



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:31 am BST

PDB ID : 3PTO
Title : Crystal Structure of an empty Vesicular Stomatitis Virus Nucleocapsid Protein Complex
Authors : Luo, M.; Green, T.J.; Rowse, M.
Deposited on : 2010-12-03
Resolution : 3.01 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

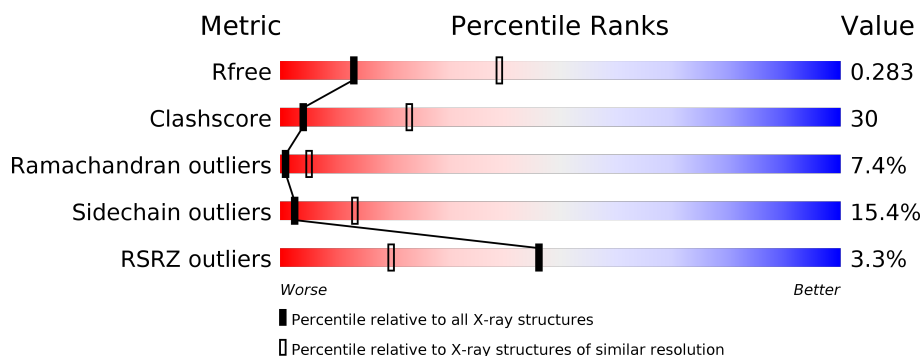
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	421	<div> <div>0%</div> <div> <div>51%</div> <div>35%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	421	<div> <div>3%</div> <div> <div>51%</div> <div>36%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	421	<div> <div>3%</div> <div> <div>50%</div> <div>36%</div> <div>10%</div> <div>..</div> </div> </div>
1	D	421	<div> <div>5%</div> <div> <div>51%</div> <div>36%</div> <div>10%</div> <div>..</div> </div> </div>
1	E	421	<div> <div>4%</div> <div> <div>51%</div> <div>36%</div> <div>10%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

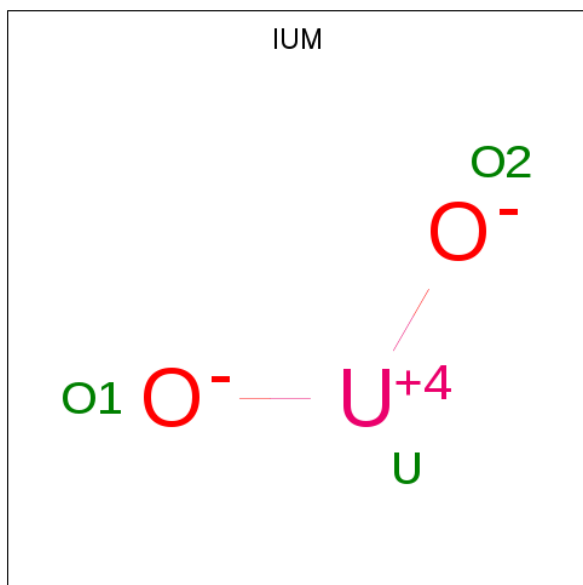
There are 2 unique types of molecules in this entry. The entry contains 16467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3298	2101	553	626	18			
1	B	415	Total	C	N	O	S	0	0	0
			3290	2097	552	623	18			
1	C	413	Total	C	N	O	S	0	0	0
			3275	2089	550	618	18			
1	D	416	Total	C	N	O	S	0	0	0
			3298	2103	553	624	18			
1	E	415	Total	C	N	O	S	0	0	0
			3291	2097	552	624	18			

- Molecule 2 is URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	U	0	0
			1	1		

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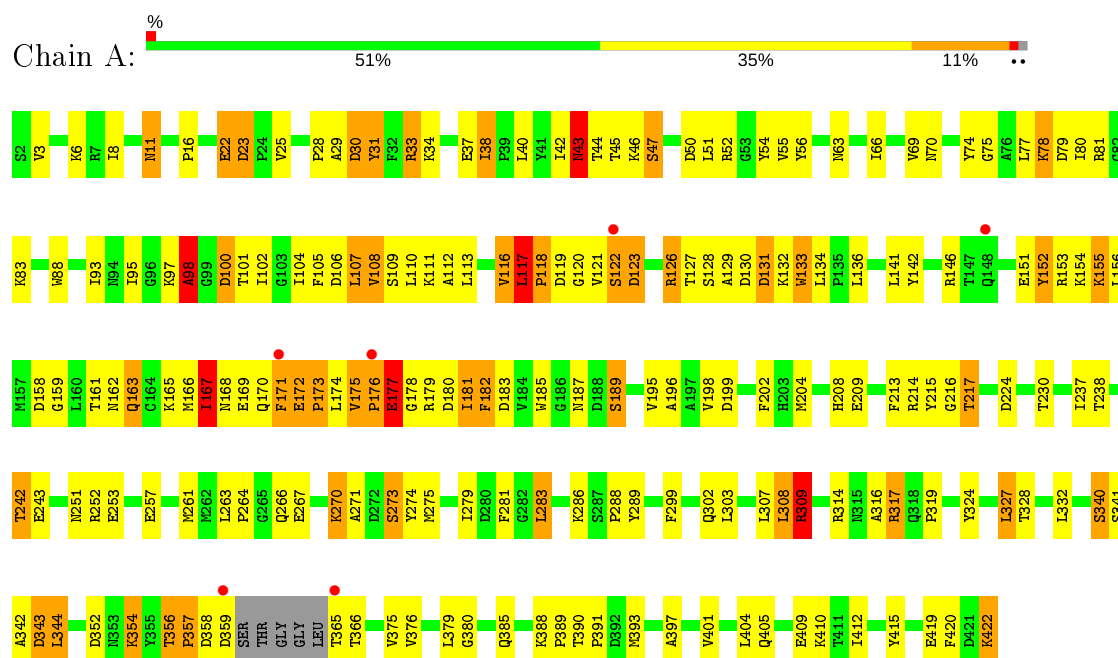
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	U 1	0	0
2	A	1	Total 1	U 1	0	0
2	A	1	Total 1	U 1	0	0
2	B	1	Total 1	U 1	0	0
2	B	1	Total 1	U 1	0	0
2	B	1	Total 1	U 1	0	0
2	C	1	Total 1	U 1	0	0
2	C	1	Total 1	U 1	0	0
2	C	1	Total 1	U 1	0	0
2	D	1	Total 1	U 1	0	0
2	D	1	Total 1	U 1	0	0
2	D	1	Total 1	U 1	0	0
2	E	1	Total 1	U 1	0	0
2	E	1	Total 1	U 1	0	0

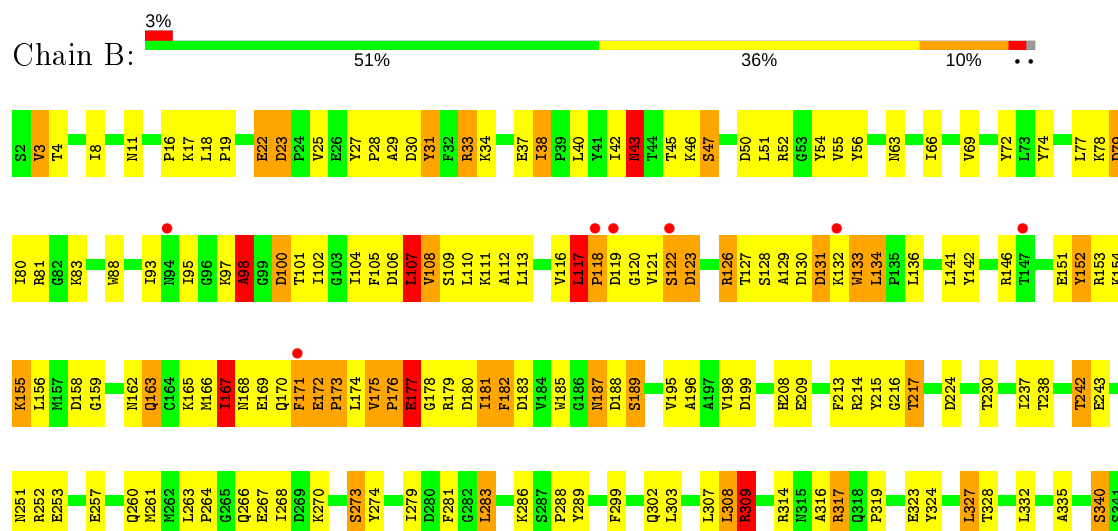
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Nucleoprotein

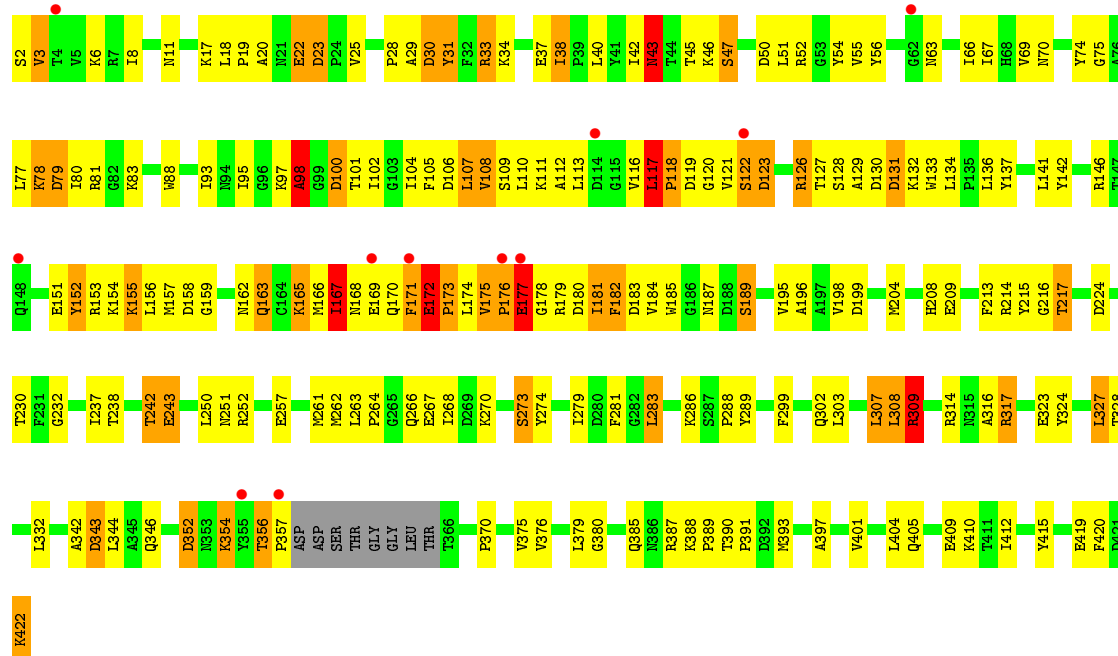


• Molecule 1: Nucleoprotein

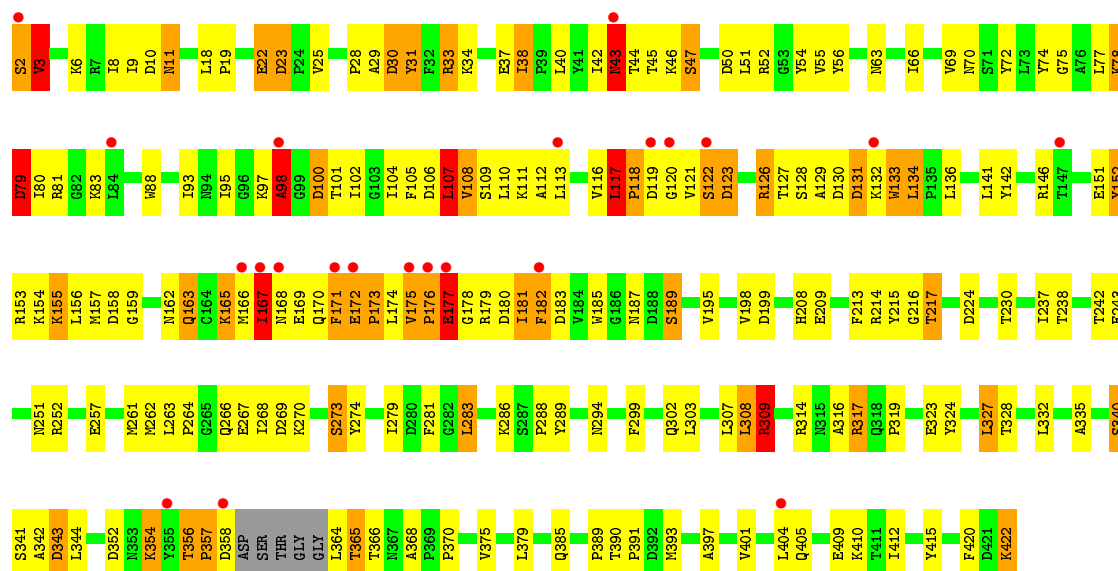




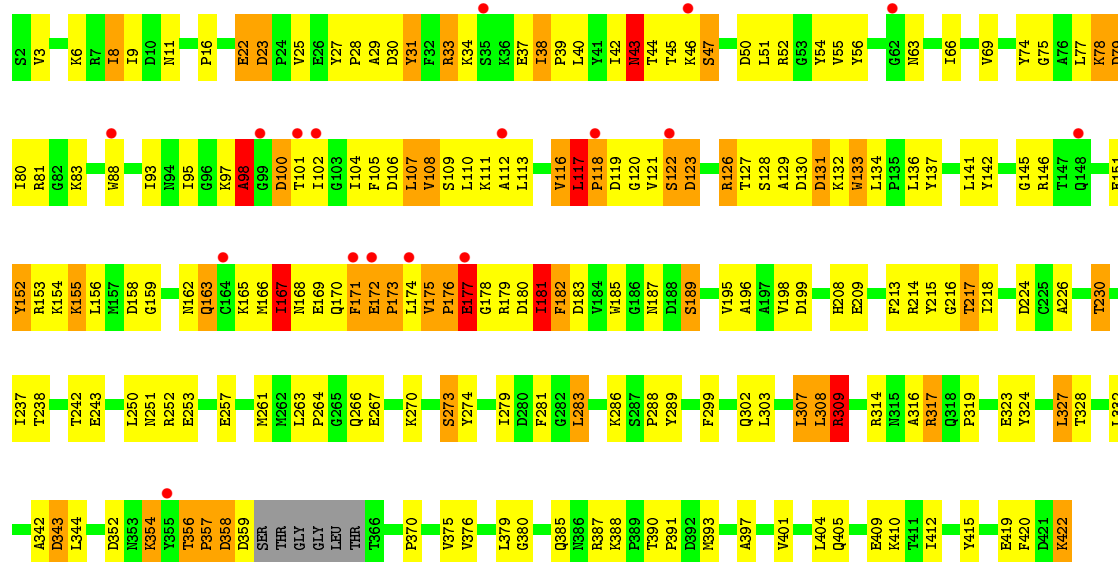
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.64Å 234.06Å 75.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.76 – 3.01 38.76 – 3.01	Depositor EDS
% Data completeness (in resolution range)	82.3 (38.76-3.01) 82.4 (38.76-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6.1 _357	Depositor
R, R_{free}	0.258 , 0.291 0.252 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16467	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.54	1/3373 (0.0%)	0.68	1/4565 (0.0%)
1	B	0.54	0/3365	0.69	3/4554 (0.1%)
1	C	0.55	1/3350 (0.0%)	0.68	1/4533 (0.0%)
1	D	0.56	1/3373 (0.0%)	0.69	3/4565 (0.1%)
1	E	0.54	0/3366	0.68	1/4555 (0.0%)
All	All	0.55	3/16827 (0.0%)	0.69	9/22772 (0.0%)

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
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	3
1	E	0	2
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ASP	CB-CG	6.10	1.64	1.51
1	C	30	ASP	CB-CG	5.94	1.64	1.51
1	D	30	ASP	CB-CG	5.84	1.64	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	177	GLU	N-CA-C	-7.00	92.11	111.00
1	D	177	GLU	N-CA-C	-6.87	92.45	111.00
1	E	177	GLU	N-CA-C	-6.78	92.69	111.00
1	B	177	GLU	N-CA-C	-6.76	92.75	111.00
1	A	177	GLU	N-CA-C	-6.40	93.72	111.00
1	B	3	VAL	CG1-CB-CG2	5.74	120.08	110.90
1	D	107	LEU	CB-CG-CD1	5.18	119.81	111.00
1	D	30	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	107	LEU	CB-CG-CD1	5.10	119.67	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LEU	Peptide
1	A	98	ALA	Peptide
1	B	107	LEU	Peptide
1	B	98	ALA	Peptide
1	C	107	LEU	Peptide
1	C	2	SER	Peptide
1	C	98	ALA	Peptide
1	D	107	LEU	Peptide
1	D	2	SER	Peptide
1	D	98	ALA	Peptide
1	E	107	LEU	Peptide
1	E	98	ALA	Peptide

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	3298	0	3257	203	0
1	B	3290	0	3253	216	0
1	C	3275	0	3242	210	0
1	D	3298	0	3264	200	0
1	E	3291	0	3250	196	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	16467	0	16266	974	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 30.

All (974) 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:C:376:VAL:HG13	1:D:354:LYS:HB2	1.26	1.14
1:B:317:ARG:HD2	1:B:317:ARG:H	1.10	1.13
1:D:117:LEU:HB3	1:D:118:PRO:HD2	1.29	1.12
1:C:117:LEU:HB3	1:C:118:PRO:HD2	1.27	1.12
1:D:2:SER:N	1:D:3:VAL:HG23	1.63	1.12
1:C:317:ARG:HD2	1:C:317:ARG:H	1.13	1.11
1:E:117:LEU:HB3	1:E:118:PRO:HD2	1.28	1.11
1:D:317:ARG:H	1:D:317:ARG:HD2	1.07	1.09
1:E:317:ARG:H	1:E:317:ARG:HD2	1.05	1.09
1:A:117:LEU:HB3	1:A:118:PRO:HD2	1.28	1.09
1:A:376:VAL:HG13	1:B:354:LYS:HB2	1.33	1.08
1:B:117:LEU:HB3	1:B:118:PRO:HD2	1.29	1.08
1:A:317:ARG:HD2	1:A:317:ARG:H	1.07	1.07
1:A:354:LYS:HB2	1:E:376:VAL:HG13	1.34	1.05
1:E:214:ARG:HA	1:E:217:THR:HG22	1.34	1.05
1:C:214:ARG:HA	1:C:217:THR:HG22	1.35	1.03
1:D:214:ARG:HA	1:D:217:THR:HG22	1.38	1.03
1:A:214:ARG:HA	1:A:217:THR:HG22	1.33	1.03
1:B:214:ARG:HA	1:B:217:THR:HG22	1.36	1.02
1:B:380:GLY:HA2	1:C:354:LYS:NZ	1.80	0.96
1:B:356:THR:HG23	1:B:357:PRO:HD3	1.46	0.96
1:D:129:ALA:HB1	1:D:133:TRP:HE1	1.30	0.95
1:C:117:LEU:HB3	1:C:118:PRO:CD	1.97	0.95
1:B:117:LEU:HB3	1:B:118:PRO:CD	1.97	0.95
1:D:317:ARG:N	1:D:317:ARG:HD2	1.81	0.94
1:A:117:LEU:HB3	1:A:118:PRO:CD	1.98	0.94
1:D:356:THR:HG23	1:D:357:PRO:HD3	1.48	0.94
1:E:117:LEU:HB3	1:E:118:PRO:CD	1.98	0.94
1:A:356:THR:HG23	1:A:357:PRO:HD3	1.46	0.94
1:D:117:LEU:HB3	1:D:118:PRO:CD	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ALA:HB1	1:C:133:TRP:HE1	1.33	0.93
1:B:129:ALA:HB1	1:B:133:TRP:HE1	1.32	0.93
1:E:37:GLU:HB2	1:E:108:VAL:HG11	1.50	0.93
1:A:129:ALA:HB1	1:A:133:TRP:HE1	1.34	0.92
1:E:317:ARG:HD2	1:E:317:ARG:N	1.85	0.92
1:B:365:THR:HG23	1:B:366:THR:H	1.34	0.92
1:A:37:GLU:HB2	1:A:108:VAL:HG11	1.52	0.91
1:E:356:THR:HG23	1:E:357:PRO:HD3	1.48	0.91
1:D:317:ARG:H	1:D:317:ARG:CD	1.82	0.91
1:C:356:THR:HG23	1:C:357:PRO:HD3	1.50	0.91
1:E:129:ALA:HB1	1:E:133:TRP:HE1	1.34	0.91
1:A:324:TYR:O	1:A:328:THR:HG23	1.70	0.91
1:C:181:ILE:HD12	1:C:181:ILE:H	1.33	0.91
1:C:324:TYR:O	1:C:328:THR:HG23	1.69	0.90
1:B:317:ARG:HD2	1:B:317:ARG:N	1.86	0.89
1:A:317:ARG:CD	1:A:317:ARG:H	1.85	0.88
1:B:317:ARG:CD	1:B:317:ARG:H	1.86	0.88
1:B:37:GLU:HB2	1:B:108:VAL:HG11	1.56	0.88
1:A:317:ARG:N	1:A:317:ARG:HD2	1.86	0.88
1:A:365:THR:HG23	1:A:366:THR:H	1.36	0.88
1:B:181:ILE:H	1:B:181:ILE:HD12	1.37	0.88
1:D:181:ILE:H	1:D:181:ILE:HD12	1.37	0.87
1:E:181:ILE:H	1:E:181:ILE:HD12	1.39	0.87
1:D:324:TYR:O	1:D:328:THR:HG23	1.73	0.87
1:E:317:ARG:H	1:E:317:ARG:CD	1.87	0.87
1:B:187:ASN:ND2	1:C:165:LYS:HD3	1.89	0.86
1:B:141:LEU:HD13	1:B:182:PHE:HD2	1.40	0.86
1:C:385:GLN:HG2	1:C:390:THR:HG22	1.58	0.86
1:A:385:GLN:HG2	1:A:390:THR:HG22	1.57	0.85
1:E:385:GLN:HG2	1:E:390:THR:HG22	1.57	0.85
1:A:181:ILE:H	1:A:181:ILE:HD12	1.38	0.85
1:C:152:TYR:HE1	1:C:153:ARG:HH11	1.25	0.85
1:B:385:GLN:HG2	1:B:390:THR:HG22	1.57	0.84
1:B:324:TYR:O	1:B:328:THR:HG23	1.76	0.84
1:D:37:GLU:HB2	1:D:108:VAL:HG11	1.56	0.84
1:C:37:GLU:HB2	1:C:108:VAL:HG11	1.57	0.84
1:D:141:LEU:HD13	1:D:182:PHE:HD2	1.42	0.84
1:E:88:TRP:CD2	1:E:95:ILE:HD11	2.13	0.83
1:A:88:TRP:CD2	1:A:95:ILE:HD11	2.14	0.83
1:D:365:THR:HG23	1:D:366:THR:H	1.44	0.82
1:C:317:ARG:CD	1:C:317:ARG:H	1.91	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:HA	1:A:217:THR:CG2	2.09	0.82
1:D:385:GLN:HG2	1:D:390:THR:HG22	1.60	0.82
1:C:141:LEU:HD13	1:C:182:PHE:HD2	1.42	0.82
1:E:141:LEU:HD13	1:E:182:PHE:HD2	1.43	0.81
1:B:88:TRP:CD2	1:B:95:ILE:HD11	2.16	0.81
1:C:317:ARG:HD2	1:C:317:ARG:N	1.93	0.80
1:D:126:ARG:HD3	1:D:127:THR:H	1.46	0.80
1:A:152:TYR:HE1	1:A:153:ARG:HH11	1.29	0.80
1:E:152:TYR:HE1	1:E:153:ARG:HH11	1.30	0.80
1:A:141:LEU:HD13	1:A:182:PHE:HD2	1.45	0.80
1:C:88:TRP:CD2	1:C:95:ILE:HD11	2.17	0.80
1:C:155:LYS:O	1:C:158:ASP:HB3	1.83	0.79
1:E:214:ARG:HA	1:E:217:THR:CG2	2.12	0.79
1:B:3:VAL:HG22	1:B:4:THR:H	1.48	0.78
1:B:376:VAL:HG13	1:C:354:LYS:HB2	1.65	0.78
1:B:152:TYR:HE1	1:B:153:ARG:HH11	1.32	0.78
1:A:126:ARG:HD3	1:A:127:THR:H	1.49	0.78
1:A:155:LYS:O	1:A:158:ASP:HB3	1.83	0.77
1:C:152:TYR:CZ	1:C:153:ARG:HD3	2.18	0.77
1:C:126:ARG:HD3	1:C:127:THR:H	1.49	0.77
1:C:152:TYR:CE1	1:C:153:ARG:NH1	2.52	0.77
1:B:126:ARG:HD3	1:B:127:THR:H	1.48	0.77
1:B:214:ARG:HA	1:B:217:THR:CG2	2.13	0.76
1:D:43:ASN:HA	1:D:112:ALA:H	1.50	0.76
1:D:152:TYR:HE1	1:D:153:ARG:HH11	1.34	0.76
1:D:364:LEU:O	1:D:365:THR:HG22	1.86	0.75
1:B:155:LYS:O	1:B:158:ASP:HB3	1.86	0.75
1:A:152:TYR:CZ	1:A:153:ARG:HD3	2.20	0.75
1:C:184:VAL:HG11	1:D:165:LYS:HA	1.69	0.75
1:E:155:LYS:O	1:E:158:ASP:HB3	1.85	0.75
1:E:324:TYR:O	1:E:328:THR:HG23	1.86	0.75
1:A:43:ASN:HA	1:A:112:ALA:H	1.51	0.74
1:C:214:ARG:HA	1:C:217:THR:CG2	2.14	0.74
1:E:126:ARG:HD3	1:E:127:THR:H	1.51	0.74
1:A:314:ARG:HD2	1:A:404:LEU:HD22	1.69	0.74
1:B:152:TYR:CZ	1:B:153:ARG:HD3	2.22	0.74
1:D:172:GLU:HB3	1:D:173:PRO:HD3	1.70	0.74
1:D:214:ARG:HA	1:D:217:THR:CG2	2.16	0.74
1:C:172:GLU:HB3	1:C:173:PRO:HD3	1.70	0.74
1:D:88:TRP:CD2	1:D:95:ILE:HD11	2.22	0.74
1:E:47:SER:HB2	1:E:50:ASP:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ASN:HA	1:E:112:ALA:H	1.52	0.74
1:B:106:ASP:C	1:B:107:LEU:HG	2.09	0.74
1:D:155:LYS:O	1:D:158:ASP:HB3	1.88	0.74
1:E:152:TYR:CZ	1:E:153:ARG:HD3	2.21	0.73
1:D:152:TYR:CZ	1:D:153:ARG:HD3	2.23	0.73
1:B:47:SER:HB2	1:B:50:ASP:HB2	1.70	0.73
1:C:47:SER:HB2	1:C:50:ASP:HB2	1.69	0.73
1:A:152:TYR:CE1	1:A:153:ARG:NH1	2.57	0.73
1:A:380:GLY:HA2	1:B:354:LYS:NZ	2.04	0.73
1:D:314:ARG:HD2	1:D:404:LEU:HD22	1.70	0.73
1:C:152:TYR:HE1	1:C:153:ARG:NH1	1.87	0.73
1:B:18:LEU:HD22	1:C:232:GLY:HA2	1.70	0.72
1:D:81:ARG:HB3	1:D:208:HIS:HE2	1.54	0.72
1:A:47:SER:HB2	1:A:50:ASP:HB2	1.70	0.72
1:B:152:TYR:CE1	1:B:153:ARG:NH1	2.57	0.72
1:D:47:SER:HB2	1:D:50:ASP:HB2	1.72	0.72
1:C:43:ASN:HA	1:C:112:ALA:H	1.55	0.72
1:E:172:GLU:HB3	1:E:173:PRO:HD3	1.70	0.72
1:A:172:GLU:HB3	1:A:173:PRO:HD3	1.70	0.72
1:A:388:LYS:HE2	1:B:340:SER:HB2	1.72	0.72
1:B:172:GLU:HB3	1:B:173:PRO:HD3	1.71	0.71
1:E:152:TYR:CE1	1:E:153:ARG:NH1	2.57	0.71
1:E:199:ASP:HB2	1:E:217:THR:HG23	1.73	0.71
1:A:299:PHE:HE1	1:A:328:THR:HG22	1.56	0.71
1:A:299:PHE:CE1	1:A:328:THR:HG22	2.26	0.70
1:B:43:ASN:HA	1:B:112:ALA:H	1.53	0.70
1:E:314:ARG:HD2	1:E:404:LEU:HD22	1.74	0.70
1:A:422:LYS:NZ	1:A:422:LYS:HA	2.06	0.70
1:C:29:ALA:H	1:C:266:GLN:HE22	1.40	0.70
1:E:88:TRP:CE2	1:E:95:ILE:HD11	2.27	0.70
1:C:314:ARG:HD2	1:C:404:LEU:HD22	1.73	0.70
1:B:177:GLU:HG2	1:B:183:ASP:OD1	1.91	0.69
1:D:106:ASP:C	1:D:107:LEU:HG	2.12	0.69
1:B:34:LYS:N	1:B:34:LYS:HD2	2.08	0.69
1:C:106:ASP:C	1:C:107:LEU:HG	2.13	0.69
1:A:106:ASP:C	1:A:107:LEU:HG	2.13	0.69
1:C:34:LYS:N	1:C:34:LYS:HD2	2.07	0.69
1:B:422:LYS:HA	1:B:422:LYS:NZ	2.08	0.69
1:C:177:GLU:HG2	1:C:183:ASP:OD1	1.92	0.69
1:E:179:ARG:HA	1:E:183:ASP:CG	2.13	0.68
1:B:380:GLY:HA2	1:C:354:LYS:HZ3	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:LEU:O	1:C:309:ARG:HB2	1.92	0.68
1:A:88:TRP:CE2	1:A:95:ILE:HD11	2.28	0.68
1:A:376:VAL:CG1	1:B:354:LYS:HB2	2.19	0.68
1:C:179:ARG:HA	1:C:183:ASP:CG	2.13	0.67
1:D:2:SER:CA	1:D:3:VAL:HG23	2.23	0.67
1:E:106:ASP:C	1:E:107:LEU:HG	2.12	0.67
1:E:177:GLU:HG2	1:E:183:ASP:OD1	1.94	0.67
1:A:177:GLU:HG2	1:A:183:ASP:OD1	1.94	0.67
1:D:117:LEU:CB	1:D:118:PRO:HD2	2.18	0.67
1:B:88:TRP:CE2	1:B:95:ILE:HD11	2.29	0.67
1:A:152:TYR:HE1	1:A:153:ARG:NH1	1.91	0.67
1:C:199:ASP:HB2	1:C:217:THR:HG23	1.76	0.67
1:D:299:PHE:CE1	1:D:328:THR:HG22	2.29	0.67
1:E:385:GLN:HG2	1:E:390:THR:CG2	2.25	0.67
1:C:388:LYS:HE2	1:D:340:SER:HB2	1.77	0.67
1:D:34:LYS:HD2	1:D:34:LYS:N	2.10	0.67
1:D:51:LEU:O	1:D:55:VAL:HG22	1.95	0.67
1:B:314:ARG:HD2	1:B:404:LEU:HD22	1.75	0.67
1:D:152:TYR:CE1	1:D:153:ARG:NH1	2.61	0.67
1:D:299:PHE:HE1	1:D:328:THR:HG22	1.58	0.66
1:B:117:LEU:CB	1:B:118:PRO:HD2	2.18	0.66
1:B:141:LEU:HD13	1:B:182:PHE:CD2	2.28	0.66
1:C:141:LEU:HD13	1:C:182:PHE:CD2	2.29	0.66
1:A:179:ARG:HA	1:A:183:ASP:CG	2.15	0.66
1:B:299:PHE:HE1	1:B:328:THR:HG22	1.60	0.66
1:B:299:PHE:CE1	1:B:328:THR:HG22	2.30	0.66
1:E:299:PHE:CE1	1:E:328:THR:HG22	2.30	0.66
1:E:152:TYR:HE1	1:E:153:ARG:NH1	1.91	0.66
1:E:34:LYS:N	1:E:34:LYS:HD2	2.10	0.66
1:C:181:ILE:HD12	1:C:181:ILE:N	2.08	0.66
1:C:376:VAL:CG1	1:D:354:LYS:HB2	2.17	0.66
1:B:152:TYR:HE1	1:B:153:ARG:NH1	1.92	0.66
1:A:81:ARG:HB3	1:A:208:HIS:HE2	1.60	0.65
1:C:267:GLU:OE2	1:C:273:SER:HB2	1.95	0.65
1:D:179:ARG:HA	1:D:183:ASP:CG	2.17	0.65
1:D:83:LYS:HE2	1:D:101:THR:HG22	1.79	0.65
1:D:81:ARG:CB	1:D:208:HIS:HE2	2.08	0.65
1:B:81:ARG:CB	1:B:208:HIS:HE2	2.10	0.65
1:C:299:PHE:HE1	1:C:328:THR:HG22	1.62	0.65
1:D:2:SER:N	1:D:3:VAL:CG2	2.53	0.65
1:A:288:PRO:HG2	1:A:289:TYR:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:ARG:HD3	1:D:127:THR:N	2.12	0.65
1:C:299:PHE:CE1	1:C:328:THR:HG22	2.32	0.65
1:D:385:GLN:HG2	1:D:390:THR:CG2	2.26	0.65
1:D:422:LYS:NZ	1:D:422:LYS:HA	2.12	0.65
1:A:29:ALA:H	1:A:266:GLN:HE22	1.44	0.65
1:A:79:ASP:OD2	1:A:79:ASP:O	2.15	0.65
1:A:267:GLU:OE2	1:A:273:SER:HB2	1.97	0.65
1:A:34:LYS:N	1:A:34:LYS:HD2	2.11	0.65
1:D:136:LEU:O	1:D:136:LEU:HD23	1.96	0.65
1:C:184:VAL:CG1	1:D:165:LYS:HA	2.27	0.65
1:C:105:PHE:C	1:C:107:LEU:H	2.01	0.64
1:E:267:GLU:OE2	1:E:273:SER:HB2	1.96	0.64
1:B:51:LEU:O	1:B:55:VAL:HG22	1.96	0.64
1:D:50:ASP:OD1	1:D:121:VAL:HA	1.97	0.64
1:D:141:LEU:HD13	1:D:182:PHE:CD2	2.31	0.64
1:A:385:GLN:HG2	1:A:390:THR:CG2	2.26	0.64
1:A:105:PHE:C	1:A:107:LEU:H	2.00	0.64
1:A:81:ARG:CB	1:A:208:HIS:HE2	2.09	0.64
1:C:88:TRP:CE2	1:C:95:ILE:HD11	2.32	0.64
1:D:79:ASP:OD2	1:D:79:ASP:O	2.16	0.64
1:B:238:THR:HG22	1:B:308:LEU:HD23	1.78	0.64
1:D:177:GLU:HG2	1:D:183:ASP:OD1	1.98	0.64
1:E:81:ARG:CB	1:E:208:HIS:HE2	2.10	0.64
1:B:181:ILE:N	1:B:181:ILE:HD12	2.13	0.64
1:E:117:LEU:CB	1:E:118:PRO:HD2	2.18	0.64
1:E:81:ARG:HB3	1:E:208:HIS:HE2	1.63	0.64
1:B:79:ASP:O	1:B:79:ASP:OD2	2.16	0.63
1:C:81:ARG:HB3	1:C:208:HIS:HE2	1.62	0.63
1:C:422:LYS:NZ	1:C:422:LYS:HA	2.12	0.63
1:A:182:PHE:HD1	1:A:183:ASP:N	1.95	0.63
1:B:105:PHE:C	1:B:107:LEU:H	2.01	0.63
1:B:308:LEU:O	1:B:309:ARG:HB2	1.98	0.63
1:C:385:GLN:HG2	1:C:390:THR:CG2	2.28	0.63
1:D:152:TYR:HE1	1:D:153:ARG:NH1	1.96	0.63
1:E:354:LYS:HE3	1:E:356:THR:HA	1.80	0.63
1:A:340:SER:HB2	1:E:388:LYS:HE2	1.78	0.63
1:C:81:ARG:CB	1:C:208:HIS:HE2	2.10	0.63
1:B:385:GLN:HG2	1:B:390:THR:CG2	2.26	0.63
1:E:159:GLY:O	1:E:163:GLN:NE2	2.31	0.63
1:B:179:ARG:HA	1:B:183:ASP:CG	2.18	0.63
1:B:81:ARG:HB3	1:B:208:HIS:HE2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:LYS:HE3	1:C:356:THR:HA	1.81	0.63
1:B:97:LYS:O	1:B:98:ALA:C	2.37	0.63
1:B:267:GLU:OE2	1:B:273:SER:HB2	1.97	0.63
1:C:79:ASP:OD2	1:C:79:ASP:O	2.16	0.63
1:A:199:ASP:HB2	1:A:217:THR:HG23	1.80	0.63
1:A:308:LEU:O	1:A:309:ARG:HB2	1.98	0.63
1:C:238:THR:HG22	1:C:308:LEU:HD23	1.81	0.62
1:D:267:GLU:OE2	1:D:273:SER:HB2	1.99	0.62
1:D:152:TYR:CE1	1:D:177:GLU:HB2	2.34	0.62
1:D:328:THR:HG21	1:D:415:TYR:OH	1.99	0.62
1:A:141:LEU:HD13	1:A:182:PHE:CD2	2.32	0.62
1:D:159:GLY:O	1:D:163:GLN:NE2	2.32	0.62
1:A:181:ILE:HD12	1:A:181:ILE:N	2.13	0.62
1:D:105:PHE:C	1:D:107:LEU:H	2.03	0.62
1:D:97:LYS:O	1:D:98:ALA:C	2.37	0.62
1:B:66:ILE:HD12	1:B:69:VAL:CG2	2.29	0.62
1:E:422:LYS:HA	1:E:422:LYS:NZ	2.15	0.62
1:E:141:LEU:HD13	1:E:182:PHE:CD2	2.30	0.62
1:A:238:THR:HG22	1:A:308:LEU:HD23	1.81	0.62
1:A:354:LYS:HE3	1:A:356:THR:HA	1.82	0.62
1:C:159:GLY:O	1:C:163:GLN:NE2	2.32	0.62
1:C:45:THR:C	1:C:46:LYS:HD2	2.19	0.62
1:D:29:ALA:H	1:D:266:GLN:HE22	1.48	0.62
1:D:181:ILE:HD12	1:D:181:ILE:N	2.14	0.62
1:E:299:PHE:HE1	1:E:328:THR:HG22	1.64	0.62
1:B:288:PRO:HG2	1:B:289:TYR:CE2	2.34	0.61
1:C:83:LYS:HE2	1:C:101:THR:HG22	1.82	0.61
1:C:51:LEU:O	1:C:55:VAL:HG22	2.00	0.61
1:E:83:LYS:HE2	1:E:101:THR:HG22	1.82	0.61
1:B:50:ASP:OD1	1:B:121:VAL:HA	1.99	0.61
1:B:126:ARG:HD3	1:B:127:THR:N	2.16	0.61
1:B:152:TYR:CE1	1:B:177:GLU:HB2	2.35	0.61
1:C:172:GLU:HB3	1:C:173:PRO:CD	2.29	0.61
1:B:354:LYS:HE3	1:B:356:THR:HA	1.83	0.61
1:D:199:ASP:HB2	1:D:217:THR:HG23	1.83	0.61
1:E:29:ALA:H	1:E:266:GLN:HE22	1.47	0.61
1:B:380:GLY:HA2	1:C:354:LYS:HZ2	1.64	0.61
1:E:105:PHE:C	1:E:107:LEU:H	2.03	0.61
1:E:281:PHE:HB3	1:E:283:LEU:HD21	1.83	0.61
1:B:136:LEU:O	1:B:136:LEU:HD23	2.01	0.61
1:E:182:PHE:HD1	1:E:183:ASP:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ILE:HD12	1:E:74:TYR:HB2	1.82	0.61
1:A:117:LEU:CB	1:A:118:PRO:HD2	2.18	0.61
1:C:182:PHE:HD1	1:C:183:ASP:N	1.99	0.61
1:D:172:GLU:HB3	1:D:173:PRO:CD	2.31	0.61
1:C:376:VAL:HG13	1:D:354:LYS:CB	2.18	0.60
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.82	0.60
1:E:136:LEU:O	1:E:136:LEU:HD23	2.01	0.60
1:E:172:GLU:HB3	1:E:173:PRO:CD	2.30	0.60
1:E:66:ILE:HD12	1:E:69:VAL:CG2	2.31	0.60
1:B:38:ILE:O	1:B:108:VAL:HB	2.00	0.60
1:C:117:LEU:CB	1:C:118:PRO:HD2	2.17	0.60
1:C:97:LYS:O	1:C:98:ALA:C	2.39	0.60
1:D:33:ARG:NH1	1:D:33:ARG:HG2	2.15	0.60
1:E:166:MET:O	1:E:167:ILE:HG23	2.01	0.60
1:E:45:THR:C	1:E:46:LYS:HD2	2.22	0.60
1:B:159:GLY:O	1:B:163:GLN:NE2	2.35	0.60
1:C:42:ILE:HD12	1:C:74:TYR:HB2	1.83	0.60
1:A:83:LYS:HE2	1:A:101:THR:HG22	1.84	0.60
1:E:303:LEU:HA	1:E:412:ILE:HD13	1.83	0.60
1:E:79:ASP:O	1:E:79:ASP:OD2	2.19	0.60
1:A:172:GLU:HB3	1:A:173:PRO:CD	2.30	0.60
1:C:66:ILE:HD12	1:C:69:VAL:CG2	2.30	0.60
1:E:181:ILE:N	1:E:181:ILE:HD12	2.15	0.60
1:E:33:ARG:NH1	1:E:33:ARG:HG2	2.16	0.60
1:B:172:GLU:HB3	1:B:173:PRO:CD	2.32	0.60
1:E:288:PRO:HG2	1:E:289:TYR:CE2	2.37	0.60
1:A:51:LEU:O	1:A:55:VAL:HG22	2.01	0.59
1:B:199:ASP:HB2	1:B:217:THR:HG23	1.82	0.59
1:A:136:LEU:O	1:A:136:LEU:HD23	2.02	0.59
1:A:303:LEU:HA	1:A:412:ILE:HD13	1.83	0.59
1:B:375:VAL:HG12	1:B:379:LEU:HD12	1.84	0.59
1:D:308:LEU:O	1:D:309:ARG:HB2	2.01	0.59
1:E:126:ARG:HD3	1:E:127:THR:N	2.17	0.59
1:B:401:VAL:HG21	1:B:420:PHE:HB2	1.85	0.59
1:C:136:LEU:HD23	1:C:136:LEU:O	2.02	0.59
1:D:33:ARG:HH11	1:D:33:ARG:HG2	1.66	0.59
1:E:97:LYS:O	1:E:98:ALA:C	2.40	0.59
1:B:129:ALA:HB1	1:B:133:TRP:NE1	2.12	0.59
1:B:141:LEU:HD22	1:B:182:PHE:CE2	2.37	0.59
1:C:166:MET:O	1:C:167:ILE:HG23	2.02	0.59
1:E:152:TYR:CE1	1:E:177:GLU:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:THR:HG21	1:E:415:TYR:OH	2.03	0.59
1:A:152:TYR:CE1	1:A:177:GLU:HB2	2.37	0.59
1:A:97:LYS:O	1:A:98:ALA:C	2.40	0.59
1:B:166:MET:O	1:B:167:ILE:HG23	2.02	0.59
1:D:365:THR:HG23	1:D:366:THR:N	2.16	0.59
1:A:328:THR:HG21	1:A:415:TYR:OH	2.03	0.59
1:C:152:TYR:CE1	1:C:177:GLU:HB2	2.38	0.59
1:A:129:ALA:HB1	1:A:133:TRP:NE1	2.13	0.59
1:C:288:PRO:HG2	1:C:289:TYR:CE2	2.38	0.59
1:C:328:THR:HG21	1:C:415:TYR:OH	2.03	0.59
1:D:129:ALA:HB1	1:D:133:TRP:NE1	2.10	0.59
1:B:83:LYS:HE2	1:B:101:THR:HG22	1.85	0.59
1:D:354:LYS:HE3	1:D:356:THR:HA	1.85	0.59
1:A:375:VAL:HG12	1:A:379:LEU:HD12	1.85	0.58
1:B:17:LYS:HG3	1:C:268:ILE:HD11	1.85	0.58
1:C:126:ARG:HD3	1:C:127:THR:N	2.16	0.58
1:A:159:GLY:O	1:A:163:GLN:NE2	2.36	0.58
1:C:42:ILE:HD12	1:C:74:TYR:CD2	2.38	0.58
1:D:281:PHE:HB3	1:D:283:LEU:HD21	1.85	0.58
1:E:51:LEU:O	1:E:55:VAL:HG22	2.03	0.58
1:B:29:ALA:C	1:B:31:TYR:H	2.06	0.58
1:B:182:PHE:HD1	1:B:183:ASP:N	2.01	0.58
1:D:288:PRO:HG2	1:D:289:TYR:CE2	2.39	0.58
1:D:42:ILE:HD12	1:D:74:TYR:HB2	1.85	0.58
1:A:214:ARG:CA	1:A:217:THR:HG22	2.22	0.58
1:D:238:THR:HG22	1:D:308:LEU:HD23	1.83	0.58
1:A:126:ARG:HD3	1:A:127:THR:N	2.16	0.58
1:A:422:LYS:CE	1:A:422:LYS:HA	2.33	0.58
1:A:66:ILE:HD12	1:A:69:VAL:CG2	2.33	0.58
1:C:33:ARG:NH1	1:C:33:ARG:HG2	2.18	0.58
1:E:238:THR:HG22	1:E:308:LEU:HD23	1.85	0.58
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.18	0.57
1:B:356:THR:CG2	1:B:357:PRO:HD3	2.28	0.57
1:D:29:ALA:C	1:D:31:TYR:H	2.07	0.57
1:D:182:PHE:HD1	1:D:183:ASP:N	2.01	0.57
1:A:356:THR:CG2	1:A:357:PRO:HD3	2.28	0.57
1:B:45:THR:C	1:B:46:LYS:HD2	2.24	0.57
1:A:281:PHE:HB3	1:A:283:LEU:HD21	1.87	0.57
1:B:281:PHE:HB3	1:B:283:LEU:HD21	1.86	0.57
1:A:50:ASP:OD1	1:A:121:VAL:HA	2.04	0.57
1:C:42:ILE:CD1	1:C:74:TYR:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:C	1:A:46:LYS:HD2	2.24	0.57
1:D:88:TRP:CE2	1:D:95:ILE:HD11	2.40	0.57
1:E:29:ALA:C	1:E:31:TYR:H	2.08	0.57
1:B:33:ARG:HG2	1:B:33:ARG:HH11	1.70	0.57
1:C:141:LEU:HD22	1:C:182:PHE:CE2	2.39	0.57
1:D:141:LEU:HD22	1:D:182:PHE:CE2	2.40	0.57
1:E:38:ILE:O	1:E:108:VAL:HB	2.05	0.57
1:E:308:LEU:O	1:E:309:ARG:HB2	2.05	0.56
1:C:303:LEU:HA	1:C:412:ILE:HD13	1.85	0.56
1:C:33:ARG:HH11	1:C:33:ARG:HG2	1.70	0.56
1:A:33:ARG:HH11	1:A:33:ARG:HG2	1.70	0.56
1:B:42:ILE:HD12	1:B:74:TYR:HB2	1.85	0.56
1:D:66:ILE:HD12	1:D:69:VAL:CG2	2.35	0.56
1:E:50:ASP:OD1	1:E:121:VAL:HA	2.05	0.56
1:E:214:ARG:CA	1:E:217:THR:HG22	2.24	0.56
1:B:33:ARG:HG2	1:B:33:ARG:NH1	2.19	0.56
1:D:422:LYS:HA	1:D:422:LYS:CE	2.36	0.56
1:A:42:ILE:HD12	1:A:74:TYR:HB2	1.86	0.56
1:B:422:LYS:HA	1:B:422:LYS:CE	2.35	0.56
1:A:29:ALA:C	1:A:31:TYR:H	2.09	0.56
1:A:376:VAL:HG13	1:B:354:LYS:CB	2.21	0.56
1:B:29:ALA:H	1:B:266:GLN:HE22	1.52	0.56
1:B:342:ALA:HB1	1:B:344:LEU:HD23	1.87	0.56
1:D:356:THR:CG2	1:D:357:PRO:HD3	2.29	0.56
1:E:422:LYS:HA	1:E:422:LYS:CE	2.36	0.56
1:A:166:MET:O	1:A:167:ILE:HG23	2.06	0.55
1:C:422:LYS:HA	1:C:422:LYS:CE	2.36	0.55
1:A:43:ASN:HB3	1:A:112:ALA:O	2.06	0.55
1:B:328:THR:HG21	1:B:415:TYR:OH	2.06	0.55
1:D:153:ARG:HH21	1:D:171:PHE:HZ	1.55	0.55
1:E:33:ARG:HH11	1:E:33:ARG:HG2	1.69	0.55
1:D:166:MET:O	1:D:167:ILE:HG23	2.06	0.55
1:B:365:THR:HG23	1:B:366:THR:N	2.14	0.55
1:C:38:ILE:O	1:C:108:VAL:HB	2.04	0.55
1:A:38:ILE:O	1:A:108:VAL:HB	2.06	0.55
1:D:257:GLU:O	1:D:261:MET:HG3	2.07	0.55
1:D:38:ILE:O	1:D:108:VAL:HB	2.06	0.55
1:E:42:ILE:CD1	1:E:74:TYR:HB2	2.36	0.55
1:A:409:GLU:O	1:A:410:LYS:HB2	2.06	0.55
1:D:45:THR:C	1:D:46:LYS:HD2	2.26	0.55
1:E:141:LEU:HD22	1:E:182:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLU:O	1:C:410:LYS:HB2	2.07	0.55
1:A:401:VAL:HG21	1:A:420:PHE:HB2	1.90	0.54
1:B:43:ASN:CA	1:B:112:ALA:H	2.20	0.54
1:A:342:ALA:HB1	1:A:344:LEU:HD23	1.89	0.54
1:C:302:GLN:HG2	1:C:316:ALA:CB	2.36	0.54
1:C:342:ALA:HB1	1:C:344:LEU:HD23	1.89	0.54
1:E:104:ILE:HD13	1:E:198:VAL:HG22	1.89	0.54
1:D:31:TYR:CD1	1:D:31:TYR:C	2.80	0.54
1:B:383:GLU:HG3	1:C:354:LYS:HE2	1.89	0.54
1:C:50:ASP:OD1	1:C:121:VAL:HA	2.07	0.54
1:D:153:ARG:NH2	1:D:171:PHE:HZ	2.05	0.54
1:E:409:GLU:O	1:E:410:LYS:HB2	2.07	0.54
1:B:42:ILE:CD1	1:B:74:TYR:HB2	2.38	0.54
1:B:66:ILE:HD12	1:B:69:VAL:HG21	1.88	0.54
1:C:175:VAL:HG13	1:C:181:ILE:HG12	1.88	0.54
1:E:302:GLN:HG2	1:E:316:ALA:CB	2.38	0.54
1:E:43:ASN:CA	1:E:112:ALA:H	2.20	0.53
1:B:18:LEU:HD22	1:C:232:GLY:CA	2.38	0.53
1:E:401:VAL:HG21	1:E:420:PHE:HB2	1.91	0.53
1:C:129:ALA:HB1	1:C:133:TRP:NE1	2.14	0.53
1:C:401:VAL:HG21	1:C:420:PHE:HB2	1.89	0.53
1:D:107:LEU:CD2	1:D:274:TYR:OH	2.57	0.53
1:E:31:TYR:C	1:E:31:TYR:CD1	2.81	0.53
1:C:257:GLU:O	1:C:261:MET:HG3	2.09	0.53
1:D:214:ARG:CA	1:D:217:THR:HG22	2.27	0.53
1:D:29:ALA:O	1:D:31:TYR:N	2.42	0.53
1:E:199:ASP:CB	1:E:217:THR:HG23	2.39	0.53
1:B:303:LEU:HA	1:B:412:ILE:HD13	1.89	0.53
1:B:31:TYR:C	1:B:31:TYR:CD1	2.81	0.53
1:C:123:ASP:N	1:C:123:ASP:OD1	2.42	0.53
1:C:163:GLN:O	1:C:167:ILE:HG13	2.09	0.53
1:C:375:VAL:HG12	1:C:379:LEU:HD12	1.91	0.53
1:E:356:THR:CG2	1:E:357:PRO:HD3	2.30	0.53
1:D:342:ALA:HB1	1:D:344:LEU:HD23	1.91	0.53
1:D:42:ILE:CD1	1:D:74:TYR:HB2	2.39	0.53
1:B:153:ARG:NH2	1:B:171:PHE:HZ	2.07	0.53
1:A:365:THR:HG23	1:A:366:THR:N	2.15	0.52
1:D:308:LEU:HD13	1:D:335:ALA:HB1	1.91	0.52
1:A:380:GLY:HA2	1:B:354:LYS:HZ3	1.73	0.52
1:C:153:ARG:HH21	1:C:171:PHE:HZ	1.57	0.52
1:D:163:GLN:O	1:D:167:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:CD1	1:E:250:LEU:HD13	2.40	0.52
1:A:43:ASN:CA	1:A:112:ALA:H	2.20	0.52
1:B:29:ALA:O	1:B:31:TYR:N	2.42	0.52
1:B:42:ILE:HD12	1:B:74:TYR:CD2	2.44	0.52
1:C:356:THR:CG2	1:C:357:PRO:HD3	2.32	0.52
1:E:129:ALA:HB1	1:E:133:TRP:NE1	2.14	0.52
1:E:175:VAL:HG13	1:E:181:ILE:HG12	1.90	0.52
1:E:75:GLY:HA2	1:E:78:LYS:HD2	1.91	0.52
1:A:175:VAL:HG13	1:A:181:ILE:HG12	1.91	0.52
1:B:56:TYR:CE1	1:B:126:ARG:CZ	2.92	0.52
1:C:42:ILE:HG22	1:C:42:ILE:O	2.09	0.52
1:E:163:GLN:O	1:E:167:ILE:HG13	2.09	0.52
1:E:169:GLU:O	1:E:170:GLN:HG2	2.08	0.52
1:A:163:GLN:O	1:A:167:ILE:HG13	2.10	0.52
1:A:354:LYS:HB2	1:E:376:VAL:CG1	2.24	0.52
1:A:52:ARG:HD3	1:A:127:THR:O	2.09	0.52
1:B:106:ASP:O	1:B:107:LEU:HG	2.09	0.52
1:C:43:ASN:OD1	1:C:112:ALA:HB3	2.09	0.52
1:D:175:VAL:HG13	1:D:181:ILE:HG12	1.91	0.52
1:E:109:SER:O	1:E:110:LEU:HD23	2.09	0.52
1:B:153:ARG:HH21	1:B:171:PHE:HZ	1.57	0.52
1:B:52:ARG:HD3	1:B:127:THR:O	2.09	0.52
1:D:56:TYR:CE1	1:D:126:ARG:CZ	2.93	0.52
1:D:52:ARG:HD3	1:D:127:THR:O	2.10	0.52
1:E:375:VAL:HG12	1:E:379:LEU:HD12	1.92	0.52
1:A:354:LYS:NZ	1:E:380:GLY:HA2	2.24	0.52
1:E:317:ARG:O	1:E:319:PRO:HD3	2.10	0.52
1:E:33:ARG:HH11	1:E:33:ARG:CG	2.23	0.52
1:A:141:LEU:HD22	1:A:182:PHE:CE2	2.45	0.51
1:B:178:GLY:O	1:B:179:ARG:HB2	2.09	0.51
1:B:302:GLN:HG2	1:B:316:ALA:CB	2.40	0.51
1:C:281:PHE:HB3	1:C:283:LEU:HD21	1.92	0.51
1:A:107:LEU:CD2	1:A:274:TYR:OH	2.58	0.51
1:A:302:GLN:HG2	1:A:316:ALA:CB	2.39	0.51
1:A:66:ILE:HD12	1:A:69:VAL:HG21	1.91	0.51
1:A:42:ILE:CD1	1:A:74:TYR:HB2	2.39	0.51
1:C:29:ALA:C	1:C:31:TYR:H	2.14	0.51
1:D:178:GLY:O	1:D:179:ARG:HB2	2.11	0.51
1:D:66:ILE:HD12	1:D:69:VAL:HG21	1.92	0.51
1:A:169:GLU:O	1:A:170:GLN:HG2	2.10	0.51
1:C:66:ILE:HD12	1:C:69:VAL:HG21	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ARG:HD3	1:E:127:THR:O	2.10	0.51
1:E:42:ILE:O	1:E:42:ILE:HG22	2.09	0.51
1:C:52:ARG:HD3	1:C:127:THR:O	2.10	0.51
1:C:419:GLU:O	1:C:419:GLU:HG3	2.11	0.51
1:D:303:LEU:HA	1:D:412:ILE:HD13	1.91	0.51
1:E:342:ALA:HB1	1:E:344:LEU:HD23	1.92	0.51
1:C:56:TYR:CE1	1:C:126:ARG:CZ	2.93	0.51
1:A:106:ASP:O	1:A:107:LEU:HG	2.10	0.51
1:D:302:GLN:HG2	1:D:316:ALA:CB	2.40	0.51
1:D:33:ARG:CG	1:D:33:ARG:HH11	2.23	0.51
1:E:390:THR:HB	1:E:391:PRO:HD2	1.93	0.51
1:C:169:GLU:O	1:C:170:GLN:HG2	2.10	0.51
1:C:31:TYR:CD1	1:C:31:TYR:C	2.84	0.51
1:D:43:ASN:CA	1:D:112:ALA:H	2.22	0.51
1:E:43:ASN:OD1	1:E:112:ALA:HB3	2.11	0.51
1:E:42:ILE:HD12	1:E:74:TYR:CD2	2.45	0.51
1:A:182:PHE:HD1	1:A:183:ASP:H	1.59	0.51
1:A:42:ILE:HD12	1:A:74:TYR:CD2	2.45	0.51
1:C:107:LEU:CD2	1:C:274:TYR:OH	2.59	0.51
1:A:31:TYR:CD1	1:A:31:TYR:C	2.84	0.51
1:D:176:PRO:O	1:D:177:GLU:HB2	2.11	0.51
1:D:43:ASN:HB3	1:D:112:ALA:O	2.11	0.51
1:E:106:ASP:O	1:E:107:LEU:HG	2.10	0.51
1:C:397:ALA:O	1:C:401:VAL:HG22	2.11	0.51
1:D:123:ASP:OD1	1:D:123:ASP:N	2.44	0.51
1:C:109:SER:O	1:C:110:LEU:HD23	2.11	0.50
1:E:123:ASP:N	1:E:123:ASP:OD1	2.43	0.50
1:B:169:GLU:O	1:B:170:GLN:HG2	2.11	0.50
1:D:375:VAL:HG12	1:D:379:LEU:HD12	1.92	0.50
1:A:257:GLU:O	1:A:261:MET:HG3	2.12	0.50
1:A:342:ALA:CB	1:A:344:LEU:HD23	2.40	0.50
1:B:342:ALA:CB	1:B:344:LEU:HD23	2.41	0.50
1:C:43:ASN:CA	1:C:112:ALA:H	2.23	0.50
1:E:107:LEU:CD2	1:E:274:TYR:OH	2.59	0.50
1:A:161:THR:HG22	1:E:179:ARG:O	2.12	0.50
1:B:175:VAL:HG13	1:B:181:ILE:HG12	1.92	0.50
1:C:196:ALA:HB3	1:C:281:PHE:CE1	2.47	0.50
1:A:42:ILE:O	1:A:42:ILE:HG22	2.11	0.50
1:D:106:ASP:O	1:D:107:LEU:HG	2.12	0.50
1:E:153:ARG:NH2	1:E:171:PHE:HZ	2.10	0.50
1:B:163:GLN:O	1:B:167:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ILE:O	1:B:42:ILE:HG22	2.12	0.50
1:C:342:ALA:CB	1:C:344:LEU:HD23	2.42	0.50
1:D:42:ILE:HG22	1:D:42:ILE:O	2.11	0.50
1:E:142:TYR:CD1	1:E:195:VAL:HG11	2.46	0.50
1:A:75:GLY:HA2	1:A:78:LYS:HD2	1.93	0.49
1:B:376:VAL:HG21	1:C:352:ASP:OD1	2.11	0.49
1:C:75:GLY:HA2	1:C:78:LYS:HD2	1.94	0.49
1:A:123:ASP:OD1	1:A:123:ASP:N	2.44	0.49
1:D:25:VAL:HG21	1:D:288:PRO:HB3	1.93	0.49
1:E:257:GLU:O	1:E:261:MET:HG3	2.12	0.49
1:A:283:LEU:N	1:A:283:LEU:HD23	2.28	0.49
1:B:176:PRO:O	1:B:177:GLU:HB2	2.11	0.49
1:B:397:ALA:O	1:B:401:VAL:HG22	2.12	0.49
1:D:126:ARG:CD	1:D:127:THR:N	2.75	0.49
1:D:151:GLU:O	1:D:154:LYS:HB3	2.13	0.49
1:D:43:ASN:OD1	1:D:112:ALA:HB3	2.12	0.49
1:A:33:ARG:HH11	1:A:33:ARG:CG	2.25	0.49
1:A:199:ASP:OD1	1:A:217:THR:HG23	2.11	0.49
1:C:153:ARG:NH2	1:C:171:PHE:HZ	2.10	0.49
1:E:153:ARG:HH21	1:E:171:PHE:HZ	1.60	0.49
1:A:93:ILE:HG22	1:A:95:ILE:HG22	1.95	0.49
1:C:43:ASN:HB3	1:C:112:ALA:O	2.13	0.49
1:D:397:ALA:O	1:D:401:VAL:HG22	2.13	0.49
1:E:151:GLU:O	1:E:151:GLU:HG2	2.12	0.49
1:A:153:ARG:NH2	1:A:171:PHE:HZ	2.11	0.49
1:B:151:GLU:O	1:B:151:GLU:HG2	2.12	0.49
1:B:17:LYS:O	1:C:262:MET:HE1	2.12	0.49
1:D:169:GLU:O	1:D:170:GLN:HG2	2.12	0.49
1:E:43:ASN:HB3	1:E:112:ALA:O	2.13	0.49
1:C:33:ARG:HH11	1:C:33:ARG:CG	2.25	0.49
1:E:66:ILE:HD12	1:E:69:VAL:HG21	1.94	0.49
1:E:23:ASP:HB2	1:E:286:LYS:HE3	1.95	0.49
1:A:153:ARG:HH21	1:A:171:PHE:HZ	1.60	0.48
1:B:123:ASP:OD1	1:B:123:ASP:N	2.46	0.48
1:B:33:ARG:CG	1:B:33:ARG:HH11	2.25	0.48
1:B:43:ASN:HB3	1:B:112:ALA:O	2.12	0.48
1:C:29:ALA:H	1:C:266:GLN:NE2	2.08	0.48
1:E:56:TYR:CE1	1:E:126:ARG:CZ	2.95	0.48
1:B:104:ILE:HD13	1:B:198:VAL:HG22	1.94	0.48
1:C:199:ASP:CB	1:C:217:THR:HG23	2.43	0.48
1:D:81:ARG:O	1:D:102:ILE:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ARG:HA	1:E:126:ARG:HH11	1.78	0.48
1:C:250:LEU:HD13	1:D:344:LEU:CD1	2.43	0.48
1:B:257:GLU:O	1:B:261:MET:HG3	2.13	0.48
1:B:383:GLU:HG3	1:C:354:LYS:NZ	2.29	0.48
1:A:133:TRP:HB3	1:A:167:ILE:HD12	1.95	0.48
1:B:107:LEU:CD2	1:B:274:TYR:OH	2.62	0.48
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.29	0.48
1:D:43:ASN:HA	1:D:111:LYS:HB3	1.96	0.48
1:E:176:PRO:O	1:E:177:GLU:HB2	2.12	0.48
1:E:28:PRO:HD2	1:E:266:GLN:NE2	2.29	0.48
1:A:317:ARG:O	1:A:319:PRO:HD3	2.14	0.48
1:D:133:TRP:HB3	1:D:167:ILE:HD12	1.95	0.48
1:A:56:TYR:CE1	1:A:126:ARG:CZ	2.96	0.48
1:A:199:ASP:CB	1:A:217:THR:HG23	2.43	0.48
1:B:214:ARG:CA	1:B:217:THR:HG22	2.25	0.48
1:E:342:ALA:CB	1:E:344:LEU:HD23	2.43	0.48
1:A:109:SER:O	1:A:110:LEU:HD23	2.14	0.48
1:A:273:SER:OG	1:A:274:TYR:N	2.46	0.48
1:B:43:ASN:OD1	1:B:112:ALA:HB3	2.13	0.48
1:B:18:LEU:CD2	1:C:232:GLY:HA2	2.42	0.48
1:E:196:ALA:HB3	1:E:281:PHE:CE1	2.49	0.48
1:A:270:LYS:HD2	1:A:271:ALA:H	1.79	0.48
1:B:409:GLU:O	1:B:410:LYS:HB2	2.12	0.48
1:E:358:ASP:O	1:E:359:ASP:CB	2.61	0.48
1:A:151:GLU:HG2	1:A:151:GLU:O	2.13	0.47
1:A:142:TYR:CD1	1:A:195:VAL:HG11	2.49	0.47
1:C:182:PHE:HD1	1:C:183:ASP:H	1.62	0.47
1:E:263:LEU:HA	1:E:264:PRO:HD3	1.64	0.47
1:E:93:ILE:HG22	1:E:95:ILE:HG22	1.96	0.47
1:C:93:ILE:HG22	1:C:95:ILE:HG22	1.95	0.47
1:E:177:GLU:HA	1:E:181:ILE:CD1	2.45	0.47
1:E:29:ALA:O	1:E:31:TYR:N	2.45	0.47
1:E:358:ASP:O	1:E:359:ASP:HB2	2.13	0.47
1:B:3:VAL:CG2	1:B:4:THR:H	2.23	0.47
1:D:182:PHE:N	1:D:182:PHE:CD1	2.80	0.47
1:D:28:PRO:HD2	1:D:266:GLN:NE2	2.29	0.47
1:D:342:ALA:CB	1:D:344:LEU:HD23	2.45	0.47
1:D:389:PRO:HA	1:D:393:MET:HE1	1.95	0.47
1:E:25:VAL:HG21	1:E:288:PRO:HB3	1.95	0.47
1:C:126:ARG:HH11	1:C:126:ARG:HA	1.79	0.47
1:D:126:ARG:HH11	1:D:126:ARG:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ARG:N	1:D:317:ARG:CD	2.55	0.47
1:D:42:ILE:HD12	1:D:74:TYR:CD2	2.50	0.47
1:E:136:LEU:HB2	1:E:213:PHE:CE2	2.50	0.47
1:A:136:LEU:HB2	1:A:213:PHE:HE2	1.79	0.47
1:A:136:LEU:HB2	1:A:213:PHE:CE2	2.49	0.47
1:C:43:ASN:HA	1:C:111:LYS:HB3	1.97	0.47
1:C:169:GLU:CG	1:C:170:GLN:H	2.28	0.47
1:C:224:ASP:HB2	1:C:279:ILE:HG13	1.97	0.47
1:C:56:TYR:HE1	1:C:126:ARG:NH1	2.13	0.47
1:D:23:ASP:HB2	1:D:286:LYS:HE3	1.96	0.47
1:B:343:ASP:HB2	1:B:344:LEU:H	1.48	0.47
1:C:23:ASP:HB2	1:C:286:LYS:HE3	1.97	0.47
1:D:177:GLU:HA	1:D:181:ILE:CD1	2.45	0.47
1:D:104:ILE:HD13	1:D:198:VAL:HG22	1.95	0.47
1:A:327:LEU:HA	1:A:327:LEU:HD12	1.78	0.47
1:A:126:ARG:HH11	1:A:126:ARG:HA	1.80	0.47
1:C:175:VAL:O	1:C:181:ILE:HG12	2.15	0.47
1:D:182:PHE:HD1	1:D:183:ASP:H	1.61	0.47
1:D:66:ILE:HD13	1:D:185:TRP:CD1	2.50	0.47
1:A:175:VAL:O	1:A:181:ILE:HG12	2.15	0.47
1:A:43:ASN:HA	1:A:111:LYS:HB3	1.97	0.47
1:B:23:ASP:HB2	1:B:286:LYS:HE3	1.97	0.47
1:B:389:PRO:HA	1:B:393:MET:HE1	1.97	0.47
1:C:127:THR:OG1	1:C:128:SER:N	2.46	0.47
1:E:178:GLY:O	1:E:179:ARG:HB2	2.15	0.47
1:A:66:ILE:HD13	1:A:185:TRP:CD1	2.49	0.47
1:B:28:PRO:HD2	1:B:266:GLN:NE2	2.30	0.47
1:B:383:GLU:HG3	1:C:354:LYS:CE	2.44	0.47
1:D:364:LEU:O	1:D:365:THR:CG2	2.62	0.47
1:E:253:GLU:O	1:E:257:GLU:HG3	2.15	0.47
1:A:151:GLU:O	1:A:154:LYS:HB3	2.14	0.46
1:A:56:TYR:HE1	1:A:126:ARG:NH1	2.13	0.46
1:B:188:ASP:HA	1:C:166:MET:CE	2.45	0.46
1:C:106:ASP:O	1:C:107:LEU:HG	2.15	0.46
1:C:380:GLY:HA2	1:D:354:LYS:NZ	2.30	0.46
1:D:136:LEU:HB2	1:D:213:PHE:CE2	2.50	0.46
1:C:142:TYR:CD1	1:C:195:VAL:HG11	2.51	0.46
1:D:390:THR:HB	1:D:391:PRO:HD2	1.96	0.46
1:D:409:GLU:O	1:D:410:LYS:HB2	2.15	0.46
1:D:56:TYR:HE1	1:D:126:ARG:NH1	2.13	0.46
1:D:97:LYS:HB2	1:D:97:LYS:NZ	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PRO:O	1:A:177:GLU:HB2	2.13	0.46
1:A:29:ALA:H	1:A:266:GLN:NE2	2.12	0.46
1:B:100:ASP:OD1	1:B:100:ASP:N	2.48	0.46
1:B:182:PHE:HD1	1:B:183:ASP:H	1.62	0.46
1:B:16:PRO:HB2	1:C:242:THR:OG1	2.16	0.46
1:B:379:LEU:CD1	1:C:346:GLN:HB2	2.46	0.46
1:C:104:ILE:HD13	1:C:198:VAL:HG22	1.97	0.46
1:D:199:ASP:CB	1:D:217:THR:HG23	2.46	0.46
1:A:344:LEU:HD12	1:E:250:LEU:HD13	1.97	0.46
1:A:43:ASN:OD1	1:A:112:ALA:HB3	2.16	0.46
1:B:181:ILE:H	1:B:181:ILE:CD1	2.16	0.46
1:C:389:PRO:HA	1:C:393:MET:HE1	1.97	0.46
1:D:263:LEU:HA	1:D:264:PRO:HD3	1.61	0.46
1:E:182:PHE:HD1	1:E:183:ASP:H	1.62	0.46
1:E:28:PRO:HD2	1:E:266:GLN:HE21	1.81	0.46
1:A:105:PHE:C	1:A:107:LEU:N	2.68	0.46
1:C:308:LEU:O	1:C:309:ARG:CB	2.64	0.46
1:A:182:PHE:CD1	1:A:183:ASP:N	2.81	0.46
1:D:127:THR:OG1	1:D:128:SER:N	2.47	0.46
1:E:6:LYS:NZ	1:E:11:ASN:HD21	2.14	0.46
1:E:181:ILE:H	1:E:181:ILE:CD1	2.18	0.46
1:A:177:GLU:HA	1:A:181:ILE:CD1	2.46	0.46
1:B:126:ARG:HH11	1:B:126:ARG:HA	1.81	0.46
1:B:166:MET:C	1:B:167:ILE:HG12	2.34	0.46
1:B:56:TYR:HE1	1:B:126:ARG:NH1	2.13	0.46
1:C:177:GLU:HA	1:C:181:ILE:CD1	2.46	0.46
1:E:156:LEU:O	1:E:156:LEU:HD23	2.16	0.46
1:D:224:ASP:HB2	1:D:279:ILE:HG13	1.98	0.46
1:E:397:ALA:O	1:E:401:VAL:HG22	2.15	0.46
1:A:166:MET:C	1:A:167:ILE:HG12	2.36	0.46
1:B:130:ASP:CG	1:B:131:ASP:H	2.18	0.46
1:C:283:LEU:N	1:C:283:LEU:HD23	2.31	0.46
1:C:28:PRO:HG2	1:C:266:GLN:HE21	1.81	0.46
1:D:79:ASP:C	1:D:81:ARG:H	2.20	0.46
1:E:151:GLU:O	1:E:154:LYS:HB3	2.15	0.46
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.31	0.45
1:B:317:ARG:O	1:B:319:PRO:HD3	2.17	0.45
1:C:151:GLU:O	1:C:154:LYS:HB3	2.16	0.45
1:A:127:THR:OG1	1:A:128:SER:N	2.49	0.45
1:B:127:THR:OG1	1:B:128:SER:N	2.49	0.45
1:D:136:LEU:HB2	1:D:213:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:LYS:HE3	1:E:83:LYS:HB2	1.62	0.45
1:A:43:ASN:HB3	1:A:112:ALA:C	2.37	0.45
1:A:79:ASP:C	1:A:81:ARG:H	2.20	0.45
1:B:43:ASN:HA	1:B:111:LYS:HB3	1.99	0.45
1:B:177:GLU:HA	1:B:181:ILE:CD1	2.46	0.45
1:B:199:ASP:CB	1:B:217:THR:HG23	2.47	0.45
1:B:263:LEU:HA	1:B:264:PRO:HD3	1.63	0.45
1:C:130:ASP:CG	1:C:131:ASP:H	2.19	0.45
1:C:151:GLU:HG2	1:C:151:GLU:O	2.17	0.45
1:B:126:ARG:CD	1:B:127:THR:N	2.80	0.45
1:C:327:LEU:HA	1:C:327:LEU:HD12	1.74	0.45
1:C:390:THR:HB	1:C:391:PRO:HD2	1.98	0.45
1:D:75:GLY:HA2	1:D:78:LYS:HD2	1.99	0.45
1:E:43:ASN:HA	1:E:111:LYS:HB3	1.98	0.45
1:C:178:GLY:O	1:C:179:ARG:HB2	2.17	0.45
1:C:17:LYS:O	1:D:262:MET:HE1	2.16	0.45
1:D:109:SER:O	1:D:110:LEU:HD23	2.16	0.45
1:E:81:ARG:O	1:E:102:ILE:O	2.35	0.45
1:E:166:MET:C	1:E:167:ILE:HG12	2.35	0.45
1:A:419:GLU:OE2	1:B:309:ARG:HD3	2.17	0.45
1:C:6:LYS:NZ	1:C:11:ASN:HD21	2.15	0.45
1:D:122:SER:OG	1:D:123:ASP:OD1	2.35	0.45
1:D:18:LEU:HB2	1:D:19:PRO:HD2	1.98	0.45
1:A:344:LEU:HD13	1:E:250:LEU:HB3	1.99	0.45
1:E:412:ILE:O	1:E:412:ILE:HD12	2.16	0.45
1:A:81:ARG:O	1:A:102:ILE:O	2.34	0.45
1:A:23:ASP:HB2	1:A:286:LYS:HE3	1.99	0.45
1:B:136:LEU:HB2	1:B:213:PHE:CE2	2.51	0.45
1:C:182:PHE:N	1:C:182:PHE:CD1	2.80	0.45
1:C:343:ASP:HB2	1:C:344:LEU:H	1.49	0.45
1:C:415:TYR:C	1:C:415:TYR:CD1	2.89	0.45
1:D:181:ILE:CD1	1:D:181:ILE:H	2.16	0.45
1:E:136:LEU:HB2	1:E:213:PHE:HE2	1.82	0.45
1:B:122:SER:OG	1:B:123:ASP:OD1	2.34	0.45
1:B:66:ILE:HD13	1:B:185:TRP:CD1	2.52	0.45
1:D:126:ARG:CD	1:D:127:THR:H	2.24	0.45
1:E:28:PRO:O	1:E:31:TYR:HB3	2.17	0.45
1:A:130:ASP:CG	1:A:131:ASP:H	2.19	0.45
1:A:169:GLU:CG	1:A:170:GLN:H	2.30	0.45
1:B:105:PHE:C	1:B:107:LEU:N	2.70	0.45
1:B:109:SER:O	1:B:110:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:ILE:HG22	1:D:95:ILE:HG22	1.98	0.45
1:E:66:ILE:HD13	1:E:185:TRP:CD1	2.51	0.45
1:E:224:ASP:HB2	1:E:279:ILE:HG13	1.99	0.45
1:A:178:GLY:O	1:A:179:ARG:HB2	2.17	0.45
1:A:25:VAL:HG21	1:A:288:PRO:HB3	1.98	0.45
1:B:22:GLU:O	1:B:23:ASP:C	2.56	0.45
1:B:93:ILE:N	1:B:93:ILE:HD12	2.32	0.45
1:C:136:LEU:HB2	1:C:213:PHE:HE2	1.83	0.45
1:C:214:ARG:CA	1:C:217:THR:HG22	2.26	0.45
1:C:307:LEU:HA	1:C:307:LEU:HD12	1.81	0.45
1:C:42:ILE:O	1:C:43:ASN:C	2.55	0.45
1:E:175:VAL:O	1:E:181:ILE:HG12	2.17	0.45
1:E:93:ILE:N	1:E:93:ILE:HD12	2.32	0.45
1:A:29:ALA:O	1:A:31:TYR:N	2.50	0.44
1:A:397:ALA:O	1:A:401:VAL:HG22	2.17	0.44
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.74	0.44
1:C:100:ASP:OD1	1:C:100:ASP:N	2.50	0.44
1:D:142:TYR:CD1	1:D:195:VAL:HG11	2.52	0.44
1:E:127:THR:OG1	1:E:128:SER:N	2.50	0.44
1:E:169:GLU:CG	1:E:170:GLN:H	2.29	0.44
1:E:97:LYS:NZ	1:E:97:LYS:HB2	2.31	0.44
1:B:56:TYR:CE1	1:B:126:ARG:NH2	2.85	0.44
1:C:18:LEU:HB2	1:C:19:PRO:HD2	1.99	0.44
1:D:33:ARG:NH1	1:D:33:ARG:CG	2.81	0.44
1:E:38:ILE:HA	1:E:39:PRO:HD2	1.81	0.44
1:A:182:PHE:CD1	1:A:182:PHE:N	2.82	0.44
1:B:151:GLU:O	1:B:154:LYS:HB3	2.17	0.44
1:B:83:LYS:HB2	1:B:83:LYS:HE3	1.59	0.44
1:C:136:LEU:HB2	1:C:213:PHE:CE2	2.51	0.44
1:C:170:GLN:HB3	1:C:171:PHE:H	1.62	0.44
1:E:327:LEU:HD12	1:E:327:LEU:HA	1.71	0.44
1:A:196:ALA:HB3	1:A:281:PHE:CE1	2.52	0.44
1:B:224:ASP:HB2	1:B:279:ILE:HG13	2.00	0.44
1:B:79:ASP:C	1:B:81:ARG:H	2.21	0.44
1:C:176:PRO:O	1:C:177:GLU:HB2	2.17	0.44
1:C:42:ILE:HD12	1:C:74:TYR:HD2	1.81	0.44
1:D:83:LYS:HB2	1:D:83:LYS:HE3	1.61	0.44
1:A:263:LEU:HA	1:A:264:PRO:HD3	1.68	0.44
1:D:151:GLU:O	1:D:151:GLU:HG2	2.18	0.44
1:D:343:ASP:HB2	1:D:344:LEU:H	1.48	0.44
1:E:130:ASP:CG	1:E:131:ASP:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HB	1:A:391:PRO:HD2	1.99	0.44
1:C:88:TRP:CD2	1:C:204:MET:HE2	2.52	0.44
1:B:28:PRO:HG2	1:B:266:GLN:HE21	1.83	0.44
1:C:169:GLU:HG3	1:C:170:GLN:H	1.83	0.44
1:D:156:LEU:HD23	1:D:156:LEU:O	2.17	0.44
1:E:199:ASP:OD1	1:E:218:ILE:HA	2.18	0.44
1:A:28:PRO:HG2	1:A:266:GLN:HE21	1.83	0.44
1:B:170:GLN:HB3	1:B:171:PHE:H	1.62	0.44
1:E:283:LEU:N	1:E:283:LEU:HD23	2.33	0.44
1:A:224:ASP:HB2	1:A:279:ILE:HG13	2.00	0.44
1:B:136:LEU:HB2	1:B:213:PHE:HE2	1.83	0.44
1:B:213:PHE:C	1:B:215:TYR:H	2.21	0.44
1:B:25:VAL:HG21	1:B:288:PRO:HB3	1.99	0.44
1:D:213:PHE:C	1:D:215:TYR:H	2.20	0.44
1:D:54:TYR:CZ	1:D:122:SER:HB2	2.53	0.44
1:E:182:PHE:N	1:E:182:PHE:CD1	2.82	0.44
1:A:126:ARG:CD	1:A:127:THR:N	2.81	0.43
1:A:170:GLN:HB3	1:A:171:PHE:H	1.62	0.43
1:C:156:LEU:O	1:C:156:LEU:HD23	2.17	0.43
1:A:242:THR:OG1	1:E:16:PRO:HB2	2.18	0.43
1:A:6:LYS:NZ	1:A:11:ASN:HD21	2.15	0.43
1:A:88:TRP:CD2	1:A:204:MET:HE2	2.53	0.43
1:C:105:PHE:C	1:C:107:LEU:N	2.70	0.43
1:C:182:PHE:CD1	1:C:183:ASP:N	2.84	0.43
1:D:182:PHE:CD1	1:D:183:ASP:N	2.86	0.43
1:D:28:PRO:HD2	1:D:266:GLN:HE21	1.83	0.43
1:D:77:LEU:C	1:D:79:ASP:H	2.22	0.43
1:E:213:PHE:C	1:E:215:TYR:H	2.22	0.43
1:C:56:TYR:CE1	1:C:126:ARG:NH2	2.87	0.43
1:C:133:TRP:HB3	1:C:167:ILE:HD12	1.99	0.43
1:E:22:GLU:O	1:E:23:ASP:C	2.56	0.43
1:E:343:ASP:HB2	1:E:344:LEU:H	1.47	0.43
1:A:389:PRO:HA	1:A:393:MET:HE1	2.01	0.43
1:B:156:LEU:O	1:B:156:LEU:HD23	2.18	0.43
1:B:182:PHE:CD1	1:B:182:PHE:N	2.81	0.43
1:D:364:LEU:HB3	1:D:368:ALA:HB2	2.00	0.43
1:D:56:TYR:CE1	1:D:126:ARG:NH2	2.87	0.43
1:C:263:LEU:HA	1:C:264:PRO:HD3	1.64	0.43
1:D:175:VAL:HA	1:D:176:PRO:HD2	1.71	0.43
1:E:273:SER:OG	1:E:274:TYR:N	2.52	0.43
1:A:354:LYS:HZ3	1:E:380:GLY:HA2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ASP:C	1:E:81:ARG:H	2.22	0.43
1:B:268:ILE:HD13	1:B:268:ILE:HG21	1.71	0.43
1:B:42:ILE:O	1:B:43:ASN:C	2.57	0.43
1:D:6:LYS:NZ	1:D:11:ASN:HD21	2.17	0.43
1:C:122:SER:OG	1:C:123:ASP:OD1	2.33	0.43
1:D:199:ASP:OD1	1:D:214:ARG:NE	2.44	0.43
1:E:100:ASP:N	1:E:100:ASP:OD1	2.51	0.43
1:E:199:ASP:OD1	1:E:217:THR:HG23	2.18	0.43
1:B:72:TYR:CE1	1:B:134:LEU:CD1	3.02	0.43
1:B:175:VAL:O	1:B:181:ILE:HG12	2.18	0.43
1:B:28:PRO:HD2	1:B:266:GLN:HE21	1.84	0.43
1:C:308:LEU:HD12	1:C:308:LEU:HA	1.76	0.43
1:C:77:LEU:C	1:C:79:ASP:H	2.22	0.43
1:D:153:ARG:O	1:D:157:MET:HG3	2.18	0.43
1:A:341:SER:HB2	1:E:387:ARG:NH2	2.34	0.43
1:A:22:GLU:HB3	1:A:23:ASP:H	1.69	0.43
1:B:18:LEU:HB2	1:B:19:PRO:HD2	2.00	0.43
1:B:390:THR:HB	1:B:391:PRO:HD2	2.00	0.43
1:C:66:ILE:HD13	1:C:185:TRP:CD1	2.54	0.43
1:C:213:PHE:C	1:C:215:TYR:H	2.23	0.43
1:E:43:ASN:HB3	1:E:112:ALA:C	2.39	0.43
1:A:77:LEU:C	1:A:79:ASP:H	2.21	0.43
1:B:376:VAL:HG21	1:C:352:ASP:CG	2.38	0.43
1:B:81:ARG:O	1:B:102:ILE:O	2.37	0.42
1:B:327:LEU:HA	1:B:327:LEU:HD12	1.78	0.42
1:D:43:ASN:HB2	1:D:44:THR:H	1.67	0.42
1:A:104:ILE:HD13	1:A:198:VAL:HG22	2.01	0.42
1:A:42:ILE:O	1:A:43:ASN:C	2.58	0.42
1:C:97:LYS:HB2	1:C:97:LYS:NZ	2.30	0.42
1:D:117:LEU:O	1:D:118:PRO:O	2.37	0.42
1:D:283:LEU:HD23	1:D:283:LEU:N	2.34	0.42
1:B:142:TYR:CD1	1:B:195:VAL:HG11	2.54	0.42
1:B:93:ILE:HG22	1:B:95:ILE:HG22	2.01	0.42
1:D:28:PRO:O	1:D:31:TYR:HB3	2.19	0.42
1:E:169:GLU:HG3	1:E:170:GLN:H	1.83	0.42
1:B:257:GLU:O	1:B:260:GLN:HB3	2.19	0.42
1:D:130:ASP:CG	1:D:131:ASP:H	2.23	0.42
1:E:28:PRO:HG2	1:E:266:GLN:HE21	1.85	0.42
1:A:22:GLU:O	1:A:23:ASP:C	2.57	0.42
1:C:54:TYR:HE1	1:C:118:PRO:HB2	1.85	0.42
1:D:29:ALA:C	1:D:31:TYR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:HD3	1:E:419:GLU:OE2	2.19	0.42
1:A:422:LYS:HZ2	1:A:422:LYS:HA	1.83	0.42
1:A:93:ILE:HD12	1:A:93:ILE:N	2.34	0.42
1:B:308:LEU:HD13	1:B:335:ALA:HB1	2.01	0.42
1:E:54:TYR:CZ	1:E:122:SER:HB2	2.54	0.42
1:A:28:PRO:HD2	1:A:266:GLN:NE2	2.35	0.42
1:A:83:LYS:HE3	1:A:83:LYS:HB2	1.63	0.42
1:B:54:TYR:CZ	1:B:122:SER:HB2	2.55	0.42
1:B:29:ALA:C	1:B:31:TYR:N	2.73	0.42
1:C:56:TYR:CE1	1:C:126:ARG:NH1	2.87	0.42
1:D:72:TYR:CE1	1:D:134:LEU:CD1	3.03	0.42
1:E:307:LEU:HD12	1:E:307:LEU:HA	1.77	0.42
1:A:54:TYR:CZ	1:A:122:SER:HB2	2.54	0.42
1:B:308:LEU:O	1:B:309:ARG:CB	2.64	0.42
1:D:43:ASN:HB3	1:D:112:ALA:C	2.40	0.42
1:D:56:TYR:CE1	1:D:126:ARG:NH1	2.88	0.42
1:D:107:LEU:HD22	1:D:274:TYR:OH	2.19	0.42
1:E:107:LEU:C	1:E:108:VAL:HG23	2.40	0.42
1:E:56:TYR:HE1	1:E:126:ARG:NH1	2.18	0.42
1:E:77:LEU:C	1:E:79:ASP:H	2.22	0.42
1:A:43:ASN:HB2	1:A:44:THR:H	1.71	0.42
1:B:117:LEU:CB	1:B:118:PRO:CD	2.79	0.42
1:B:141:LEU:HD22	1:B:182:PHE:CD2	2.55	0.42
1:B:419:GLU:O	1:B:419:GLU:HG3	2.20	0.42
1:D:175:VAL:O	1:D:181:ILE:HG12	2.20	0.42
1:D:323:GLU:O	1:D:327:LEU:HB2	2.20	0.42
1:A:343:ASP:HB2	1:A:344:LEU:H	1.47	0.42
1:A:415:TYR:C	1:A:415:TYR:CD1	2.93	0.42
1:B:43:ASN:HB3	1:B:112:ALA:C	2.39	0.42
1:B:133:TRP:HB3	1:B:167:ILE:HD12	2.00	0.42
1:B:188:ASP:HA	1:C:166:MET:HE3	2.02	0.42
1:B:283:LEU:HD23	1:B:283:LEU:N	2.35	0.42
1:D:42:ILE:O	1:D:43:ASN:C	2.58	0.42
1:E:145:GLY:HA2	1:E:183:ASP:HB3	2.02	0.42
1:C:137:TYR:O	1:C:141:LEU:HG	2.20	0.41
1:C:181:ILE:HB	1:C:182:PHE:H	1.66	0.41
1:D:105:PHE:C	1:D:107:LEU:N	2.71	0.41
1:E:226:ALA:O	1:E:230:THR:HG23	2.20	0.41
1:E:390:THR:O	1:E:393:MET:HG2	2.20	0.41
1:A:100:ASP:OD1	1:A:100:ASP:N	2.52	0.41
1:B:253:GLU:OE2	1:B:253:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ASN:HB3	1:C:112:ALA:C	2.40	0.41
1:E:181:ILE:HB	1:E:182:PHE:H	1.64	0.41
1:E:27:TYR:HB3	1:E:266:GLN:NE2	2.35	0.41
1:E:42:ILE:O	1:E:43:ASN:C	2.59	0.41
1:A:275:MET:C	1:A:275:MET:SD	2.98	0.41
1:C:323:GLU:O	1:C:327:LEU:HB2	2.19	0.41
1:D:29:ALA:H	1:D:266:GLN:NE2	2.15	0.41
1:D:69:VAL:HG23	1:D:70:ASN:N	2.35	0.41
1:B:323:GLU:O	1:B:327:LEU:HB2	2.20	0.41
1:C:126:ARG:CD	1:C:127:THR:N	2.82	0.41
1:D:54:TYR:CE2	1:D:122:SER:HB2	2.56	0.41
1:A:122:SER:OG	1:A:123:ASP:OD1	2.34	0.41
1:A:107:LEU:HD22	1:A:274:TYR:OH	2.21	0.41
1:A:288:PRO:HG2	1:A:289:TYR:CD2	2.55	0.41
1:B:176:PRO:HB2	1:B:177:GLU:H	1.70	0.41
1:C:20:ALA:HB2	1:D:269:ASP:O	2.20	0.41
1:A:117:LEU:O	1:A:118:PRO:O	2.38	0.41
1:A:156:LEU:O	1:A:156:LEU:HD23	2.20	0.41
1:A:253:GLU:O	1:A:257:GLU:HG3	2.21	0.41
1:B:27:TYR:HB3	1:B:266:GLN:NE2	2.36	0.41
1:D:169:GLU:CG	1:D:170:GLN:H	2.32	0.41
1:E:29:ALA:H	1:E:266:GLN:NE2	2.14	0.41
1:A:56:TYR:CE1	1:A:126:ARG:NH1	2.88	0.41
1:B:117:LEU:O	1:B:118:PRO:O	2.38	0.41
1:B:54:TYR:HE1	1:B:118:PRO:HB2	1.85	0.41
1:C:25:VAL:HG21	1:C:288:PRO:HB3	2.02	0.41
1:C:81:ARG:O	1:C:102:ILE:O	2.39	0.41
1:C:93:ILE:HD12	1:C:93:ILE:N	2.36	0.41
1:D:9:ILE:HG23	1:D:10:ASP:N	2.36	0.41
1:A:54:TYR:HE1	1:A:118:PRO:HB2	1.86	0.41
1:B:169:GLU:CG	1:B:170:GLN:H	2.33	0.41
1:C:181:ILE:CD1	1:C:181:ILE:H	2.14	0.41
1:C:79:ASP:C	1:C:81:ARG:H	2.24	0.41
1:A:16:PRO:HB2	1:B:242:THR:OG1	2.20	0.41
1:A:69:VAL:HG23	1:A:70:ASN:N	2.36	0.41
1:B:286:LYS:HE2	1:B:286:LYS:HB2	1.91	0.41
1:B:29:ALA:H	1:B:266:GLN:NE2	2.18	0.41
1:D:364:LEU:CB	1:D:368:ALA:HB2	2.51	0.41
1:E:122:SER:OG	1:E:123:ASP:OD1	2.36	0.41
1:E:142:TYR:CE1	1:E:195:VAL:HG11	2.56	0.41
1:A:44:THR:HG21	1:A:116:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:TYR:CE1	1:B:126:ARG:NH1	2.89	0.41
1:C:166:MET:C	1:C:167:ILE:HG12	2.37	0.41
1:D:93:ILE:HD12	1:D:93:ILE:N	2.36	0.41
1:E:137:TYR:O	1:E:141:LEU:HG	2.21	0.41
1:E:182:PHE:CD1	1:E:183:ASP:N	2.84	0.41
1:E:354:LYS:CE	1:E:356:THR:HA	2.50	0.41
1:B:365:THR:CG2	1:B:366:THR:H	2.14	0.41
1:C:199:ASP:OD1	1:C:217:THR:HG23	2.20	0.41
1:B:376:VAL:CG1	1:C:354:LYS:HB2	2.44	0.41
1:C:387:ARG:NH2	1:D:341:SER:HB2	2.35	0.41
1:D:100:ASP:OD1	1:D:100:ASP:N	2.52	0.41
1:D:268:ILE:HG21	1:D:268:ILE:HD13	1.71	0.41
1:E:44:THR:HG21	1:E:116:VAL:HG22	2.03	0.41
1:E:126:ARG:CD	1:E:127:THR:N	2.83	0.41
1:E:133:TRP:HB3	1:E:167:ILE:HD12	2.03	0.41
1:C:107:LEU:HD22	1:C:274:TYR:OH	2.21	0.40
1:C:28:PRO:O	1:C:31:TYR:HB3	2.21	0.40
1:C:29:ALA:O	1:C:31:TYR:N	2.54	0.40
1:B:54:TYR:CE1	1:B:118:PRO:HB2	2.56	0.40
1:B:199:ASP:OD1	1:B:217:THR:HG23	2.21	0.40
1:D:317:ARG:O	1:D:319:PRO:HD3	2.21	0.40
1:E:323:GLU:O	1:E:327:LEU:HB2	2.21	0.40
1:A:202:PHE:HB2	1:A:214:ARG:HD3	2.04	0.40
1:B:196:ALA:HB3	1:B:281:PHE:CE1	2.56	0.40
1:B:77:LEU:C	1:B:79:ASP:H	2.24	0.40
1:C:54:TYR:CE1	1:C:118:PRO:HB2	2.56	0.40
1:D:257:GLU:HB3	1:D:294:ASN:OD1	2.21	0.40
1:A:50:ASP:HB3	1:A:54:TYR:HE2	1.87	0.40
1:A:54:TYR:CE2	1:A:122:SER:HB2	2.57	0.40
1:B:81:ARG:HB2	1:B:208:HIS:HE2	1.84	0.40
1:C:153:ARG:O	1:C:157:MET:HG3	2.21	0.40
1:C:69:VAL:HG23	1:C:70:ASN:N	2.36	0.40
1:D:199:ASP:OD1	1:D:217:THR:HG23	2.20	0.40
1:D:22:GLU:O	1:D:23:ASP:C	2.59	0.40
1:E:105:PHE:C	1:E:107:LEU:N	2.71	0.40
1:E:22:GLU:HB3	1:E:23:ASP:H	1.70	0.40
1:E:8:ILE:O	1:E:9:ILE:C	2.59	0.40
1:A:175:VAL:HA	1:A:176:PRO:HD2	1.72	0.40
1:A:213:PHE:C	1:A:215:TYR:H	2.25	0.40
1:B:317:ARG:CD	1:B:317:ARG:N	2.60	0.40
1:C:22:GLU:HB3	1:C:23:ASP:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:GLU:H	1:C:243:GLU:HG2	1.65	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	412/421 (98%)	329 (80%)	54 (13%)	29 (7%)	1	6
1	B	411/421 (98%)	327 (80%)	54 (13%)	30 (7%)	1	5
1	C	409/421 (97%)	325 (80%)	55 (13%)	29 (7%)	1	5
1	D	412/421 (98%)	328 (80%)	51 (12%)	33 (8%)	1	4
1	E	411/421 (98%)	324 (79%)	56 (14%)	31 (8%)	1	5
All	All	2055/2105 (98%)	1633 (80%)	270 (13%)	152 (7%)	1	5

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	118	PRO
1	A	122	SER
1	A	168	ASN
1	A	171	PHE
1	A	176	PRO
1	A	177	GLU
1	A	343	ASP
1	B	43	ASN
1	B	118	PRO
1	B	168	ASN
1	B	171	PHE
1	B	176	PRO

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Mol	Chain	Res	Type
1	B	177	GLU
1	B	343	ASP
1	C	43	ASN
1	C	108	VAL
1	C	118	PRO
1	C	122	SER
1	C	168	ASN
1	C	171	PHE
1	C	176	PRO
1	C	177	GLU
1	C	343	ASP
1	D	43	ASN
1	D	118	PRO
1	D	122	SER
1	D	168	ASN
1	D	171	PHE
1	D	176	PRO
1	D	177	GLU
1	D	343	ASP
1	E	43	ASN
1	E	118	PRO
1	E	122	SER
1	E	168	ASN
1	E	171	PHE
1	E	176	PRO
1	E	177	GLU
1	E	343	ASP
1	A	63	ASN
1	A	108	VAL
1	A	113	LEU
1	A	165	LYS
1	A	167	ILE
1	A	172	GLU
1	B	30	ASP
1	B	63	ASN
1	B	98	ALA
1	B	108	VAL
1	B	122	SER
1	B	165	LYS
1	B	167	ILE
1	B	172	GLU
1	B	189	SER

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Mol	Chain	Res	Type
1	C	63	ASN
1	C	165	LYS
1	C	167	ILE
1	C	172	GLU
1	D	30	ASP
1	D	63	ASN
1	D	98	ALA
1	D	108	VAL
1	D	165	LYS
1	D	167	ILE
1	D	172	GLU
1	E	30	ASP
1	E	63	ASN
1	E	108	VAL
1	E	165	LYS
1	E	167	ILE
1	E	172	GLU
1	A	98	ALA
1	B	113	LEU
1	B	132	LYS
1	C	30	ASP
1	C	98	ALA
1	C	113	LEU
1	C	120	GLY
1	D	80	ILE
1	D	113	LEU
1	D	120	GLY
1	D	189	SER
1	E	98	ALA
1	E	113	LEU
1	A	30	ASP
1	A	80	ILE
1	A	120	GLY
1	A	189	SER
1	A	309	ARG
1	B	47	SER
1	B	80	ILE
1	B	120	GLY
1	B	131	ASP
1	B	309	ARG
1	C	80	ILE
1	C	189	SER

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Mol	Chain	Res	Type
1	C	216	GLY
1	C	309	ARG
1	D	3	VAL
1	D	47	SER
1	D	117	LEU
1	D	309	ARG
1	D	357	PRO
1	D	365	THR
1	E	47	SER
1	E	80	ILE
1	E	120	GLY
1	E	132	LYS
1	E	189	SER
1	A	23	ASP
1	A	47	SER
1	A	117	LEU
1	A	132	LYS
1	A	357	PRO
1	B	23	ASP
1	B	117	LEU
1	B	133	TRP
1	B	357	PRO
1	C	23	ASP
1	C	47	SER
1	C	117	LEU
1	C	131	ASP
1	C	173	PRO
1	D	23	ASP
1	D	79	ASP
1	D	132	LYS
1	D	133	TRP
1	E	23	ASP
1	E	117	LEU
1	E	131	ASP
1	E	133	TRP
1	E	309	ARG
1	E	357	PRO
1	A	131	ASP
1	A	133	TRP
1	A	173	PRO
1	A	216	GLY
1	B	216	GLY

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Mol	Chain	Res	Type
1	C	132	LYS
1	D	131	ASP
1	D	173	PRO
1	D	216	GLY
1	D	370	PRO
1	E	173	PRO
1	E	216	GLY
1	E	370	PRO
1	B	173	PRO
1	C	370	PRO
1	B	370	PRO
1	C	3	VAL
1	E	181	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	359/362 (99%)	302 (84%)	57 (16%)	2	12
1	B	358/362 (99%)	304 (85%)	54 (15%)	3	14
1	C	356/362 (98%)	301 (85%)	55 (15%)	2	13
1	D	359/362 (99%)	303 (84%)	56 (16%)	2	13
1	E	358/362 (99%)	304 (85%)	54 (15%)	3	14
All	All	1790/1810 (99%)	1514 (85%)	276 (15%)	2	13

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	8	ILE
1	A	11	ASN
1	A	22	GLU
1	A	31	TYR
1	A	33	ARG

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	40	LEU
1	A	43	ASN
1	A	78	LYS
1	A	100	ASP
1	A	116	VAL
1	A	117	LEU
1	A	119	ASP
1	A	123	ASP
1	A	126	ARG
1	A	134	LEU
1	A	146	ARG
1	A	152	TYR
1	A	155	LYS
1	A	162	ASN
1	A	163	GLN
1	A	167	ILE
1	A	174	LEU
1	A	175	VAL
1	A	177	GLU
1	A	180	ASP
1	A	181	ILE
1	A	182	PHE
1	A	187	ASN
1	A	189	SER
1	A	209	GLU
1	A	217	THR
1	A	230	THR
1	A	237	ILE
1	A	242	THR
1	A	243	GLU
1	A	251	ASN
1	A	252	ARG
1	A	270	LYS
1	A	273	SER
1	A	283	LEU
1	A	307	LEU
1	A	308	LEU
1	A	309	ARG
1	A	317	ARG
1	A	327	LEU
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	340	SER
1	A	344	LEU
1	A	352	ASP
1	A	354	LYS
1	A	356	THR
1	A	358	ASP
1	A	359	ASP
1	A	405	GLN
1	A	422	LYS
1	B	8	ILE
1	B	11	ASN
1	B	22	GLU
1	B	31	TYR
1	B	33	ARG
1	B	38	ILE
1	B	40	LEU
1	B	43	ASN
1	B	78	LYS
1	B	79	ASP
1	B	100	ASP
1	B	116	VAL
1	B	117	LEU
1	B	119	ASP
1	B	123	ASP
1	B	126	ARG
1	B	134	LEU
1	B	146	ARG
1	B	152	TYR
1	B	155	LYS
1	B	162	ASN
1	B	163	GLN
1	B	167	ILE
1	B	174	LEU
1	B	175	VAL
1	B	177	GLU
1	B	180	ASP
1	B	181	ILE
1	B	182	PHE
1	B	187	ASN
1	B	189	SER
1	B	209	GLU
1	B	217	THR

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Mol	Chain	Res	Type
1	B	230	THR
1	B	237	ILE
1	B	242	THR
1	B	243	GLU
1	B	251	ASN
1	B	252	ARG
1	B	270	LYS
1	B	273	SER
1	B	283	LEU
1	B	307	LEU
1	B	308	LEU
1	B	309	ARG
1	B	317	ARG
1	B	327	LEU
1	B	332	LEU
1	B	340	SER
1	B	352	ASP
1	B	354	LYS
1	B	356	THR
1	B	405	GLN
1	B	422	LYS
1	C	3	VAL
1	C	8	ILE
1	C	22	GLU
1	C	31	TYR
1	C	33	ARG
1	C	38	ILE
1	C	40	LEU
1	C	43	ASN
1	C	67	ILE
1	C	78	LYS
1	C	79	ASP
1	C	100	ASP
1	C	116	VAL
1	C	117	LEU
1	C	119	ASP
1	C	123	ASP
1	C	126	ARG
1	C	134	LEU
1	C	146	ARG
1	C	152	TYR
1	C	155	LYS

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Mol	Chain	Res	Type
1	C	162	ASN
1	C	163	GLN
1	C	167	ILE
1	C	172	GLU
1	C	174	LEU
1	C	175	VAL
1	C	177	GLU
1	C	180	ASP
1	C	181	ILE
1	C	182	PHE
1	C	187	ASN
1	C	189	SER
1	C	209	GLU
1	C	217	THR
1	C	230	THR
1	C	237	ILE
1	C	242	THR
1	C	243	GLU
1	C	251	ASN
1	C	252	ARG
1	C	270	LYS
1	C	273	SER
1	C	283	LEU
1	C	307	LEU
1	C	308	LEU
1	C	309	ARG
1	C	317	ARG
1	C	327	LEU
1	C	332	LEU
1	C	352	ASP
1	C	354	LYS
1	C	356	THR
1	C	405	GLN
1	C	422	LYS
1	D	3	VAL
1	D	8	ILE
1	D	11	ASN
1	D	22	GLU
1	D	31	TYR
1	D	33	ARG
1	D	38	ILE
1	D	40	LEU

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Mol	Chain	Res	Type
1	D	43	ASN
1	D	78	LYS
1	D	79	ASP
1	D	100	ASP
1	D	116	VAL
1	D	117	LEU
1	D	119	ASP
1	D	123	ASP
1	D	126	ARG
1	D	134	LEU
1	D	146	ARG
1	D	152	TYR
1	D	155	LYS
1	D	162	ASN
1	D	163	GLN
1	D	167	ILE
1	D	174	LEU
1	D	175	VAL
1	D	177	GLU
1	D	180	ASP
1	D	181	ILE
1	D	182	PHE
1	D	187	ASN
1	D	189	SER
1	D	209	GLU
1	D	217	THR
1	D	230	THR
1	D	237	ILE
1	D	242	THR
1	D	243	GLU
1	D	251	ASN
1	D	252	ARG
1	D	270	LYS
1	D	273	SER
1	D	283	LEU
1	D	307	LEU
1	D	308	LEU
1	D	309	ARG
1	D	317	ARG
1	D	327	LEU
1	D	332	LEU
1	D	340	SER

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Mol	Chain	Res	Type
1	D	352	ASP
1	D	354	LYS
1	D	356	THR
1	D	358	ASP
1	D	405	GLN
1	D	422	LYS
1	E	3	VAL
1	E	8	ILE
1	E	22	GLU
1	E	31	TYR
1	E	33	ARG
1	E	38	ILE
1	E	40	LEU
1	E	43	ASN
1	E	78	LYS
1	E	79	ASP
1	E	100	ASP
1	E	116	VAL
1	E	117	LEU
1	E	119	ASP
1	E	123	ASP
1	E	126	ARG
1	E	134	LEU
1	E	146	ARG
1	E	152	TYR
1	E	155	LYS
1	E	162	ASN
1	E	163	GLN
1	E	167	ILE
1	E	174	LEU
1	E	175	VAL
1	E	177	GLU
1	E	180	ASP
1	E	181	ILE
1	E	182	PHE
1	E	187	ASN
1	E	189	SER
1	E	209	GLU
1	E	217	THR
1	E	230	THR
1	E	237	ILE
1	E	242	THR

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Mol	Chain	Res	Type
1	E	243	GLU
1	E	251	ASN
1	E	252	ARG
1	E	270	LYS
1	E	273	SER
1	E	283	LEU
1	E	307	LEU
1	E	308	LEU
1	E	309	ARG
1	E	317	ARG
1	E	327	LEU
1	E	332	LEU
1	E	352	ASP
1	E	354	LYS
1	E	356	THR
1	E	358	ASP
1	E	405	GLN
1	E	422	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	70	ASN
1	A	163	GLN
1	A	203	HIS
1	A	266	GLN
1	A	347	GLN
1	B	11	ASN
1	B	70	ASN
1	B	163	GLN
1	B	187	ASN
1	B	266	GLN
1	B	347	GLN
1	C	11	ASN
1	C	70	ASN
1	C	203	HIS
1	C	266	GLN
1	C	347	GLN
1	C	395	GLN
1	D	11	ASN
1	D	70	ASN

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Mol	Chain	Res	Type
1	D	163	GLN
1	D	203	HIS
1	D	266	GLN
1	D	347	GLN
1	E	11	ASN
1	E	70	ASN
1	E	187	ASN
1	E	203	HIS
1	E	266	GLN
1	E	347	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 15 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	416/421 (98%)	-0.11	6 (1%)	75 49	62, 93, 152, 180	0
1	B	415/421 (98%)	-0.05	12 (2%)	51 23	63, 93, 151, 164	0
1	C	413/421 (98%)	-0.02	11 (2%)	54 26	62, 93, 150, 164	0
1	D	416/421 (98%)	0.11	22 (5%)	26 10	63, 93, 152, 164	0
1	E	415/421 (98%)	0.03	17 (4%)	37 14	62, 94, 152, 175	0
All	All	2075/2105 (98%)	-0.01	68 (3%)	46 20	62, 93, 152, 180	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	GLN	6.2
1	D	119	ASP	6.2
1	D	166	MET	6.1
1	D	2	SER	6.0
1	C	171	PHE	5.9
1	B	119	ASP	5.6
1	A	171	PHE	4.8
1	C	357	PRO	4.8
1	D	147	THR	4.5
1	A	122	SER	4.4
1	C	122	SER	4.1
1	E	148	GLN	4.0
1	B	132	LYS	3.9
1	D	132	LYS	3.7
1	C	176	PRO	3.6
1	C	177	GLU	3.5
1	D	43	ASN	3.5
1	E	171	PHE	3.4
1	E	172	GLU	3.3
1	D	171	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	3.1
1	D	98	ALA	3.1
1	E	112	ALA	3.1
1	B	171	PHE	3.1
1	E	35	SER	2.8
1	B	386	ASN	2.8
1	B	365	THR	2.8
1	D	167	ILE	2.7
1	E	88	TRP	2.7
1	E	101	THR	2.7
1	A	176	PRO	2.6
1	D	355	TYR	2.5
1	D	122	SER	2.5
1	B	118	PRO	2.5
1	E	46	LYS	2.5
1	B	122	SER	2.5
1	D	113	LEU	2.5
1	E	102	ILE	2.5
1	B	147	THR	2.5
1	E	62	GLY	2.4
1	C	148	GLN	2.4
1	E	99	GLY	2.2
1	E	122	SER	2.2
1	B	355	TYR	2.2
1	C	355	TYR	2.2
1	D	172	GLU	2.2
1	D	177	GLU	2.2
1	D	404	LEU	2.2
1	B	357	PRO	2.2
1	E	174	LEU	2.2
1	D	182	PHE	2.2
1	D	84	LEU	2.1
1	E	118	PRO	2.1
1	C	114	ASP	2.1
1	C	4	THR	2.1
1	D	176	PRO	2.1
1	C	169	GLU	2.1
1	B	353	ASN	2.1
1	E	177	GLU	2.1
1	D	358	ASP	2.1
1	D	120	GLY	2.1
1	D	168	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	164	CYS	2.0
1	E	355	TYR	2.0
1	B	94	ASN	2.0
1	D	175	VAL	2.0
1	C	62	GLY	2.0
1	A	365	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IUM	B	423	1/3	0.78	0.09	225,225,225,225	0
2	IUM	B	425	1/3	0.85	0.05	229,229,229,229	0
2	IUM	D	423	1/3	0.91	0.09	224,224,224,224	0
2	IUM	A	1	1/3	0.94	0.06	212,212,212,212	0
2	IUM	A	424	1/3	0.94	0.05	204,204,204,204	0
2	IUM	E	424	1/3	0.95	0.09	232,232,232,232	0
2	IUM	C	423	1/3	0.96	0.04	170,170,170,170	0
2	IUM	C	425	1/3	0.96	0.04	177,177,177,177	0
2	IUM	E	423	1/3	0.96	0.06	197,197,197,197	0
2	IUM	A	425	1/3	0.98	0.03	192,192,192,192	0
2	IUM	D	425	1/3	0.99	0.12	111,111,111,111	0
2	IUM	D	424	1/3	0.99	0.13	117,117,117,117	0
2	IUM	B	424	1/3	1.00	0.14	116,116,116,116	0
2	IUM	A	423	1/3	1.00	0.15	116,116,116,116	0
2	IUM	C	424	1/3	1.00	0.12	110,110,110,110	0

6.5 Other polymers

There are no such residues in this entry.