



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:48 AM UTC

PDB ID : 1LS5 / pdb_00001ls5
Title : Crystal structure of plasmepsin IV from *P. falciparum* in complex with pepstatin A
Authors : Asojo, O.A.; Gulnik, S.V.; Afonina, E.; Yu, B.; Ellman, J.A.; Haque, T.S.; Silva, A.M.
Deposited on : 2002-05-16
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

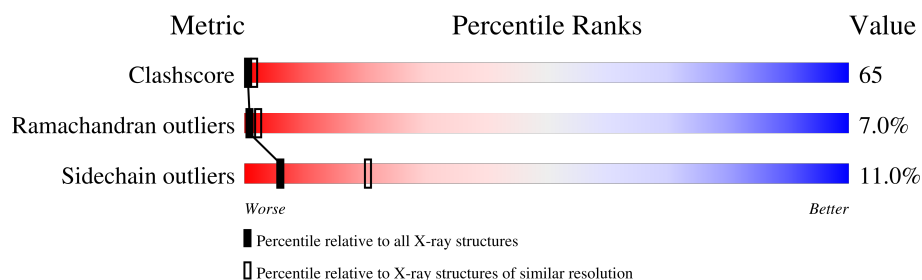
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

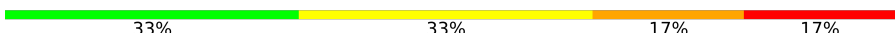
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	
1	B	328	
2	C	6	
2	D	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5342 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 plasmepsin IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2609	1686	397	515	11			
1	B	328	Total	C	N	O	S	0	0	0
			2609	1686	397	515	11			

- Molecule 2 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			48	34	5	9			
2	D	6	Total	C	N	O	0	0	0
			48	34	5	9			

- Molecule 3 is water.

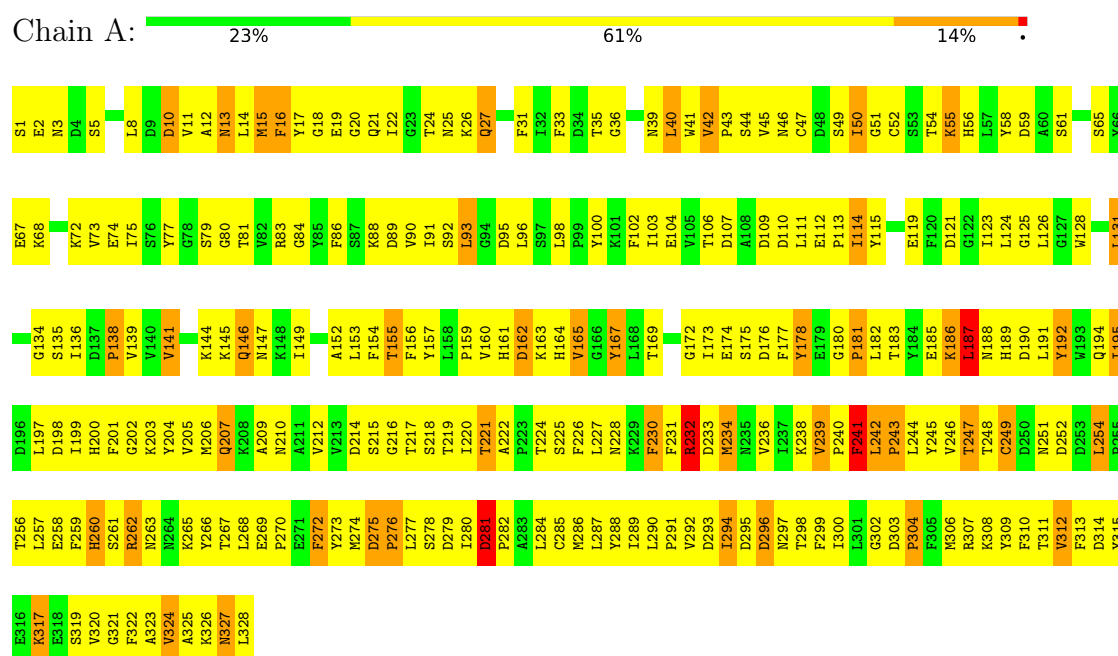
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	10	Total	O	0	0
			10	10		

3 Residue-property plots

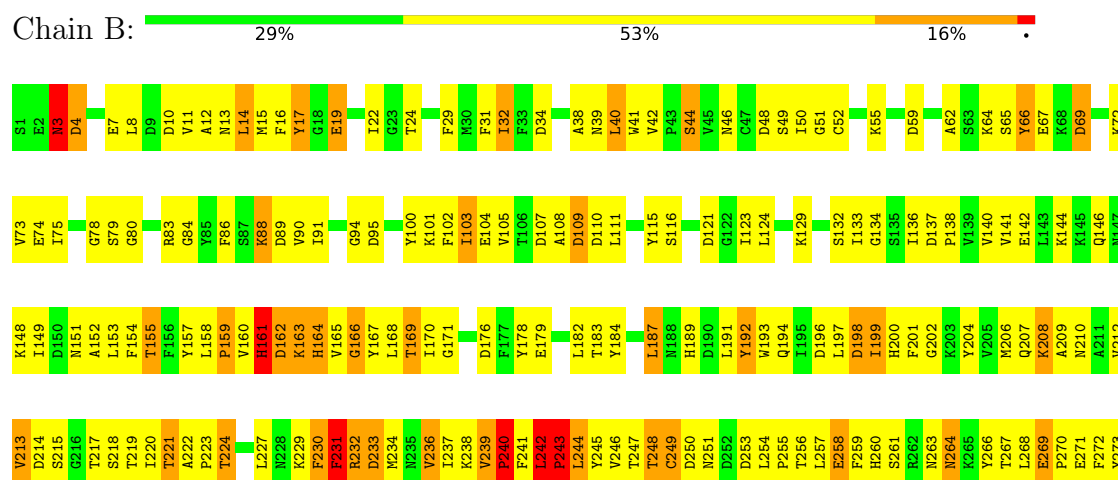
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: plasmepsin IV

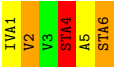


- Molecule 1: plasmepsin IV

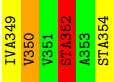
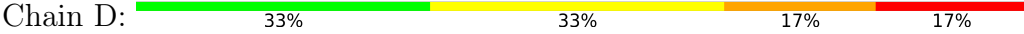




● Molecule 2: Pepstatin



● Molecule 2: Pepstatin



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.93Å 101.93Å 123.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5342	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/2677	1.11	25/3637 (0.7%)
1	B	0.54	0/2677	1.12	22/3637 (0.6%)
2	C	0.81	0/17	2.05	1/21 (4.8%)
2	D	0.80	0/17	2.23	1/21 (4.8%)
All	All	0.53	0/5388	1.12	49/7316 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	PHE	N-CA-C	-10.92	99.96	113.18
1	A	180	GLY	CA-C-N	10.67	133.17	119.84
1	A	180	GLY	C-N-CA	10.67	133.17	119.84
1	B	242	LEU	N-CA-C	8.20	127.93	109.81
1	B	34	ASP	N-CA-C	7.80	121.79	107.99
1	B	198	ASP	N-CA-C	-7.72	96.70	108.67
1	B	148	LYS	N-CA-C	-7.66	104.08	113.50
1	A	221	THR	N-CA-C	7.45	121.89	108.48
1	A	254	LEU	CA-C-N	7.30	129.21	120.23
1	A	254	LEU	C-N-CA	7.30	129.21	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	CYS	N-CA-C	6.93	120.27	109.52
1	A	55	LYS	N-CA-C	6.91	119.25	108.96
1	B	298	THR	N-CA-C	6.55	119.92	109.24
1	B	134	GLY	N-CA-C	-6.50	105.63	115.00
1	A	311	THR	N-CA-C	6.24	120.22	110.17
1	A	192	TYR	N-CA-C	-6.19	101.31	110.48
1	B	214	ASP	N-CA-C	6.16	118.89	107.99
2	D	350	VAL	CG1-CB-CG2	-6.16	97.25	110.80
1	B	89	ASP	N-CA-C	6.11	117.17	108.74
1	A	207	GLN	N-CA-C	6.06	118.53	109.25
1	B	192	TYR	N-CA-C	-6.04	102.01	110.35
1	B	32	ILE	N-CA-C	-6.02	98.54	107.51
1	A	272	PHE	N-CA-C	5.96	117.86	111.36
2	C	2	VAL	CG1-CB-CG2	-5.88	97.85	110.80
1	A	232	ARG	N-CA-C	-5.85	105.24	112.38
1	B	69	ASP	N-CA-C	-5.84	98.35	110.80
1	B	167	TYR	N-CA-C	5.77	118.51	108.76
1	A	106	THR	N-CA-C	-5.69	107.33	114.56
1	B	3	ASN	CB-CA-C	-5.68	108.39	116.34
1	A	175	SER	N-CA-C	5.67	119.67	112.87
1	A	214	ASP	N-CA-C	5.66	117.62	108.34
1	A	173	ILE	CB-CA-C	-5.59	105.87	111.80
1	A	187	LEU	N-CA-C	5.59	122.71	110.80
1	B	275	ASP	CA-C-N	-5.55	114.00	119.99
1	B	275	ASP	C-N-CA	-5.55	114.00	119.99
1	B	297	ASN	N-CA-C	-5.47	104.05	111.55
1	B	269	GLU	CA-C-N	5.44	126.64	119.84
1	B	269	GLU	C-N-CA	5.44	126.64	119.84
1	A	27	GLN	CA-C-N	5.41	125.32	119.85
1	A	27	GLN	C-N-CA	5.41	125.32	119.85
1	A	50	ILE	N-CA-C	5.34	115.97	110.36
1	A	203	LYS	N-CA-C	-5.20	105.40	112.26
1	A	173	ILE	N-CA-C	5.18	114.73	107.37
1	A	131	LEU	N-CA-C	-5.17	107.35	113.97
1	B	215	SER	N-CA-C	-5.16	106.93	113.18
1	A	138	PRO	N-CA-C	5.16	119.67	111.26
1	A	249	CYS	N-CA-C	5.04	119.14	112.89
1	A	167	TYR	N-CA-C	5.04	117.46	109.50
1	B	199	ILE	N-CA-C	5.00	115.51	108.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	4	STA	Peptide,Mainchain
2	D	352	STA	Peptide,Mainchain

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	2609	0	2501	408	8
1	B	2609	0	2501	281	7
2	C	48	0	60	11	0
2	D	48	0	60	6	0
3	A	18	0	0	5	0
3	B	10	0	0	1	0
All	All	5342	0	5122	678	8

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 65.

All (678) 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:B:277:LEU:HD22	1:B:280:ILE:HD13	1.33	1.09
1:B:310:PHE:HB2	1:B:325:ALA:HB2	1.39	1.04
1:A:74:GLU:HG2	1:A:83:ARG:HG2	1.38	1.04
1:B:221:THR:HB	1:B:300:ILE:HB	1.39	1.02
1:A:307:ARG:HH11	1:A:307:ARG:HB2	1.26	1.00
1:A:251:ASN:HD22	1:A:252:ASP:H	1.08	0.99
1:B:247:THR:HG22	1:B:248:THR:H	1.29	0.97
1:A:269:GLU:H	1:A:308:LYS:HZ1	1.09	0.96
1:A:251:ASN:ND2	1:A:252:ASP:H	1.63	0.95
1:A:307:ARG:HB2	1:A:307:ARG:NH1	1.83	0.94
1:B:178:TYR:HA	1:B:325:ALA:HA	1.50	0.93
1:A:281:ASP:OD2	1:B:281:ASP:HB2	1.66	0.93
1:A:5:SER:HB3	1:A:169:THR:HG22	1.49	0.92
1:A:275:ASP:H	1:A:285:CYS:HB2	1.33	0.92
1:A:244:LEU:HD21	1:A:288:TYR:HD2	1.33	0.91
1:B:19:GLU:H	1:B:19:GLU:CD	1.79	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:HB3	1:B:260:HIS:HB2	1.52	0.91
1:A:13:ASN:HB2	1:A:307:ARG:HH21	1.36	0.90
1:A:236:VAL:HG12	1:A:245:TYR:HB3	1.51	0.90
1:B:294:ILE:HD12	1:B:294:ILE:H	1.33	0.89
1:A:314:ASP:OD2	1:A:317:LYS:HD2	1.72	0.88
1:A:144:LYS:HG2	1:A:152:ALA:HB2	1.52	0.88
1:B:241:PHE:O	1:B:243:PRO:HD3	1.74	0.87
1:A:27:GLN:HE22	1:A:59:ASP:H	1.23	0.85
1:B:138:PRO:HB2	1:B:141:VAL:HG23	1.58	0.85
1:A:221:THR:HB	1:A:300:ILE:HB	1.59	0.85
1:B:303:ASP:O	1:B:307:ARG:HG2	1.76	0.84
1:A:114:ILE:H	1:A:114:ILE:HD12	1.40	0.84
1:A:251:ASN:HD22	1:A:252:ASP:N	1.75	0.83
1:B:247:THR:HG22	1:B:248:THR:N	1.94	0.82
1:A:277:LEU:HD21	1:A:286:MET:HG2	1.63	0.81
1:A:13:ASN:HB3	1:A:161:HIS:HA	1.61	0.81
1:A:79:SER:HB3	1:A:114:ILE:HG12	1.63	0.81
1:A:303:ASP:HB3	1:A:307:ARG:HH12	1.45	0.80
1:A:244:LEU:HD21	1:A:288:TYR:HA	1.64	0.80
1:A:293:ASP:HB2	1:B:50:ILE:HD11	1.63	0.80
1:A:326:LYS:O	1:A:328:LEU:N	2.13	0.79
1:B:276:PRO:HA	1:B:285:CYS:SG	2.22	0.79
1:A:236:VAL:CG1	1:A:245:TYR:HB3	2.13	0.79
1:A:18:GLY:HA3	1:A:33:PHE:HE1	1.47	0.79
1:A:199:ILE:HD13	1:A:209:ALA:HB3	1.63	0.79
1:B:263:ASN:O	1:B:264:ASN:HB2	1.83	0.79
1:A:17:TYR:CE2	1:A:119:GLU:HB2	2.19	0.78
1:A:293:ASP:HB2	1:B:50:ILE:CD1	2.14	0.78
1:A:234:MET:HE3	1:A:254:LEU:HD22	1.65	0.78
1:A:185:GLU:O	1:A:319:SER:HB2	1.84	0.78
1:B:258:GLU:HB3	1:B:267:THR:HG22	1.64	0.77
1:B:142:GLU:HG3	1:B:146:GLN:HE21	1.48	0.77
1:B:268:LEU:HD23	1:B:308:LYS:HD2	1.66	0.77
1:A:277:LEU:HD13	1:A:285:CYS:HA	1.65	0.77
1:A:12:ALA:O	1:A:14:LEU:HD12	1.84	0.77
1:A:275:ASP:N	1:A:285:CYS:HB2	2.00	0.77
1:A:242:LEU:HD12	1:A:243:PRO:HA	1.67	0.77
1:B:236:VAL:HB	1:B:287:LEU:HD22	1.65	0.77
1:B:239:VAL:HG13	1:B:240:PRO:HD2	1.67	0.77
1:B:251:ASN:HB3	1:B:254:LEU:HD11	1.67	0.75
1:A:209:ALA:HA	1:A:297:ASN:HD21	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LEU:HG	1:B:286:MET:HE1	1.68	0.75
1:A:209:ALA:HA	1:A:297:ASN:ND2	2.02	0.74
1:A:284:LEU:HD22	1:B:280:ILE:HG23	1.67	0.74
1:A:281:ASP:HB2	1:A:284:LEU:HD13	1.69	0.74
1:A:198:ASP:OD1	1:A:207:GLN:HA	1.86	0.74
1:A:242:LEU:HD12	1:A:243:PRO:CA	2.17	0.74
1:B:270:PRO:HB3	1:B:274:MET:HE2	1.69	0.74
1:A:290:LEU:HD23	1:A:291:PRO:HD2	1.68	0.73
1:A:293:ASP:HB2	1:B:50:ILE:CG1	2.17	0.73
1:B:12:ALA:HB3	1:B:14:LEU:HD11	1.69	0.73
1:B:308:LYS:HD3	1:B:309:TYR:CE2	2.23	0.73
1:B:200:HIS:HB2	1:B:258:GLU:HG3	1.70	0.73
1:A:244:LEU:CD2	1:A:288:TYR:HA	2.19	0.73
1:A:221:THR:O	1:A:299:PHE:HA	1.89	0.73
1:A:160:VAL:HG23	1:A:163:LYS:HZ1	1.54	0.72
1:A:178:TYR:HE2	1:A:182:LEU:HB2	1.54	0.72
1:B:73:VAL:HG11	1:B:86:PHE:CE2	2.24	0.72
1:A:270:PRO:HA	1:A:273:TYR:CZ	2.25	0.71
1:A:5:SER:CB	1:A:169:THR:HG22	2.21	0.71
1:A:13:ASN:HD22	1:A:307:ARG:CZ	2.04	0.71
1:A:178:TYR:C	1:A:326:LYS:HD2	2.15	0.71
1:B:91:ILE:HD13	1:B:100:TYR:HB3	1.72	0.71
1:B:239:VAL:HG12	1:B:243:PRO:HG2	1.71	0.70
1:B:277:LEU:HB2	1:B:284:LEU:O	1.91	0.70
1:A:96:LEU:HD11	1:A:149:ILE:HD13	1.73	0.70
1:A:219:THR:HG22	1:A:220:ILE:O	1.92	0.70
1:A:40:LEU:HD12	1:A:41:TRP:N	2.07	0.70
1:B:244:LEU:HD13	1:B:244:LEU:H	1.56	0.70
1:A:5:SER:HA	1:A:169:THR:HA	1.72	0.70
1:A:178:TYR:CE2	1:A:182:LEU:HB2	2.26	0.69
1:A:293:ASP:HB2	1:B:50:ILE:HG12	1.74	0.69
1:B:246:VAL:HG12	1:B:247:THR:N	2.07	0.69
1:A:246:VAL:HB	1:A:286:MET:SD	2.32	0.69
1:B:155:THR:N	1:B:169:THR:O	2.22	0.68
1:B:163:LYS:HG3	1:B:164:HIS:NE2	2.08	0.68
1:A:220:ILE:HB	1:A:289:ILE:HD13	1.76	0.68
1:A:27:GLN:HE22	1:A:59:ASP:N	1.91	0.68
1:B:103:ILE:HD12	1:B:103:ILE:N	2.09	0.68
1:B:144:LYS:HA	1:B:149:ILE:HG22	1.76	0.68
1:B:222:ALA:HB3	1:B:227:LEU:HD13	1.76	0.68
1:B:44:SER:HB2	1:B:104:GLU:OE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LEU:HD11	1:B:289:ILE:HG22	1.76	0.67
1:B:40:LEU:HD12	1:B:41:TRP:N	2.08	0.67
1:A:294:ILE:HG23	2:C:6:STA:HD13	1.74	0.67
1:B:165:VAL:HG13	1:B:165:VAL:O	1.93	0.67
1:B:221:THR:CG2	1:B:292:VAL:HB	2.25	0.67
1:B:247:THR:CG2	1:B:248:THR:H	2.05	0.67
1:A:24:THR:C	1:A:26:LYS:H	2.02	0.66
1:A:160:VAL:HG22	1:A:307:ARG:HG3	1.78	0.66
1:B:227:LEU:CD2	1:B:291:PRO:HB3	2.25	0.66
1:B:254:LEU:HD12	1:B:254:LEU:N	2.10	0.66
1:B:178:TYR:CA	1:B:325:ALA:HA	2.26	0.66
1:A:307:ARG:HH11	1:A:307:ARG:CB	2.06	0.66
1:A:244:LEU:HD21	1:A:288:TYR:CD2	2.25	0.65
1:B:59:ASP:OD2	1:B:62:ALA:HB2	1.97	0.65
1:A:42:VAL:HG11	1:A:58:TYR:HB2	1.78	0.65
1:A:73:VAL:HG21	1:A:103:ILE:HD13	1.79	0.65
1:B:221:THR:HB	1:B:300:ILE:CB	2.22	0.65
1:B:275:ASP:HB2	1:B:286:MET:HB2	1.79	0.65
1:A:153:LEU:HB2	1:A:313:PHE:O	1.96	0.65
1:A:27:GLN:NE2	1:A:59:ASP:H	1.94	0.65
1:A:124:LEU:HD23	1:A:125:GLY:O	1.95	0.64
1:A:200:HIS:HB2	1:A:204:TYR:O	1.97	0.64
1:A:222:ALA:HB3	1:A:227:LEU:CD1	2.27	0.64
1:B:242:LEU:O	1:B:243:PRO:C	2.40	0.64
1:A:269:GLU:N	1:A:308:LYS:HZ1	1.89	0.64
1:A:67:GLU:HB2	1:A:88:LYS:NZ	2.12	0.64
1:A:268:LEU:HA	1:A:308:LYS:HE3	1.77	0.64
1:A:269:GLU:H	1:A:308:LYS:NZ	1.91	0.64
1:B:200:HIS:CB	1:B:258:GLU:HG3	2.27	0.64
1:A:55:LYS:HB2	1:A:121:ASP:OD1	1.97	0.64
1:A:188:ASN:C	1:A:189:HIS:ND1	2.56	0.64
1:A:2:GLU:O	1:A:3:ASN:ND2	2.31	0.63
1:A:260:HIS:HB3	1:A:265:LYS:CB	2.29	0.63
1:A:268:LEU:HD12	1:A:308:LYS:HE2	1.79	0.63
1:B:111:LEU:HG	1:B:115:TYR:HB2	1.79	0.63
1:A:13:ASN:HD22	1:A:307:ARG:NH2	1.96	0.63
1:A:239:VAL:HG22	1:A:246:VAL:HG12	1.79	0.63
1:A:12:ALA:O	1:A:13:ASN:OD1	2.17	0.63
1:B:3:ASN:HB3	1:B:170:ILE:O	1.98	0.63
1:B:206:MET:HA	1:B:206:MET:HE3	1.81	0.63
1:A:234:MET:HB3	1:A:236:VAL:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:HB3	1:A:227:LEU:HD13	1.81	0.62
1:A:73:VAL:HG11	1:A:86:PHE:CE2	2.33	0.62
1:A:281:ASP:HB2	1:A:284:LEU:CD1	2.28	0.62
1:B:163:LYS:HG3	1:B:164:HIS:CE1	2.34	0.62
1:B:218:SER:HA	1:B:303:ASP:OD2	1.99	0.62
1:A:18:GLY:HA3	1:A:33:PHE:CE1	2.31	0.62
1:B:305:PHE:HD2	1:B:305:PHE:O	1.81	0.62
1:A:144:LYS:CG	1:A:152:ALA:HB2	2.27	0.62
1:A:260:HIS:N	1:A:260:HIS:CD2	2.68	0.62
2:C:2:VAL:HG11	2:C:4:STA:HD23	1.82	0.62
1:A:174:GLU:HB3	1:A:177:PHE:CE2	2.34	0.61
1:A:251:ASN:ND2	1:A:252:ASP:N	2.39	0.61
2:C:2:VAL:HG12	2:C:4:STA:HB2	1.83	0.61
1:A:210:ASN:HD22	1:A:298:THR:HG23	1.66	0.61
1:A:244:LEU:O	1:A:286:MET:HE1	2.01	0.61
1:A:278:SER:HA	1:A:282:PRO:HA	1.82	0.61
1:A:174:GLU:CD	1:A:176:ASP:H	2.08	0.61
1:A:238:LYS:HB2	1:A:245:TYR:CE2	2.36	0.61
1:A:159:PRO:HB3	1:A:164:HIS:ND1	2.16	0.61
1:A:192:TYR:O	1:A:194:GLN:HG2	2.01	0.61
1:A:73:VAL:HG21	1:A:103:ILE:CD1	2.30	0.61
1:B:14:LEU:HD23	1:B:288:TYR:CE2	2.36	0.61
1:A:284:LEU:HD12	1:A:284:LEU:N	2.16	0.60
1:A:304:PRO:HD2	3:A:366:HOH:O	2.01	0.60
1:B:238:LYS:HD2	1:B:242:LEU:H	1.66	0.60
1:B:204:TYR:CE2	1:B:229:LYS:HB3	2.36	0.60
1:B:281:ASP:OD2	1:B:283:ALA:HB3	2.02	0.60
1:A:177:PHE:O	1:A:326:LYS:HG2	2.02	0.60
1:A:234:MET:HB3	1:A:236:VAL:CG2	2.32	0.60
1:A:241:PHE:CD2	1:A:241:PHE:N	2.70	0.60
1:A:256:THR:HG23	1:A:268:LEU:O	2.02	0.60
1:A:277:LEU:HB2	1:A:284:LEU:O	2.02	0.60
1:A:218:SER:HA	1:A:303:ASP:OD2	2.02	0.60
1:B:178:TYR:O	1:B:326:LYS:HE2	2.01	0.59
1:B:187:LEU:HB3	1:B:189:HIS:O	2.02	0.59
1:A:163:LYS:HG2	1:A:164:HIS:CG	2.38	0.59
1:B:159:PRO:O	1:B:160:VAL:HG23	2.03	0.59
1:B:248:THR:HG23	1:B:250:ASP:OD1	2.03	0.59
1:B:210:ASN:O	1:B:298:THR:HA	2.03	0.59
1:B:237:ILE:N	1:B:246:VAL:O	2.35	0.59
1:B:242:LEU:HD23	1:B:242:LEU:C	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLN:HE22	1:A:58:TYR:HA	1.66	0.59
1:A:309:TYR:HA	1:A:325:ALA:H	1.67	0.59
1:A:221:THR:CG2	1:A:292:VAL:HB	2.32	0.59
1:B:239:VAL:CG1	1:B:243:PRO:HG2	2.31	0.59
1:A:293:ASP:CB	1:B:50:ILE:HD11	2.31	0.59
1:B:17:TYR:HB3	1:B:32:ILE:HD13	1.84	0.59
1:B:84:GLY:HA3	1:B:104:GLU:O	2.02	0.59
1:B:159:PRO:HB3	1:B:164:HIS:ND1	2.18	0.59
1:B:253:ASP:CG	1:B:253:ASP:O	2.45	0.59
1:A:20:GLY:HA3	1:A:31:PHE:CD2	2.38	0.58
1:A:178:TYR:HD2	1:A:323:ALA:HB1	1.68	0.58
1:B:3:ASN:O	1:B:4:ASP:HB2	2.03	0.58
1:A:14:LEU:O	1:A:15:MET:HB3	2.02	0.58
1:A:303:ASP:O	1:A:307:ARG:N	2.36	0.58
1:A:326:LYS:C	1:A:328:LEU:H	2.10	0.58
1:B:14:LEU:O	1:B:218:SER:OG	2.16	0.58
1:A:50:ILE:C	1:A:52:CYS:H	2.10	0.58
1:B:238:LYS:NZ	1:B:241:PHE:HA	2.19	0.58
1:A:187:LEU:O	1:A:189:HIS:N	2.33	0.58
1:B:40:LEU:HG	1:B:102:PHE:CB	2.34	0.58
1:B:199:ILE:HD12	1:B:209:ALA:HB3	1.84	0.58
1:A:19:GLU:N	1:A:19:GLU:OE1	2.36	0.58
1:A:36:GLY:HA3	2:C:4:STA:HM2	1.84	0.58
1:B:227:LEU:HD23	1:B:291:PRO:HB3	1.85	0.58
1:A:220:ILE:HG22	1:A:221:THR:N	2.18	0.58
1:A:89:ASP:OD1	1:A:90:VAL:N	2.34	0.57
1:B:244:LEU:C	1:B:245:TYR:CD1	2.82	0.57
1:A:174:GLU:OE1	1:A:176:ASP:HB2	2.04	0.57
1:A:189:HIS:HB2	1:A:194:GLN:OE1	2.03	0.57
1:A:27:GLN:NE2	1:A:58:TYR:HA	2.18	0.57
1:B:29:PHE:CD2	1:B:42:VAL:HG21	2.39	0.57
1:A:188:ASN:OD1	1:A:195:ILE:HA	2.05	0.57
1:B:241:PHE:C	1:B:243:PRO:HD3	2.29	0.57
1:A:187:LEU:HD23	1:A:190:ASP:OD1	2.03	0.57
1:A:83:ARG:NH1	1:A:107:ASP:OD1	2.38	0.57
1:A:232:ARG:HA	1:A:232:ARG:HH11	1.70	0.57
1:A:10:ASP:OD2	1:A:16:PHE:CE2	2.58	0.57
1:B:153:LEU:C	1:B:153:LEU:HD12	2.30	0.57
1:B:272:PHE:CD2	1:B:308:LYS:HB2	2.39	0.56
1:A:13:ASN:CB	1:A:307:ARG:HH21	2.14	0.56
1:A:177:PHE:C	1:A:326:LYS:HG2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HG22	1:A:248:THR:H	1.70	0.56
1:B:4:ASP:OD2	1:B:94:GLY:HA3	2.04	0.56
1:B:163:LYS:HG3	1:B:164:HIS:CD2	2.40	0.56
1:A:155:THR:HB	1:A:169:THR:OG1	2.05	0.56
1:B:142:GLU:HG3	1:B:146:GLN:NE2	2.18	0.56
2:D:350:VAL:HG11	2:D:352:STA:HD23	1.87	0.56
1:A:176:ASP:O	1:A:326:LYS:HD3	2.05	0.56
1:B:4:ASP:OD1	1:B:95:ASP:OD2	2.23	0.56
1:B:246:VAL:CG1	1:B:247:THR:N	2.69	0.56
1:B:15:MET:HE3	2:D:350:VAL:HG21	1.88	0.56
1:B:244:LEU:HD13	1:B:244:LEU:N	2.21	0.56
1:A:210:ASN:ND2	1:A:298:THR:HG23	2.21	0.56
1:A:35:THR:HG23	1:A:215:SER:OG	2.06	0.56
1:A:162:ASP:CG	1:A:163:LYS:H	2.12	0.56
1:B:294:ILE:HG12	1:B:298:THR:O	2.05	0.56
1:A:275:ASP:CB	1:A:276:PRO:HA	2.36	0.56
1:A:279:ASP:HB3	1:B:237:ILE:HD13	1.87	0.56
1:A:197:LEU:HD23	1:A:261:SER:HB3	1.89	0.55
1:B:219:THR:HG22	1:B:288:TYR:HB3	1.87	0.55
1:A:74:GLU:HG2	1:A:83:ARG:CG	2.24	0.55
1:B:12:ALA:O	1:B:13:ASN:HB2	2.06	0.55
1:B:249:CYS:HB2	1:B:283:ALA:O	2.06	0.55
1:A:162:ASP:CG	1:A:163:LYS:N	2.63	0.55
1:A:14:LEU:HD22	2:C:1:IVA:HG13	1.88	0.55
1:B:138:PRO:HB2	1:B:141:VAL:CG2	2.36	0.55
1:A:295:ASP:O	1:A:296:ASP:HB2	2.05	0.55
1:B:29:PHE:CE2	1:B:42:VAL:HG21	2.42	0.55
1:A:312:VAL:O	1:A:321:GLY:N	2.37	0.55
1:A:79:SER:OG	2:C:2:VAL:HG13	2.07	0.55
1:A:224:THR:HG22	1:A:228:ASN:HD21	1.72	0.55
1:B:206:MET:HG2	1:B:209:ALA:HB2	1.88	0.55
1:B:306:MET:C	1:B:308:LYS:H	2.13	0.55
1:B:12:ALA:HB3	1:B:14:LEU:CD1	2.35	0.54
1:A:79:SER:O	1:A:114:ILE:HD13	2.07	0.54
1:A:178:TYR:CE2	1:A:182:LEU:HD13	2.42	0.54
1:A:256:THR:HG23	1:A:268:LEU:C	2.33	0.54
1:A:21:GLN:HB2	1:A:92:SER:HB2	1.90	0.54
1:A:221:THR:HG21	1:A:292:VAL:HB	1.88	0.54
1:A:284:LEU:HD22	1:B:280:ILE:CG2	2.36	0.54
1:B:40:LEU:HG	1:B:102:PHE:HB2	1.89	0.54
1:B:83:ARG:NH1	1:B:107:ASP:OD2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:HA	1:A:285:CYS:HB2	1.89	0.54
1:A:280:ILE:HA	1:B:284:LEU:HD12	1.90	0.54
1:B:236:VAL:HG23	1:B:246:VAL:O	2.07	0.54
1:A:17:TYR:HE2	1:A:119:GLU:HB2	1.70	0.54
1:A:146:GLN:O	1:A:147:ASN:C	2.51	0.54
1:A:314:ASP:CG	1:A:317:LYS:H	2.15	0.54
1:B:160:VAL:O	1:B:162:ASP:N	2.40	0.54
1:A:182:LEU:HD12	1:A:323:ALA:HB2	1.89	0.54
1:B:256:THR:HG22	1:B:267:THR:HB	1.90	0.54
1:B:230:PHE:CD1	1:B:234:MET:HE3	2.42	0.54
1:A:16:PHE:CD1	1:A:16:PHE:N	2.75	0.54
1:A:74:GLU:OE1	1:A:83:ARG:HD2	2.08	0.54
1:A:92:SER:C	1:A:93:LEU:HD13	2.33	0.54
1:A:13:ASN:OD1	1:A:14:LEU:HD12	2.09	0.53
1:A:15:MET:C	1:A:16:PHE:CD1	2.86	0.53
1:A:219:THR:HG21	1:A:290:LEU:H	1.73	0.53
1:A:162:ASP:O	1:A:163:LYS:HB3	2.09	0.53
1:A:276:PRO:C	1:A:277:LEU:HD12	2.33	0.53
1:A:277:LEU:HD22	1:A:285:CYS:C	2.33	0.53
1:B:24:THR:HG23	1:B:65:SER:OG	2.08	0.53
1:A:13:ASN:O	1:A:307:ARG:NH2	2.41	0.53
1:A:113:PRO:HG3	1:B:78:GLY:O	2.07	0.53
1:A:303:ASP:HB2	1:A:304:PRO:HD3	1.90	0.53
1:B:7:GLU:OE1	1:B:165:VAL:HG11	2.09	0.53
1:A:40:LEU:HG	1:A:102:PHE:HB2	1.91	0.53
1:A:65:SER:HB2	1:A:90:VAL:HG23	1.91	0.53
1:A:131:LEU:HB2	1:A:191:LEU:HD13	1.90	0.53
1:A:278:SER:O	1:A:279:ASP:C	2.52	0.53
1:A:24:THR:C	1:A:26:LYS:N	2.65	0.53
1:A:242:LEU:HD12	1:A:243:PRO:CB	2.39	0.53
1:A:245:TYR:HB2	1:A:287:LEU:HD23	1.89	0.53
1:B:11:VAL:HG21	1:B:17:TYR:OH	2.08	0.53
1:B:227:LEU:HD22	1:B:291:PRO:HB3	1.91	0.53
1:A:260:HIS:HB3	1:A:265:LYS:HA	1.89	0.53
1:A:275:ASP:CA	1:A:285:CYS:HB2	2.39	0.53
1:A:163:LYS:HG2	1:A:164:HIS:N	2.24	0.52
1:B:67:GLU:HB3	1:B:88:LYS:HB2	1.90	0.52
1:A:197:LEU:CD2	1:A:261:SER:HB3	2.40	0.52
1:A:277:LEU:HD13	1:A:286:MET:H	1.74	0.52
1:A:83:ARG:HB2	1:A:107:ASP:HB3	1.92	0.52
1:A:114:ILE:H	1:A:114:ILE:CD1	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:O	1:A:226:PHE:CD1	2.63	0.52
1:A:236:VAL:HG11	1:A:287:LEU:HD22	1.92	0.52
1:A:244:LEU:HD12	1:A:286:MET:CE	2.40	0.52
1:B:179:GLU:OE2	1:B:326:LYS:HA	2.09	0.52
1:B:230:PHE:O	1:B:234:MET:HE2	2.09	0.52
1:A:268:LEU:HA	1:A:308:LYS:CE	2.40	0.52
1:B:193:TRP:O	1:B:213:VAL:HG23	2.09	0.52
1:B:199:ILE:CD1	1:B:209:ALA:HB3	2.40	0.52
1:A:91:ILE:HD12	1:A:91:ILE:N	2.25	0.52
1:A:176:ASP:C	1:A:326:LYS:HD3	2.35	0.52
1:A:49:SER:O	1:A:52:CYS:HB2	2.10	0.52
1:A:277:LEU:CD1	1:A:286:MET:H	2.23	0.52
1:B:210:ASN:N	1:B:297:ASN:O	2.41	0.52
1:B:219:THR:CG2	1:B:288:TYR:CD2	2.93	0.52
1:A:160:VAL:C	1:A:162:ASP:H	2.15	0.51
1:A:257:LEU:HB3	1:A:259:PHE:CZ	2.45	0.51
1:B:201:PHE:HA	1:B:257:LEU:HD22	1.92	0.51
1:B:206:MET:SD	1:B:297:ASN:OD1	2.68	0.51
1:A:174:GLU:HB3	1:A:177:PHE:CD2	2.45	0.51
1:A:178:TYR:OH	1:A:182:LEU:HD22	2.10	0.51
1:A:155:THR:HG23	1:A:310:PHE:CE1	2.45	0.51
1:A:260:HIS:HB3	1:A:265:LYS:HB2	1.91	0.51
1:A:310:PHE:HB2	1:A:325:ALA:HA	1.91	0.51
1:B:158:LEU:HB2	1:B:307:ARG:HA	1.92	0.51
1:B:251:ASN:CB	1:B:254:LEU:HD11	2.38	0.51
1:A:8:LEU:HD11	1:A:156:PHE:HE1	1.75	0.51
1:A:185:GLU:O	1:A:319:SER:CB	2.56	0.51
1:B:12:ALA:HA	1:B:161:HIS:CE1	2.45	0.51
1:B:317:LYS:O	1:B:318:GLU:C	2.54	0.51
1:A:157:TYR:HB2	1:A:310:PHE:CD1	2.45	0.51
1:A:294:ILE:HD12	2:C:6:STA:CD1	2.40	0.51
1:B:193:TRP:CZ2	1:B:313:PHE:HB3	2.45	0.51
1:B:209:ALA:HA	1:B:297:ASN:HB3	1.92	0.51
1:A:55:LYS:HD2	1:A:115:TYR:CZ	2.45	0.51
1:B:66:TYR:CG	1:B:67:GLU:N	2.78	0.51
1:A:10:ASP:OD1	1:A:11:VAL:N	2.44	0.51
1:A:242:LEU:HD12	1:A:243:PRO:HB3	1.93	0.51
1:A:281:ASP:CG	1:B:281:ASP:HB2	2.35	0.51
1:B:157:TYR:O	1:B:158:LEU:HD23	2.11	0.51
1:B:230:PHE:CE1	1:B:234:MET:HE3	2.45	0.51
1:B:256:THR:HG22	1:B:256:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:HA3	1:A:104:GLU:O	2.11	0.50
1:A:219:THR:CG2	1:A:290:LEU:H	2.24	0.50
1:A:145:LYS:C	1:A:147:ASN:H	2.18	0.50
1:A:280:ILE:N	1:A:280:ILE:HD12	2.26	0.50
1:B:305:PHE:C	1:B:305:PHE:CD2	2.89	0.50
1:A:275:ASP:H	1:A:285:CYS:CB	2.17	0.50
1:A:192:TYR:HB2	1:A:212:VAL:HG22	1.92	0.50
1:A:201:PHE:CD1	1:A:202:GLY:N	2.78	0.50
1:A:254:LEU:HD13	1:A:274:MET:HE1	1.94	0.50
1:A:294:ILE:HD12	2:C:6:STA:HD11	1.94	0.50
1:A:114:ILE:HD12	1:A:114:ILE:N	2.18	0.50
1:A:138:PRO:HG2	1:A:141:VAL:CG2	2.42	0.50
1:A:201:PHE:HB3	1:A:257:LEU:HA	1.94	0.50
1:B:183:THR:O	1:B:321:GLY:HA2	2.12	0.50
1:A:163:LYS:HD2	1:A:327:ASN:OD1	2.11	0.50
1:A:312:VAL:HB	1:A:321:GLY:HA3	1.93	0.50
1:B:80:GLY:HA3	1:B:111:LEU:CD1	2.41	0.50
1:A:95:ASP:OD2	1:A:96:LEU:HG	2.12	0.50
1:B:152:ALA:HB3	1:B:316:GLU:HG3	1.93	0.50
1:B:236:VAL:HB	1:B:287:LEU:CD2	2.39	0.49
1:B:305:PHE:HD2	1:B:305:PHE:C	2.20	0.49
1:A:230:PHE:CE2	1:A:234:MET:SD	3.05	0.49
1:A:277:LEU:HD12	1:A:277:LEU:N	2.27	0.49
1:B:219:THR:HA	1:B:304:PRO:CD	2.42	0.49
1:A:47:CYS:SG	1:A:49:SER:HB3	2.52	0.49
1:A:231:PHE:C	1:A:233:ASP:N	2.70	0.49
1:A:258:GLU:HB3	1:A:265:LYS:HZ3	1.78	0.49
1:B:44:SER:C	1:B:46:ASN:H	2.21	0.49
1:B:206:MET:CG	1:B:209:ALA:HB2	2.41	0.49
1:A:92:SER:O	1:A:93:LEU:HD13	2.12	0.49
1:A:187:LEU:C	1:A:188:ASN:OD1	2.55	0.49
1:A:275:ASP:OD2	1:A:285:CYS:HB3	2.13	0.49
1:B:50:ILE:N	1:B:50:ILE:HD12	2.28	0.49
1:B:301:LEU:HD13	1:B:305:PHE:CD1	2.48	0.49
1:A:224:THR:HG22	1:A:228:ASN:ND2	2.28	0.49
1:B:74:GLU:C	1:B:75:ILE:HD12	2.37	0.49
1:B:294:ILE:HG12	1:B:298:THR:HB	1.93	0.49
1:A:42:VAL:CG1	1:A:58:TYR:HB2	2.42	0.49
1:A:280:ILE:O	1:A:280:ILE:HG22	2.12	0.49
1:B:165:VAL:O	1:B:166:GLY:O	2.31	0.49
1:A:210:ASN:HD22	1:A:298:THR:CG2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:O	1:B:234:MET:HB2	2.13	0.49
1:B:231:PHE:O	1:B:231:PHE:CD1	2.66	0.49
1:B:273:TYR:O	1:B:288:TYR:HB2	2.13	0.49
1:A:67:GLU:HB3	1:A:88:LYS:HB3	1.94	0.49
1:A:80:GLY:HA3	1:A:111:LEU:HD12	1.94	0.49
1:A:221:THR:HB	1:A:300:ILE:CB	2.37	0.49
1:B:227:LEU:HD22	1:B:291:PRO:CA	2.43	0.49
1:B:276:PRO:C	1:B:278:SER:H	2.20	0.49
1:A:20:GLY:HA3	1:A:31:PHE:HD2	1.78	0.48
1:A:25:ASN:HD21	1:A:27:GLN:HG2	1.78	0.48
1:B:272:PHE:O	1:B:307:ARG:NH1	2.45	0.48
1:B:83:ARG:H	1:B:105:VAL:HG13	1.79	0.48
1:A:152:ALA:O	1:A:314:ASP:OD1	2.32	0.48
1:A:310:PHE:H	1:A:325:ALA:N	2.12	0.48
1:B:124:LEU:C	1:B:124:LEU:HD23	2.38	0.48
1:B:178:TYR:HA	1:B:325:ALA:CA	2.31	0.48
1:B:251:ASN:O	1:B:254:LEU:HD13	2.13	0.48
1:B:286:MET:SD	1:B:288:TYR:HE1	2.36	0.48
1:B:303:ASP:N	1:B:304:PRO:CD	2.76	0.48
1:B:305:PHE:O	1:B:305:PHE:CD2	2.65	0.48
1:A:13:ASN:HB3	1:A:161:HIS:CA	2.40	0.48
1:B:55:LYS:HB3	1:B:121:ASP:OD1	2.13	0.48
1:B:67:GLU:HB3	1:B:88:LYS:CB	2.43	0.48
1:A:178:TYR:CA	1:A:326:LYS:HD2	2.44	0.48
1:A:272:PHE:CE2	1:A:308:LYS:HA	2.48	0.48
1:A:260:HIS:HB3	1:A:265:LYS:CA	2.44	0.48
1:B:238:LYS:CD	1:B:242:LEU:H	2.26	0.48
1:A:178:TYR:N	1:A:326:LYS:HD2	2.29	0.48
1:B:247:THR:OG1	1:B:287:LEU:HD22	2.13	0.48
1:A:326:LYS:C	1:A:328:LEU:HD12	2.39	0.48
1:B:80:GLY:HA3	1:B:111:LEU:HD13	1.96	0.48
1:B:223:PRO:O	1:B:224:THR:C	2.57	0.48
1:A:157:TYR:HB2	1:A:310:PHE:CE1	2.49	0.47
1:A:83:ARG:HD2	3:A:358:HOH:O	2.14	0.47
1:A:174:GLU:CD	1:A:174:GLU:C	2.82	0.47
1:A:221:THR:HB	1:A:300:ILE:H	1.79	0.47
1:B:221:THR:HG23	1:B:292:VAL:HB	1.94	0.47
1:A:2:GLU:C	1:A:2:GLU:CD	2.83	0.47
1:A:138:PRO:HG2	1:A:141:VAL:HB	1.96	0.47
1:A:217:THR:HG22	1:A:219:THR:H	1.77	0.47
1:A:239:VAL:HG12	1:A:240:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:PHE:O	1:B:255:PRO:HB2	2.14	0.47
1:B:313:PHE:CD1	1:B:313:PHE:N	2.82	0.47
1:B:276:PRO:O	1:B:278:SER:N	2.46	0.47
1:A:55:LYS:HD2	1:A:115:TYR:OH	2.15	0.47
1:A:77:TYR:HA	2:C:5:ALA:HA	1.96	0.47
1:A:98:LEU:N	1:A:98:LEU:HD23	2.29	0.47
1:B:227:LEU:HD11	1:B:289:ILE:CG2	2.43	0.47
1:A:220:ILE:HB	1:A:289:ILE:CD1	2.45	0.47
1:B:212:VAL:HG23	1:B:298:THR:HG23	1.97	0.47
1:B:306:MET:C	1:B:308:LYS:N	2.73	0.47
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.96	0.47
1:A:185:GLU:O	1:A:186:LYS:O	2.32	0.47
1:B:39:ASN:HD21	1:B:133:ILE:H	1.62	0.47
1:B:40:LEU:HG	1:B:102:PHE:HB3	1.96	0.47
1:B:69:ASP:HB3	1:B:86:PHE:O	2.15	0.47
1:B:241:PHE:C	1:B:243:PRO:CD	2.88	0.47
1:A:199:ILE:N	1:A:199:ILE:HD12	2.30	0.47
1:B:196:ASP:HB3	1:B:208:LYS:HD2	1.97	0.47
1:B:244:LEU:HB2	3:B:355:HOH:O	2.15	0.47
1:A:44:SER:C	1:A:46:ASN:N	2.70	0.47
1:A:275:ASP:HB3	1:A:276:PRO:HA	1.97	0.47
1:A:302:GLY:HA3	3:A:366:HOH:O	2.15	0.47
1:B:219:THR:O	1:B:302:GLY:HA3	2.15	0.47
1:A:244:LEU:HD12	1:A:286:MET:HE3	1.97	0.46
1:B:302:GLY:C	1:B:304:PRO:HD2	2.40	0.46
1:A:56:HIS:HD2	1:A:121:ASP:OD2	1.99	0.46
1:A:257:LEU:N	1:A:268:LEU:O	2.48	0.46
1:B:103:ILE:N	1:B:103:ILE:CD1	2.78	0.46
1:B:279:ASP:OD1	1:B:280:ILE:HD12	2.16	0.46
1:A:10:ASP:OD2	1:A:16:PHE:HE2	1.97	0.46
1:A:245:TYR:O	1:A:287:LEU:HB3	2.15	0.46
1:A:280:ILE:CG2	1:B:280:ILE:HG21	2.46	0.46
1:B:246:VAL:HG12	1:B:247:THR:H	1.80	0.46
1:A:77:TYR:HB3	2:C:4:STA:HD13	1.97	0.46
1:A:278:SER:C	1:A:280:ILE:N	2.70	0.46
1:A:177:PHE:HB3	1:A:310:PHE:CD1	2.51	0.46
1:A:216:GLY:HA3	2:C:4:STA:OH	2.15	0.46
1:A:226:PHE:O	1:A:227:LEU:HD12	2.15	0.46
1:A:220:ILE:CG2	1:A:221:THR:N	2.78	0.46
1:B:294:ILE:H	1:B:294:ILE:CD1	2.08	0.46
1:A:22:ILE:HG12	1:A:91:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:CB	1:A:88:LYS:HE2	2.45	0.46
1:A:322:PHE:O	1:A:323:ALA:HB2	2.15	0.46
1:B:140:VAL:HG21	1:B:154:PHE:CD2	2.51	0.46
1:A:241:PHE:O	1:A:242:LEU:HB3	2.15	0.46
1:A:258:GLU:HB3	1:A:265:LYS:NZ	2.31	0.46
1:A:260:HIS:ND1	1:A:265:LYS:HD2	2.31	0.46
1:B:19:GLU:CD	1:B:19:GLU:N	2.60	0.46
1:A:159:PRO:HD3	1:A:165:VAL:O	2.16	0.45
1:A:198:ASP:HA	1:A:206:MET:O	2.16	0.45
1:A:326:LYS:C	1:A:328:LEU:N	2.71	0.45
1:B:12:ALA:O	1:B:14:LEU:HG	2.16	0.45
1:B:162:ASP:O	1:B:163:LYS:C	2.58	0.45
1:B:278:SER:C	1:B:280:ILE:H	2.23	0.45
1:A:100:TYR:OH	1:A:138:PRO:HA	2.16	0.45
1:A:160:VAL:HG13	1:A:307:ARG:HD3	1.97	0.45
1:A:192:TYR:HB3	3:A:351:HOH:O	2.15	0.45
1:A:200:HIS:HB3	1:A:205:VAL:HA	1.96	0.45
1:A:239:VAL:HG22	1:A:246:VAL:CG1	2.45	0.45
1:A:81:THR:O	1:A:110:ASP:HB2	2.16	0.45
1:A:268:LEU:HD12	1:A:308:LYS:CE	2.45	0.45
1:B:327:ASN:HB2	1:B:328:LEU:H	1.53	0.45
1:A:222:ALA:HB3	1:A:227:LEU:HD11	1.97	0.45
1:A:233:ASP:O	1:A:234:MET:HB2	2.16	0.45
1:B:278:SER:O	1:B:280:ILE:N	2.41	0.45
1:A:320:VAL:HG12	1:A:321:GLY:N	2.30	0.45
1:B:159:PRO:HB2	1:B:163:LYS:HB3	1.98	0.45
1:A:154:PHE:N	1:A:154:PHE:CD2	2.85	0.45
1:A:160:VAL:H	1:A:163:LYS:CE	2.29	0.45
1:A:200:HIS:HB2	1:A:204:TYR:C	2.41	0.45
1:B:91:ILE:N	1:B:91:ILE:HD12	2.31	0.45
1:B:246:VAL:CG1	1:B:247:THR:H	2.29	0.45
1:A:40:LEU:HD12	1:A:40:LEU:C	2.41	0.45
1:A:50:ILE:C	1:A:52:CYS:N	2.74	0.45
1:A:227:LEU:O	1:A:230:PHE:HB2	2.17	0.45
1:A:265:LYS:NZ	1:A:267:THR:HG22	2.31	0.45
1:B:259:PHE:N	1:B:266:TYR:O	2.45	0.45
1:A:109:ASP:O	1:A:112:GLU:HG2	2.16	0.45
1:A:303:ASP:CB	1:A:307:ARG:HH12	2.24	0.45
1:B:101:LYS:HE3	1:B:136:ILE:HD11	1.98	0.45
1:B:140:VAL:HG21	1:B:154:PHE:HD2	1.81	0.45
1:A:178:TYR:O	1:A:326:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:H	1:A:241:PHE:HD2	1.62	0.45
1:A:272:PHE:CE2	1:A:308:LYS:HB2	2.52	0.44
1:A:163:LYS:HD2	1:A:164:HIS:NE2	2.31	0.44
1:B:51:GLY:HA2	1:B:116:SER:HB3	2.00	0.44
1:B:304:PRO:HA	1:B:307:ARG:NH1	2.31	0.44
1:A:134:GLY:O	1:A:135:SER:HB3	2.16	0.44
1:A:219:THR:CG2	1:A:220:ILE:N	2.80	0.44
1:A:260:HIS:N	1:A:260:HIS:HD2	2.13	0.44
1:B:230:PHE:C	1:B:232:ARG:N	2.71	0.44
1:A:20:GLY:HA3	1:A:31:PHE:CE2	2.53	0.44
1:A:75:ILE:HD11	1:A:103:ILE:HD12	1.99	0.44
1:A:244:LEU:HD22	1:A:289:ILE:H	1.82	0.44
2:D:350:VAL:CG1	2:D:352:STA:HD23	2.47	0.44
1:A:284:LEU:CD2	1:B:280:ILE:HG23	2.41	0.44
1:A:294:ILE:HG22	1:A:295:ASP:H	1.81	0.44
1:B:155:THR:OG1	1:B:312:VAL:HG22	2.18	0.44
1:A:13:ASN:OD1	1:A:14:LEU:CD1	2.66	0.44
1:B:230:PHE:C	1:B:232:ARG:H	2.21	0.44
1:A:188:ASN:HD21	1:A:195:ILE:C	2.25	0.44
1:B:22:ILE:HA	1:B:90:VAL:O	2.17	0.44
1:B:40:LEU:HD12	1:B:40:LEU:C	2.41	0.44
1:B:210:ASN:O	1:B:298:THR:HG23	2.17	0.44
1:A:40:LEU:HA	1:A:123:ILE:O	2.17	0.44
1:A:44:SER:C	1:A:46:ASN:H	2.26	0.44
1:A:186:LYS:HG3	1:A:187:LEU:H	1.82	0.44
1:B:236:VAL:HB	1:B:247:THR:OG1	2.18	0.44
1:B:239:VAL:HG13	1:B:240:PRO:CD	2.44	0.44
1:A:125:GLY:O	1:A:126:LEU:HG	2.18	0.43
1:A:186:LYS:HG3	1:A:187:LEU:N	2.32	0.43
1:A:243:PRO:O	1:A:290:LEU:HD21	2.18	0.43
1:A:276:PRO:O	1:A:277:LEU:HB2	2.18	0.43
1:A:303:ASP:O	1:A:304:PRO:C	2.61	0.43
1:B:179:GLU:OE2	1:B:326:LYS:HB3	2.17	0.43
1:A:13:ASN:HB2	1:A:307:ARG:NH2	2.18	0.43
1:A:219:THR:HG22	1:A:220:ILE:N	2.32	0.43
1:A:50:ILE:O	1:A:52:CYS:N	2.50	0.43
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.75	0.43
1:A:165:VAL:HG21	1:A:167:TYR:OH	2.18	0.43
1:A:192:TYR:O	1:A:194:GLN:N	2.51	0.43
1:A:199:ILE:HG21	1:A:299:PHE:CD2	2.53	0.43
1:A:200:HIS:CE1	1:A:258:GLU:OE2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASP:HB2	1:A:280:ILE:HD12	1.99	0.43
1:B:108:ALA:O	1:B:109:ASP:C	2.62	0.43
1:B:129:LYS:HD3	1:B:137:ASP:OD1	2.18	0.43
1:B:239:VAL:HB	1:B:243:PRO:HB2	1.99	0.43
1:B:305:PHE:CE2	1:B:309:TYR:CD2	3.06	0.43
1:A:5:SER:HB2	1:A:167:TYR:HB3	2.01	0.43
1:A:79:SER:HB3	1:A:114:ILE:CG1	2.41	0.43
1:A:153:LEU:HB3	1:A:314:ASP:CB	2.49	0.43
1:A:257:LEU:HB2	1:A:268:LEU:HB3	2.00	0.43
1:A:259:PHE:O	1:A:266:TYR:N	2.35	0.43
1:A:269:GLU:N	1:A:269:GLU:OE1	2.52	0.43
1:B:197:LEU:HD13	1:B:259:PHE:HB3	2.00	0.43
1:B:271:GLU:HG3	1:B:272:PHE:N	2.33	0.43
1:B:217:THR:HG22	1:B:219:THR:H	1.83	0.43
1:A:197:LEU:HD13	1:A:259:PHE:HB3	2.00	0.43
1:B:198:ASP:CB	1:B:260:HIS:HB2	2.35	0.43
1:B:261:SER:C	1:B:263:ASN:H	2.27	0.43
1:B:41:TRP:CE3	1:B:105:VAL:HG21	2.54	0.43
1:B:165:VAL:O	1:B:165:VAL:CG1	2.65	0.43
1:A:178:TYR:CZ	1:A:182:LEU:HD22	2.54	0.43
1:B:199:ILE:HG23	1:B:259:PHE:CE1	2.54	0.43
1:B:242:LEU:HD23	1:B:243:PRO:N	2.33	0.43
1:A:128:TRP:CZ2	1:A:315:TYR:HA	2.54	0.43
1:B:149:ILE:HG13	1:B:171:GLY:HA2	2.01	0.43
1:B:207:GLN:O	1:B:208:LYS:C	2.61	0.43
1:B:286:MET:SD	1:B:288:TYR:CE1	3.12	0.43
1:B:290:LEU:HD11	2:D:349:IVA:HG22	2.00	0.43
1:A:3:ASN:ND2	1:A:172:GLY:H	2.17	0.42
1:A:188:ASN:O	1:A:189:HIS:ND1	2.51	0.42
1:A:278:SER:O	1:A:281:ASP:N	2.52	0.42
1:A:160:VAL:C	1:A:162:ASP:N	2.77	0.42
1:A:178:TYR:CD2	1:A:323:ALA:CB	3.03	0.42
1:A:309:TYR:HD1	1:A:324:VAL:HA	1.84	0.42
1:B:14:LEU:HD23	1:B:288:TYR:CZ	2.55	0.42
1:B:184:TYR:HD1	1:B:319:SER:HG	1.67	0.42
1:A:73:VAL:CG2	1:A:103:ILE:HD13	2.48	0.42
1:A:231:PHE:C	1:A:233:ASP:H	2.26	0.42
1:B:221:THR:CG2	1:B:300:ILE:HG12	2.49	0.42
1:A:182:LEU:HD12	1:A:323:ALA:CB	2.50	0.42
1:A:201:PHE:HB3	1:A:257:LEU:HD23	2.02	0.42
1:B:14:LEU:HB3	1:B:288:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ALA:HB1	1:B:297:ASN:O	2.19	0.42
1:B:244:LEU:CG	1:B:286:MET:HE1	2.45	0.42
1:B:302:GLY:C	1:B:304:PRO:CD	2.93	0.42
1:A:200:HIS:CE1	1:A:260:HIS:NE2	2.88	0.42
1:B:191:LEU:HB3	1:B:192:TYR:HD1	1.83	0.42
1:A:320:VAL:HG11	1:A:322:PHE:CE2	2.54	0.42
1:B:221:THR:HG21	1:B:300:ILE:HG12	2.02	0.42
1:A:190:ASP:O	1:A:191:LEU:HD22	2.19	0.42
1:A:221:THR:HG23	1:A:292:VAL:HB	1.99	0.42
1:A:303:ASP:O	1:A:306:MET:N	2.53	0.42
1:B:69:ASP:HB2	1:B:88:LYS:NZ	2.34	0.42
1:B:220:ILE:HA	1:B:300:ILE:O	2.20	0.42
1:A:239:VAL:O	1:A:240:PRO:C	2.62	0.42
1:B:8:LEU:HD12	1:B:166:GLY:C	2.45	0.42
1:A:80:GLY:CA	1:A:111:LEU:HD12	2.50	0.42
1:A:277:LEU:HD22	1:A:285:CYS:CA	2.49	0.42
1:B:10:ASP:CG	1:B:16:PHE:CE2	2.98	0.42
1:B:49:SER:O	1:B:52:CYS:HB2	2.20	0.42
1:B:254:LEU:N	1:B:254:LEU:CD1	2.81	0.42
1:B:256:THR:CG2	1:B:269:GLU:HG3	2.50	0.42
1:A:12:ALA:O	1:A:14:LEU:CD1	2.60	0.41
1:A:67:GLU:HB3	1:A:88:LYS:HE2	2.01	0.41
1:A:199:ILE:HG21	1:A:299:PHE:CE2	2.55	0.41
1:A:262:ARG:HA	3:A:362:HOH:O	2.19	0.41
1:A:277:LEU:HD13	1:A:286:MET:N	2.35	0.41
1:A:295:ASP:O	1:A:296:ASP:CB	2.67	0.41
1:B:151:ASN:HB2	1:B:171:GLY:O	2.20	0.41
1:B:244:LEU:C	1:B:244:LEU:HD22	2.45	0.41
1:A:14:LEU:HB3	1:A:218:SER:HB2	2.02	0.41
1:A:244:LEU:HD22	1:A:288:TYR:HA	1.98	0.41
1:A:278:SER:O	1:A:280:ILE:N	2.52	0.41
1:B:66:TYR:CD1	1:B:67:GLU:N	2.87	0.41
1:A:236:VAL:HG13	1:A:247:THR:OG1	2.20	0.41
1:A:238:LYS:HD2	1:A:239:VAL:O	2.19	0.41
1:B:48:ASP:O	1:B:49:SER:C	2.60	0.41
1:B:144:LYS:CA	1:B:149:ILE:HG22	2.47	0.41
1:B:162:ASP:O	1:B:164:HIS:N	2.53	0.41
1:B:196:ASP:O	1:B:197:LEU:HD23	2.20	0.41
1:B:233:ASP:O	1:B:234:MET:C	2.64	0.41
1:A:79:SER:CB	1:A:114:ILE:HG12	2.42	0.41
1:B:123:ILE:HD11	2:D:352:STA:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HA	1:B:194:GLN:O	2.20	0.41
1:A:113:PRO:HG3	1:B:79:SER:HA	2.02	0.41
1:A:314:ASP:OD2	1:A:317:LYS:CD	2.58	0.41
1:B:15:MET:CE	2:D:350:VAL:HG21	2.48	0.41
1:B:279:ASP:C	1:B:280:ILE:HD12	2.44	0.41
1:A:24:THR:O	1:A:26:LYS:N	2.54	0.41
1:A:25:ASN:ND2	1:A:27:GLN:HG2	2.36	0.41
1:A:187:LEU:O	1:A:194:GLN:O	2.39	0.41
1:A:14:LEU:O	1:A:218:SER:HB3	2.20	0.41
1:A:200:HIS:CB	1:A:205:VAL:HA	2.51	0.41
1:B:144:LYS:HA	1:B:144:LYS:HD2	1.88	0.41
1:A:1:SER:O	1:A:3:ASN:OD1	2.39	0.41
1:A:67:GLU:HB2	1:A:88:LYS:CE	2.51	0.41
1:A:128:TRP:CE3	1:A:190:ASP:HB3	2.56	0.41
1:B:10:ASP:OD2	1:B:10:ASP:C	2.64	0.41
1:B:38:ALA:HB3	1:B:132:SER:HB3	2.03	0.41
1:B:109:ASP:O	1:B:111:LEU:N	2.53	0.41
1:B:319:SER:OG	1:B:320:VAL:N	2.52	0.41
1:A:124:LEU:HD23	1:A:124:LEU:C	2.46	0.41
1:A:230:PHE:HD2	1:A:230:PHE:HA	1.74	0.41
1:A:236:VAL:CG1	1:A:245:TYR:CB	2.92	0.41
1:B:73:VAL:HG11	1:B:86:PHE:CD2	2.56	0.41
1:A:10:ASP:CG	1:A:16:PHE:CE2	2.99	0.40
1:A:153:LEU:HD23	1:A:314:ASP:CG	2.46	0.40
1:A:240:PRO:O	1:A:241:PHE:C	2.64	0.40
1:B:274:MET:HA	1:B:286:MET:O	2.20	0.40
1:B:277:LEU:O	1:B:278:SER:C	2.63	0.40
1:A:277:LEU:HD13	1:A:285:CYS:CA	2.44	0.40
1:A:281:ASP:N	1:A:281:ASP:OD1	2.54	0.40
1:A:295:ASP:CG	1:A:296:ASP:OD1	2.63	0.40
1:B:44:SER:C	1:B:46:ASN:N	2.79	0.40
1:B:140:VAL:HB	1:B:315:TYR:CE2	2.55	0.40
1:A:174:GLU:OE2	1:A:176:ASP:OD1	2.38	0.40
1:A:26:LYS:O	1:A:27:GLN:C	2.62	0.40
1:A:159:PRO:HA	1:A:164:HIS:HE1	1.86	0.40
1:A:177:PHE:HB3	1:A:310:PHE:CE1	2.57	0.40
1:B:31:PHE:CZ	1:B:40:LEU:HD11	2.56	0.40
1:B:80:GLY:HA3	1:B:111:LEU:HA	2.02	0.40
1:B:149:ILE:HD11	1:B:171:GLY:HA3	2.04	0.40
1:B:155:THR:O	1:B:168:LEU:HA	2.21	0.40
1:B:263:ASN:O	1:B:264:ASN:CB	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:HE1	1:A:123:ILE:HD12	1.87	0.40
1:A:74:GLU:C	1:A:75:ILE:HG13	2.47	0.40
1:A:290:LEU:CD2	1:A:291:PRO:HD2	2.46	0.40
1:A:295:ASP:OD2	1:A:296:ASP:OD1	2.39	0.40
1:B:227:LEU:HD22	1:B:291:PRO:CB	2.50	0.40
1:B:253:ASP:C	1:B:254:LEU:HD12	2.46	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD2	1:B:232:ARG:NH2[3_454]	1.23	0.97
1:A:207:GLN:NE2	1:B:233:ASP:O[3_454]	1.59	0.61
1:A:198:ASP:CG	1:B:232:ARG:NH2[3_454]	1.64	0.56
1:A:145:LYS:CE	1:B:163:LYS:NZ[5_665]	1.97	0.23
1:A:134:GLY:CA	1:B:282:PRO:CB[5_665]	2.01	0.19
1:A:68:LYS:O	1:B:64:LYS:O[2_665]	2.15	0.05
1:A:72:LYS:NZ	1:A:248:THR:OG1[5_665]	2.17	0.03
1:A:198:ASP:OD2	1:B:232:ARG:CZ[3_454]	2.19	0.01

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	326/328 (99%)	251 (77%)	53 (16%)	22 (7%)	1	3
1	B	326/328 (99%)	259 (79%)	43 (13%)	24 (7%)	1	2
2	C	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	D	3/6 (50%)	3 (100%)	0	0	100	100
All	All	658/668 (98%)	515 (78%)	97 (15%)	46 (7%)	1	2

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	181	PRO
1	A	186	LYS
1	A	276	PRO
1	A	327	ASN
1	B	159	PRO
1	B	161	HIS
1	B	163	LYS
1	B	166	GLY
1	B	242	LEU
1	B	243	PRO
1	B	278	SER
1	B	279	ASP
1	B	296	ASP
1	A	10	ASP
1	A	162	ASP
1	A	241	PHE
1	A	296	ASP
1	B	4	ASP
1	B	110	ASP
1	B	176	ASP
1	B	230	PHE
1	B	264	ASN
1	B	277	LEU
1	A	51	GLY
1	A	61	SER
1	A	275	ASP
1	A	294	ILE
1	B	109	ASP
1	B	208	LYS
1	B	232	ARG
1	B	240	PRO
1	B	280	ILE
1	A	139	VAL
1	A	146	GLN
1	A	234	MET
1	A	281	ASP
1	A	324	VAL
1	B	224	THR
1	B	233	ASP
1	A	187	LEU
1	A	242	LEU
1	B	66	TYR

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Mol	Chain	Res	Type
1	A	165	VAL
1	B	202	GLY
1	A	114	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	293/293 (100%)	263 (90%)	30 (10%)	7	23
1	B	293/293 (100%)	258 (88%)	35 (12%)	5	17
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	590/590 (100%)	525 (89%)	65 (11%)	6	20

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	16	PHE
1	A	39	ASN
1	A	40	LEU
1	A	42	VAL
1	A	45	VAL
1	A	54	THR
1	A	93	LEU
1	A	136	ILE
1	A	141	VAL
1	A	155	THR
1	A	178	TYR
1	A	181	PRO
1	A	183	THR
1	A	195	ILE
1	A	225	SER
1	A	230	PHE
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	241	PHE
1	A	243	PRO
1	A	247	THR
1	A	249	CYS
1	A	260	HIS
1	A	262	ARG
1	A	263	ASN
1	A	281	ASP
1	A	304	PRO
1	A	312	VAL
1	A	317	LYS
1	B	3	ASN
1	B	14	LEU
1	B	17	TYR
1	B	19	GLU
1	B	40	LEU
1	B	44	SER
1	B	72	LYS
1	B	88	LYS
1	B	103	ILE
1	B	155	THR
1	B	161	HIS
1	B	162	ASP
1	B	164	HIS
1	B	169	THR
1	B	182	LEU
1	B	187	LEU
1	B	213	VAL
1	B	221	THR
1	B	231	PHE
1	B	236	VAL
1	B	239	VAL
1	B	240	PRO
1	B	243	PRO
1	B	244	LEU
1	B	248	THR
1	B	249	CYS
1	B	258	GLU
1	B	277	LEU
1	B	286	MET
1	B	287	LEU

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Mol	Chain	Res	Type
1	B	292	VAL
1	B	294	ILE
1	B	308	LYS
1	B	311	THR
1	B	318	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	13	ASN
1	A	21	GLN
1	A	25	ASN
1	A	27	GLN
1	A	46	ASN
1	A	56	HIS
1	A	147	ASN
1	A	161	HIS
1	A	200	HIS
1	A	228	ASN
1	A	235	ASN
1	A	251	ASN
1	A	263	ASN
1	B	161	HIS
1	B	188	ASN
1	B	194	GLN
1	B	210	ASN
1	B	228	ASN
1	B	235	ASN
1	B	263	ASN
1	B	264	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	STA	C	6	2	11,11,11	2.26	3 (27%)	11,14,14	1.43	2 (18%)
2	STA	C	4	2	10,10,11	1.03	1 (10%)	9,12,14	1.66	2 (22%)
2	STA	D	354	2	11,11,11	2.31	2 (18%)	11,14,14	1.22	2 (18%)
2	STA	D	352	2	10,10,11	0.97	1 (10%)	9,12,14	1.28	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STA	C	6	2	-	2/12/12/12	-
2	STA	C	4	2	-	2/11/11/12	-
2	STA	D	354	2	-	0/12/12/12	-
2	STA	D	352	2	-	2/11/11/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	STA	CH-CA	5.49	1.58	1.53
2	C	6	STA	CH-CA	5.47	1.58	1.53
2	D	354	STA	OH-CH	4.60	1.53	1.43
2	C	6	STA	OH-CH	3.83	1.51	1.43
2	C	4	STA	CH-CA	3.14	1.56	1.53
2	D	352	STA	CH-CA	2.69	1.56	1.53
2	C	6	STA	CB-CA	2.01	1.56	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	STA	OH-CH-CM	-3.43	101.34	109.24
2	C	6	STA	CM-CH-CA	-3.40	107.67	112.93
2	D	352	STA	OH-CH-CM	-2.66	103.12	109.24
2	C	6	STA	OH-CH-CM	2.34	115.08	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	STA	CG-CB-CA	2.22	120.55	115.76
2	D	354	STA	OH-CH-CM	2.21	114.77	109.45
2	D	354	STA	CM-CH-CA	-2.10	109.68	112.93

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	STA	CH-CA-CB-CG
2	D	352	STA	CH-CA-CB-CG
2	D	352	STA	O-C-CM-CH
2	C	4	STA	O-C-CM-CH
2	C	6	STA	OXT-C-CM-CH
2	C	6	STA	O-C-CM-CH

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	STA	3	0
2	C	4	STA	5	0
2	D	352	STA	3	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.