:A:45:LEU:HA	1:A:495:ARG:NH1	1.76	1.00
1:A:3:THR:HG22	1:A:6:GLU:H	1.28	0.98
2:B:609:THR:HG22	2:B:611:GLU:H	1.30	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:ARG:NH1	2:B:1092:ASN:HD22	1.66	0.94
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.47	0.93
2:B:854:ARG:HH12	2:B:866:ALA:HB2	1.33	0.92
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.10	0.92
3:C:39:GLN:HE21	3:C:39:GLN:HA	1.32	0.91
1:A:290:ILE:HG21	1:A:355:THR:HG23	1.54	0.90
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.50	0.90
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.55	0.89
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.55	0.88
1:A:508:THR:HB	1:A:512:ASN:HD21	1.38	0.87
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.55	0.87
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.40	0.87
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.56	0.86
1:A:722:VAL:HG22	1:A:723:ASN:H	1.41	0.85
3:C:2:VAL:HG12	3:C:3:LEU:N	1.92	0.84
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.58	0.84
2:B:992:LEU:O	2:B:1052:LEU:HD12	1.78	0.83
3:C:2:VAL:CG1	3:C:3:LEU:H	1.91	0.83
1:A:118:GLU:HB2	1:A:495:ARG:HD2	1.60	0.83
1:A:407:GLU:HG3	1:A:445:GLN:HG2	1.59	0.83
2:B:602:LEU:HA	2:B:605:MET:HE3	1.60	0.82
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.62	0.82
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.61	0.82
2:B:760:HIS:NE2	2:B:788:GLN:HG2	1.94	0.81
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.10	0.81
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.62	0.80
1:A:238:MET:O	1:A:241:THR:HG22	1.81	0.80
2:B:955:GLU:OE1	2:B:955:GLU:N	2.15	0.80
2:B:879:ARG:HH12	2:B:1092:ASN:HD22	1.29	0.79
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.65	0.79
2:B:382:ASN:ND2	2:B:384:GLU:H	1.81	0.78
3:C:113:ILE:O	3:C:116:ASP:HB2	1.83	0.78
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.01	0.78
2:B:423:VAL:HG23	2:B:488:ILE:HD11	1.65	0.77
1:A:181:GLU:O	1:A:183:ILE:N	2.16	0.77
2:B:1074:THR:HG23	2:B:1076:SER:H	1.47	0.77
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.66	0.77
1:A:313:TRP:O	1:A:316:ILE:HG22	1.84	0.77
2:B:854:ARG:NH1	2:B:866:ALA:HB2	1.99	0.76
1:A:296:GLN:HA	1:A:300:MET:HE2	1.66	0.76
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.27	0.75
1:A:297:GLY:H	1:A:300:MET:CE	1.99	0.75
2:B:382:ASN:HD22	2:B:384:GLU:H	1.33	0.75
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.68	0.74
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.23	0.74
2:B:916:THR:HG22	2:B:917:ASN:N	2.03	0.74
2:B:671:ASP:OD2	2:B:675:LYS:HE3	1.86	0.74
1:A:168:THR:HG21	1:A:247:LEU:HD21	1.70	0.73
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.18	0.73
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.69	0.73
1:A:508:THR:HB	1:A:512:ASN:ND2	2.02	0.73
2:B:642:PRO:HD2	2:B:649:LEU:HD12	1.71	0.73
3:C:81:LYS:HD3	3:C:81:LYS:H	1.54	0.73
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.54	0.72
1:A:596:SER:OG	1:A:599:GLU:HG3	1.88	0.72
1:A:5:LEU:O	1:A:9:GLN:HG3	1.88	0.72
2:B:438:ILE:HD12	2:B:442:VAL:HG11	1.71	0.72
1:A:101:ILE:HD11	1:A:107:PRO:CD	2.20	0.71
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.72	0.71
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.26	0.70
1:A:543:LEU:HD22	1:A:585:ARG:HB2	1.71	0.70
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.73	0.70
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.72	0.70
2:B:666:MET:HE3	2:B:856:MET:CE	2.22	0.70
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.74	0.70
2:B:750:ARG:HD3	2:B:772:ASP:O	1.91	0.70
2:B:1059:SER:H	2:B:1060:PRO:HD3	1.57	0.69
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.22	0.69
2:B:358:ASN:HA	2:B:972:GLN:HE22	1.56	0.69
2:B:879:ARG:HH12	2:B:1092:ASN:ND2	1.90	0.69
1:A:559:GLU:O	1:A:568:PHE:HA	1.93	0.69
2:B:770:SER:O	2:B:771:THR:C	2.36	0.69
2:B:954:ASP:C	2:B:956:GLY:H	1.98	0.69
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.75	0.68
1:A:287:MET:HA	1:A:346:ASP:HB2	1.74	0.68
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.75	0.68
2:B:1063:ALA:C	2:B:1065:PHE:H	1.99	0.68
1:A:58:PRO:O	1:A:59:VAL:HB	1.92	0.68
2:B:620:LEU:HD22	2:B:634:MET:CE	2.24	0.68
2:B:759:ILE:HG23	2:B:787:VAL:CG1	2.24	0.68
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLY:HA3	1:A:450:GLY:O	1.94	0.68
3:C:20:MET:SD	3:C:30:LEU:HD11	2.34	0.68
2:B:425:SER:HB3	2:B:427:THR:O	1.94	0.68
2:B:382:ASN:HD22	2:B:382:ASN:C	2.03	0.67
3:C:113:ILE:HD13	3:C:113:ILE:H	1.60	0.67
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.24	0.67
2:B:830:THR:HG22	2:B:833:ASP:H	1.57	0.67
2:B:747:ALA:HB2	2:B:809:TYR:CB	2.25	0.67
2:B:909:GLN:HG2	2:B:911:SER:H	1.59	0.67
2:B:407:LEU:HG	2:B:789:MET:HG3	1.76	0.67
2:B:964:THR:O	2:B:965:ILE:HB	1.94	0.67
1:A:28:ARG:HH11	1:A:28:ARG:HB3	1.60	0.66
1:A:80:ALA:O	1:A:82:LEU:HG	1.96	0.66
2:B:411:LEU:N	2:B:411:LEU:HD23	2.11	0.66
2:B:958:LEU:HD23	2:B:958:LEU:O	1.95	0.66
1:A:297:GLY:H	1:A:300:MET:HE3	1.57	0.66
1:A:147:LEU:HG	1:A:151:MET:HE2	1.78	0.66
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.77	0.66
1:A:649:LEU:HD12	1:A:649:LEU:C	2.21	0.66
2:B:496:TYR:HD1	2:B:818:ILE:HD11	1.61	0.66
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.11	0.65
1:A:98:TYR:O	1:A:101:ILE:HB	1.96	0.65
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.79	0.65
1:A:624:TYR:CE2	1:A:634:PRO:HG3	2.32	0.64
2:B:1020:PRO:HG3	2:B:1062:LYS:NZ	2.13	0.64
2:B:496:TYR:CD1	2:B:818:ILE:HD11	2.33	0.64
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.32	0.64
1:A:316:ILE:HD13	1:A:316:ILE:O	1.96	0.64
2:B:879:ARG:NH1	2:B:1092:ASN:ND2	2.42	0.64
2:B:412:HIS:HE1	2:B:781:PRO:O	1.80	0.64
2:B:634:MET:HE3	2:B:636:VAL:HG21	1.79	0.64
1:A:524:ILE:CG1	1:A:615:SER:HB3	2.28	0.64
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.34	0.63
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.33	0.63
1:A:4:TYR:O	1:A:8:ILE:HG13	1.99	0.63
1:A:198:LYS:O	1:A:202:GLU:HG3	1.99	0.63
2:B:567:MET:HE2	2:B:569:ILE:HD11	1.79	0.63
1:A:116:SER:HA	1:A:496:VAL:O	1.98	0.62
1:A:650:MET:HE1	1:A:718:LEU:HA	1.81	0.62
1:A:224:PRO:HB2	5:A:869:HOH:O	1.99	0.62
1:A:3:THR:HG22	1:A:6:GLU:N	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:GLN:HG2	2:B:939:MET:HE2	1.80	0.62
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.81	0.62
1:A:528:ARG:HA	1:A:608:MET:HE1	1.81	0.62
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.82	0.62
2:B:1041:TRP:O	2:B:1045:GLN:HG2	1.98	0.62
1:A:148:LYS:O	1:A:152:GLN:HG3	1.99	0.62
2:B:504:PRO:HG2	2:B:542:THR:HA	1.81	0.62
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.15	0.62
1:A:410:THR:HB	1:A:414:ILE:HB	1.81	0.61
1:A:404:GLY:HA2	1:A:484:GLN:O	2.01	0.61
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.30	0.61
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.64	0.61
3:C:128:ASP:OD1	3:C:130:ARG:HG2	2.01	0.61
2:B:454:LEU:HG	2:B:754:THR:H	1.65	0.61
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.82	0.60
3:C:35:SER:O	3:C:39:GLN:HG2	2.01	0.60
1:A:583:HIS:HD2	1:A:620:GLN:HE21	1.45	0.60
1:A:259:ARG:NH2	1:A:308:THR:O	2.34	0.60
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.36	0.60
2:B:352:ASN:O	2:B:356:GLU:HG2	2.02	0.60
2:B:652:ARG:NH2	5:B:218:HOH:O	2.34	0.60
1:A:593:PHE:O	1:A:594:ASN:HB2	2.02	0.60
2:B:348:LEU:HG	2:B:348:LEU:O	1.99	0.60
2:B:438:ILE:O	2:B:438:ILE:HG23	2.00	0.60
2:B:958:LEU:HA	2:B:964:THR:HA	1.83	0.60
2:B:959:ASN:O	2:B:961:SER:N	2.33	0.60
1:A:611:ASP:HB2	5:A:819:HOH:O	2.00	0.60
1:A:288:MET:HG2	1:A:290:ILE:CD1	2.32	0.60
1:A:227:ASN:HD21	1:A:278:THR:HB	1.67	0.60
1:A:452:SER:HB2	1:A:453:PRO:CD	2.32	0.59
1:A:268:LEU:HG	1:A:288:MET:SD	2.42	0.59
2:B:1054:VAL:O	2:B:1056:ARG:N	2.35	0.59
2:B:382:ASN:HD22	2:B:383:PRO:N	2.01	0.59
1:A:475:GLY:O	1:A:476:ARG:HB2	2.02	0.59
1:A:339:ALA:HB1	1:A:424:VAL:HG21	1.85	0.59
2:B:666:MET:HE3	2:B:856:MET:HE1	1.83	0.59
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.68	0.59
1:A:549:GLN:HE22	1:A:552:ARG:HH11	1.49	0.59
2:B:916:THR:CG2	2:B:917:ASN:N	2.65	0.59
3:C:63:TYR:CD1	3:C:63:TYR:C	2.81	0.59
2:B:936:VAL:O	2:B:940:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLU:HG3	1:A:445:GLN:CG	2.32	0.58
1:A:560:TYR:CD2	1:A:560:TYR:N	2.71	0.58
2:B:602:LEU:CA	2:B:605:MET:HE3	2.30	0.58
2:B:747:ALA:HB2	2:B:809:TYR:HB3	1.84	0.58
1:A:475:GLY:HA2	1:A:503:TRP:HB2	1.84	0.58
2:B:1021:MET:N	2:B:1055:ILE:HG12	2.14	0.58
2:B:558:LEU:CD2	2:B:565:PRO:HB3	2.33	0.58
2:B:1064:ASN:HA	5:B:89:HOH:O	2.01	0.58
1:A:381:LEU:HA	1:A:702:MET:HE2	1.85	0.58
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.33	0.58
2:B:916:THR:HG22	2:B:917:ASN:H	1.66	0.58
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.18	0.58
1:A:293:PRO:HA	1:A:355:THR:O	2.04	0.58
2:B:445:LEU:C	2:B:447:GLN:H	2.12	0.58
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.85	0.58
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.86	0.58
1:A:560:TYR:N	1:A:560:TYR:HD2	2.01	0.58
2:B:871:VAL:HG11	2:B:1087:ILE:HD13	1.84	0.58
1:A:393:ASP:C	1:A:395:HIS:H	2.12	0.57
2:B:430:ARG:O	2:B:431:CYS:C	2.47	0.57
2:B:1051:ILE:H	2:B:1051:ILE:HD13	1.69	0.57
2:B:439:ASN:HB2	2:B:440:PRO:CD	2.34	0.57
2:B:433:SER:OG	2:B:457:ARG:HD3	2.03	0.57
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.86	0.57
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.86	0.57
2:B:412:HIS:HD2	5:B:22:HOH:O	1.87	0.57
2:B:702:LEU:O	2:B:705:ILE:HG22	2.04	0.57
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.35	0.57
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.86	0.57
2:B:576:VAL:HG12	2:B:577:PHE:N	2.18	0.57
1:A:3:THR:HB	1:A:6:GLU:HG3	1.87	0.57
2:B:634:MET:HE2	2:B:687:VAL:HG13	1.87	0.57
1:A:652:THR:O	1:A:653:PHE:C	2.47	0.57
2:B:916:THR:CG2	2:B:917:ASN:H	2.17	0.57
1:A:45:LEU:CD1	1:A:451:LEU:HD13	2.36	0.56
2:B:641:LEU:HD23	2:B:642:PRO:HD2	1.86	0.56
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.87	0.56
2:B:666:MET:HE1	2:B:927:MET:HE1	1.88	0.56
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.81	0.56
3:C:39:GLN:HE21	3:C:39:GLN:CA	2.09	0.56
3:C:50:THR:O	3:C:51:ARG:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HE	1:A:49:PRO:HD2	1.70	0.56
1:A:519:GLN:HG2	5:A:810:HOH:O	2.04	0.56
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.87	0.56
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.87	0.56
1:A:54:ILE:HG23	1:A:56:TYR:CE2	2.41	0.56
2:B:854:ARG:HH12	2:B:866:ALA:CB	2.14	0.56
1:A:171:ARG:HG2	1:A:172:MET:HE2	1.88	0.56
2:B:375:ASP:O	2:B:378:LYS:HG2	2.06	0.56
2:B:772:ASP:O	2:B:773:LEU:HB2	2.06	0.56
3:C:127:ILE:HG22	3:C:127:ILE:O	2.04	0.56
1:A:45:LEU:CA	1:A:495:ARG:HH12	1.99	0.56
1:A:289:PHE:C	1:A:290:ILE:HD12	2.31	0.56
1:A:686:GLN:HG2	1:A:690:ASP:OD1	2.06	0.56
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.86	0.56
2:B:958:LEU:HB3	2:B:964:THR:CG2	2.27	0.56
3:C:30:LEU:O	3:C:34:GLN:HB2	2.06	0.56
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.21	0.56
2:B:634:MET:HE3	2:B:636:VAL:CG2	2.36	0.56
2:B:964:THR:O	2:B:965:ILE:CB	2.54	0.56
2:B:1055:ILE:HG22	2:B:1062:LYS:HD2	1.88	0.56
2:B:492:ALA:HB1	2:B:496:TYR:HB2	1.87	0.56
3:C:20:MET:SD	3:C:30:LEU:HD21	2.46	0.56
1:A:76:VAL:HG21	1:A:110:LEU:HD13	1.88	0.56
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.40	0.56
3:C:4:LEU:HD23	3:C:74:LEU:CB	2.36	0.56
1:A:44:PRO:O	1:A:495:ARG:NH1	2.39	0.55
1:A:426:LEU:O	1:A:427:ASN:C	2.49	0.55
1:A:56:TYR:HD1	1:A:57:GLU:O	1.89	0.55
1:A:495:ARG:HH11	1:A:495:ARG:HG2	1.71	0.55
2:B:429:VAL:HB	2:B:438:ILE:CG2	2.36	0.55
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.06	0.55
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.41	0.55
1:A:345:ILE:HG21	1:A:363:CYS:HB3	1.87	0.55
1:A:108:ALA:HB1	1:A:114:PHE:HD1	1.71	0.55
1:A:78:TYR:HD1	1:A:78:TYR:H	1.53	0.55
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.89	0.55
3:C:94:GLU:HG2	3:C:118:PHE:CD2	2.42	0.55
1:A:101:ILE:HD13	1:A:102:SER:H	1.72	0.55
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.88	0.55
1:A:155:LEU:HD22	1:A:240:LEU:HD13	1.88	0.54
2:B:1032:SER:O	2:B:1036:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HE2	1:A:154:SER:HA	1.89	0.54
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.29	0.54
1:A:418:GLY:HA3	1:A:438:ILE:O	2.07	0.54
2:B:360:LEU:HB3	2:B:972:GLN:HG2	1.88	0.54
2:B:1074:THR:HG23	2:B:1076:SER:N	2.21	0.54
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.42	0.54
2:B:513:SER:O	2:B:517:VAL:HG23	2.08	0.54
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.90	0.54
3:C:56:ALA:HB2	3:C:153:ILE:CG2	2.36	0.54
2:B:409:LEU:C	2:B:410:LEU:HD12	2.32	0.54
2:B:915:GLY:HA3	2:B:1076:SER:OG	2.07	0.54
2:B:1063:ALA:C	2:B:1065:PHE:N	2.66	0.54
2:B:615:ALA:O	2:B:618:PRO:HD2	2.08	0.54
3:C:61:PHE:CZ	3:C:74:LEU:HD13	2.43	0.54
1:A:24:TRP:HB3	1:A:25:PRO:HD2	1.90	0.54
1:A:101:ILE:HD11	1:A:107:PRO:HD2	1.87	0.54
1:A:529:LEU:O	1:A:533:ARG:HG3	2.08	0.54
1:A:687:ALA:N	1:A:688:PRO:HD2	2.23	0.54
2:B:351:VAL:CG1	2:B:356:GLU:HG3	2.38	0.54
1:A:190:ARG:NH2	2:B:577:PHE:HB3	2.23	0.53
2:B:348:LEU:CD1	2:B:836:LEU:HD21	2.39	0.53
3:C:4:LEU:HD12	3:C:20:MET:HG2	1.90	0.53
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.38	0.53
1:A:76:VAL:HG12	1:A:77:ASP:N	2.23	0.53
2:B:446:ASP:O	2:B:448:ARG:N	2.42	0.53
2:B:480:ARG:HG3	2:B:480:ARG:HH11	1.73	0.53
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.89	0.53
2:B:779:VAL:HA	5:B:82:HOH:O	2.08	0.53
2:B:932:ASN:ND2	5:B:2:HOH:O	2.40	0.53
2:B:936:VAL:HG13	2:B:937:TYR:N	2.23	0.53
2:B:954:ASP:C	2:B:956:GLY:N	2.65	0.53
2:B:1074:THR:HG22	2:B:1077:ALA:CB	2.35	0.53
2:B:991:VAL:HG12	2:B:1051:ILE:HD11	1.91	0.53
2:B:997:GLY:O	2:B:1000:CYS:HB2	2.07	0.53
1:A:393:ASP:O	1:A:395:HIS:N	2.40	0.53
2:B:845:GLY:HA2	2:B:938:LEU:CD2	2.38	0.53
3:C:81:LYS:HD3	3:C:81:LYS:N	2.22	0.53
2:B:423:VAL:HG12	2:B:425:SER:H	1.73	0.53
2:B:734:GLU:HG2	2:B:1048:PHE:CE2	2.44	0.53
3:C:62:HIS:O	3:C:73:VAL:HG12	2.08	0.53
1:A:524:ILE:HG13	1:A:615:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:VAL:HG13	5:B:111:HOH:O	2.08	0.53
1:A:41:LEU:HD21	1:A:524:ILE:HG21	1.90	0.53
1:A:346:ASP:HB3	1:A:348:TYR:CE1	2.44	0.53
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.44	0.53
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.91	0.53
2:B:654:GLU:OE2	2:B:919:ARG:HB3	2.09	0.53
1:A:3:THR:CG2	1:A:6:GLU:HG3	2.38	0.53
2:B:420:LEU:HD21	2:B:489:GLU:HB2	1.90	0.53
1:A:695:ILE:C	1:A:697:HIS:H	2.16	0.53
2:B:454:LEU:HD11	2:B:802:SER:HB2	1.90	0.53
2:B:429:VAL:HB	2:B:438:ILE:HG21	1.91	0.52
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.09	0.52
2:B:634:MET:HE2	2:B:687:VAL:CG1	2.39	0.52
1:A:179:GLY:CA	1:A:239:ASN:HD22	2.22	0.52
1:A:283:GLY:H	1:A:486:GLN:NE2	2.07	0.52
2:B:539:ASN:ND2	2:B:813:LYS:HA	2.24	0.52
2:B:696:TYR:CE1	2:B:920:LEU:HD23	2.44	0.52
1:A:58:PRO:HA	1:A:119:TYR:CE2	2.45	0.52
2:B:620:LEU:HD22	2:B:634:MET:HE1	1.90	0.52
2:B:1020:PRO:HG3	2:B:1062:LYS:HZ1	1.73	0.52
3:C:81:LYS:H	3:C:81:LYS:CD	2.16	0.52
2:B:666:MET:HB3	2:B:856:MET:HE1	1.92	0.52
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.35	0.52
1:A:45:LEU:O	1:A:453:PRO:HA	2.09	0.52
1:A:126:GLN:NE2	1:A:491:GLN:HG2	2.25	0.52
2:B:1019:GLN:CG	2:B:1020:PRO:HD3	2.39	0.52
1:A:288:MET:HG2	1:A:290:ILE:HD11	1.90	0.52
1:A:476:ARG:HA	1:A:501:ARG:O	2.10	0.52
2:B:395:GLN:NE2	2:B:796:THR:HA	2.24	0.52
1:A:3:THR:CG2	1:A:6:GLU:H	2.12	0.52
2:B:550:ASP:OD1	2:B:551:SER:N	2.42	0.52
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.10	0.52
1:A:25:PRO:HD3	1:A:34:MET:HE3	1.91	0.52
1:A:195:LEU:HD22	1:A:203:MET:CE	2.31	0.52
1:A:586:ARG:HB2	1:A:586:ARG:NH1	2.25	0.52
2:B:465:PHE:CE1	2:B:480:ARG:HG2	2.44	0.52
2:B:641:LEU:HD21	2:B:649:LEU:HB2	1.92	0.52
3:C:31:GLN:CG	3:C:32:GLN:N	2.72	0.52
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.91	0.51
1:A:250:ASP:OD2	1:A:251:PRO:HD2	2.10	0.51
1:A:262:ARG:HG2	1:A:264:SER:OG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:VAL:HG12	2:B:483:VAL:O	2.10	0.51
2:B:601:THR:HG22	2:B:605:MET:HE2	1.91	0.51
2:B:760:HIS:HE2	2:B:788:GLN:HG2	1.73	0.51
2:B:916:THR:HG22	2:B:918:ALA:H	1.75	0.51
3:C:4:LEU:HD23	3:C:74:LEU:HB2	1.92	0.51
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.75	0.51
1:A:153:MET:HE2	1:A:153:MET:C	2.36	0.51
2:B:609:THR:HG21	5:B:24:HOH:O	2.10	0.51
3:C:55:GLU:HB2	3:C:152:ASN:HD22	1.75	0.51
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.93	0.51
2:B:1054:VAL:C	2:B:1056:ARG:N	2.65	0.51
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.45	0.51
2:B:960:ILE:HG21	2:B:963:ARG:HH12	1.76	0.51
1:A:536:THR:O	1:A:537:GLU:C	2.53	0.51
1:A:76:VAL:HG12	1:A:77:ASP:H	1.76	0.51
1:A:384:GLN:O	1:A:388:ARG:HG2	2.10	0.51
2:B:573:ILE:HG22	5:B:136:HOH:O	2.11	0.51
3:C:61:PHE:HD2	3:C:72:LEU:HD11	1.74	0.51
3:C:148:ILE:HG22	3:C:149:MET:N	2.24	0.51
1:A:58:PRO:O	1:A:59:VAL:CB	2.57	0.51
2:B:447:GLN:O	2:B:447:GLN:HG2	2.11	0.51
2:B:981:ASP:OD1	2:B:999:ASN:ND2	2.43	0.51
1:A:126:GLN:HE22	1:A:491:GLN:HG2	1.76	0.50
2:B:753:CYS:HB3	2:B:803:PHE:HD1	1.76	0.50
2:B:831:LEU:HD22	2:B:835:PHE:CE1	2.46	0.50
2:B:1074:THR:HG22	2:B:1077:ALA:N	2.27	0.50
3:C:62:HIS:HB2	3:C:73:VAL:CG1	2.40	0.50
1:A:183:ILE:CD1	2:B:565:PRO:HG2	2.41	0.50
2:B:381:CYS:HB2	2:B:822:THR:O	2.11	0.50
1:A:168:THR:HG21	1:A:247:LEU:CD2	2.40	0.50
2:B:638:GLN:HE21	2:B:640:GLN:H	1.60	0.50
2:B:360:LEU:HB3	2:B:972:GLN:CG	2.42	0.50
1:A:180:CYS:SG	1:A:185:LYS:HE2	2.52	0.50
2:B:348:LEU:HD13	2:B:836:LEU:HD21	1.93	0.50
2:B:602:LEU:N	2:B:605:MET:HE3	2.27	0.50
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.93	0.50
2:B:498:LEU:N	2:B:498:LEU:HD12	2.26	0.50
2:B:1079:SER:OG	2:B:1082:GLU:HG3	2.11	0.50
3:C:108:ARG:HB2	3:C:111:SER:OG	2.12	0.50
3:C:153:ILE:HG23	3:C:154:GLU:N	2.27	0.50
1:A:180:CYS:O	1:A:181:GLU:CG	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:O	1:A:445:GLN:HA	2.12	0.50
1:A:618:MET:HG2	1:A:653:PHE:HB3	1.94	0.50
1:A:658:ILE:HD12	1:A:705:TYR:OH	2.11	0.50
3:C:10:VAL:HG23	3:C:68:GLY:O	2.11	0.50
3:C:39:GLN:HA	3:C:39:GLN:NE2	2.13	0.49
1:A:313:TRP:HE3	1:A:316:ILE:HG21	1.77	0.49
1:A:536:THR:O	1:A:536:THR:HG22	2.12	0.49
1:A:162:ALA:O	1:A:233:VAL:HG23	2.11	0.49
1:A:266:VAL:HA	1:A:269:SER:OG	2.12	0.49
1:A:649:LEU:C	1:A:649:LEU:CD1	2.85	0.49
2:B:1055:ILE:HG21	2:B:1062:LYS:CD	2.42	0.49
3:C:79:PHE:CD1	3:C:80:PRO:HD2	2.47	0.49
1:A:71:ASN:OD1	1:A:73:LEU:HB2	2.12	0.49
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.42	0.49
3:C:92:HIS:C	3:C:92:HIS:CD2	2.91	0.49
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.28	0.49
2:B:425:SER:C	2:B:427:THR:H	2.20	0.49
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.48	0.49
2:B:425:SER:C	2:B:427:THR:N	2.71	0.49
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.94	0.49
2:B:963:ARG:HH11	2:B:963:ARG:HB2	1.77	0.49
1:A:575:SER:O	1:A:578:PRO:HD2	2.12	0.49
1:A:583:HIS:HD2	1:A:620:GLN:NE2	2.09	0.49
2:B:446:ASP:C	2:B:448:ARG:N	2.71	0.49
1:A:190:ARG:NH1	2:B:575:ASP:OD1	2.46	0.49
1:A:364:PRO:O	1:A:367:THR:O	2.31	0.49
1:A:3:THR:CG2	1:A:5:LEU:H	2.26	0.49
2:B:420:LEU:HD12	2:B:421:PRO:HD2	1.94	0.49
2:B:411:LEU:HB2	2:B:413:PRO:HD3	1.95	0.48
1:A:88:CYS:SG	1:A:90:GLN:HB3	2.53	0.48
2:B:439:ASN:O	2:B:442:VAL:HG13	2.13	0.48
1:A:63:ARG:O	1:A:64:THR:C	2.56	0.48
1:A:369:GLY:O	1:A:609:ARG:NH2	2.46	0.48
1:A:583:HIS:CD2	1:A:620:GLN:HG3	2.49	0.48
2:B:753:CYS:HB2	2:B:803:PHE:CD1	2.48	0.48
3:C:50:THR:C	3:C:51:ARG:HG2	2.38	0.48
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.94	0.48
1:A:259:ARG:NH1	1:A:306:LEU:HD23	2.27	0.48
1:A:510:ILE:HD13	1:A:556:LYS:HE2	1.94	0.48
2:B:802:SER:HA	2:B:823:LEU:O	2.13	0.48
1:A:88:CYS:C	1:A:90:GLN:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:O	1:A:722:VAL:HG12	2.13	0.48
3:C:65:ILE:C	3:C:66:GLU:HG2	2.39	0.48
2:B:352:ASN:HD21	2:B:889:GLY:HA3	1.79	0.48
2:B:498:LEU:N	2:B:498:LEU:CD1	2.77	0.48
2:B:1055:ILE:O	2:B:1057:ASP:N	2.47	0.48
1:A:753:MET:O	1:A:757:LYS:HG3	2.14	0.48
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.43	0.48
2:B:773:LEU:HD12	2:B:773:LEU:HA	1.71	0.48
2:B:958:LEU:HD23	2:B:958:LEU:C	2.39	0.48
1:A:495:ARG:NH1	1:A:495:ARG:HG2	2.29	0.48
1:A:297:GLY:CA	1:A:300:MET:HB2	2.43	0.48
2:B:601:THR:CG2	2:B:605:MET:HE2	2.44	0.48
2:B:913:GLN:NE2	2:B:916:THR:HG21	2.29	0.48
1:A:564:ASP:OD2	1:A:567:SER:HB3	2.14	0.47
3:C:10:VAL:HG23	3:C:68:GLY:C	2.39	0.47
3:C:80:PRO:HB3	3:C:82:LYS:HE3	1.95	0.47
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.26	0.47
3:C:19:SER:C	3:C:20:MET:HG3	2.39	0.47
2:B:358:ASN:CA	2:B:972:GLN:HE22	2.24	0.47
2:B:958:LEU:H	2:B:958:LEU:HD22	1.79	0.47
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.78	0.47
3:C:53:THR:O	3:C:150:VAL:HA	2.14	0.47
2:B:386:PHE:CE1	2:B:409:LEU:HD13	2.49	0.47
1:A:78:TYR:CD1	1:A:78:TYR:N	2.82	0.47
1:A:722:VAL:HG22	1:A:723:ASN:N	2.19	0.47
2:B:450:TRP:CE2	2:B:459:ASN:HB2	2.50	0.47
2:B:559:GLN:HG2	2:B:583:ASN:ND2	2.29	0.47
2:B:573:ILE:CG2	2:B:618:PRO:HG2	2.35	0.47
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.97	0.47
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.97	0.47
2:B:916:THR:HG22	2:B:918:ALA:N	2.30	0.47
1:A:51:LEU:HD22	1:A:52:PRO:HD2	1.96	0.47
1:A:524:ILE:HG12	1:A:615:SER:HB3	1.94	0.47
1:A:562:LYS:HB3	1:A:562:LYS:HZ2	1.80	0.47
1:A:577:TYR:N	1:A:578:PRO:CD	2.78	0.47
1:A:282:THR:HG22	5:A:825:HOH:O	2.15	0.47
1:A:417:SER:O	1:A:437:GLU:HA	2.15	0.47
2:B:368:PRO:HD2	2:B:839:ASP:OD2	2.14	0.47
2:B:493:PRO:HD2	2:B:496:TYR:CG	2.50	0.47
2:B:879:ARG:NH1	2:B:1092:ASN:HB3	2.30	0.47
1:A:238:MET:C	1:A:241:THR:HG22	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:VAL:HG21	2:B:482:GLU:HG3	1.96	0.47
2:B:452:CYS:O	2:B:456:TYR:HA	2.15	0.47
2:B:453:ASN:C	2:B:454:LEU:HD12	2.39	0.47
2:B:674:LYS:O	2:B:678:LEU:HG	2.15	0.47
2:B:993:MET:CE	2:B:1065:PHE:HA	2.45	0.47
2:B:1049:PHE:C	2:B:1049:PHE:CD2	2.92	0.47
2:B:1055:ILE:HG21	2:B:1062:LYS:NZ	2.30	0.47
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.50	0.46
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.49	0.46
1:A:664:ILE:HG22	1:A:664:ILE:O	2.15	0.46
2:B:505:VAL:HG21	2:B:630:THR:OG1	2.15	0.46
2:B:807:LEU:O	2:B:818:ILE:HA	2.15	0.46
2:B:1059:SER:N	2:B:1060:PRO:CD	2.78	0.46
1:A:185:LYS:CB	2:B:567:MET:HB3	2.45	0.46
1:A:617:ILE:HG12	1:A:622:ILE:CD1	2.45	0.46
2:B:752:ARG:HA	5:B:184:HOH:O	2.15	0.46
2:B:854:ARG:HH11	2:B:854:ARG:HG2	1.79	0.46
2:B:1005:LEU:HD13	2:B:1013:ASN:HA	1.97	0.46
2:B:1011:VAL:HG12	2:B:1012:GLN:N	2.29	0.46
1:A:39:ALA:CB	1:A:525:LEU:HD13	2.36	0.46
1:A:191:GLY:HA3	1:A:263:SER:CB	2.45	0.46
2:B:641:LEU:HD23	2:B:642:PRO:CD	2.46	0.46
2:B:909:GLN:HG2	2:B:910:LYS:N	2.31	0.46
2:B:913:GLN:HE22	2:B:916:THR:HG21	1.79	0.46
2:B:1059:SER:H	2:B:1060:PRO:CD	2.27	0.46
3:C:33:TYR:HB3	3:C:74:LEU:HD22	1.97	0.46
1:A:19:PHE:HA	1:A:39:ALA:O	2.15	0.46
2:B:768:VAL:HG22	2:B:774:LEU:HD22	1.97	0.46
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.51	0.46
1:A:757:LYS:O	1:A:761:VAL:HG22	2.16	0.46
2:B:753:CYS:O	2:B:754:THR:O	2.33	0.46
2:B:991:VAL:HG12	2:B:1051:ILE:CD1	2.45	0.46
1:A:609:ARG:HG3	5:A:805:HOH:O	2.16	0.46
1:A:612:LEU:O	1:A:613:THR:C	2.55	0.46
2:B:439:ASN:HB2	2:B:440:PRO:HD2	1.97	0.46
2:B:576:VAL:CG1	2:B:577:PHE:N	2.78	0.46
1:A:12:GLU:CD	1:A:18:ARG:HD2	2.40	0.46
2:B:656:ASN:OD1	2:B:658:ARG:HB3	2.15	0.46
1:A:649:LEU:HD12	1:A:650:MET:N	2.30	0.46
1:A:680:ASN:CG	1:A:681:PHE:H	2.24	0.46
2:B:521:TYR:CG	2:B:522:LEU:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:MET:O	2:B:628:SER:C	2.59	0.46
2:B:763:HIS:HB3	2:B:849:ASN:OD1	2.16	0.46
2:B:993:MET:HE3	2:B:1064:ASN:OD1	2.16	0.46
3:C:3:LEU:HD22	3:C:127:ILE:HD13	1.98	0.46
1:A:559:GLU:O	1:A:560:TYR:HB3	2.16	0.46
2:B:555:PHE:HE2	2:B:570:VAL:HG11	1.81	0.46
1:A:101:ILE:HD13	1:A:102:SER:N	2.31	0.45
1:A:680:ASN:CG	1:A:681:PHE:N	2.74	0.45
2:B:457:ARG:HG3	2:B:458:VAL:N	2.31	0.45
2:B:753:CYS:CB	2:B:803:PHE:HD1	2.29	0.45
3:C:94:GLU:HG2	3:C:118:PHE:CE2	2.51	0.45
1:A:15:ASP:OD1	1:A:497:THR:HG23	2.16	0.45
1:A:183:ILE:O	2:B:565:PRO:O	2.34	0.45
2:B:382:ASN:ND2	2:B:382:ASN:C	2.74	0.45
2:B:666:MET:HE2	2:B:855:SER:HB3	1.97	0.45
2:B:734:GLU:HA	2:B:1048:PHE:HE2	1.81	0.45
2:B:854:ARG:NH1	2:B:866:ALA:CB	2.76	0.45
2:B:631:GLY:HA2	2:B:685:VAL:CG2	2.46	0.45
3:C:19:SER:O	3:C:20:MET:HG3	2.16	0.45
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.52	0.45
1:A:302:VAL:HG22	1:A:303:GLY:H	1.81	0.45
2:B:923:ARG:O	2:B:927:MET:HG3	2.17	0.45
1:A:63:ARG:HH11	1:A:88:CYS:HB2	1.82	0.45
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.46	0.45
2:B:359:MET:HE3	2:B:359:MET:H	1.81	0.45
1:A:560:TYR:HD1	1:A:761:VAL:HG12	1.81	0.45
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.99	0.45
2:B:666:MET:HE1	2:B:927:MET:CE	2.46	0.45
1:A:190:ARG:C	1:A:192:THR:H	2.24	0.45
1:A:700:PHE:O	1:A:701:PRO:C	2.57	0.45
2:B:749:MET:HA	2:B:806:ALA:O	2.16	0.45
2:B:779:VAL:O	2:B:779:VAL:HG13	2.15	0.45
3:C:155:GLU:O	3:C:156:VAL:C	2.59	0.45
1:A:457:LEU:N	1:A:457:LEU:HD22	2.32	0.45
2:B:1051:ILE:HD13	2:B:1051:ILE:N	2.32	0.45
1:A:183:ILE:HG23	1:A:184:SER:N	2.32	0.44
2:B:494:SER:HA	2:B:497:MET:HE3	1.98	0.44
2:B:639:THR:O	2:B:693:SER:HA	2.17	0.44
2:B:934:PRO:O	2:B:935:LEU:C	2.60	0.44
1:A:180:CYS:O	1:A:181:GLU:HG2	2.18	0.44
1:A:250:ASP:OD2	1:A:252:TRP:HD1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG22	1:A:303:GLY:N	2.32	0.44
2:B:397:GLN:OE1	2:B:790:SER:HB2	2.17	0.44
1:A:275:LEU:HA	1:A:278:THR:OG1	2.18	0.44
1:A:638:ASP:HB3	1:A:640:SER:OG	2.17	0.44
2:B:395:GLN:HE21	2:B:796:THR:HA	1.83	0.44
2:B:446:ASP:C	2:B:448:ARG:H	2.25	0.44
1:A:342:GLY:HA2	1:A:449:CYS:SG	2.57	0.44
1:A:508:THR:O	1:A:512:ASN:ND2	2.51	0.44
1:A:747:VAL:HG12	1:A:748:SER:N	2.32	0.44
2:B:1078:LEU:HB3	2:B:1082:GLU:HB2	1.99	0.44
3:C:58:ALA:O	3:C:59:MET:HE2	2.17	0.44
3:C:61:PHE:CD1	3:C:153:ILE:HD12	2.52	0.44
1:A:297:GLY:H	1:A:300:MET:HE2	1.81	0.44
1:A:313:TRP:CZ2	1:A:597:PRO:HA	2.52	0.44
1:A:661:GLY:O	1:A:662:GLU:C	2.59	0.44
2:B:449:ARG:HA	2:B:459:ASN:O	2.18	0.44
2:B:913:GLN:NE2	2:B:918:ALA:HB2	2.32	0.44
3:C:3:LEU:HD13	3:C:123:LYS:HD3	2.00	0.44
2:B:1064:ASN:CA	5:B:89:HOH:O	2.63	0.44
1:A:700:PHE:O	1:A:702:MET:N	2.51	0.44
2:B:972:GLN:HB3	2:B:1071:GLU:OE2	2.18	0.44
3:C:131:ALA:C	3:C:132:ARG:HG2	2.42	0.44
2:B:747:ALA:CB	2:B:809:TYR:HB3	2.45	0.44
2:B:753:CYS:CB	2:B:803:PHE:CD1	3.01	0.44
1:A:196:SER:HA	5:A:842:HOH:O	2.17	0.44
1:A:509:GLN:O	1:A:513:ILE:HG13	2.17	0.43
2:B:369:VAL:O	2:B:370:PRO:C	2.60	0.43
2:B:420:LEU:HA	2:B:421:PRO:HD3	1.89	0.43
2:B:551:SER:HA	2:B:644:LEU:HD23	1.99	0.43
2:B:1066:LEU:C	2:B:1068:ASN:N	2.75	0.43
3:C:57:GLY:C	3:C:59:MET:H	2.25	0.43
1:A:666:GLN:H	1:A:666:GLN:HG3	1.59	0.43
2:B:853:ASP:O	2:B:857:THR:HB	2.18	0.43
1:A:159:PRO:HD3	1:A:398:PHE:CE1	2.53	0.43
1:A:651:ASP:OD1	1:A:651:ASP:C	2.61	0.43
2:B:561:SER:HB3	5:B:122:HOH:O	2.18	0.43
1:A:88:CYS:SG	1:A:90:GLN:CB	3.07	0.43
1:A:177:GLU:OE1	1:A:185:LYS:HE3	2.19	0.43
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.33	0.43
1:A:560:TYR:CD1	1:A:761:VAL:HA	2.54	0.43
2:B:350:VAL:HG12	2:B:351:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:HIS:CE1	2:B:781:PRO:O	2.67	0.43
2:B:544:ILE:HG13	2:B:545:GLY:N	2.33	0.43
2:B:680:CYS:HB3	2:B:685:VAL:O	2.19	0.43
2:B:894:PHE:O	2:B:897:ARG:HD3	2.17	0.43
2:B:1057:ASP:O	2:B:1060:PRO:HD3	2.18	0.43
3:C:31:GLN:CD	3:C:32:GLN:N	2.76	0.43
3:C:52:CYS:SG	3:C:53:THR:N	2.91	0.43
3:C:114:GLU:C	3:C:116:ASP:H	2.26	0.43
1:A:114:PHE:HB3	1:A:117:ILE:HD12	2.00	0.43
1:A:153:MET:HE3	1:A:157:LEU:HD11	2.00	0.43
1:A:362:CYS:HA	1:A:365:ASN:HB2	2.00	0.43
1:A:393:ASP:C	1:A:395:HIS:N	2.77	0.43
1:A:662:GLU:HG3	1:A:710:HIS:HD2	1.83	0.43
2:B:351:VAL:O	2:B:891:MET:HA	2.18	0.43
2:B:652:ARG:HB2	2:B:696:TYR:CZ	2.52	0.43
2:B:393:ILE:HA	2:B:394:PRO:HD3	1.90	0.43
2:B:584:LEU:HD23	2:B:584:LEU:HA	1.79	0.43
2:B:848:ALA:O	2:B:852:VAL:HG23	2.19	0.43
3:C:54:LEU:HA	3:C:151:ALA:O	2.18	0.43
1:A:17:VAL:O	1:A:18:ARG:HG3	2.19	0.43
2:B:564:GLN:HB2	2:B:565:PRO:HD2	2.00	0.43
2:B:609:THR:HG22	2:B:610:LEU:N	2.33	0.43
2:B:750:ARG:HD3	2:B:772:ASP:C	2.43	0.43
1:A:126:GLN:H	1:A:126:GLN:HG3	1.54	0.43
1:A:12:GLU:OE1	1:A:18:ARG:HD2	2.19	0.43
2:B:479:ARG:HD2	2:B:479:ARG:HA	1.68	0.43
1:A:159:PRO:HA	1:A:160:PRO:HD3	1.91	0.42
1:A:297:GLY:HA3	1:A:300:MET:HB2	2.01	0.42
2:B:501:PRO:HB3	2:B:810:THR:HG23	2.01	0.42
2:B:1054:VAL:O	2:B:1055:ILE:C	2.61	0.42
3:C:110:TYR:C	3:C:112:PHE:H	2.27	0.42
1:A:255:PRO:HG2	1:A:258:LYS:CG	2.39	0.42
1:A:571:SER:C	1:A:573:THR:N	2.74	0.42
2:B:445:LEU:O	2:B:447:GLN:N	2.51	0.42
2:B:871:VAL:CG1	2:B:1087:ILE:HD13	2.47	0.42
2:B:993:MET:HE2	2:B:1065:PHE:HA	2.01	0.42
3:C:4:LEU:HD23	3:C:74:LEU:HB3	2.01	0.42
3:C:63:TYR:HD1	3:C:64:ILE:N	2.17	0.42
3:C:80:PRO:HB2	3:C:83:LEU:HG	2.01	0.42
2:B:502:GLN:HG2	2:B:746:GLU:CD	2.44	0.42
3:C:1:MET:HA	3:C:79:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:LEU:HG	3:C:34:GLN:HE21	1.83	0.42
3:C:61:PHE:CE1	3:C:74:LEU:HD13	2.54	0.42
1:A:3:THR:HG22	1:A:5:LEU:N	2.35	0.42
1:A:227:ASN:HD22	1:A:230:LEU:HD12	1.85	0.42
1:A:368:GLY:C	1:A:609:ARG:HH22	2.27	0.42
1:A:541:ASP:HB3	1:A:544:ARG:HD2	2.01	0.42
1:A:650:MET:CE	1:A:718:LEU:HA	2.48	0.42
2:B:876:SER:HA	2:B:1091:VAL:HG13	2.00	0.42
2:B:977:LYS:HE3	5:B:114:HOH:O	2.19	0.42
3:C:20:MET:CG	3:C:30:LEU:HD11	2.49	0.42
3:C:74:LEU:O	3:C:75:CYS:HB3	2.20	0.42
1:A:30:GLU:OE1	1:A:30:GLU:HA	2.19	0.42
1:A:264:SER:HB2	1:A:294:ALA:HB2	2.02	0.42
1:A:409:LYS:HB2	1:A:480:GLN:HB3	2.01	0.42
2:B:359:MET:HE2	5:B:14:HOH:O	2.19	0.42
2:B:440:PRO:HA	2:B:483:VAL:HG13	2.02	0.42
2:B:1054:VAL:C	2:B:1056:ARG:H	2.26	0.42
1:A:521:ALA:HA	1:A:612:LEU:HD12	2.01	0.42
3:C:31:GLN:CD	3:C:32:GLN:H	2.26	0.42
3:C:128:ASP:OD1	3:C:130:ARG:CG	2.66	0.42
1:A:63:ARG:O	1:A:65:THR:N	2.53	0.42
1:A:157:LEU:HD12	1:A:390:PHE:HB2	2.02	0.42
1:A:361:LYS:O	1:A:364:PRO:HD2	2.19	0.42
3:C:101:LYS:HE3	3:C:101:LYS:HA	2.01	0.42
3:C:148:ILE:CG2	3:C:149:MET:N	2.83	0.42
1:A:191:GLY:HA3	1:A:263:SER:HB3	2.01	0.42
1:A:17:VAL:HG22	1:A:18:ARG:N	2.34	0.42
1:A:147:LEU:HD11	1:A:289:PHE:CD2	2.54	0.42
1:A:363:CYS:HB2	1:A:364:PRO:HD3	2.01	0.42
1:A:519:GLN:NE2	1:A:576:LEU:HB2	2.35	0.42
2:B:654:GLU:HA	2:B:655:PRO:HD3	1.89	0.42
3:C:3:LEU:CD2	3:C:127:ILE:HD13	2.50	0.42
3:C:31:GLN:HG2	3:C:32:GLN:N	2.32	0.42
3:C:72:LEU:HD12	3:C:73:VAL:H	1.84	0.42
1:A:164:VAL:O	1:A:230:LEU:HA	2.20	0.41
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.91	0.41
2:B:360:LEU:CB	2:B:972:GLN:HG2	2.50	0.41
2:B:998:LYS:C	2:B:1000:CYS:H	2.27	0.41
1:A:3:THR:HB	1:A:6:GLU:CG	2.49	0.41
1:A:25:PRO:HD3	1:A:34:MET:CE	2.49	0.41
1:A:452:SER:CB	1:A:453:PRO:CD	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:PHE:CD1	1:A:700:PHE:C	2.97	0.41
2:B:412:HIS:N	2:B:413:PRO:CD	2.82	0.41
1:A:258:LYS:HA	1:A:304:ASP:O	2.20	0.41
1:A:425:SER:C	1:A:427:ASN:H	2.27	0.41
2:B:530:LEU:HD21	2:B:599:LEU:HB2	2.02	0.41
3:C:39:GLN:CB	3:C:157:LEU:HD22	2.50	0.41
1:A:203:MET:HB3	2:B:571:SER:OG	2.21	0.41
1:A:280:PRO:O	1:A:281:ASN:HB2	2.20	0.41
2:B:361:PRO:HG3	2:B:365:LEU:CD2	2.51	0.41
2:B:445:LEU:C	2:B:447:GLN:N	2.78	0.41
2:B:904:LEU:CD2	2:B:1080:TYR:HA	2.50	0.41
1:A:561:HIS:O	1:A:562:LYS:C	2.63	0.41
1:A:633:GLU:HA	1:A:634:PRO:HD3	1.84	0.41
2:B:408:GLY:HA2	2:B:789:MET:HG2	2.03	0.41
2:B:558:LEU:HD13	2:B:595:VAL:HG12	2.02	0.41
2:B:655:PRO:HD3	2:B:920:LEU:HD13	2.02	0.41
2:B:1078:LEU:HA	2:B:1082:GLU:OE1	2.21	0.41
3:C:2:VAL:CG1	3:C:3:LEU:N	2.59	0.41
3:C:130:ARG:O	3:C:130:ARG:HG3	2.21	0.41
1:A:158:LEU:HA	1:A:159:PRO:HD3	1.89	0.41
2:B:410:LEU:C	2:B:411:LEU:HD23	2.45	0.41
1:A:259:ARG:HB2	1:A:304:ASP:HA	2.03	0.41
1:A:290:ILE:HD12	1:A:290:ILE:N	2.36	0.41
1:A:551:ILE:O	1:A:555:GLN:HG3	2.21	0.41
1:A:686:GLN:HG2	1:A:686:GLN:O	2.21	0.41
2:B:357:ARG:NH2	2:B:1081:TYR:HB2	2.36	0.41
2:B:904:LEU:HD11	2:B:908:LYS:HE3	2.02	0.41
2:B:911:SER:OG	2:B:926:ALA:HB1	2.21	0.41
2:B:933:GLN:HA	2:B:934:PRO:HD3	1.82	0.41
3:C:80:PRO:HB3	3:C:82:LYS:CE	2.51	0.41
1:A:180:CYS:C	1:A:181:GLU:HG2	2.45	0.41
1:A:368:GLY:C	1:A:609:ARG:NH2	2.78	0.41
1:A:701:PRO:O	1:A:702:MET:C	2.63	0.41
1:A:708:THR:HB	1:A:714:GLN:HB2	2.03	0.41
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.54	0.41
1:A:695:ILE:C	1:A:697:HIS:N	2.79	0.40
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.93	0.40
2:B:411:LEU:N	2:B:411:LEU:CD2	2.81	0.40
2:B:420:LEU:HD12	2:B:421:PRO:CD	2.51	0.40
3:C:155:GLU:HG2	3:C:156:VAL:N	2.35	0.40
1:A:127:MET:HE2	1:A:127:MET:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:585:LEU:HD23	2:B:585:LEU:HA	1.89	0.40
2:B:831:LEU:HD22	2:B:835:PHE:HE1	1.84	0.40
2:B:1017:ILE:HA	2:B:1018:PRO:HD2	1.80	0.40
2:B:1043:ARG:HB3	2:B:1050:PRO:HD2	2.03	0.40
1:A:3:THR:HG23	1:A:5:LEU:H	1.86	0.40
1:A:499:ILE:C	1:A:499:ILE:HD12	2.46	0.40
2:B:348:LEU:O	2:B:348:LEU:CG	2.64	0.40
2:B:1019:GLN:O	2:B:1055:ILE:HG23	2.21	0.40
1:A:297:GLY:N	1:A:300:MET:CE	2.78	0.40
1:A:398:PHE:HB3	1:A:400:MET:CG	2.49	0.40
1:A:586:ARG:CB	1:A:586:ARG:HH11	2.33	0.40
1:A:687:ALA:N	1:A:688:PRO:CD	2.84	0.40
1:A:722:VAL:HG13	1:A:723:ASN:N	2.37	0.40
2:B:963:ARG:HB2	2:B:963:ARG:NH1	2.37	0.40
2:B:1066:LEU:C	2:B:1068:ASN:H	2.28	0.40
3:C:114:GLU:HG3	5:C:201:HOH:O	2.21	0.40
1:A:3:THR:CB	1:A:6:GLU:HG3	2.49	0.40
1:A:57:GLU:CG	1:A:58:PRO:HD2	2.51	0.40
1:A:237:ASP:O	1:A:241:THR:HB	2.22	0.40
1:A:618:MET:HE2	1:A:653:PHE:CE2	2.57	0.40
2:B:432:ARG:HD2	2:B:457:ARG:NH2	2.36	0.40
2:B:730:LYS:HE2	2:B:734:GLU:OE2	2.21	0.40
2:B:879:ARG:C	2:B:881:SER:N	2.79	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	687/769 (89%)	607 (88%)	61 (9%)	19 (3%)	4	14
2	B	723/753 (96%)	638 (88%)	64 (9%)	21 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	131/196 (67%)	107 (82%)	19 (14%)	5 (4%)	2	9
All	All	1541/1718 (90%)	1352 (88%)	144 (9%)	45 (3%)	3	13

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	64	THR
1	A	105	ASN
1	A	182	GLY
1	A	197	ALA
1	A	394	MET
2	B	447	GLN
2	B	754	THR
2	B	769	ARG
2	B	773	LEU
2	B	961	SER
2	B	1019	GLN
3	C	4	LEU
3	C	131	ALA
1	A	59	VAL
1	A	66	CYS
1	A	196	SER
1	A	747	VAL
2	B	446	ASP
2	B	456	TYR
2	B	960	ILE
2	B	1055	ILE
2	B	1056	ARG
1	A	123	ARG
1	A	181	GLU
1	A	427	ASN
1	A	696	LEU
2	B	772	ASP
2	B	797	ASP
2	B	1059	SER
3	C	92	HIS
1	A	109	GLU
1	A	184	SER
1	A	476	ARG
1	A	700	PHE
2	B	431	CYS

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Mol	Chain	Res	Type
2	B	464	GLU
2	B	771	THR
2	B	965	ILE
2	B	1018	PRO
3	C	75	CYS
1	A	722	VAL
2	B	438	ILE
2	B	915	GLY
3	C	156	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/667 (92%)	583 (96%)	27 (4%)	25	59
2	B	662/684 (97%)	620 (94%)	42 (6%)	16	45
3	C	120/171 (70%)	105 (88%)	15 (12%)	4	15
All	All	1392/1522 (92%)	1308 (94%)	84 (6%)	17	47

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	28	ARG
1	A	30	GLU
1	A	101	ILE
1	A	105	ASN
1	A	153	MET
1	A	161	THR
1	A	164	VAL
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU

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Mol	Chain	Res	Type
1	A	316	ILE
1	A	328	THR
1	A	355	THR
1	A	414	ILE
1	A	451	LEU
1	A	508	THR
1	A	524	ILE
1	A	544	ARG
1	A	560	TYR
1	A	569	ARG
1	A	570	PHE
1	A	649	LEU
1	A	723	ASN
1	A	754	ASP
2	B	359	MET
2	B	382	ASN
2	B	411	LEU
2	B	431	CYS
2	B	455	CYS
2	B	498	LEU
2	B	511	ASP
2	B	522	LEU
2	B	544	ILE
2	B	570	VAL
2	B	607	THR
2	B	608	LYS
2	B	640	GLN
2	B	641	LEU
2	B	650	LYS
2	B	652	ARG
2	B	712	SER
2	B	713	VAL
2	B	751	ILE
2	B	789	MET
2	B	798	THR
2	B	799	GLN
2	B	807	LEU
2	B	816	ARG
2	B	831	LEU
2	B	857	THR
2	B	906	LEU
2	B	920	LEU

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Mol	Chain	Res	Type
2	B	935	LEU
2	B	958	LEU
2	B	961	SER
2	B	993	MET
2	B	1001	THR
2	B	1002	GLN
2	B	1034	ARG
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1057	ASP
2	B	1060	PRO
2	B	1075	GLU
2	B	1085	LEU
3	C	1	MET
3	C	3	LEU
3	C	31	GLN
3	C	34	GLN
3	C	39	GLN
3	C	46	GLU
3	C	47	GLN
3	C	63	TYR
3	C	64	ILE
3	C	67	GLN
3	C	81	LYS
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	106	GLN
1	A	113	GLN
1	A	126	GLN
1	A	174	GLN
1	A	227	ASN
1	A	239	ASN
1	A	256	GLN
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	509	GLN
1	A	512	ASN
1	A	519	GLN
1	A	549	GLN
1	A	583	HIS
1	A	595	ASN
1	A	606	HIS
1	A	610	GLN
1	A	614	GLN
1	A	620	GLN
1	A	710	HIS
1	A	723	ASN
2	B	355	GLN
2	B	382	ASN
2	B	412	HIS
2	B	439	ASN
2	B	502	GLN
2	B	514	HIS
2	B	515	ASN
2	B	583	ASN
2	B	589	ASN
2	B	613	GLN
2	B	638	GLN
2	B	683	GLN
2	B	721	HIS
2	B	778	ASN
2	B	832	ASN
2	B	841	GLN
2	B	913	GLN
2	B	917	ASN
2	B	932	ASN
2	B	967	GLN
2	B	972	GLN
2	B	1002	GLN
2	B	1003	ASN
2	B	1007	GLN
2	B	1067	GLN
2	B	1092	ASN
3	C	36	GLN

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Mol	Chain	Res	Type
3	C	39	GLN
3	C	152	ASN

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](#)

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](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	699/769 (90%)	-0.35	4 (0%) 85 80	10, 35, 75, 103	0
2	B	731/753 (97%)	-0.47	6 (0%) 82 75	8, 29, 74, 98	0
3	C	137/196 (69%)	0.14	0 100 100	24, 63, 91, 111	0
All	All	1567/1718 (91%)	-0.36	10 (0%) 85 80	8, 33, 79, 111	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1057	ASP	3.1
2	B	772	ASP	3.0
1	A	49	PRO	2.6
2	B	959	ASN	2.6
2	B	466	LEU	2.4
2	B	1055	ILE	2.3
1	A	94	PHE	2.2
1	A	510	ILE	2.1
2	B	662	LYS	2.0
1	A	747	VAL	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	A	800	1/1	0.99	0.04	47,47,47,47	0
4	ZN	B	1100	1/1	0.99	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.