



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:44 AM UTC

PDB ID : 3EWE / pdb_00003ewe
Title : Crystal Structure of the Nup85/Seh1 Complex
Authors : Brohawn, S.G.; Leksa, N.C.; Rajashankar, K.R.; Schwartz, T.U.
Deposited on : 2008-10-14
Resolution : 3.50 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

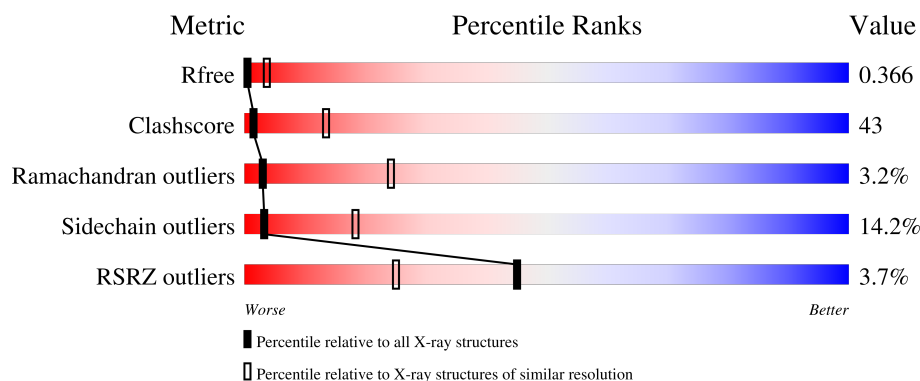
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	349	4% 30% 38% 6% 27%
1	C	349	2% 31% 37% 6% 27%
2	B	564	2% 28% 36% 6% 30%
2	D	564	2% 30% 33% 7% 30%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9689 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1869	1198	304	358	9			
1	C	255	Total	C	N	O	S	0	0	0
			1872	1201	304	358	9			

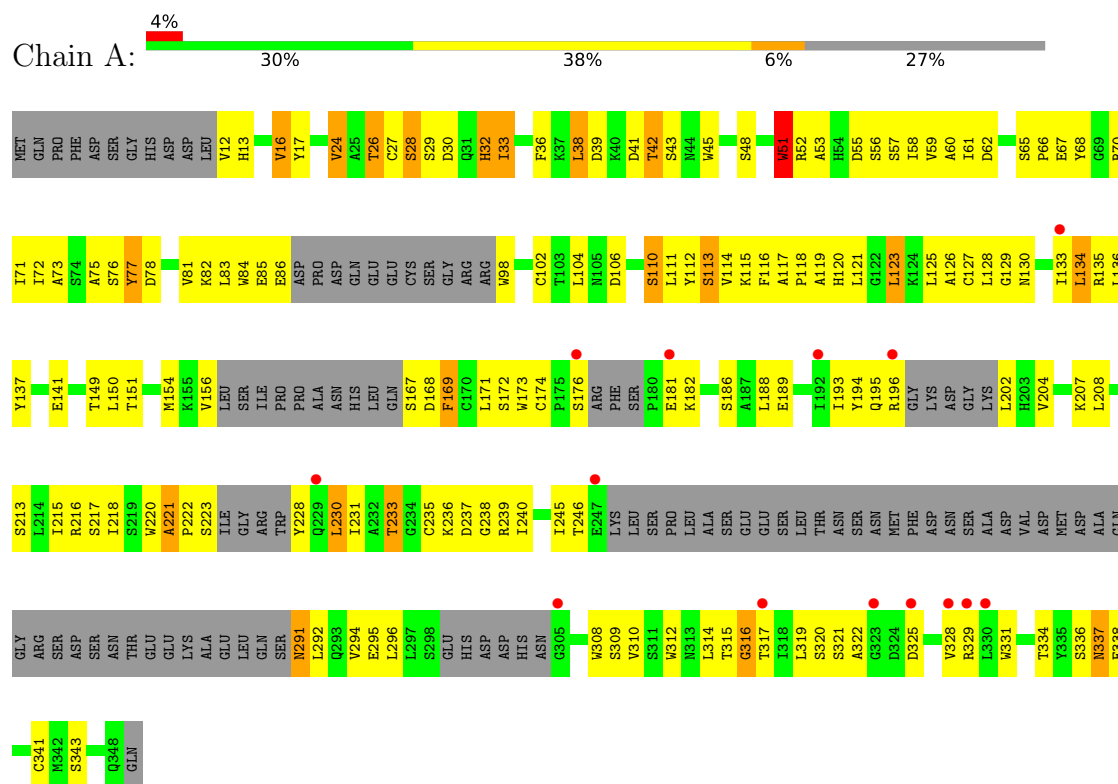
- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			2974	1941	452	560	21			
2	D	395	Total	C	N	O	S	0	0	0
			2974	1941	452	560	21			

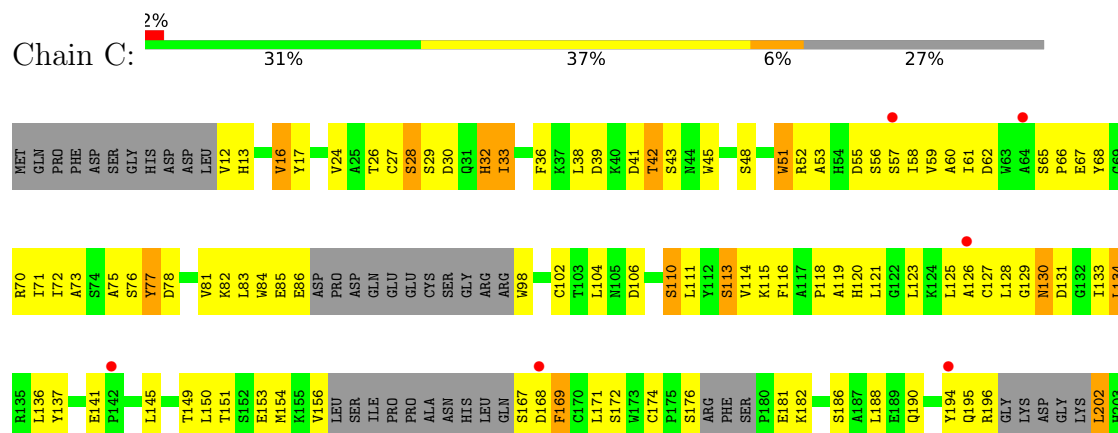
3 Residue-property plots

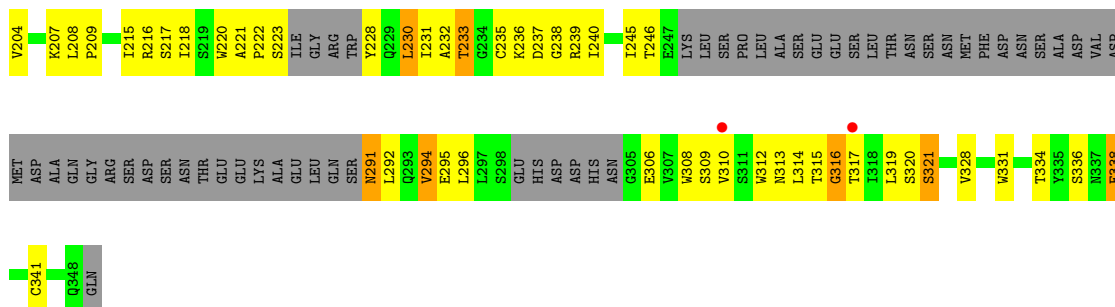
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoporin SEH1

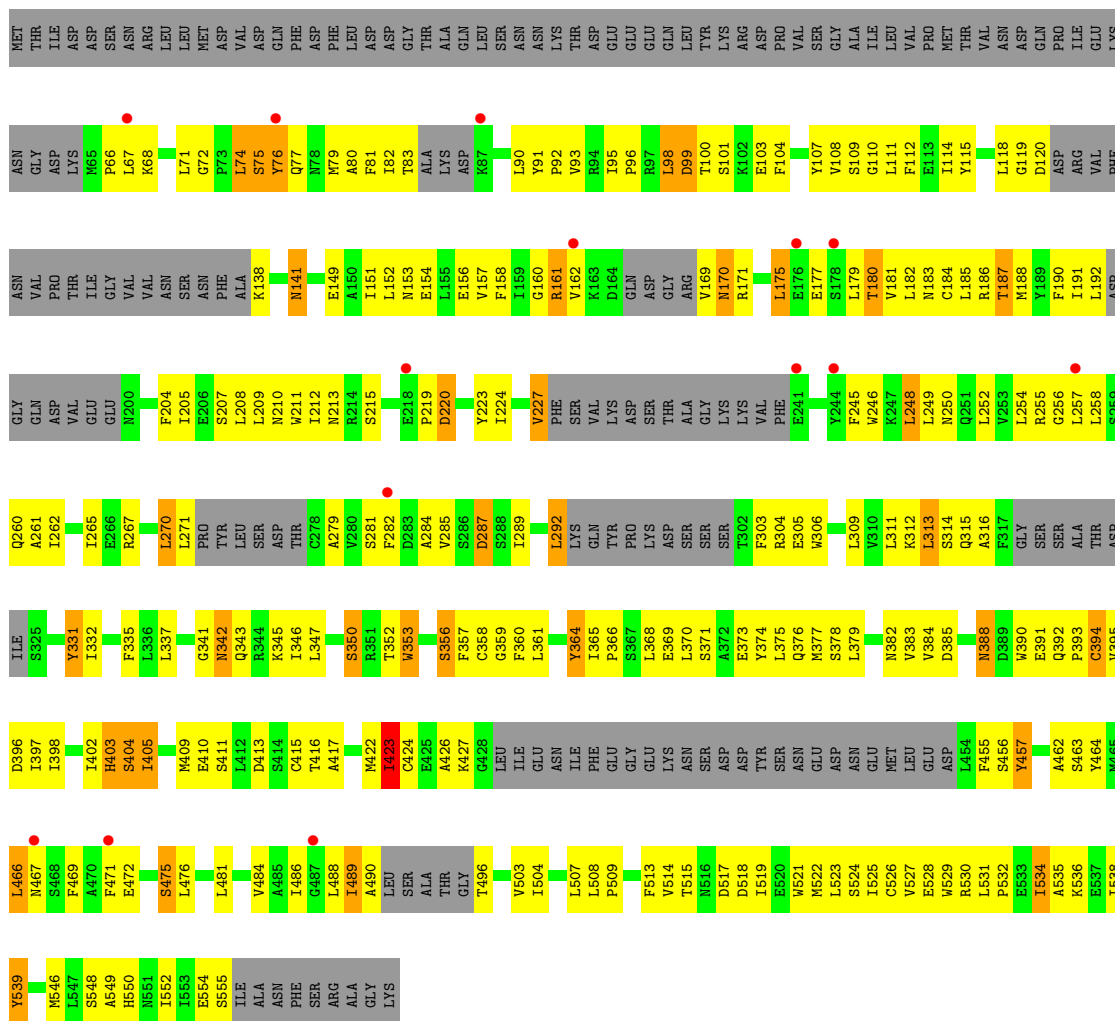
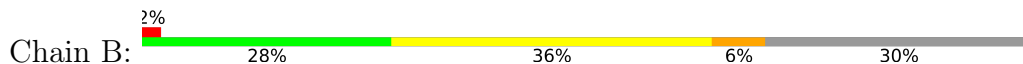


• Molecule 1: Nucleoporin SEH1

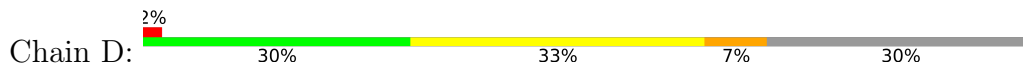




• Molecule 2: Nucleoporin NUP85



• Molecule 2: Nucleoporin NUP85



S548	L473	I398	Y331	G263	THR	ASN
I552	C474	I402	I332	C264	ILE	GLY
I553	S475	H403	E333	I265	GLY	ASP
E554	L481	S404	F335	D269	VAL	LYS
S555	L481	I405	L336	N200	VAL	M65
ILE	V484	E410	L337	R201	ASN	P66
ALA	A485	S411			SER	K68
ASN	I486	E411	G341	F204	ASN	F69
PHE	G487	A485	N342	I205	PHE	K70
ARG	L488	L412	N342	E206	ALA	L71
ARG	I489	D413	Q343	S207	K138	G72
ALA	A490	S414	R344	L208		P73
GLY	LEU	C415	K345	L209	M141	L74
LYS	SER	T416	I346	N210		S75
	ALA	M422	L347	W210	M148	Y76
	THR	I423	S350	I212	E149	Q77
	T496		R351	N213	A150	
	V503	A426	T352		I151	A80
	I504	G428	W353	G217	L152	F81
	E505				M153	I82
	E506	K427			E154	T83
	L507				L155	
	L508	LEU	S356		E156	ALA
	P509	GLY	F357		V157	LYS
	H510	GLU	C358		F158	ASP
	Y511	GLU	G359		I159	K87
		GLY	L361		G160	
	V514	GLU	Y364		R161	L90
	T515	GLY	I365		V162	Y91
		LYS	P366		K163	P92
	D518	ASN	S367		D164	V93
		SER	L368		GLN	R94
		ASP	E369		ASP	I95
		ASP	L370		GLY	
		TYR	S371		ARG	L98
	M521	SER	A372		V169	D99
	M522	ASN	E373		M170	
	L523	ASN	Y374		R171	E103
	S524	GLY	L375			F104
	I525	ASP			L176	
	G526	ASN	Q376		E176	Y107
	V527	GLU	M377		E177	V108
	E528	MET	S378		S178	S109
	W529	LEU	L379		L179	G110
	B530	GLY			T180	L111
	L531	ASP	N382		V181	F112
	P532	GLY	V383		L182	E113
		ASP	V384		M183	I114
	K536	F455	D385		C184	Y115
	E537	S456			L185	
	I538	Y457	F317		L186	L118
	V539		GLY		R186	G119
	T540	A462	SER		T187	D120
	T541	S463	SER		M188	ASP
	L542	Y464	ALA		Y189	ARG
	G543	M465	THR		F190	VAL
	P544	L466	ASP		L191	PHE
	N544	M467	ILE		L192	ASN
	Q545	C394			ASP	VAL
	M546	V395	S325		Q260	ASN
	L547	D396			A261	PRO
		E471	D330		I262	

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.56Å 112.56Å 350.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.50 29.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.75-3.50) 96.2 (29.75-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.326 , 0.369 0.315 , 0.366	Depositor DCC
R_{free} test set	1955 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	117.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 103.1	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	0.89	EDS
Total number of atoms	9689	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/1909	0.96	5/2610 (0.2%)
1	C	0.50	0/1912	0.93	3/2614 (0.1%)
2	B	0.54	0/3033	0.87	2/4137 (0.0%)
2	D	0.55	0/3033	0.90	3/4137 (0.1%)
All	All	0.54	0/9887	0.91	13/13498 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	71	LEU	N-CA-C	10.96	119.27	108.75
1	A	316	GLY	N-CA-C	-10.05	101.86	114.92
1	C	316	GLY	N-CA-C	-9.11	103.36	115.21
2	B	220	ASP	N-CA-C	6.05	118.37	111.11
1	A	169	PHE	N-CA-C	5.71	116.08	108.38
1	A	221	ALA	CA-C-N	5.63	125.34	119.82
1	A	221	ALA	C-N-CA	5.63	125.34	119.82
2	B	423	ILE	CB-CA-C	-5.52	104.82	111.88
1	C	169	PHE	N-CA-C	5.41	115.68	108.38
2	D	475	SER	N-CA-C	-5.26	105.18	113.02
1	C	338	GLU	N-CA-C	-5.25	101.91	110.20
1	A	51	TRP	N-CA-C	5.14	117.06	108.99
2	D	201	ARG	N-CA-C	5.09	117.56	111.71

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	1869	0	1709	175	0
1	C	1872	0	1718	176	0
2	B	2974	0	2765	250	0
2	D	2974	0	2765	235	0
All	All	9689	0	8957	808	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 43.

All (808) 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:239:ARG:HD3	1:A:296:LEU:HD11	1.17	1.15
1:C:239:ARG:HD3	1:C:296:LEU:HD11	1.25	1.09
2:B:279:ALA:HA	2:B:282:PHE:HD2	1.22	1.03
1:C:118:PRO:HB2	1:C:120:HIS:HD2	1.23	1.03
1:C:154:MET:CB	1:C:202:LEU:HD13	1.89	1.02
1:C:154:MET:HB2	1:C:202:LEU:CD1	1.89	1.02
1:A:118:PRO:HB2	1:A:120:HIS:HD2	1.23	1.01
2:D:262:ILE:HA	2:D:265:ILE:HD12	1.40	0.99
2:D:279:ALA:HA	2:D:282:PHE:HD2	1.29	0.98
1:C:154:MET:HB2	1:C:202:LEU:HD13	0.98	0.97
1:A:58:ILE:HD13	1:A:76:SER:HB2	1.45	0.97
2:D:413:ASP:OD2	2:D:416:THR:HG23	1.65	0.94
2:B:413:ASP:OD2	2:B:416:THR:HG23	1.69	0.93
1:C:60:ALA:HB3	1:C:75:ALA:HB3	1.52	0.92
2:D:360:PHE:HB3	2:D:374:TYR:CE1	2.04	0.92
2:B:74:LEU:HD23	2:B:475:SER:O	1.69	0.92
2:D:74:LEU:HG	2:D:75:SER:H	1.34	0.92
1:A:51:TRP:N	1:A:51:TRP:HE3	1.69	0.90
2:B:370:LEU:HB3	2:B:374:TYR:CE2	2.06	0.90
2:B:262:ILE:HA	2:B:265:ILE:HD12	1.52	0.90
2:B:74:LEU:HG	2:B:75:SER:H	1.35	0.90
2:D:360:PHE:HB3	2:D:374:TYR:CD1	2.08	0.88
1:A:60:ALA:HB3	1:A:75:ALA:HB3	1.56	0.88
2:B:370:LEU:CB	2:B:374:TYR:HE2	1.87	0.88
2:B:67:LEU:HA	2:B:82:ILE:HG13	1.55	0.87
1:C:58:ILE:HD13	1:C:76:SER:HB2	1.54	0.87
1:A:239:ARG:HD3	1:A:296:LEU:CD1	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:MET:HG3	1:C:202:LEU:HD22	1.55	0.87
1:A:81:VAL:HG23	1:A:111:LEU:HD12	1.55	0.86
2:D:258:LEU:HD13	2:D:289:ILE:HG23	1.56	0.86
2:D:74:LEU:HD11	2:D:98:LEU:HG	1.58	0.86
1:C:27:CYS:HB2	1:C:58:ILE:HB	1.56	0.86
1:A:118:PRO:HB2	1:A:120:HIS:CD2	2.11	0.85
2:B:74:LEU:HG	2:B:75:SER:N	1.92	0.84
1:C:51:TRP:HE3	1:C:51:TRP:N	1.75	0.84
1:C:169:PHE:HB2	1:C:186:SER:O	1.77	0.84
2:D:74:LEU:HG	2:D:75:SER:N	1.93	0.83
1:A:51:TRP:HE3	1:A:51:TRP:H	1.24	0.83
2:D:292:LEU:C	2:D:292:LEU:HD23	2.03	0.83
2:D:220:ASP:HA	2:D:223:TYR:HD2	1.44	0.82
2:B:74:LEU:HD11	2:B:98:LEU:HG	1.61	0.82
2:B:220:ASP:HA	2:B:223:TYR:HD2	1.44	0.82
1:C:32:HIS:C	1:C:33:ILE:HD13	2.05	0.82
1:A:169:PHE:HB2	1:A:186:SER:O	1.81	0.80
2:B:509:PRO:HD3	2:B:534:ILE:HD11	1.63	0.80
1:A:51:TRP:N	1:A:51:TRP:CE3	2.50	0.80
2:B:258:LEU:HD13	2:B:289:ILE:HG23	1.64	0.80
2:D:245:PHE:CE2	2:D:249:LEU:HD11	2.17	0.80
1:C:118:PRO:HB2	1:C:120:HIS:CD2	2.12	0.79
1:A:331:TRP:CZ3	1:A:341:CYS:HB2	2.18	0.79
1:C:239:ARG:HD3	1:C:296:LEU:CD1	2.09	0.79
2:B:107:TYR:OH	2:B:416:THR:HG22	1.83	0.78
1:C:331:TRP:CZ3	1:C:341:CYS:HB2	2.19	0.78
1:A:27:CYS:HB2	1:A:58:ILE:HB	1.64	0.77
1:C:60:ALA:HB1	1:C:114:VAL:HG12	1.67	0.77
2:D:220:ASP:HA	2:D:223:TYR:CD2	2.19	0.76
2:B:279:ALA:HA	2:B:282:PHE:CD2	2.14	0.76
1:C:51:TRP:HE3	1:C:51:TRP:H	1.32	0.76
1:C:291:ASN:O	1:C:292:LEU:HD23	1.85	0.75
2:B:98:LEU:HD22	2:B:99:ASP:N	2.00	0.75
2:D:67:LEU:HA	2:D:82:ILE:HG13	1.66	0.75
2:B:220:ASP:HA	2:B:223:TYR:CD2	2.21	0.74
1:C:51:TRP:N	1:C:51:TRP:CE3	2.56	0.74
2:B:360:PHE:HB3	2:B:374:TYR:CD1	2.22	0.74
1:C:81:VAL:HG23	1:C:111:LEU:HD12	1.68	0.74
2:B:368:LEU:HD23	2:B:368:LEU:H	1.51	0.74
2:B:360:PHE:HB3	2:B:374:TYR:CE1	2.22	0.74
1:A:291:ASN:O	1:A:292:LEU:HD23	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:C	1:A:33:ILE:HD13	2.14	0.73
1:A:315:THR:HB	2:B:471:PHE:HB3	1.70	0.73
1:A:56:SER:CB	1:A:77:TYR:HB2	2.19	0.73
2:D:279:ALA:HA	2:D:282:PHE:CD2	2.20	0.72
1:C:26:THR:HG21	2:D:90:LEU:HD11	1.71	0.72
2:D:250:ASN:HD21	2:D:335:PHE:HD1	1.37	0.72
2:B:422:MET:SD	2:B:466:LEU:HD11	2.29	0.72
2:B:370:LEU:HB2	2:B:374:TYR:HE2	1.54	0.72
2:B:385:ASP:HB2	2:B:391:GLU:OE1	1.88	0.71
1:A:33:ILE:HD11	1:A:58:ILE:HG13	1.71	0.71
2:B:370:LEU:CB	2:B:374:TYR:CE2	2.68	0.71
2:D:98:LEU:HD22	2:D:99:ASP:N	2.05	0.71
1:A:16:VAL:HG12	1:A:17:TYR:H	1.54	0.71
2:B:81:PHE:C	2:B:82:ILE:HD12	2.16	0.71
1:C:315:THR:HB	2:D:471:PHE:HB3	1.72	0.70
2:B:188:MET:HE2	2:B:398:ILE:HG12	1.74	0.70
1:C:33:ILE:HD11	1:C:58:ILE:HG13	1.73	0.70
2:D:537:GLU:O	2:D:541:THR:HG23	1.92	0.70
1:A:27:CYS:SG	1:A:61:ILE:HD11	2.32	0.70
2:B:353:TRP:HE1	2:B:391:GLU:HG2	1.55	0.70
2:D:368:LEU:HD23	2:D:368:LEU:H	1.56	0.70
2:B:504:ILE:HG22	2:B:531:LEU:HD21	1.72	0.70
2:B:74:LEU:HD13	2:B:95:ILE:HD12	1.73	0.69
2:D:422:MET:SD	2:D:466:LEU:HD11	2.32	0.69
1:C:16:VAL:HG12	1:C:17:TYR:H	1.57	0.69
2:D:360:PHE:CB	2:D:374:TYR:CD1	2.76	0.69
1:A:45:TRP:CZ2	2:B:77:GLN:HG2	2.28	0.69
1:A:45:TRP:HZ2	2:B:77:GLN:HG2	1.57	0.69
2:B:245:PHE:CE2	2:B:249:LEU:HD11	2.28	0.69
2:D:285:VAL:HG23	2:D:313:LEU:HD21	1.74	0.69
2:D:541:THR:HA	2:D:544:ASN:HD22	1.58	0.68
2:D:74:LEU:CD1	2:D:98:LEU:HG	2.23	0.68
1:C:56:SER:CB	1:C:77:TYR:HB2	2.24	0.68
2:D:524:SER:O	2:D:527:VAL:HG12	1.93	0.68
2:B:185:LEU:HD23	2:B:190:PHE:CE1	2.29	0.68
2:B:248:LEU:HD12	2:B:248:LEU:O	1.94	0.68
1:C:150:LEU:H	1:C:150:LEU:HD23	1.57	0.67
1:A:26:THR:HG21	2:B:90:LEU:HD11	1.76	0.67
1:C:310:VAL:HA	1:C:320:SER:O	1.94	0.67
2:D:114:ILE:HD11	2:D:154:GLU:HG3	1.75	0.67
1:A:51:TRP:CZ2	1:A:98:TRP:HB2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD22	2:B:82:ILE:HG12	1.76	0.67
2:B:246:TRP:CZ3	2:B:249:LEU:HD12	2.30	0.67
1:C:114:VAL:O	1:C:115:LYS:HG3	1.94	0.67
2:D:481:LEU:O	2:D:484:VAL:HB	1.94	0.67
2:D:370:LEU:CB	2:D:374:TYR:HE2	2.08	0.67
2:B:177:GLU:CG	2:B:390:TRP:HB3	2.25	0.67
1:A:60:ALA:C	1:A:61:ILE:HG13	2.20	0.66
1:A:167:SER:HA	1:A:188:LEU:HD21	1.76	0.66
2:B:67:LEU:O	2:B:68:LYS:HG2	1.95	0.66
2:B:515:THR:HG22	2:B:517:ASP:H	1.59	0.66
2:D:107:TYR:OH	2:D:416:THR:HG22	1.95	0.66
1:C:334:THR:HG23	1:C:338:GLU:O	1.95	0.66
2:D:67:LEU:HD22	2:D:82:ILE:HG12	1.76	0.66
2:D:530:ARG:C	2:D:532:PRO:HD3	2.21	0.66
2:B:185:LEU:CD2	2:B:190:PHE:HE1	2.08	0.66
2:D:74:LEU:HD23	2:D:475:SER:O	1.94	0.66
1:A:60:ALA:HB1	1:A:114:VAL:HG12	1.78	0.66
2:D:74:LEU:HD13	2:D:95:ILE:HD12	1.77	0.66
1:A:126:ALA:HB2	1:A:136:LEU:HD12	1.76	0.66
2:B:185:LEU:HD23	2:B:190:PHE:HE1	1.60	0.66
2:D:370:LEU:HB2	2:D:374:TYR:HE2	1.60	0.66
2:D:341:GLY:HA2	2:D:346:ILE:HD11	1.78	0.66
1:A:174:CYS:HB2	1:A:220:TRP:CE2	2.31	0.66
1:A:51:TRP:CD1	1:A:84:TRP:HZ3	2.13	0.65
1:A:83:LEU:HD12	1:A:102:CYS:HB2	1.77	0.65
1:C:195:GLN:HG2	1:C:196:ARG:H	1.61	0.65
1:C:167:SER:HA	1:C:188:LEU:HD21	1.76	0.65
2:D:385:ASP:HB2	2:D:391:GLU:OE1	1.96	0.65
2:D:246:TRP:CZ3	2:D:249:LEU:HD12	2.32	0.65
2:B:250:ASN:HD21	2:B:335:PHE:HD1	1.43	0.65
2:B:285:VAL:HG23	2:B:313:LEU:HD21	1.77	0.65
2:B:375:LEU:HD22	2:B:398:ILE:HB	1.79	0.65
1:C:45:TRP:HZ2	2:D:77:GLN:HG2	1.61	0.65
1:C:65:SER:CB	1:C:119:ALA:HB2	2.27	0.65
2:D:522:MET:HE3	2:D:538:ILE:HD13	1.79	0.65
1:C:125:LEU:O	1:C:136:LEU:HD12	1.96	0.65
1:A:310:VAL:HA	1:A:320:SER:O	1.96	0.65
2:B:341:GLY:HA2	2:B:346:ILE:HD11	1.79	0.65
2:B:529:TRP:HB3	2:B:531:LEU:HD11	1.79	0.65
2:D:110:GLY:O	2:D:114:ILE:HG13	1.97	0.65
1:A:65:SER:CB	1:A:119:ALA:HB2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:LEU:CD2	2:B:190:PHE:CE1	2.80	0.64
1:A:53:ALA:HB2	1:A:84:TRP:CH2	2.32	0.64
1:C:45:TRP:CZ2	2:D:77:GLN:HG2	2.33	0.64
1:C:208:LEU:HD23	1:C:292:LEU:HD13	1.80	0.64
2:B:114:ILE:HD11	2:B:154:GLU:HG3	1.79	0.64
2:B:526:CYS:SG	2:B:534:ILE:CG2	2.86	0.64
1:C:27:CYS:SG	1:C:61:ILE:HD11	2.38	0.64
2:B:279:ALA:CA	2:B:282:PHE:HD2	2.07	0.63
2:D:75:SER:O	2:D:76:TYR:HB3	1.97	0.63
2:B:74:LEU:CD1	2:B:98:LEU:HG	2.26	0.63
2:D:81:PHE:C	2:D:82:ILE:HD12	2.23	0.63
2:D:248:LEU:HD12	2:D:248:LEU:O	1.99	0.63
1:C:291:ASN:C	1:C:292:LEU:HD23	2.24	0.63
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.34	0.63
1:A:195:GLN:HG2	1:A:196:ARG:H	1.62	0.63
1:A:174:CYS:HB2	1:A:220:TRP:CD2	2.34	0.63
2:B:527:VAL:HG13	2:B:528:GLU:N	2.12	0.63
2:B:74:LEU:HD13	2:B:95:ILE:CD1	2.28	0.62
2:B:530:ARG:C	2:B:532:PRO:HD3	2.24	0.62
1:C:51:TRP:CZ2	1:C:98:TRP:HB2	2.33	0.62
2:D:212:ILE:HD13	2:D:358:CYS:SG	2.39	0.62
1:A:245:ILE:HG12	1:A:292:LEU:CD2	2.30	0.62
2:D:375:LEU:HD22	2:D:398:ILE:HB	1.80	0.62
1:A:13:HIS:HB2	1:A:59:VAL:HA	1.81	0.62
1:C:86:GLU:HA	1:C:98:TRP:HA	1.82	0.62
1:C:316:GLY:O	1:C:317:THR:C	2.42	0.62
1:C:110:SER:O	1:C:129:GLY:HA3	2.00	0.62
1:A:106:ASP:HB2	1:A:137:TYR:OH	1.99	0.61
1:C:312:TRP:CZ3	1:C:317:THR:HG22	2.35	0.61
2:D:393:PRO:HB3	2:D:405:ILE:HD12	1.81	0.61
1:C:245:ILE:HG12	1:C:292:LEU:CD2	2.30	0.61
1:A:334:THR:HG23	1:A:338:GLU:O	2.00	0.61
2:D:219:PRO:HB2	2:D:223:TYR:CZ	2.36	0.61
1:A:125:LEU:O	1:A:136:LEU:HD12	2.00	0.61
1:A:58:ILE:CD1	1:A:76:SER:HB2	2.27	0.61
1:A:150:LEU:H	1:A:150:LEU:HD23	1.65	0.61
1:C:28:SER:HB2	1:C:30:ASP:OD1	2.01	0.61
2:D:360:PHE:CG	2:D:374:TYR:HD1	2.18	0.61
1:A:114:VAL:O	1:A:115:LYS:HG3	2.01	0.60
1:C:55:ASP:OD1	1:C:78:ASP:HB3	2.01	0.60
1:C:83:LEU:HD12	1:C:102:CYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TRP:CE2	2:B:66:PRO:HB3	2.36	0.60
1:A:55:ASP:OD1	1:A:78:ASP:HB3	2.01	0.60
1:A:312:TRP:CZ3	1:A:317:THR:HG22	2.37	0.60
2:D:303:PHE:O	2:D:306:TRP:N	2.34	0.60
2:B:75:SER:O	2:B:76:TYR:HB3	2.01	0.60
2:B:524:SER:O	2:B:527:VAL:HG12	2.02	0.60
2:B:82:ILE:CG2	2:B:83:THR:N	2.65	0.60
2:D:471:PHE:HE2	2:D:489:ILE:HD11	1.66	0.60
2:D:67:LEU:O	2:D:68:LYS:HG2	2.02	0.60
2:D:99:ASP:N	2:D:99:ASP:OD1	2.34	0.60
2:B:373:GLU:O	2:B:377:MET:HG3	2.02	0.59
1:A:221:ALA:HB2	1:A:230:LEU:HD12	1.84	0.59
2:B:115:TYR:CE2	2:B:488:LEU:HD23	2.37	0.59
1:A:39:ASP:C	1:A:41:ASP:H	2.09	0.59
1:C:126:ALA:HB2	1:C:136:LEU:HD12	1.83	0.59
2:D:185:LEU:O	2:D:185:LEU:HD23	2.02	0.59
1:A:56:SER:O	1:A:57:SER:C	2.46	0.59
1:A:110:SER:O	1:A:129:GLY:HA3	2.02	0.59
1:A:111:LEU:HD13	1:A:127:CYS:SG	2.42	0.59
2:B:107:TYR:CZ	2:B:111:LEU:HD11	2.38	0.59
2:B:187:THR:OG1	2:B:207:SER:HB3	2.03	0.59
2:B:394:CYS:HA	2:B:397:ILE:HD12	1.85	0.59
2:B:536:LYS:O	2:B:539:TYR:HB3	2.03	0.59
1:C:27:CYS:CB	1:C:58:ILE:HB	2.30	0.59
2:D:74:LEU:CG	2:D:75:SER:H	2.13	0.59
2:D:152:LEU:O	2:D:156:GLU:HG3	2.03	0.59
1:A:86:GLU:HA	1:A:98:TRP:HA	1.85	0.58
2:B:99:ASP:N	2:B:99:ASP:OD1	2.36	0.58
1:C:174:CYS:HB2	1:C:220:TRP:CE2	2.38	0.58
1:C:308:TRP:CE2	2:D:66:PRO:HB3	2.37	0.58
1:C:42:THR:O	1:C:43:SER:HB2	2.03	0.58
1:C:60:ALA:C	1:C:61:ILE:HG13	2.28	0.58
2:D:402:ILE:O	2:D:404:SER:N	2.37	0.58
2:B:393:PRO:HB3	2:B:405:ILE:HD12	1.84	0.58
1:C:27:CYS:CB	1:C:61:ILE:HD11	2.33	0.58
2:D:279:ALA:CA	2:D:282:PHE:HD2	2.12	0.58
2:B:303:PHE:O	2:B:306:TRP:N	2.36	0.58
2:D:250:ASN:ND2	2:D:335:PHE:HD1	2.02	0.58
2:B:177:GLU:HG2	2:B:390:TRP:HB3	1.85	0.58
2:D:392:GLN:HB3	2:D:393:PRO:HD3	1.85	0.58
1:A:295:GLU:N	1:A:295:GLU:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:PHE:CB	2:D:374:TYR:HD1	2.15	0.58
1:C:77:TYR:HA	1:C:110:SER:OG	2.03	0.57
2:B:250:ASN:ND2	2:B:335:PHE:HD1	2.03	0.57
2:D:115:TYR:CE2	2:D:488:LEU:HD23	2.38	0.57
2:B:82:ILE:CG2	2:B:83:THR:HG23	2.35	0.57
1:C:51:TRP:CD1	1:C:84:TRP:HZ3	2.22	0.57
2:B:98:LEU:HD22	2:B:99:ASP:H	1.69	0.57
1:C:27:CYS:HB3	1:C:61:ILE:HD11	1.85	0.57
2:D:74:LEU:HD13	2:D:95:ILE:CD1	2.35	0.57
2:D:522:MET:HE3	2:D:538:ILE:CD1	2.34	0.57
1:A:316:GLY:O	1:A:317:THR:C	2.47	0.57
2:B:409:MET:HB3	2:B:417:ALA:HB2	1.86	0.57
1:C:39:ASP:C	1:C:41:ASP:H	2.10	0.57
1:C:295:GLU:N	1:C:295:GLU:OE1	2.38	0.57
1:A:208:LEU:HD23	1:A:292:LEU:HD13	1.86	0.57
2:B:385:ASP:HB2	2:B:388:ASN:HD21	1.70	0.57
1:A:60:ALA:O	1:A:61:ILE:HG13	2.05	0.56
1:C:13:HIS:HB2	1:C:59:VAL:HA	1.87	0.56
2:D:370:LEU:HB3	2:D:374:TYR:CE2	2.40	0.56
2:D:393:PRO:O	2:D:405:ILE:HD11	2.06	0.56
2:B:303:PHE:O	2:B:306:TRP:HB3	2.05	0.56
2:D:248:LEU:HD12	2:D:248:LEU:C	2.31	0.56
2:D:508:LEU:HD22	2:D:522:MET:HG3	1.87	0.56
2:D:541:THR:HA	2:D:544:ASN:ND2	2.18	0.56
1:A:27:CYS:CB	1:A:61:ILE:HD11	2.34	0.56
1:A:28:SER:HB2	1:A:30:ASP:OD1	2.06	0.56
1:C:77:TYR:HA	1:C:110:SER:CB	2.35	0.56
1:C:133:ILE:O	1:C:133:ILE:HG23	2.05	0.56
1:C:60:ALA:CB	1:C:114:VAL:HG12	2.36	0.56
1:C:65:SER:OG	1:C:119:ALA:HB2	2.05	0.56
1:C:85:GLU:C	1:C:98:TRP:HE3	2.12	0.56
1:C:120:HIS:NE2	1:C:121:LEU:HG	2.20	0.56
1:C:217:SER:HB3	1:C:310:VAL:HG12	1.86	0.56
1:C:104:LEU:HD13	1:C:137:TYR:CD2	2.40	0.56
2:D:245:PHE:CE2	2:D:249:LEU:CD1	2.88	0.56
2:B:171:ARG:O	2:B:175:LEU:HB2	2.06	0.56
1:A:320:SER:OG	2:B:71:LEU:HD11	2.06	0.56
2:B:292:LEU:C	2:B:292:LEU:HD12	2.30	0.56
1:C:174:CYS:HB2	1:C:220:TRP:CD2	2.40	0.56
2:D:82:ILE:CG2	2:D:83:THR:N	2.68	0.56
2:B:353:TRP:HE1	2:B:391:GLU:CG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:TYR:CE1	1:C:204:VAL:HG22	2.40	0.56
2:D:82:ILE:CG2	2:D:83:THR:HG23	2.36	0.56
2:B:393:PRO:O	2:B:405:ILE:HD11	2.06	0.55
1:C:33:ILE:CD1	1:C:58:ILE:HG13	2.35	0.55
1:A:68:TYR:CE1	1:A:123:LEU:HG	2.41	0.55
1:A:240:ILE:O	1:A:296:LEU:HD12	2.06	0.55
2:B:152:LEU:O	2:B:156:GLU:HG3	2.05	0.55
2:D:530:ARG:O	2:D:532:PRO:HD3	2.06	0.55
1:A:42:THR:HG23	1:A:42:THR:O	2.07	0.55
2:B:392:GLN:HB3	2:B:393:PRO:HD3	1.87	0.55
2:D:75:SER:O	2:D:76:TYR:CB	2.54	0.55
1:A:51:TRP:NE1	1:A:84:TRP:CZ3	2.74	0.55
1:C:33:ILE:HD13	1:C:33:ILE:N	2.20	0.55
1:C:56:SER:O	1:C:57:SER:C	2.49	0.55
1:C:85:GLU:C	1:C:98:TRP:CE3	2.84	0.55
1:A:134:LEU:HB3	1:A:154:MET:O	2.06	0.55
1:C:53:ALA:HB2	1:C:84:TRP:CH2	2.41	0.55
1:C:85:GLU:HG2	1:C:86:GLU:H	1.71	0.55
1:A:217:SER:HB3	1:A:310:VAL:HG12	1.88	0.55
1:C:83:LEU:C	1:C:84:TRP:CD1	2.85	0.55
1:C:104:LEU:HD13	1:C:137:TYR:CG	2.42	0.55
2:D:394:CYS:O	2:D:398:ILE:HG13	2.07	0.55
2:B:463:SER:O	2:B:467:ASN:ND2	2.38	0.55
2:B:508:LEU:HD22	2:B:522:MET:HG3	1.89	0.55
2:D:177:GLU:HG2	2:D:390:TRP:HB3	1.87	0.55
1:C:60:ALA:HB2	1:C:113:SER:HA	1.88	0.55
2:D:177:GLU:CG	2:D:390:TRP:HB3	2.37	0.55
2:B:410:GLU:HG3	2:B:411:SER:N	2.22	0.54
2:D:527:VAL:HG13	2:D:528:GLU:N	2.23	0.54
1:A:120:HIS:NE2	1:A:121:LEU:HG	2.22	0.54
1:A:83:LEU:C	1:A:84:TRP:CD1	2.86	0.54
2:D:303:PHE:O	2:D:306:TRP:HB3	2.07	0.54
2:D:529:TRP:HB3	2:D:531:LEU:HD11	1.89	0.54
1:A:33:ILE:CD1	1:A:58:ILE:HG13	2.37	0.54
1:A:60:ALA:HB2	1:A:113:SER:HA	1.88	0.54
2:D:330:ASP:C	2:D:330:ASP:OD1	2.50	0.54
2:D:356:SER:O	2:D:357:PHE:C	2.50	0.54
2:B:160:GLY:O	2:B:162:VAL:N	2.41	0.54
2:B:188:MET:CE	2:B:398:ILE:HG23	2.38	0.54
2:B:248:LEU:HD12	2:B:248:LEU:C	2.33	0.54
2:D:356:SER:HB2	2:D:378:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:THR:O	1:A:43:SER:HB2	2.08	0.53
2:B:81:PHE:O	2:B:82:ILE:HD12	2.08	0.53
2:D:250:ASN:ND2	2:D:335:PHE:CD1	2.75	0.53
2:D:370:LEU:CB	2:D:374:TYR:CE2	2.90	0.53
1:C:68:TYR:CE1	1:C:123:LEU:HG	2.43	0.53
1:A:27:CYS:HB3	1:A:61:ILE:HD11	1.90	0.53
2:D:490:ALA:CB	2:D:529:TRP:HZ2	2.22	0.53
1:A:85:GLU:C	1:A:98:TRP:HE3	2.17	0.53
1:A:291:ASN:C	1:A:292:LEU:HD23	2.34	0.53
2:D:292:LEU:C	2:D:292:LEU:CD2	2.74	0.53
1:A:53:ALA:HB2	1:A:84:TRP:CZ2	2.44	0.53
2:D:246:TRP:CD1	2:D:331:TYR:CG	2.96	0.53
1:C:106:ASP:HB2	1:C:137:TYR:OH	2.08	0.53
2:B:346:ILE:O	2:B:350:SER:HB2	2.09	0.53
2:B:282:PHE:CE1	2:B:332:ILE:HD13	2.44	0.53
1:C:111:LEU:HD23	1:C:129:GLY:HA3	1.91	0.53
1:C:111:LEU:HD13	1:C:127:CYS:SG	2.48	0.53
2:D:179:LEU:O	2:D:183:ASN:N	2.41	0.53
1:A:65:SER:OG	1:A:119:ALA:HB2	2.09	0.52
2:D:342:ASN:O	2:D:345:LYS:N	2.36	0.52
2:B:212:ILE:HD13	2:B:358:CYS:SG	2.49	0.52
2:D:353:TRP:HE1	2:D:391:GLU:HG2	1.75	0.52
2:D:375:LEU:HD11	2:D:395:VAL:HG13	1.92	0.52
1:A:27:CYS:CB	1:A:58:ILE:HB	2.36	0.52
1:A:27:CYS:HA	1:A:33:ILE:HG23	1.91	0.52
2:B:99:ASP:HB2	2:B:104:PHE:CD1	2.44	0.52
2:B:224:ILE:HA	2:B:227:VAL:HG23	1.90	0.52
1:A:33:ILE:HD13	1:A:33:ILE:N	2.24	0.52
2:B:95:ILE:O	2:B:98:LEU:CB	2.57	0.52
2:D:187:THR:OG1	2:D:207:SER:HB3	2.10	0.52
1:A:85:GLU:C	1:A:98:TRP:CE3	2.87	0.52
2:D:68:LYS:HD2	2:D:81:PHE:CZ	2.44	0.52
2:B:481:LEU:O	2:B:484:VAL:HB	2.09	0.52
2:D:390:TRP:C	2:D:393:PRO:HD2	2.35	0.52
2:B:402:ILE:O	2:B:404:SER:N	2.43	0.52
2:D:185:LEU:CD2	2:D:190:PHE:CE1	2.93	0.52
2:D:345:LYS:C	2:D:347:LEU:H	2.18	0.52
1:A:186:SER:HB2	1:A:218:ILE:HG13	1.92	0.52
2:B:527:VAL:HG13	2:B:528:GLU:H	1.75	0.52
1:A:67:GLU:CD	1:A:68:TYR:CE1	2.88	0.51
2:D:98:LEU:HD22	2:D:99:ASP:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ILE:HG22	2:B:83:THR:HG23	1.92	0.51
2:B:158:PHE:CE1	2:B:175:LEU:HD21	2.45	0.51
2:B:281:SER:HB2	2:B:313:LEU:HD11	1.93	0.51
2:B:284:ALA:O	2:B:287:ASP:HB2	2.10	0.51
2:B:356:SER:O	2:B:357:PHE:C	2.53	0.51
2:B:360:PHE:CB	2:B:374:TYR:CD1	2.93	0.51
2:D:188:MET:CE	2:D:398:ILE:HG23	2.40	0.51
1:A:51:TRP:NE1	1:A:84:TRP:HZ3	2.09	0.51
1:A:310:VAL:HG22	1:A:319:LEU:HD11	1.92	0.51
1:C:154:MET:HE2	1:C:202:LEU:CD2	2.39	0.51
1:C:154:MET:CG	1:C:202:LEU:HD22	2.33	0.51
1:A:56:SER:HB3	1:A:77:TYR:HB2	1.89	0.51
1:A:228:TYR:HE1	2:B:457:TYR:HE2	1.58	0.51
1:C:174:CYS:HB3	1:C:182:LYS:O	2.09	0.51
1:C:67:GLU:O	1:C:67:GLU:HG2	2.11	0.51
1:A:126:ALA:HB2	1:A:136:LEU:CD1	2.40	0.51
1:A:194:TYR:CE1	1:A:204:VAL:HG22	2.45	0.51
2:B:422:MET:SD	2:B:466:LEU:HD21	2.50	0.51
2:B:548:SER:O	2:B:552:ILE:HG12	2.10	0.51
2:B:370:LEU:O	2:B:374:TYR:HD2	1.93	0.51
1:A:32:HIS:HB3	1:A:52:ARG:CA	2.40	0.51
2:B:250:ASN:ND2	2:B:335:PHE:CD1	2.79	0.51
2:B:292:LEU:C	2:B:292:LEU:CD1	2.84	0.51
1:C:42:THR:O	1:C:42:THR:HG23	2.11	0.51
1:C:168:ASP:H	1:C:188:LEU:HD11	1.75	0.51
2:D:157:VAL:O	2:D:161:ARG:HG2	2.11	0.51
1:C:70:ARG:O	1:C:98:TRP:HZ3	1.94	0.51
2:D:394:CYS:HA	2:D:397:ILE:HD12	1.93	0.51
2:B:75:SER:O	2:B:76:TYR:CB	2.59	0.50
2:D:306:TRP:O	2:D:310:VAL:HG23	2.11	0.50
1:A:32:HIS:HB3	1:A:52:ARG:HA	1.91	0.50
1:A:85:GLU:HG2	1:A:86:GLU:H	1.76	0.50
2:B:471:PHE:HE2	2:B:489:ILE:HD11	1.75	0.50
2:D:423:ILE:O	2:D:426:ALA:HB3	2.11	0.50
1:A:70:ARG:O	1:A:98:TRP:HZ3	1.95	0.50
2:B:160:GLY:C	2:B:162:VAL:N	2.69	0.50
2:B:394:CYS:O	2:B:398:ILE:HG13	2.11	0.50
1:C:134:LEU:HB3	1:C:154:MET:O	2.12	0.50
1:A:56:SER:HB2	1:A:77:TYR:H	1.76	0.50
1:A:315:THR:C	1:A:317:THR:H	2.20	0.50
2:D:270:LEU:N	2:D:270:LEU:HD23	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:463:SER:O	2:D:467:ASN:ND2	2.44	0.50
2:B:415:CYS:HA	2:B:469:PHE:CE1	2.46	0.50
2:D:185:LEU:CD2	2:D:190:PHE:HE1	2.24	0.50
2:D:393:PRO:O	2:D:397:ILE:HG13	2.11	0.50
1:C:104:LEU:HD21	1:C:149:THR:HG21	1.94	0.50
1:C:320:SER:OG	2:D:71:LEU:HD11	2.12	0.50
2:D:158:PHE:CE1	2:D:175:LEU:HD21	2.46	0.50
1:A:120:HIS:CD2	1:A:121:LEU:HG	2.46	0.50
2:B:74:LEU:CG	2:B:75:SER:H	2.14	0.50
2:B:179:LEU:O	2:B:183:ASN:N	2.43	0.50
1:A:39:ASP:C	1:A:41:ASP:N	2.71	0.49
1:A:53:ALA:CB	1:A:84:TRP:CZ2	2.94	0.49
2:B:246:TRP:HA	2:B:246:TRP:CE3	2.47	0.49
2:D:360:PHE:HB3	2:D:374:TYR:HE1	1.71	0.49
2:D:112:PHE:CD2	2:D:484:VAL:HG22	2.47	0.49
2:B:79:MET:HE2	2:B:90:LEU:HD22	1.93	0.49
2:B:526:CYS:SG	2:B:534:ILE:HG21	2.52	0.49
1:C:51:TRP:NE1	1:C:84:TRP:CZ3	2.80	0.49
1:C:67:GLU:CD	1:C:68:TYR:CE1	2.90	0.49
2:D:184:CYS:HB2	2:D:211:TRP:NE1	2.27	0.49
2:D:245:PHE:CZ	2:D:249:LEU:HD11	2.48	0.49
2:B:112:PHE:CD2	2:B:484:VAL:HG22	2.47	0.49
2:B:254:LEU:C	2:B:256:GLY:H	2.20	0.49
1:C:39:ASP:C	1:C:41:ASP:N	2.71	0.49
1:C:315:THR:C	1:C:317:THR:H	2.20	0.49
1:C:120:HIS:CD2	1:C:121:LEU:HG	2.48	0.49
2:D:80:ALA:HB3	2:D:91:TYR:HB2	1.94	0.49
2:D:82:ILE:HG22	2:D:83:THR:HG23	1.94	0.49
1:A:106:ASP:OD2	1:A:151:THR:HG21	2.12	0.49
2:B:74:LEU:HD13	2:B:95:ILE:CG1	2.42	0.49
2:B:368:LEU:H	2:B:368:LEU:CD2	2.22	0.49
2:B:394:CYS:SG	2:B:397:ILE:HD12	2.52	0.49
1:C:195:GLN:CG	1:C:196:ARG:H	2.25	0.49
1:C:236:LYS:C	1:C:238:GLY:H	2.21	0.49
1:A:12:VAL:N	1:A:29:SER:HG	2.11	0.49
2:B:311:LEU:O	2:B:312:LYS:C	2.55	0.49
1:A:77:TYR:HA	1:A:110:SER:CB	2.43	0.49
1:A:174:CYS:HB3	1:A:182:LYS:O	2.12	0.49
1:A:320:SER:OG	2:B:71:LEU:CD1	2.61	0.49
2:B:270:LEU:O	2:B:271:LEU:HD23	2.13	0.49
2:D:158:PHE:O	2:D:162:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:GLN:O	2:D:316:ALA:C	2.55	0.49
2:B:490:ALA:CB	2:B:529:TRP:HZ2	2.25	0.48
2:B:527:VAL:CG1	2:B:528:GLU:N	2.76	0.48
1:C:215:ILE:HG22	1:C:216:ARG:N	2.27	0.48
2:B:82:ILE:HG23	2:B:83:THR:N	2.28	0.48
2:B:305:GLU:O	2:B:309:LEU:HG	2.13	0.48
1:C:128:LEU:HG	1:C:171:LEU:HD23	1.95	0.48
2:D:346:ILE:HG22	2:D:346:ILE:O	2.13	0.48
2:D:388:ASN:C	2:D:390:TRP:H	2.21	0.48
2:D:181:VAL:O	2:D:184:CYS:HB3	2.13	0.48
2:B:315:GLN:O	2:B:316:ALA:C	2.55	0.48
2:B:529:TRP:CB	2:B:531:LEU:HD11	2.43	0.48
2:D:311:LEU:HA	2:D:314:SER:OG	2.13	0.48
2:D:285:VAL:CG2	2:D:313:LEU:HD21	2.42	0.48
2:B:213:ASN:ND2	2:B:257:LEU:HD21	2.29	0.48
2:D:68:LYS:HD2	2:D:81:PHE:CE1	2.49	0.48
1:A:236:LYS:C	1:A:238:GLY:H	2.22	0.48
2:B:423:ILE:O	2:B:426:ALA:HB3	2.14	0.48
2:B:365:ILE:HA	2:B:366:PRO:HD3	1.75	0.48
1:C:208:LEU:HD23	1:C:292:LEU:CD1	2.43	0.48
2:D:153:ASN:O	2:D:157:VAL:HG23	2.14	0.48
2:B:246:TRP:CE3	2:B:249:LEU:HD12	2.49	0.47
1:C:334:THR:C	1:C:336:SER:H	2.22	0.47
1:A:104:LEU:HD13	1:A:137:TYR:CD2	2.48	0.47
1:C:154:MET:CB	1:C:202:LEU:CD1	2.68	0.47
2:D:152:LEU:CD1	2:D:186:ARG:HD3	2.45	0.47
2:D:246:TRP:HA	2:D:246:TRP:CE3	2.48	0.47
1:A:17:TYR:OH	2:B:79:MET:HG2	2.14	0.47
2:D:152:LEU:HD23	2:D:152:LEU:HA	1.67	0.47
2:D:390:TRP:C	2:D:390:TRP:CD2	2.92	0.47
1:A:67:GLU:O	1:A:67:GLU:HG2	2.14	0.47
2:B:281:SER:HB2	2:B:313:LEU:CD1	2.45	0.47
1:C:310:VAL:HG22	1:C:319:LEU:HD11	1.95	0.47
2:D:95:ILE:O	2:D:98:LEU:CB	2.63	0.47
2:D:258:LEU:CD1	2:D:289:ILE:HG23	2.37	0.47
2:D:410:GLU:HG3	2:D:411:SER:N	2.29	0.47
1:A:42:THR:O	1:A:42:THR:CG2	2.62	0.47
1:A:86:GLU:O	1:A:86:GLU:HG3	2.14	0.47
1:C:126:ALA:HB2	1:C:136:LEU:CD1	2.44	0.47
1:A:66:PRO:C	1:A:68:TYR:H	2.23	0.47
2:B:138:LYS:O	2:B:141:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:PHE:C	2:B:204:PHE:CD2	2.93	0.47
2:D:284:ALA:O	2:D:287:ASP:HB2	2.15	0.47
2:D:337:LEU:HD23	2:D:337:LEU:HA	1.55	0.47
2:D:541:THR:O	2:D:545:GLN:HG3	2.15	0.47
1:A:71:ILE:C	1:A:72:ILE:HD12	2.40	0.47
1:A:171:LEU:HD12	1:A:171:LEU:O	2.14	0.47
1:C:56:SER:HB2	1:C:77:TYR:H	1.79	0.47
2:D:248:LEU:O	2:D:249:LEU:C	2.57	0.47
2:D:490:ALA:HB2	2:D:529:TRP:HZ2	1.78	0.47
2:D:508:LEU:N	2:D:509:PRO:HD2	2.30	0.47
1:A:27:CYS:CA	1:A:33:ILE:HG23	2.45	0.47
2:D:373:GLU:O	2:D:377:MET:HG3	2.15	0.47
2:D:246:TRP:CD1	2:D:331:TYR:CD1	3.02	0.47
1:A:112:TYR:HE1	1:A:168:ASP:HA	1.80	0.46
2:B:170:ASN:HD22	2:B:170:ASN:HA	1.56	0.46
2:B:345:LYS:C	2:B:347:LEU:H	2.23	0.46
1:C:240:ILE:HG12	1:C:321:SER:HB2	1.97	0.46
2:D:364:TYR:CD2	2:D:365:ILE:HG12	2.49	0.46
2:B:152:LEU:HD21	2:B:182:LEU:HG	1.98	0.46
2:B:211:TRP:CE3	2:B:212:ILE:HG13	2.51	0.46
2:B:315:GLN:HE21	1:C:207:LYS:H	1.63	0.46
2:D:151:ILE:HD12	2:D:423:ILE:HD11	1.97	0.46
1:A:117:ALA:HB2	1:A:173:TRP:CZ2	2.51	0.46
2:B:531:LEU:N	2:B:531:LEU:HD12	2.31	0.46
1:C:32:HIS:HB3	1:C:52:ARG:HA	1.96	0.46
2:B:99:ASP:HB2	2:B:104:PHE:CE1	2.51	0.46
2:B:208:LEU:O	2:B:209:LEU:C	2.59	0.46
2:D:188:MET:HE2	2:D:398:ILE:HG12	1.97	0.46
1:C:129:GLY:O	1:C:131:ASP:N	2.48	0.46
1:C:172:SER:HB3	1:C:218:ILE:HG22	1.98	0.46
2:B:152:LEU:HD23	2:B:152:LEU:HA	1.69	0.46
2:B:342:ASN:O	2:B:343:GLN:C	2.59	0.46
1:C:120:HIS:CE1	1:C:121:LEU:HD21	2.51	0.46
2:D:515:THR:HB	2:D:518:ASP:H	1.80	0.46
1:A:137:TYR:CD1	1:A:151:THR:HB	2.51	0.46
1:C:73:ALA:HB2	1:C:116:PHE:CZ	2.51	0.46
2:D:160:GLY:O	2:D:162:VAL:N	2.49	0.46
2:D:211:TRP:CE3	2:D:212:ILE:HG13	2.51	0.46
2:D:254:LEU:C	2:D:256:GLY:H	2.24	0.46
2:B:258:LEU:O	2:B:262:ILE:HG13	2.16	0.46
2:B:529:TRP:C	2:B:531:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:HIS:HB3	1:C:52:ARG:CA	2.45	0.46
1:C:125:LEU:HG	1:C:126:ALA:N	2.30	0.46
1:C:190:GLN:O	1:C:215:ILE:HD12	2.16	0.46
2:D:474:CYS:SG	2:D:507:LEU:HD13	2.56	0.46
1:A:128:LEU:HG	1:A:171:LEU:HD23	1.98	0.46
1:C:171:LEU:HD12	1:C:171:LEU:O	2.15	0.46
2:D:99:ASP:HB2	2:D:104:PHE:CD1	2.50	0.46
2:D:151:ILE:HD12	2:D:423:ILE:CD1	2.46	0.46
2:D:543:GLY:O	2:D:544:ASN:C	2.60	0.45
1:A:24:VAL:HG13	1:A:36:PHE:HB2	1.97	0.45
1:A:322:ALA:HB2	1:A:328:VAL:HG22	1.99	0.45
1:C:71:ILE:C	1:C:72:ILE:HD12	2.42	0.45
2:D:81:PHE:O	2:D:82:ILE:HD12	2.16	0.45
2:D:246:TRP:CE3	2:D:249:LEU:HD12	2.51	0.45
2:D:311:LEU:O	2:D:312:LYS:C	2.59	0.45
2:D:521:TRP:O	2:D:524:SER:HB3	2.16	0.45
1:A:104:LEU:HD13	1:A:137:TYR:CG	2.52	0.45
2:B:110:GLY:O	2:B:114:ILE:HG13	2.16	0.45
2:B:554:GLU:O	2:B:555:SER:C	2.58	0.45
1:A:28:SER:HB2	1:A:30:ASP:CG	2.42	0.45
1:A:60:ALA:O	1:A:61:ILE:CG1	2.64	0.45
1:A:71:ILE:HA	1:A:84:TRP:O	2.16	0.45
1:A:215:ILE:HG22	1:A:216:ARG:N	2.31	0.45
2:B:95:ILE:O	2:B:98:LEU:HB2	2.16	0.45
1:C:120:HIS:CE1	1:C:121:LEU:CD2	2.99	0.45
1:C:186:SER:HB2	1:C:218:ILE:HG13	1.98	0.45
2:D:345:LYS:C	2:D:347:LEU:N	2.74	0.45
2:D:346:ILE:O	2:D:350:SER:HB2	2.16	0.45
2:D:353:TRP:HE1	2:D:391:GLU:CG	2.28	0.45
2:D:385:ASP:HB2	2:D:388:ASN:HD21	1.80	0.45
1:A:189:GLU:HA	1:A:213:SER:O	2.16	0.45
2:B:80:ALA:HB3	2:B:91:TYR:HB2	1.98	0.45
2:B:246:TRP:CD1	2:B:331:TYR:CG	3.04	0.45
2:B:390:TRP:CD2	2:B:390:TRP:C	2.95	0.45
1:C:62:ASP:HB3	1:C:116:PHE:CD2	2.51	0.45
1:C:236:LYS:C	1:C:238:GLY:N	2.75	0.45
1:C:72:ILE:HD12	1:C:72:ILE:N	2.32	0.45
1:C:171:LEU:HD12	1:C:171:LEU:C	2.42	0.45
2:D:422:MET:SD	2:D:466:LEU:HD21	2.56	0.45
1:A:60:ALA:CB	1:A:114:VAL:HG12	2.44	0.45
1:A:62:ASP:HB3	1:A:116:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:C	1:A:68:TYR:N	2.73	0.45
1:A:82:LYS:CB	1:A:84:TRP:HE1	2.30	0.45
2:B:160:GLY:O	2:B:161:ARG:C	2.60	0.45
2:B:521:TRP:O	2:B:524:SER:HB3	2.17	0.45
2:B:527:VAL:CG1	2:B:528:GLU:H	2.30	0.45
1:A:16:VAL:HG12	1:A:17:TYR:N	2.28	0.45
1:A:208:LEU:HD23	1:A:292:LEU:CD1	2.46	0.45
1:A:222:PRO:O	1:A:223:SER:C	2.59	0.45
2:B:153:ASN:O	2:B:157:VAL:HG23	2.17	0.45
2:B:208:LEU:HG	2:B:212:ILE:CD1	2.46	0.45
1:C:328:VAL:HG11	2:D:69:PHE:CD1	2.52	0.45
2:D:342:ASN:O	2:D:343:GLN:C	2.60	0.45
2:D:360:PHE:CG	2:D:374:TYR:CD1	3.01	0.45
1:A:207:LYS:O	1:A:292:LEU:CD1	2.65	0.45
2:D:249:LEU:O	2:D:253:VAL:HG23	2.17	0.45
2:D:390:TRP:O	2:D:390:TRP:CE3	2.69	0.45
1:A:77:TYR:HA	1:A:110:SER:HB2	1.99	0.45
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.37	0.45
2:B:358:CYS:O	2:B:359:GLY:C	2.60	0.45
1:C:58:ILE:CD1	1:C:76:SER:HB2	2.36	0.45
1:A:236:LYS:C	1:A:238:GLY:N	2.75	0.44
2:D:74:LEU:HD13	2:D:95:ILE:CG1	2.47	0.44
2:D:529:TRP:C	2:D:531:LEU:HD12	2.41	0.44
2:D:536:LYS:C	2:D:538:ILE:N	2.74	0.44
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.78	0.44
2:B:522:MET:HE3	2:B:538:ILE:HG13	2.00	0.44
1:C:153:GLU:O	1:C:154:MET:HG2	2.18	0.44
2:D:65:MET:HA	2:D:66:PRO:HD3	1.77	0.44
2:D:171:ARG:O	2:D:175:LEU:HB2	2.17	0.44
2:D:219:PRO:HB2	2:D:223:TYR:CE2	2.53	0.44
2:B:151:ILE:HD12	2:B:423:ILE:HD11	1.98	0.44
2:D:178:SER:O	2:D:179:LEU:C	2.60	0.44
1:A:218:ILE:HD13	1:A:233:THR:HG22	1.98	0.44
1:C:27:CYS:HA	1:C:33:ILE:HG23	2.00	0.44
2:D:208:LEU:O	2:D:209:LEU:C	2.61	0.44
2:B:530:ARG:O	2:B:532:PRO:HD3	2.16	0.44
1:C:42:THR:O	1:C:42:THR:CG2	2.66	0.44
2:D:365:ILE:HA	2:D:366:PRO:HD3	1.74	0.44
1:A:104:LEU:HD21	1:A:149:THR:HG21	2.00	0.44
2:B:282:PHE:CZ	2:B:332:ILE:HD13	2.52	0.44
2:D:82:ILE:HG23	2:D:83:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:ILE:HA	2:D:227:VAL:HG23	1.98	0.44
2:D:529:TRP:O	2:D:531:LEU:HD12	2.17	0.44
1:A:168:ASP:H	1:A:188:LEU:HD11	1.83	0.44
1:C:222:PRO:O	1:C:223:SER:C	2.60	0.44
1:C:235:CYS:HB3	1:C:237:ASP:OD1	2.18	0.44
1:C:294:VAL:C	1:C:295:GLU:OE1	2.60	0.44
2:D:95:ILE:O	2:D:98:LEU:HB3	2.18	0.44
2:D:152:LEU:HD12	2:D:186:ARG:HD3	1.99	0.44
1:C:51:TRP:NE1	1:C:84:TRP:HZ3	2.15	0.44
1:C:222:PRO:HG2	1:C:313:ASN:O	2.18	0.44
1:A:112:TYR:CE1	1:A:168:ASP:HA	2.53	0.43
1:A:309:SER:CB	2:B:68:LYS:HA	2.49	0.43
2:B:92:PRO:C	2:B:93:VAL:CG2	2.91	0.43
2:B:177:GLU:HG3	2:B:390:TRP:HB3	2.00	0.43
2:B:508:LEU:N	2:B:509:PRO:HD2	2.33	0.43
1:C:82:LYS:CB	1:C:84:TRP:HE1	2.31	0.43
1:C:309:SER:HB3	2:D:68:LYS:HA	2.00	0.43
2:D:158:PHE:O	2:D:158:PHE:CD2	2.71	0.43
2:D:334:ASP:O	2:D:337:LEU:N	2.51	0.43
2:B:364:TYR:CD2	2:B:365:ILE:HG12	2.52	0.43
2:B:515:THR:HB	2:B:518:ASP:H	1.83	0.43
2:B:535:ALA:O	2:B:536:LYS:C	2.61	0.43
1:C:28:SER:HB2	1:C:30:ASP:CG	2.43	0.43
1:C:77:TYR:N	1:C:77:TYR:CD2	2.86	0.43
2:D:160:GLY:O	2:D:161:ARG:C	2.60	0.43
1:A:133:ILE:HG23	1:A:133:ILE:O	2.18	0.43
1:A:309:SER:HB3	2:B:68:LYS:HA	2.01	0.43
1:C:66:PRO:C	1:C:68:TYR:H	2.26	0.43
1:C:128:LEU:HD23	1:C:128:LEU:HA	1.80	0.43
2:D:212:ILE:CD1	2:D:358:CYS:SG	3.06	0.43
2:D:249:LEU:HD23	2:D:249:LEU:HA	1.60	0.43
1:A:325:ASP:OD2	1:A:329:ARG:NH2	2.52	0.43
2:B:74:LEU:HD13	2:B:95:ILE:HG13	1.99	0.43
2:B:337:LEU:HA	2:B:337:LEU:HD23	1.80	0.43
1:C:118:PRO:HG2	1:C:174:CYS:O	2.19	0.43
1:A:334:THR:C	1:A:336:SER:N	2.77	0.43
2:B:423:ILE:H	2:B:423:ILE:HG13	1.57	0.43
1:C:12:VAL:N	1:C:29:SER:HG	2.17	0.43
1:C:53:ALA:CB	1:C:84:TRP:CZ2	3.02	0.43
1:A:228:TYR:CE1	2:B:457:TYR:HE2	2.35	0.43
2:B:337:LEU:HD22	2:B:342:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:LEU:C	2:B:509:PRO:HD2	2.44	0.43
1:C:334:THR:C	1:C:336:SER:N	2.73	0.43
2:D:148:MET:O	2:D:149:GLU:C	2.61	0.43
2:D:368:LEU:H	2:D:368:LEU:CD2	2.28	0.43
2:D:523:LEU:C	2:D:525:ILE:N	2.76	0.43
1:A:126:ALA:HA	1:A:135:ARG:O	2.18	0.43
1:A:239:ARG:CD	1:A:296:LEU:HD11	2.13	0.43
1:C:86:GLU:O	1:C:86:GLU:HG3	2.18	0.43
1:C:145:LEU:HD12	1:C:145:LEU:HA	1.86	0.43
2:D:531:LEU:HD12	2:D:531:LEU:N	2.33	0.43
1:A:73:ALA:HB2	1:A:116:PHE:CZ	2.53	0.43
1:C:36:PHE:CD1	1:C:36:PHE:N	2.86	0.43
1:C:60:ALA:O	1:C:61:ILE:HG13	2.19	0.43
1:C:133:ILE:O	1:C:133:ILE:CG2	2.65	0.43
2:D:402:ILE:O	2:D:403:HIS:C	2.61	0.43
2:B:68:LYS:HD2	2:B:81:PHE:CZ	2.54	0.43
2:B:249:LEU:HD23	2:B:249:LEU:HA	1.59	0.43
2:B:423:ILE:O	2:B:424:CYS:C	2.61	0.43
1:C:77:TYR:HA	1:C:110:SER:HB2	1.99	0.43
1:C:221:ALA:HB2	1:C:230:LEU:HD12	2.00	0.43
1:C:320:SER:OG	2:D:71:LEU:CD1	2.67	0.43
2:D:213:ASN:ND2	2:D:257:LEU:HD21	2.34	0.43
1:A:310:VAL:CG2	1:A:319:LEU:HD11	2.49	0.43
2:B:74:LEU:CD2	2:B:475:SER:O	2.55	0.43
2:B:393:PRO:O	2:B:397:ILE:HG13	2.18	0.43
1:A:217:SER:OG	1:A:309:SER:HA	2.19	0.42
2:B:152:LEU:CD1	2:B:186:ARG:HD3	2.48	0.42
2:D:71:LEU:HB3	2:D:72:GLY:H	1.60	0.42
1:A:343:SER:OG	2:B:96:PRO:HG2	2.18	0.42
2:B:95:ILE:O	2:B:96:PRO:C	2.62	0.42
2:B:99:ASP:CB	2:B:104:PHE:CD1	3.03	0.42
2:B:508:LEU:HD23	2:B:508:LEU:HA	1.86	0.42
1:C:129:GLY:O	1:C:130:ASN:C	2.62	0.42
1:C:240:ILE:O	1:C:296:LEU:HD12	2.18	0.42
2:D:205:ILE:H	2:D:205:ILE:HG13	1.44	0.42
2:D:490:ALA:HB2	2:D:529:TRP:CZ2	2.53	0.42
2:D:554:GLU:O	2:D:555:SER:C	2.61	0.42
1:A:195:GLN:O	1:A:202:LEU:N	2.53	0.42
1:A:216:ARG:NH1	1:A:308:TRP:CE2	2.87	0.42
2:B:99:ASP:C	2:B:101:SER:H	2.27	0.42
2:B:191:ILE:O	2:B:192:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ALA:O	2:B:265:ILE:HG13	2.20	0.42
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.82	0.42
2:D:258:LEU:HD22	2:D:289:ILE:HG23	2.02	0.42
2:D:546:MET:HE3	2:D:546:MET:HB3	1.95	0.42
2:B:260:GLN:O	2:B:261:ALA:C	2.62	0.42
2:B:356:SER:HB2	2:B:378:SER:OG	2.19	0.42
2:B:471:PHE:N	2:B:471:PHE:CD2	2.87	0.42
1:C:53:ALA:HB2	1:C:84:TRP:CZ2	2.55	0.42
2:D:182:LEU:O	2:D:182:LEU:HD12	2.19	0.42
2:D:282:PHE:CE1	2:D:332:ILE:HD13	2.54	0.42
1:A:38:LEU:HD21	2:B:77:GLN:NE2	2.34	0.42
2:B:219:PRO:HB2	2:B:223:TYR:CZ	2.55	0.42
2:B:248:LEU:O	2:B:249:LEU:C	2.62	0.42
2:D:160:GLY:C	2:D:162:VAL:N	2.75	0.42
2:D:536:LYS:C	2:D:538:ILE:H	2.28	0.42
1:A:193:ILE:HD11	1:A:231:ILE:HD12	2.01	0.42
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.85	0.42
2:B:118:LEU:O	2:B:120:ASP:N	2.53	0.42
2:B:151:ILE:HD12	2:B:423:ILE:CD1	2.50	0.42
1:C:56:SER:HB3	1:C:77:TYR:HB2	1.98	0.42
2:D:357:PHE:CE1	2:D:398:ILE:HG21	2.55	0.42
2:B:375:LEU:HD11	2:B:395:VAL:HG13	2.01	0.42
2:D:473:LEU:C	2:D:475:SER:H	2.28	0.42
2:B:403:HIS:C	2:B:405:ILE:H	2.26	0.42
2:B:523:LEU:C	2:B:525:ILE:N	2.77	0.42
1:C:216:ARG:NH1	1:C:308:TRP:CE2	2.88	0.42
1:C:231:ILE:HG22	1:C:232:ALA:N	2.34	0.42
2:D:353:TRP:O	2:D:378:SER:OG	2.33	0.42
2:B:476:LEU:HD12	2:B:476:LEU:O	2.20	0.42
1:C:309:SER:CB	2:D:68:LYS:HA	2.50	0.42
2:D:118:LEU:O	2:D:119:GLY:C	2.62	0.42
1:A:27:CYS:HB2	1:A:33:ILE:HD12	2.01	0.42
1:A:27:CYS:SG	1:A:27:CYS:O	2.78	0.42
1:A:337:ASN:HD22	1:A:337:ASN:HA	1.66	0.42
2:B:180:THR:HG21	2:B:215:SER:HA	2.00	0.42
2:B:252:LEU:HD23	2:B:252:LEU:HA	1.86	0.42
1:C:56:SER:HB2	1:C:76:SER:OG	2.20	0.42
1:C:68:TYR:CZ	1:C:123:LEU:HG	2.55	0.42
2:D:204:PHE:CD2	2:D:204:PHE:C	2.98	0.42
2:D:547:LEU:O	2:D:548:SER:C	2.62	0.42
2:B:71:LEU:HB3	2:B:72:GLY:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LEU:HD12	2:B:186:ARG:HD3	2.01	0.41
2:B:462:ALA:C	2:B:464:TYR:H	2.28	0.41
2:B:554:GLU:O	2:B:555:SER:O	2.37	0.41
1:C:71:ILE:HA	1:C:84:TRP:O	2.20	0.41
1:C:208:LEU:HA	1:C:209:PRO:HD3	1.82	0.41
2:D:260:GLN:O	2:D:261:ALA:C	2.62	0.41
1:A:292:LEU:O	2:D:311:LEU:HD13	2.20	0.41
2:B:514:VAL:HG12	2:B:515:THR:N	2.35	0.41
1:C:65:SER:HA	1:C:66:PRO:HD3	1.89	0.41
2:D:185:LEU:HD23	2:D:185:LEU:C	2.45	0.41
2:B:99:ASP:O	2:B:101:SER:N	2.48	0.41
2:B:181:VAL:O	2:B:184:CYS:HB3	2.20	0.41
2:B:209:LEU:CD2	2:B:256:GLY:HA3	2.50	0.41
2:B:469:PHE:O	2:B:472:GLU:HB2	2.20	0.41
2:B:513:PHE:CD1	2:B:519:ILE:HD11	2.55	0.41
1:C:106:ASP:OD2	1:C:151:THR:HG21	2.20	0.41
2:D:138:LYS:O	2:D:141:ASN:HB2	2.20	0.41
1:A:68:TYR:CZ	1:A:123:LEU:HG	2.55	0.41
1:C:77:TYR:N	1:C:77:TYR:HD2	2.18	0.41
2:D:375:LEU:HD12	2:D:379:LEU:CD2	2.51	0.41
2:D:536:LYS:O	2:D:540:THR:HG23	2.21	0.41
1:A:308:TRP:NE1	2:B:66:PRO:HB3	2.35	0.41
2:B:184:CYS:HB2	2:B:211:TRP:NE1	2.36	0.41
2:B:360:PHE:CB	2:B:374:TYR:HD1	2.33	0.41
2:B:388:ASN:C	2:B:390:TRP:H	2.28	0.41
1:C:228:TYR:HE1	2:D:457:TYR:HE2	1.67	0.41
2:D:201:ARG:O	2:D:205:ILE:HD11	2.21	0.41
1:A:16:VAL:O	1:A:24:VAL:HG23	2.20	0.41
2:B:179:LEU:O	2:B:183:ASN:HB2	2.20	0.41
2:B:208:LEU:HG	2:B:212:ILE:HD11	2.01	0.41
2:B:392:GLN:NE2	2:B:396:ASP:OD1	2.54	0.41
1:C:86:GLU:OE1	1:C:98:TRP:CD1	2.74	0.41
2:D:290:GLU:O	2:D:290:GLU:HG2	2.20	0.41
1:A:77:TYR:N	1:A:77:TYR:CD2	2.88	0.41
2:B:95:ILE:O	2:B:98:LEU:HB3	2.20	0.41
2:B:549:ALA:O	2:B:550:HIS:C	2.62	0.41
2:D:413:ASP:O	2:D:414:SER:C	2.63	0.41
1:A:125:LEU:HG	1:A:126:ALA:N	2.35	0.41
1:A:172:SER:HB3	1:A:218:ILE:HG22	2.02	0.41
2:B:370:LEU:HB3	2:B:374:TYR:CD2	2.54	0.41
1:C:111:LEU:HA	1:C:129:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:252:LEU:HD23	2:D:252:LEU:HA	1.78	0.41
2:D:359:GLY:O	2:D:360:PHE:C	2.64	0.41
2:D:403:HIS:C	2:D:405:ILE:H	2.28	0.41
1:A:36:PHE:CD1	1:A:36:PHE:N	2.88	0.41
1:A:125:LEU:HG	1:A:126:ALA:H	1.85	0.41
1:A:235:CYS:SG	1:A:237:ASP:CG	3.04	0.41
2:B:67:LEU:C	2:B:68:LYS:CG	2.94	0.41
2:B:68:LYS:HD2	2:B:81:PHE:CE1	2.55	0.41
2:B:74:LEU:C	2:B:76:TYR:N	2.77	0.41
2:B:303:PHE:O	2:B:306:TRP:CB	2.69	0.41
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.85	0.41
2:B:345:LYS:C	2:B:347:LEU:N	2.78	0.41
2:B:359:GLY:O	2:B:360:PHE:C	2.64	0.41
2:B:471:PHE:N	2:B:471:PHE:HD2	2.19	0.41
2:B:534:ILE:O	2:B:538:ILE:HG12	2.20	0.41
1:C:125:LEU:HG	1:C:126:ALA:H	1.84	0.41
1:C:154:MET:HE2	1:C:202:LEU:HD21	2.03	0.41
2:D:67:LEU:HD22	2:D:82:ILE:CG1	2.49	0.41
2:D:261:ALA:O	2:D:265:ILE:HG13	2.20	0.41
2:D:269:ASP:O	2:D:270:LEU:C	2.62	0.41
1:A:129:GLY:C	1:A:169:PHE:HZ	2.28	0.41
2:B:370:LEU:O	2:B:374:TYR:CD2	2.74	0.41
1:C:218:ILE:HD13	1:C:233:THR:HG22	2.02	0.41
2:D:75:SER:O	2:D:75:SER:OG	2.39	0.41
1:A:235:CYS:HB3	1:A:237:ASP:OD1	2.21	0.40
1:C:236:LYS:HA	1:C:306:GLU:HG3	2.03	0.40
2:D:311:LEU:HA	2:D:311:LEU:HD23	1.82	0.40
2:D:462:ALA:C	2:D:464:TYR:H	2.29	0.40
1:A:217:SER:O	1:A:233:THR:HA	2.21	0.40
2:B:303:PHE:CG	2:B:304:ARG:N	2.89	0.40
2:B:402:ILE:O	2:B:403:HIS:C	2.63	0.40
2:D:514:VAL:HG12	2:D:515:THR:N	2.36	0.40
2:D:537:GLU:O	2:D:537:GLU:HG2	2.22	0.40
1:A:195:GLN:CG	1:A:196:ARG:H	2.28	0.40
1:A:221:ALA:HA	1:A:222:PRO:HD3	1.86	0.40
2:B:67:LEU:HD23	2:B:67:LEU:N	2.36	0.40
2:B:160:GLY:C	2:B:162:VAL:H	2.29	0.40
2:B:360:PHE:CG	2:B:374:TYR:HD1	2.39	0.40
2:D:281:SER:HB2	2:D:313:LEU:CD1	2.52	0.40
2:D:281:SER:HB2	2:D:313:LEU:HD11	2.04	0.40
1:A:68:TYR:N	1:A:68:TYR:CD1	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LEU:N	2:B:270:LEU:HD23	2.36	0.40
1:C:172:SER:HB2	1:C:218:ILE:O	2.22	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	239/349 (68%)	201 (84%)	33 (14%)	5 (2%)	5	31
1	C	239/349 (68%)	204 (85%)	30 (13%)	5 (2%)	5	31
2	B	373/564 (66%)	293 (79%)	64 (17%)	16 (4%)	2	18
2	D	373/564 (66%)	298 (80%)	62 (17%)	13 (4%)	3	23
All	All	1224/1826 (67%)	996 (81%)	189 (15%)	39 (3%)	3	24

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
2	B	270	LEU
2	B	364	TYR
2	B	403	HIS
1	C	130	ASN
2	D	270	LEU
2	D	364	TYR
2	D	403	HIS
2	D	141	ASN
1	A	28	SER
2	B	76	TYR
2	B	100	THR
2	B	141	ASN

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Mol	Chain	Res	Type
2	B	161	ARG
2	B	353	TRP
2	B	539	TYR
1	C	28	SER
1	C	181	GLU
2	D	74	LEU
2	D	76	TYR
2	D	119	GLY
2	D	161	ARG
1	A	110	SER
1	A	141	GLU
1	A	181	GLU
2	B	74	LEU
2	B	119	GLY
2	B	210	ASN
2	D	371	SER
2	D	389	ASP
2	B	108	VAL
2	B	331	TYR
1	C	110	SER
2	D	108	VAL
2	D	524	SER
2	B	255	ARG
2	B	267	ARG
1	C	141	GLU
2	D	402	ILE

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	188/305 (62%)	165 (88%)	23 (12%)	5	22
1	C	189/305 (62%)	168 (89%)	21 (11%)	6	25
2	B	304/504 (60%)	257 (84%)	47 (16%)	2	15
2	D	304/504 (60%)	255 (84%)	49 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	985/1618 (61%)	845 (86%)	140 (14%)	3 18

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	24	VAL
1	A	26	THR
1	A	32	HIS
1	A	33	ILE
1	A	38	LEU
1	A	42	THR
1	A	48	SER
1	A	51	TRP
1	A	77	TYR
1	A	113	SER
1	A	123	LEU
1	A	134	LEU
1	A	156	VAL
1	A	176	SER
1	A	230	LEU
1	A	233	THR
1	A	246	THR
1	A	291	ASN
1	A	294	VAL
1	A	314	LEU
1	A	321	SER
1	A	337	ASN
2	B	75	SER
2	B	98	LEU
2	B	99	ASP
2	B	103	GLU
2	B	109	SER
2	B	149	GLU
2	B	169	VAL
2	B	170	ASN
2	B	175	LEU
2	B	180	THR
2	B	187	THR
2	B	205	ILE
2	B	227	VAL
2	B	248	LEU

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Mol	Chain	Res	Type
2	B	287	ASP
2	B	292	LEU
2	B	313	LEU
2	B	314	SER
2	B	342	ASN
2	B	350	SER
2	B	352	THR
2	B	356	SER
2	B	361	LEU
2	B	369	GLU
2	B	371	SER
2	B	376	GLN
2	B	379	LEU
2	B	382	ASN
2	B	383	VAL
2	B	384	VAL
2	B	388	ASN
2	B	394	CYS
2	B	404	SER
2	B	405	ILE
2	B	423	ILE
2	B	427	LYS
2	B	455	PHE
2	B	456	SER
2	B	457	TYR
2	B	466	LEU
2	B	475	SER
2	B	486	ILE
2	B	489	ILE
2	B	496	THR
2	B	503	VAL
2	B	534	ILE
2	B	546	MET
1	C	16	VAL
1	C	24	VAL
1	C	32	HIS
1	C	33	ILE
1	C	38	LEU
1	C	42	THR
1	C	48	SER
1	C	51	TRP
1	C	77	TYR

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Mol	Chain	Res	Type
1	C	113	SER
1	C	134	LEU
1	C	156	VAL
1	C	176	SER
1	C	202	LEU
1	C	230	LEU
1	C	233	THR
1	C	246	THR
1	C	291	ASN
1	C	294	VAL
1	C	314	LEU
1	C	321	SER
2	D	71	LEU
2	D	75	SER
2	D	93	VAL
2	D	98	LEU
2	D	99	ASP
2	D	103	GLU
2	D	109	SER
2	D	149	GLU
2	D	169	VAL
2	D	170	ASN
2	D	175	LEU
2	D	180	THR
2	D	187	THR
2	D	205	ILE
2	D	227	VAL
2	D	248	LEU
2	D	287	ASP
2	D	292	LEU
2	D	313	LEU
2	D	314	SER
2	D	342	ASN
2	D	350	SER
2	D	352	THR
2	D	356	SER
2	D	361	LEU
2	D	369	GLU
2	D	371	SER
2	D	376	GLN
2	D	378	SER
2	D	379	LEU

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Mol	Chain	Res	Type
2	D	382	ASN
2	D	383	VAL
2	D	384	VAL
2	D	388	ASN
2	D	394	CYS
2	D	404	SER
2	D	405	ILE
2	D	427	LYS
2	D	455	PHE
2	D	456	SER
2	D	457	TYR
2	D	466	LEU
2	D	475	SER
2	D	484	VAL
2	D	486	ILE
2	D	489	ILE
2	D	496	THR
2	D	503	VAL
2	D	552	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	337	ASN
2	B	170	ASN
2	B	250	ASN
2	B	342	ASN
2	B	376	GLN
2	B	382	ASN
2	B	388	ASN
1	C	120	HIS
1	C	337	ASN
2	D	78	ASN
2	D	170	ASN
2	D	213	ASN
2	D	250	ASN
2	D	376	GLN
2	D	382	ASN
2	D	388	ASN
2	D	403	HIS
2	D	544	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	255/349 (73%)	0.48	14 (5%)	30 18	113, 154, 229, 288	0
1	C	255/349 (73%)	0.46	8 (3%)	51 29	124, 191, 259, 320	0
2	B	395/564 (70%)	0.17	14 (3%)	47 26	106, 137, 205, 278	0
2	D	395/564 (70%)	0.27	12 (3%)	52 30	97, 134, 201, 267	0
All	All	1300/1826 (71%)	0.32	48 (3%)	45 25	97, 148, 235, 320	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	76	TYR	5.6
2	D	505	ALA	4.8
1	A	329	ARG	4.7
2	D	506	GLU	4.5
2	D	511	TYR	3.2
2	B	244	TYR	3.2
2	D	223	TYR	3.1
2	D	241	GLU	3.1
2	B	282	PHE	3.1
1	C	317	THR	3.1
1	A	328	VAL	3.1
2	B	467	ASN	2.9
2	B	67	LEU	2.8
2	B	487	GLY	2.7
2	B	218	GLU	2.7
1	A	133	ILE	2.6
2	D	245	PHE	2.5
1	C	142	PRO	2.5
2	B	87	LYS	2.5
1	A	317	THR	2.4
1	C	126	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	217	GLY	2.4
1	A	229	GLN	2.4
1	A	192	ILE	2.4
2	D	99	ASP	2.4
1	A	196	ARG	2.3
1	A	181	GLU	2.3
2	B	176	GLU	2.3
2	B	178	SER	2.3
2	B	471	PHE	2.2
1	A	247	GLU	2.2
2	D	264	CYS	2.2
1	C	64	ALA	2.2
1	C	168	ASP	2.2
2	B	257	LEU	2.1
1	A	323	GLY	2.1
1	A	176	SER	2.1
1	A	330	LEU	2.1
2	D	218	GLU	2.1
2	B	162	VAL	2.1
2	B	241	GLU	2.1
1	C	57	SER	2.0
1	C	310	VAL	2.0
2	D	181	VAL	2.0
1	A	305	GLY	2.0
1	C	194	TYR	2.0
1	A	325	ASP	2.0
2	D	120	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.