Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 12:06 AM EDT

PDB ID	:	6UFQ
Title	:	Crystal structure of D678N GoxA bound to glycine
Authors	:	Yukl, E.T.
Deposited on	:	2019-09-24
Resolution	:	2.51 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:

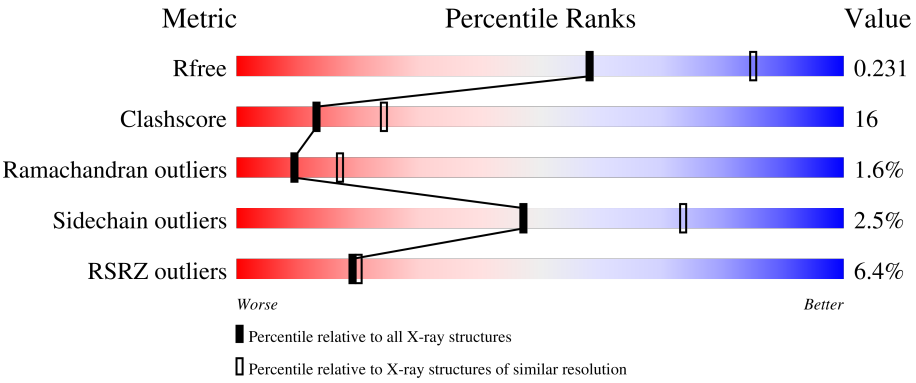
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	816	5% 70% 25%
1	B	816	6% 69% 25%
1	C	816	4% 67% 24% 7%
1	D	816	9% 70% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	A	902	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25587 atoms, of which 20 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 Glycine Oxidase GoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6247	3948	1064	1215	20			
1	B	790	Total	C	N	O	S	0	0	0
			6246	3946	1063	1217	20			
1	C	760	Total	C	N	O	S	0	0	0
			6002	3797	1021	1164	20			
1	D	787	Total	C	N	O	S	0	0	0
			6221	3931	1060	1210	20			

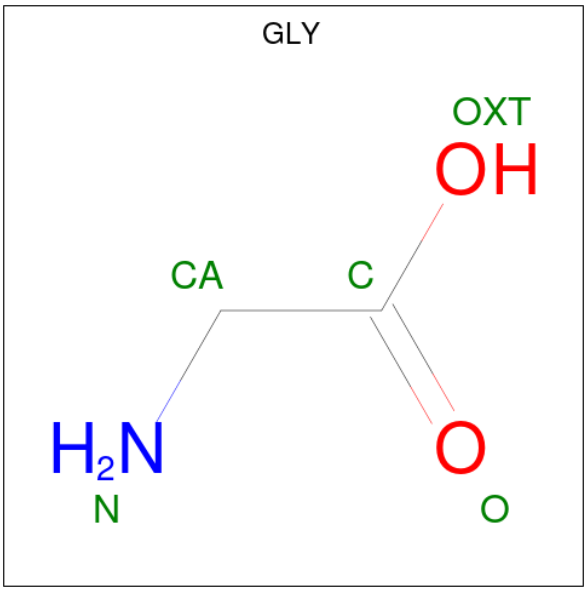
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	ASN	ASP	engineered mutation	UNP A0A161XU12
B	678	ASN	ASP	engineered mutation	UNP A0A161XU12
C	678	ASN	ASP	engineered mutation	UNP A0A161XU12
D	678	ASN	ASP	engineered mutation	UNP A0A161XU12

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	B	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	C	1	Total	C	H	N	O	0	0
			10	2	5	1	2		
3	D	1	Total	C	H	N	O	0	0
			10	2	5	1	2		

- Molecule 4 is water.

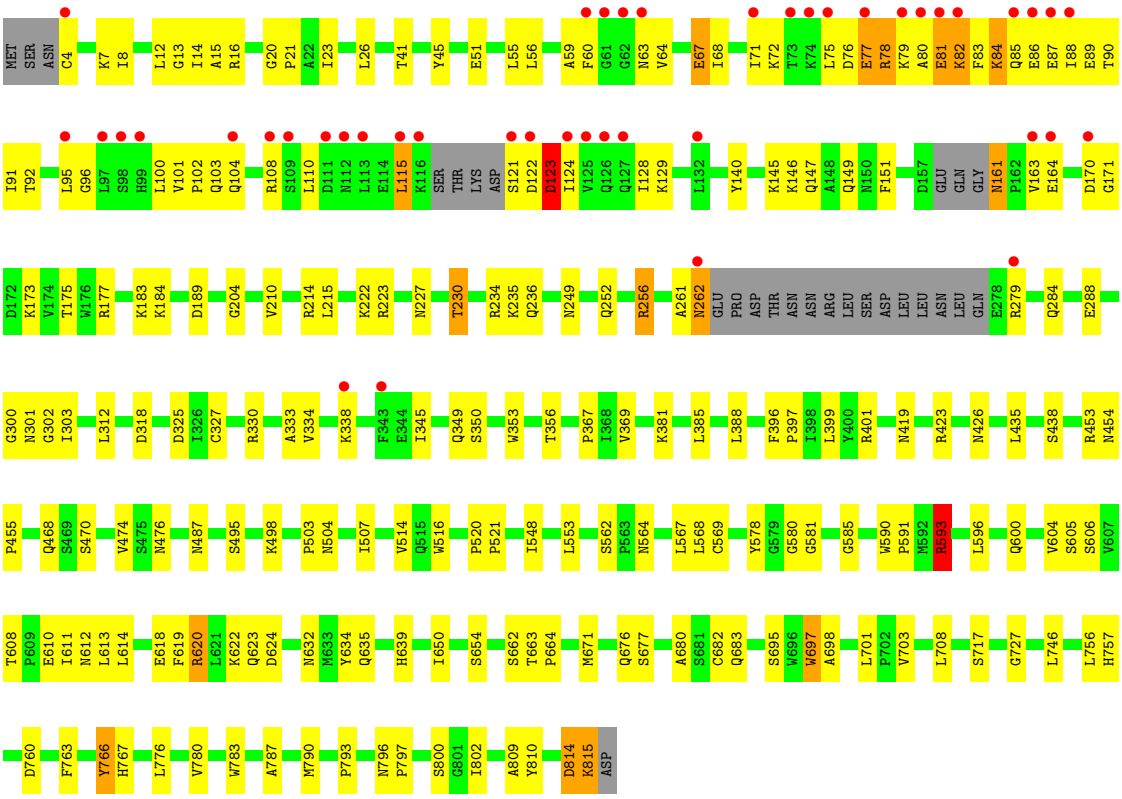
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	240	Total	O	0	0
			240	240		
4	B	215	Total	O	0	0
			215	215		
4	C	195	Total	O	0	0
			195	195		
4	D	177	Total	O	0	0
			177	177		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

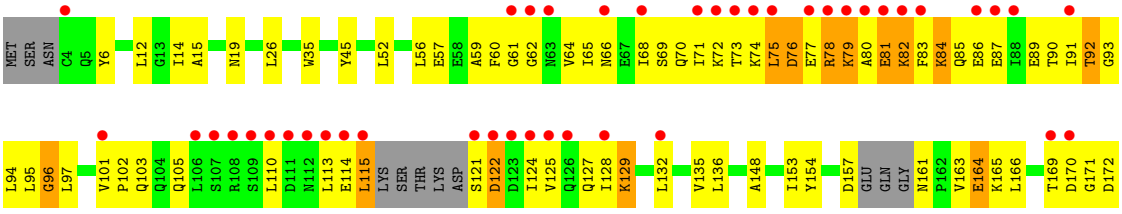
• Molecule 1: Glycine Oxidase GoxA

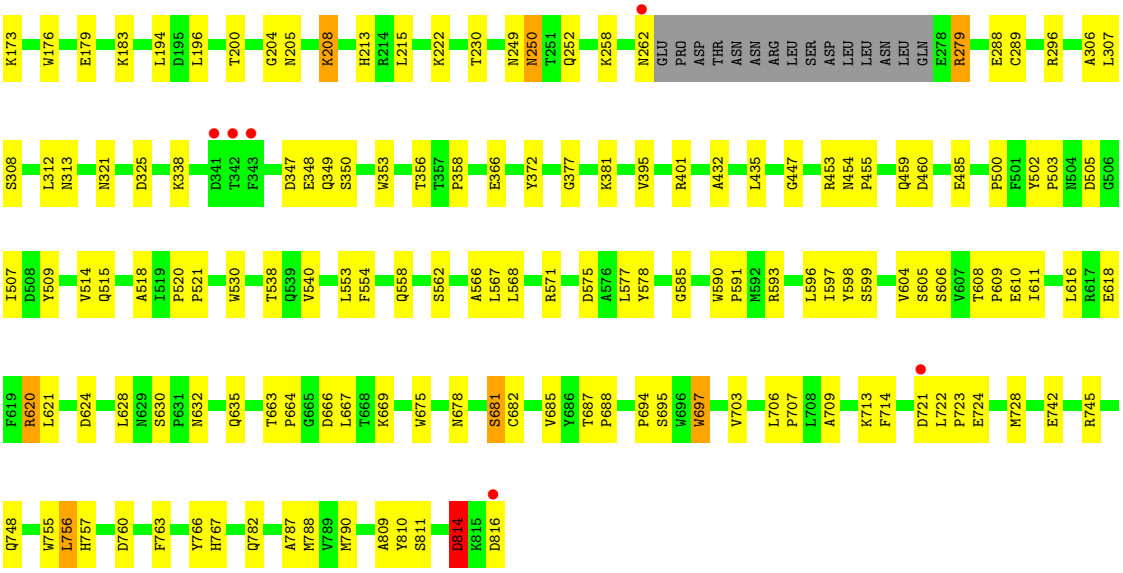
Chain A:



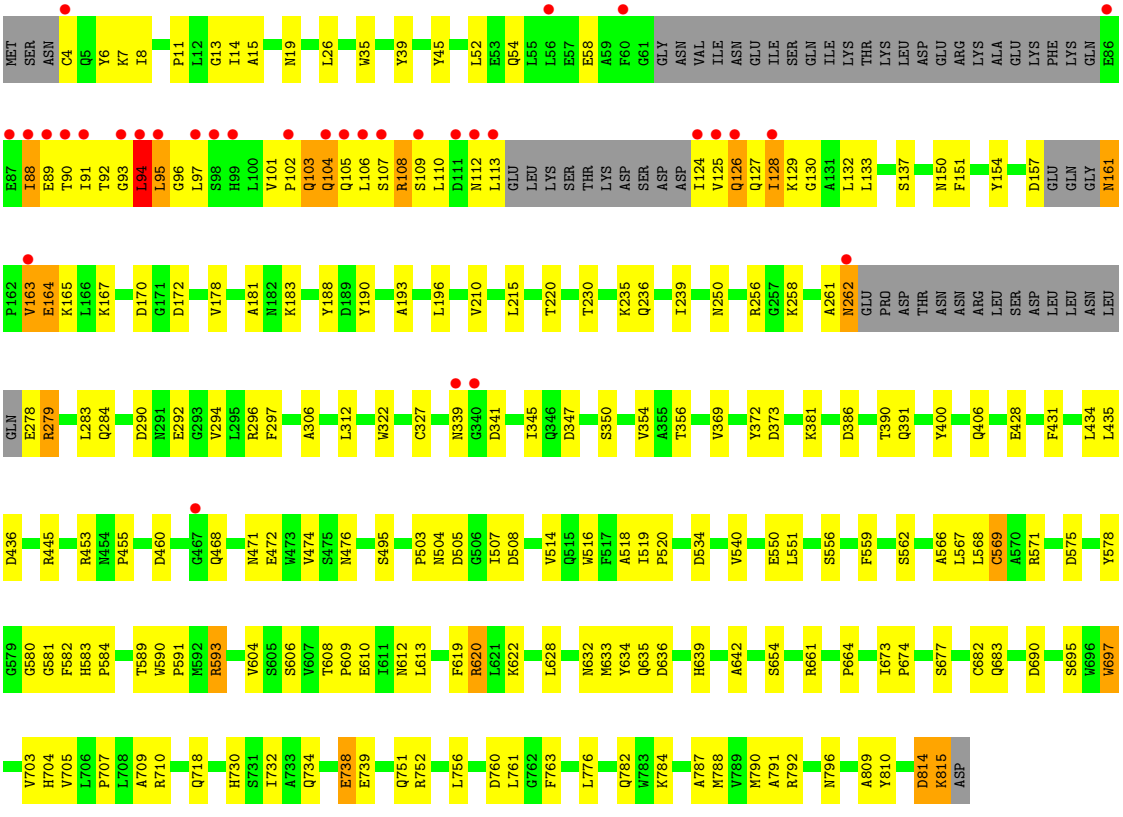
• Molecule 1: Glycine Oxidase GoxA

Chain B:

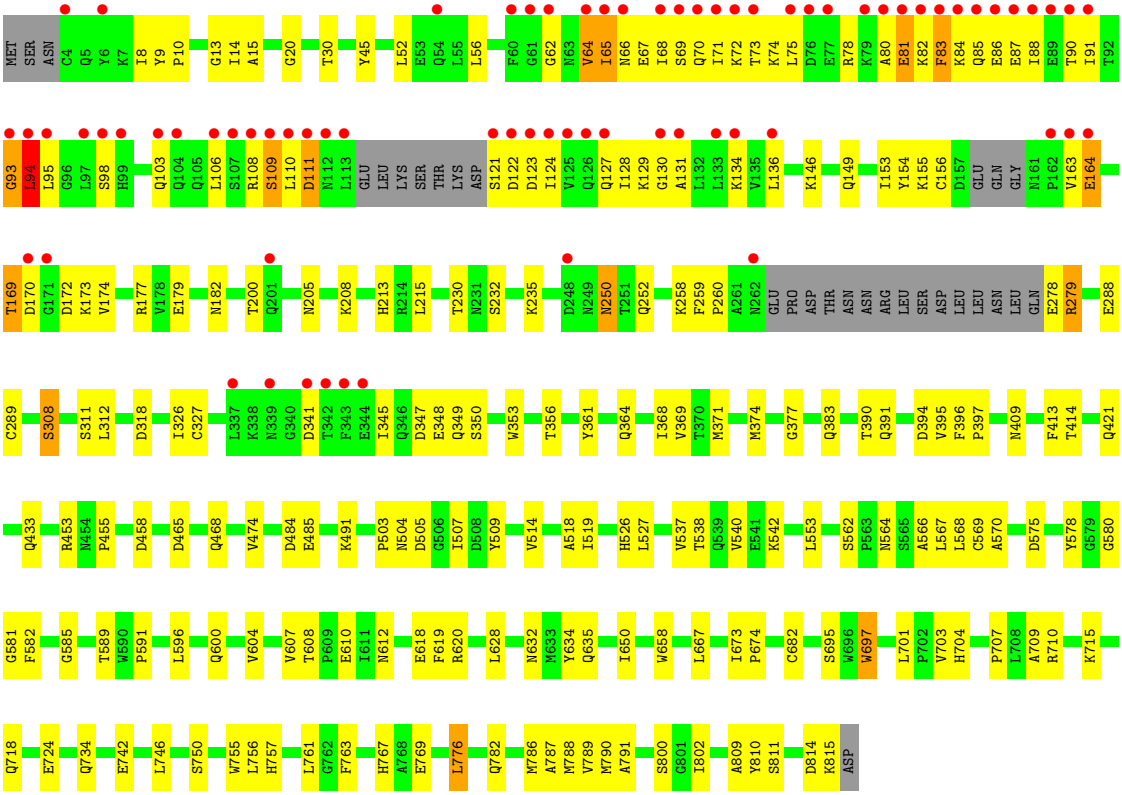




• Molecule 1: Glycine Oxidase GoxA



• Molecule 1: Glycine Oxidase GoxA


MET SER ASN C4 Q5 Y6 K7 I8 Y9 P10 G13 I14 A15 G20 T30 Y45 L52 E53 Q54 L55 L56 F60 G61 G62 N63 V64 I65 N66 E67 I68 S69 Q70 I71 K72 T73 K74 L75 D76 E77 R78 K79 A80 E81 K82 F83 K84 Q85 E86 E87 I88 E89 T90 I91 T92
G93 L94 L95 G96 L97 S98 H99 Q103 Q104 Q105 L106 S107 R108 S109 L110 D111 N112 L113 GLU LEU LYS SER THR LYS ASP S121 D122 D123 I124 V125 Q126 Q127 I128 K129 G130 A131 L132 L133 K134 V135 L136 K146 Q149 I153 Y154 K155 C156 D157 GLU GLN GLY N161 P162 V163 E164
T169 D170 G171 D172 K173 V174 R177 V178 E179 N182 T200 Q201 N205 K208 H213 R214 L215 T230 N231 S232 K235 D248 N249 N250 T251 Q252 K258 F259 P260 A261 N262 GLU PRO ASP THR ASN ASN ARG LEU SER ASP LEU LEU ASN LEU GLN E278 R279 E288
C289 S308 S311 L312 D318 I326 C327 L337 K338 N339 G340 D341 T342 F343 E344 I345 Q346 D347 E348 Q349 S350 W353 T356 Y361 Q364 I368 V369 T370 M371 M374 G377 Q383 T390 Q391 D394 V395 F396 P397 N409 F413 T414 Q421
Q433 R453 N454 P455 D458 D465 Q468 V474 D484 E485 K491 P503 N504 D505 G506 I507 D508 Y509 V514 A518 I519 H526 L527 V537 T538 Q539 V540 E541 K542 L553 S562 P563 N564 S565 A566 L567 L568 C569 A570 D575 Y578 G579 G580
G581 F582 G585 T589 W590 P591 L596 Q600 V604 V607 T608 P609 E610 I611 N612 E618 F619 R620 L628 N632 M633 Y634 Q635 I650 W658 L667 I673 P674 C682 S695 W696 W697 L701 P702 V703 H704 P707 L708 A709 R710 K715
Q718 E724 Q734 E742 L746 S750 W755 L756 H757 L761 G762 F763 H767 A768 E769 L776 Q782 M786 A787 M788 V789 M790 A791 S800 G801 I802 A809 Y810 S811 D814 K815 ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.14Å 91.57Å 178.41Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	46.87 – 2.51 46.87 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.87-2.51) 99.6 (46.87-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.176 , 0.231 0.176 , 0.231	Depositor DCC
R_{free} test set	6022 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25587	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	3/6379 (0.0%)	0.63	0/8680
1	B	0.49	2/6378 (0.0%)	0.62	3/8680 (0.0%)
1	C	0.50	5/6132 (0.1%)	0.66	4/8351 (0.0%)
1	D	0.46	0/6353	0.62	1/8646 (0.0%)
All	All	0.49	10/25242 (0.0%)	0.63	8/34357 (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	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	327	CYS	CB-SG	7.13	1.94	1.82
1	A	327	CYS	CB-SG	6.87	1.94	1.82
1	B	755	TRP	NE1-CE2	-6.12	1.29	1.37
1	A	766	TYR	CE1-CZ	-6.11	1.30	1.38
1	C	569	CYS	CB-SG	-6.00	1.72	1.82
1	C	167	LYS	CD-CE	-5.87	1.36	1.51
1	A	593	ARG	CZ-NH1	-5.66	1.25	1.33
1	B	681	SER	CB-OG	-5.37	1.35	1.42
1	C	677	SER	CB-OG	-5.23	1.35	1.42
1	C	167	LYS	CB-CG	-5.00	1.39	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	167	LYS	CD-CE-NZ	-13.56	80.51	111.70
1	C	167	LYS	CB-CG-CD	-9.30	87.41	111.60
1	B	75	LEU	CB-CG-CD1	-7.01	99.09	111.00
1	C	94	LEU	CA-CB-CG	6.85	131.06	115.30
1	D	776	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	667	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	115	LEU	CB-CG-CD2	-5.37	101.86	111.00
1	C	776	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	814	ASP	Peptide
1	C	93	GLY	Peptide
1	C	94	LEU	Peptide
1	D	94	LEU	Peptide

5.2 Too-close contacts (i)

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	6247	0	6021	192	0
1	B	6246	0	6012	209	0
1	C	6002	0	5767	200	1
1	D	6221	0	5991	207	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	5	2	3	0
3	B	5	5	2	3	0
3	C	5	5	2	2	0
3	D	5	5	2	0	0
4	A	240	0	0	13	0
4	B	215	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	195	0	0	19	0
4	D	177	0	0	18	0
All	All	25567	20	23799	790	1

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 16.

All (790) 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:91:ILE:C	1:C:94:LEU:HD13	1.22	1.50
1:C:91:ILE:O	1:C:94:LEU:HD13	1.36	1.24
1:C:91:ILE:C	1:C:94:LEU:CD1	2.06	1.23
1:A:75:LEU:HD11	1:A:80:ALA:HB3	1.23	1.16
1:D:80:ALA:CA	1:D:81:GLU:HB2	1.76	1.15
1:B:618:GLU:OE2	1:B:620:ARG:NH1	1.81	1.12
1:D:80:ALA:HA	1:D:81:GLU:HB2	1.09	1.09
1:B:80:ALA:HA	1:B:81:GLU:CB	1.82	1.08
1:B:84:LYS:O	1:B:86:GLU:N	1.89	1.06
1:A:80:ALA:HB1	1:A:81:GLU:HB3	1.39	1.03
1:C:91:ILE:CA	1:C:94:LEU:HD13	1.89	1.01
1:C:103:GLN:HA	1:C:106:LEU:HD12	1.42	1.00
1:A:71:ILE:HD11	1:A:87:GLU:HG2	1.41	0.97
1:C:709:ALA:HB2	1:C:815:LYS:HE2	1.49	0.94
1:A:80:ALA:HA	1:A:81:GLU:HB2	1.48	0.94
1:C:91:ILE:CA	1:C:94:LEU:CD1	2.46	0.94
1:D:562:SER:HB3	1:D:568:LEU:HD11	1.51	0.93
1:B:80:ALA:HA	1:B:81:GLU:HB2	1.49	0.91
1:B:447:GLY:O	4:B:1001:HOH:O	1.88	0.91
1:C:622:LYS:O	4:C:1001:HOH:O	1.90	0.90
1:A:312:LEU:HD11	1:C:312:LEU:HD11	1.53	0.89
1:A:80:ALA:CB	1:A:81:GLU:HB3	2.03	0.88
1:C:95:LEU:O	1:C:97:LEU:N	2.06	0.88
1:C:815:LYS:NZ	4:C:1003:HOH:O	2.05	0.88
1:A:87:GLU:O	1:A:90:THR:HB	1.73	0.87
1:B:80:ALA:HA	1:B:81:GLU:HB3	1.54	0.86
1:B:157:ASP:O	4:B:1002:HOH:O	1.92	0.86
1:D:673:ILE:HD12	1:D:674:PRO:HA	1.58	0.86
1:D:769:GLU:OE2	4:D:1001:HOH:O	1.92	0.86
1:D:64:VAL:O	1:D:67:GLU:HB2	1.76	0.86
1:A:683:GLN:OE1	1:A:756:LEU:HD13	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:GLN:OE1	1:C:756:LEU:HD13	1.76	0.85
1:D:66:ASN:O	1:D:70:GLN:HB2	1.75	0.85
1:D:8:ILE:O	1:D:620:ARG:NH2	2.08	0.85
1:C:109:SER:HA	1:C:112:ASN:HD21	1.40	0.85
1:D:503:PRO:HB3	1:D:507:ILE:HD12	1.57	0.84
1:B:95:LEU:HD12	1:B:95:LEU:O	1.77	0.84
1:B:65:ILE:O	1:B:68:ILE:HG22	1.77	0.84
1:B:110:LEU:HA	1:B:113:LEU:HD12	1.59	0.84
1:B:325:ASP:OD2	4:B:1003:HOH:O	1.95	0.84
1:A:75:LEU:CD1	1:A:80:ALA:HB3	2.06	0.83
3:C:902:GLY:O	1:D:767:HIS:NE2	2.11	0.83
1:A:64:VAL:O	1:A:68:ILE:HG13	1.78	0.83
1:C:258:LYS:HD2	1:C:262:ASN:ND2	1.92	0.83
1:A:75:LEU:HD22	1:A:78:ARG:HH21	1.42	0.83
1:D:66:ASN:HA	1:D:69:SER:HB2	1.60	0.82
1:D:409:ASN:OD1	4:D:1002:HOH:O	1.97	0.82
1:B:95:LEU:HD13	1:B:97:LEU:HG	1.62	0.81
1:B:86:GLU:O	1:B:89:GLU:HB3	1.81	0.81
1:D:252:GLN:HG3	1:D:288:GLU:HG3	1.61	0.81
1:A:121:SER:O	1:A:123:ASP:N	2.13	0.81
1:D:348:GLU:HG2	4:D:1072:HOH:O	1.80	0.81
1:B:608:THR:HG23	1:B:609:PRO:HD2	1.62	0.81
1:B:598:TYR:O	4:B:1004:HOH:O	1.98	0.81
1:C:102:PRO:O	1:C:105:GLN:HB3	1.81	0.81
1:B:72:LYS:NZ	4:B:1008:HOH:O	2.12	0.80
1:C:154:TYR:CE2	1:C:566:ALA:HB2	2.16	0.79
1:D:695:SER:HB2	1:D:703:VAL:HG21	1.65	0.79
1:C:540:VAL:HG12	4:C:1023:HOH:O	1.81	0.79
1:D:746:LEU:HD23	1:D:802:ILE:HG13	1.63	0.79
1:A:608:THR:HG22	1:A:610:GLU:H	1.47	0.79
1:D:88:ILE:HD13	1:D:110:LEU:HD12	1.65	0.78
1:C:709:ALA:CB	1:C:815:LYS:HE2	2.13	0.78
1:D:106:LEU:O	1:D:109:SER:OG	2.01	0.78
1:D:85:GLN:NE2	4:D:1009:HOH:O	2.15	0.78
1:D:458:ASP:OD2	4:D:1003:HOH:O	2.02	0.77
1:A:161:ASN:N	4:A:1008:HOH:O	2.16	0.77
1:A:80:ALA:HA	1:A:81:GLU:CB	2.14	0.77
1:B:593:ARG:O	4:B:1005:HOH:O	2.03	0.77
1:A:345:ILE:HG23	1:A:350:SER:HB3	1.67	0.76
1:D:80:ALA:HA	1:D:81:GLU:CB	2.04	0.76
1:C:472:GLU:OE2	4:C:1002:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:LEU:CD2	1:C:604:VAL:HG21	2.15	0.76
1:B:66:ASN:O	1:B:69:SER:OG	2.02	0.76
1:B:75:LEU:HD11	1:B:78:ARG:HD2	1.67	0.76
1:D:9:TYR:OH	1:D:618:GLU:OE1	2.03	0.76
1:D:66:ASN:O	1:D:70:GLN:N	2.19	0.75
1:A:468:GLN:HB3	1:D:635:GLN:HE22	1.52	0.74
1:C:683:GLN:HG3	1:C:756:LEU:HD11	1.69	0.74
1:D:75:LEU:HD22	1:D:80:ALA:CB	2.17	0.74
1:D:761:LEU:O	4:D:1004:HOH:O	2.04	0.74
1:A:68:ILE:HA	1:A:71:ILE:HG22	1.70	0.73
1:C:796:ASN:ND2	4:C:1018:HOH:O	2.21	0.73
1:A:227:ASN:O	4:A:1002:HOH:O	2.06	0.73
1:C:92:THR:C	1:C:94:LEU:HD12	2.09	0.73
1:A:787:ALA:HA	1:A:810:TYR:O	1.89	0.73
1:A:606:SER:HB2	1:A:608:THR:O	1.89	0.72
1:B:78:ARG:NH2	1:B:87:GLU:OE1	2.22	0.72
1:C:210:VAL:HA	1:C:215:LEU:HD22	1.71	0.72
1:B:80:ALA:CA	1:B:81:GLU:CB	2.64	0.72
1:A:284:GLN:O	4:A:1001:HOH:O	2.05	0.72
1:A:80:ALA:CA	1:A:81:GLU:CB	2.67	0.72
1:B:72:LYS:HD2	1:B:121:SER:HB2	1.71	0.72
1:A:695:SER:HB2	1:A:703:VAL:HG21	1.71	0.72
1:B:110:LEU:HD23	1:B:113:LEU:HD11	1.71	0.72
1:B:787:ALA:HB1	1:B:809:ALA:HB1	1.70	0.72
1:A:325:ASP:OD1	4:A:1003:HOH:O	2.08	0.71
1:A:75:LEU:HD11	1:A:80:ALA:CB	2.13	0.71
1:D:608:THR:HG22	1:D:610:GLU:H	1.55	0.71
1:D:87:GLU:O	1:D:91:ILE:HG13	1.90	0.71
1:D:318:ASP:O	4:D:1005:HOH:O	2.09	0.70
1:A:71:ILE:CD1	1:A:87:GLU:HG2	2.20	0.70
1:B:70:GLN:O	1:B:73:THR:N	2.24	0.70
1:C:124:ILE:HD11	1:C:127:GLN:OE1	1.91	0.70
1:D:95:LEU:HD22	1:D:95:LEU:H	1.56	0.70
1:C:8:ILE:O	1:C:620:ARG:NH2	2.24	0.70
1:C:761:LEU:O	4:C:1005:HOH:O	2.10	0.70
1:B:262:ASN:O	4:B:1006:HOH:O	2.08	0.70
1:B:453:ARG:HG2	1:B:518:ALA:HB2	1.72	0.69
1:C:91:ILE:O	1:C:94:LEU:CD1	2.26	0.69
1:A:438:SER:OG	4:A:1004:HOH:O	2.10	0.69
1:D:153:ILE:HD12	1:D:174:VAL:HG21	1.74	0.69
1:C:258:LYS:HD2	1:C:262:ASN:HD21	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ASP:OD1	4:C:1004:HOH:O	2.09	0.69
1:D:67:GLU:O	1:D:71:ILE:HG23	1.93	0.69
1:B:161:ASN:N	4:B:1011:HOH:O	2.25	0.69
1:B:249:ASN:O	1:B:250:ASN:OD1	2.10	0.69
1:D:782:GLN:OE1	4:D:1006:HOH:O	2.11	0.69
1:C:339:ASN:ND2	1:C:341:ASP:OD2	2.26	0.69
1:C:157:ASP:OD1	1:C:161:ASN:HB3	1.93	0.69
1:C:91:ILE:CA	1:C:94:LEU:HD11	2.23	0.68
1:D:88:ILE:HD11	1:D:110:LEU:HB2	1.74	0.68
1:D:179:GLU:OE2	4:D:1007:HOH:O	2.11	0.68
1:B:110:LEU:CA	1:B:113:LEU:HD12	2.24	0.68
1:D:650:ILE:O	4:D:1008:HOH:O	2.11	0.68
1:C:550:GLU:OE2	4:C:1006:HOH:O	2.11	0.68
1:B:258:LYS:NZ	1:B:279:ARG:HB3	2.08	0.68
1:C:661:ARG:O	4:C:1007:HOH:O	2.12	0.67
1:C:107:SER:C	1:C:109:SER:H	1.97	0.67
1:B:80:ALA:CA	1:B:81:GLU:HB3	2.23	0.67
1:C:582:PHE:HD2	1:C:593:ARG:NH2	1.91	0.67
1:D:67:GLU:HG3	1:D:94:LEU:HD11	1.76	0.67
1:C:589:THR:OG1	1:C:590:TRP:N	2.28	0.67
1:A:147:GLN:OE1	4:A:1005:HOH:O	2.12	0.66
1:B:59:ALA:HB1	1:B:95:LEU:CB	2.25	0.66
1:B:91:ILE:O	1:B:93:GLY:N	2.28	0.66
1:A:80:ALA:HB1	1:A:81:GLU:CB	2.22	0.66
1:C:91:ILE:HA	1:C:94:LEU:CD1	2.22	0.66
1:C:428:GLU:OE2	4:C:1008:HOH:O	2.13	0.66
1:B:562:SER:HB3	1:B:568:LEU:HD11	1.78	0.66
1:D:84:LYS:HD2	1:D:85:GLN:H	1.59	0.66
1:D:80:ALA:CB	1:D:81:GLU:HB2	2.25	0.66
1:D:64:VAL:O	1:D:67:GLU:N	2.28	0.66
3:A:902:GLY:N	1:B:697:TRQ:O6	2.29	0.66
1:B:12:LEU:HD13	1:B:353:TRP:HB3	1.78	0.65
1:C:126:GLN:HA	1:C:129:LYS:HG2	1.79	0.65
1:D:98:SER:HB3	1:D:103:GLN:NE2	2.10	0.65
1:A:15:ALA:O	1:A:356:THR:HA	1.97	0.65
1:D:756:LEU:HD22	1:D:761:LEU:HD13	1.79	0.65
1:C:92:THR:O	1:C:94:LEU:HD12	1.97	0.65
1:D:83:PHE:CZ	1:D:110:LEU:HB3	2.32	0.65
1:A:249:ASN:HB3	4:A:1011:HOH:O	1.97	0.64
1:C:683:GLN:OE1	1:C:756:LEU:CD1	2.44	0.64
1:A:60:PHE:CE2	1:A:129:LYS:HG2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:ALA:HA	1:B:810:TYR:O	1.97	0.64
1:D:75:LEU:HD22	1:D:80:ALA:HB2	1.79	0.64
1:C:13:GLY:O	1:C:14:ILE:HD13	1.96	0.64
1:B:75:LEU:HD13	1:B:78:ARG:HB3	1.80	0.64
1:D:15:ALA:O	1:D:356:THR:HA	1.98	0.64
1:D:80:ALA:CA	1:D:81:GLU:CB	2.65	0.64
1:D:83:PHE:CE1	1:D:88:ILE:HD11	2.32	0.64
1:D:78:ARG:CZ	1:D:78:ARG:HB3	2.28	0.63
1:D:673:ILE:HD12	1:D:674:PRO:CA	2.27	0.63
1:C:157:ASP:O	4:C:1009:HOH:O	2.15	0.63
1:D:88:ILE:CD1	1:D:110:LEU:HB2	2.27	0.63
1:C:163:VAL:O	1:C:164:GLU:CB	2.45	0.63
1:A:189:ASP:HA	1:A:318:ASP:OD1	1.98	0.62
1:B:722:LEU:HB3	1:B:723:PRO:HD2	1.82	0.62
1:B:200:THR:O	1:B:208:LYS:HE2	1.98	0.62
1:A:82:LYS:HA	1:A:115:LEU:HD21	1.79	0.62
1:D:567:LEU:CD2	1:D:604:VAL:HG21	2.28	0.62
1:A:585:GLY:HA2	1:A:697:TRQ:CZ2	2.30	0.62
1:C:15:ALA:O	1:C:356:THR:HA	2.00	0.61
1:C:809:ALA:O	1:C:814:ASP:OD2	2.18	0.61
1:A:210:VAL:HA	1:A:215:LEU:HD12	1.82	0.61
1:D:109:SER:OG	1:D:110:LEU:HG	2.00	0.61
1:A:76:ASP:O	1:A:78:ARG:N	2.33	0.61
1:C:406:GLN:OE1	4:C:1010:HOH:O	2.16	0.61
1:B:76:ASP:HB2	1:B:77:GLU:OE2	2.00	0.61
1:C:106:LEU:O	1:C:109:SER:OG	2.13	0.61
1:C:787:ALA:HA	1:C:810:TYR:O	2.01	0.61
1:D:814:ASP:O	1:D:815:LYS:HB2	1.99	0.61
1:C:503:PRO:HB3	1:C:507:ILE:HD12	1.82	0.61
1:D:75:LEU:HD22	1:D:80:ALA:HB3	1.81	0.61
1:D:347:ASP:OD1	1:D:350:SER:HB2	2.01	0.61
1:A:8:ILE:O	1:A:620:ARG:NH2	2.32	0.61
1:B:171:GLY:CA	1:B:338:LYS:HG2	2.30	0.61
1:B:590:TRP:O	1:B:593:ARG:HB2	2.00	0.61
1:D:121:SER:O	1:D:122:ASP:HB3	2.01	0.61
1:C:606:SER:HB2	1:C:608:THR:O	2.01	0.61
1:C:814:ASP:O	1:C:815:LYS:HB2	2.01	0.61
1:D:122:ASP:O	1:D:124:ILE:N	2.34	0.61
1:A:20:GLY:O	1:A:146:LYS:HE2	2.01	0.60
1:B:114:GLU:O	1:B:115:LEU:HG	2.01	0.60
1:B:685:VAL:O	1:B:694:PRO:HD2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:ALA:HB2	1:D:815:LYS:H	1.65	0.60
1:A:72:LYS:HA	1:A:75:LEU:HB2	1.82	0.60
1:C:682:CYS:SG	1:C:697:TRQ:HB3	2.42	0.60
1:A:84:LYS:HD2	1:A:85:GLN:H	1.65	0.60
1:B:366:GLU:HB3	1:B:401:ARG:HG2	1.83	0.60
1:B:628:LEU:HD12	1:B:664:PRO:HG2	1.82	0.60
1:B:503:PRO:HB3	1:B:507:ILE:HD12	1.82	0.60
1:C:695:SER:HB2	1:C:703:VAL:HG21	1.82	0.59
1:D:742:GLU:OE1	1:D:742:GLU:HA	2.02	0.59
1:A:68:ILE:HA	1:A:71:ILE:CG2	2.31	0.59
1:A:91:ILE:O	1:A:95:LEU:HD12	2.01	0.59
1:A:618:GLU:OE2	1:A:620:ARG:NH1	2.36	0.59
1:C:284:GLN:O	4:C:1011:HOH:O	2.16	0.59
1:B:196:LEU:HD11	1:B:505:ASP:HB3	1.84	0.59
1:C:112:ASN:OD1	1:C:112:ASN:N	2.35	0.59
1:C:763:PHE:O	4:C:1013:HOH:O	2.17	0.59
1:D:585:GLY:HA2	1:D:697:TRQ:CZ2	2.33	0.59
1:B:110:LEU:HA	1:B:113:LEU:CD1	2.32	0.59
1:B:110:LEU:HD23	1:B:113:LEU:CD1	2.31	0.59
1:A:84:LYS:HD2	1:A:85:GLN:N	2.18	0.59
1:B:95:LEU:O	1:B:95:LEU:CD1	2.50	0.59
1:B:75:LEU:CD1	1:B:78:ARG:HB3	2.33	0.59
1:B:766:TYR:OH	3:B:902:GLY:OXT	2.15	0.59
1:B:682:CYS:SG	1:B:697:TRQ:HB3	2.43	0.59
1:D:345:ILE:HG23	1:D:350:SER:HB3	1.84	0.59
1:D:787:ALA:HA	1:D:810:TYR:O	2.02	0.59
1:C:125:VAL:O	1:C:128:ILE:N	2.36	0.58
1:A:101:VAL:HG12	1:A:102:PRO:HD2	1.84	0.58
1:A:67:GLU:O	1:A:71:ILE:HG22	2.03	0.58
1:A:683:GLN:HG3	1:A:756:LEU:HD11	1.86	0.58
1:D:278:GLU:OE2	4:D:1010:HOH:O	2.17	0.58
1:C:628:LEU:HD23	1:C:664:PRO:HG2	1.84	0.58
1:C:791:ALA:O	1:C:792:ARG:HD3	2.02	0.58
1:A:82:LYS:HE3	1:A:83:PHE:N	2.18	0.58
1:D:413:PHE:CD2	1:D:414:THR:HG23	2.38	0.58
1:D:746:LEU:HG	1:D:800:SER:O	2.04	0.58
1:C:129:LYS:O	1:C:129:LYS:HG3	2.01	0.58
1:A:766:TYR:OH	3:A:902:GLY:O	2.10	0.57
1:B:635:GLN:HE22	1:C:468:GLN:HB3	1.68	0.57
1:C:172:ASP:OD2	4:C:1012:HOH:O	2.16	0.57
1:D:62:GLY:CA	1:D:65:ILE:HG13	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:LEU:O	1:D:761:LEU:HD12	2.04	0.57
1:A:84:LYS:O	1:A:87:GLU:N	2.38	0.57
1:B:65:ILE:C	1:B:68:ILE:HG22	2.24	0.57
1:A:369:VAL:HG21	1:A:520:PRO:HD3	1.87	0.57
1:A:746:LEU:HG	1:A:800:SER:O	2.04	0.57
1:C:345:ILE:HG23	1:C:350:SER:OG	2.04	0.57
1:D:746:LEU:CD2	1:D:802:ILE:HG13	2.33	0.57
1:A:256:ARG:NH2	4:A:1021:HOH:O	2.38	0.57
1:C:90:THR:C	1:C:94:LEU:HD11	2.25	0.57
1:A:4:CYS:SG	1:A:7:LYS:HE3	2.45	0.57
1:C:92:THR:HA	1:C:95:LEU:HD11	1.87	0.57
1:D:131:ALA:O	1:D:134:LYS:HB3	2.03	0.57
1:A:163:VAL:O	1:A:164:GLU:HB3	2.05	0.57
1:B:252:GLN:NE2	1:B:288:GLU:OE2	2.37	0.57
1:A:88:ILE:C	1:A:90:THR:H	2.08	0.56
1:A:92:THR:HB	1:A:103:GLN:HE22	1.70	0.56
1:D:68:ILE:HA	1:D:71:ILE:CD1	2.34	0.56
1:D:538:THR:OG1	1:D:540:VAL:HG12	2.05	0.56
1:D:718:GLN:O	1:D:734:GLN:NE2	2.38	0.56
1:D:84:LYS:HG3	1:D:86:GLU:H	1.70	0.56
1:D:88:ILE:HD13	1:D:110:LEU:CD1	2.35	0.56
1:A:82:LYS:HE3	1:A:83:PHE:H	1.69	0.56
1:A:115:LEU:HB3	1:A:124:ILE:HD11	1.86	0.56
1:A:608:THR:HG22	1:A:610:GLU:N	2.19	0.56
1:A:797:PRO:HB3	1:A:802:ILE:O	2.05	0.56
1:B:75:LEU:CD1	1:B:78:ARG:HD2	2.34	0.56
1:B:258:LYS:HZ3	1:B:279:ARG:HB3	1.69	0.56
1:C:92:THR:N	1:C:94:LEU:CD1	2.68	0.56
1:C:703:VAL:HG12	1:C:704:HIS:CE1	2.40	0.56
1:B:71:ILE:CD1	1:B:87:GLU:CD	2.74	0.56
1:B:249:ASN:O	1:B:250:ASN:CB	2.54	0.56
1:D:755:TRP:CZ2	1:D:786:MET:HB3	2.41	0.56
1:A:80:ALA:CB	1:A:81:GLU:CB	2.78	0.56
1:B:71:ILE:CD1	1:B:87:GLU:OE1	2.53	0.56
1:B:115:LEU:HD21	1:B:127:GLN:OE1	2.05	0.56
1:D:182:ASN:HA	4:D:1018:HOH:O	2.06	0.56
1:A:55:LEU:HD21	1:A:100:LEU:HD11	1.87	0.56
1:B:554:PHE:O	1:B:558:GLN:HG2	2.06	0.56
1:C:26:LEU:HD21	1:C:52:LEU:HD23	1.87	0.56
1:A:596:LEU:O	1:A:622:LYS:HE3	2.05	0.56
1:A:760:ASP:OD2	1:B:485:GLU:OE2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:GLY:HA2	1:B:697:TRQ:CZ2	2.36	0.56
1:C:589:THR:HG23	1:C:591:PRO:HD2	1.88	0.55
1:A:110:LEU:HD21	1:A:128:ILE:HG23	1.87	0.55
1:C:151:PHE:O	1:C:294:VAL:HG23	2.05	0.55
1:B:78:ARG:HH22	1:B:87:GLU:CD	2.09	0.55
1:B:114:GLU:O	1:B:114:GLU:HG2	2.03	0.55
1:C:738:GLU:HB3	1:C:739:GLU:OE1	2.06	0.55
1:D:200:THR:O	1:D:208:LYS:HE3	2.06	0.55
1:B:163:VAL:O	1:B:164:GLU:HB3	2.06	0.55
1:B:811:SER:O	1:B:814:ASP:HB2	2.07	0.55
1:C:91:ILE:N	1:C:94:LEU:HD11	2.21	0.55
1:C:188:TYR:OH	1:C:636:ASP:HB2	2.07	0.55
1:C:730:HIS:NE2	1:C:734:GLN:HG3	2.21	0.55
1:D:607:VAL:HG23	1:D:612:ASN:O	2.07	0.55
1:D:756:LEU:HD22	1:D:761:LEU:CD1	2.37	0.55
1:A:426:ASN:HD21	1:A:548:ILE:HG22	1.71	0.55
1:D:582:PHE:CD1	1:D:589:THR:HA	2.41	0.55
1:A:164:GLU:OE1	1:A:164:GLU:HA	2.07	0.55
1:A:252:GLN:HG3	1:A:288:GLU:HG3	1.88	0.55
1:C:782:GLN:OE1	4:C:1014:HOH:O	2.18	0.55
1:A:14:ILE:O	1:A:149:GLN:HB2	2.07	0.55
1:B:349:GLN:O	1:B:620:ARG:HD2	2.07	0.55
1:C:514:VAL:HG12	1:C:514:VAL:O	2.06	0.55
1:D:68:ILE:O	1:D:71:ILE:HG12	2.07	0.55
1:C:92:THR:HA	1:C:95:LEU:CD1	2.37	0.55
1:C:619:PHE:O	1:C:620:ARG:HG2	2.08	0.54
1:C:739:GLU:CD	1:C:739:GLU:H	2.09	0.54
1:D:83:PHE:CZ	1:D:88:ILE:HD11	2.43	0.54
1:A:21:PRO:HD3	1:A:140:TYR:CD1	2.42	0.54
1:A:68:ILE:CA	1:A:71:ILE:HG22	2.37	0.54
1:A:503:PRO:HB3	1:A:507:ILE:HD12	1.88	0.54
1:B:62:GLY:O	1:B:65:ILE:HG12	2.08	0.54
1:D:103:GLN:HE21	1:D:103:GLN:HA	1.71	0.54
1:C:154:TYR:CD2	1:C:566:ALA:HB2	2.43	0.54
1:D:83:PHE:HZ	1:D:110:LEU:C	2.11	0.54
1:A:590:TRP:O	1:A:593:ARG:HG3	2.07	0.54
1:C:608:THR:HG23	1:C:609:PRO:HD2	1.89	0.54
1:B:606:SER:HB3	1:B:608:THR:O	2.07	0.54
1:B:110:LEU:HD21	1:B:128:ILE:HG23	1.88	0.54
1:D:13:GLY:O	1:D:14:ILE:HD13	2.08	0.54
1:A:453:ARG:CZ	1:A:516:TRP:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:O	1:B:97:LEU:N	2.40	0.54
1:C:45:TYR:HB2	1:C:788:MET:HG2	1.89	0.54
1:B:83:PHE:O	1:B:84:LYS:HB2	2.08	0.54
1:B:628:LEU:CD1	1:B:664:PRO:HG2	2.38	0.54
1:A:80:ALA:CA	1:A:81:GLU:HB2	2.26	0.54
1:A:504:ASN:HB3	1:A:514:VAL:O	2.08	0.54
1:B:15:ALA:O	1:B:356:THR:HA	2.08	0.54
1:B:179:GLU:HB2	1:B:628:LEU:HD13	1.90	0.54
1:D:67:GLU:O	1:D:70:GLN:HB3	2.07	0.54
1:A:487:ASN:OD1	1:D:308:SER:HB2	2.08	0.53
1:B:194:LEU:HB2	1:B:590:TRP:CZ2	2.42	0.53
1:A:619:PHE:O	1:A:620:ARG:HG2	2.09	0.53
1:B:395:VAL:HG21	1:B:530:TRP:HB2	1.91	0.53
1:C:163:VAL:O	1:C:164:GLU:HB2	2.07	0.53
1:A:419:ASN:O	1:A:423:ARG:HG3	2.07	0.53
1:A:606:SER:HB3	1:A:612:ASN:HA	1.91	0.53
1:C:369:VAL:HG21	1:C:520:PRO:HD3	1.91	0.53
1:D:205:ASN:OD1	1:D:377:GLY:HA3	2.09	0.53
1:C:104:GLN:HG3	1:C:104:GLN:O	2.08	0.53
1:D:64:VAL:HA	1:D:67:GLU:HB2	1.91	0.53
1:D:814:ASP:O	1:D:815:LYS:CB	2.57	0.53
1:B:372:TYR:CD1	1:B:571:ARG:HG3	2.42	0.53
1:C:124:ILE:CD1	1:C:127:GLN:HB2	2.39	0.53
1:C:453:ARG:O	4:C:1015:HOH:O	2.19	0.53
1:D:707:PRO:HG2	1:D:710:ARG:HG2	1.91	0.53
1:B:81:GLU:O	1:B:82:LYS:HB2	2.09	0.53
1:B:92:THR:HG22	1:B:103:GLN:OE1	2.09	0.53
1:D:391:GLN:OE1	1:D:612:ASN:N	2.32	0.53
1:A:514:VAL:O	1:A:514:VAL:HG12	2.09	0.52
1:D:600:GLN:O	1:D:619:PHE:HA	2.10	0.52
1:C:154:TYR:CE1	1:C:165:LYS:HG2	2.44	0.52
1:D:682:CYS:SG	1:D:701:LEU:HD12	2.49	0.52
1:B:71:ILE:HD11	1:B:87:GLU:CD	2.30	0.52
1:C:431:PHE:CE1	1:C:434:LEU:HD12	2.44	0.52
1:A:91:ILE:HG22	1:A:95:LEU:HD11	1.91	0.52
1:A:639:HIS:HB3	1:D:509:TYR:CD1	2.43	0.52
1:A:385:LEU:O	1:A:388:LEU:HB2	2.10	0.52
1:C:4:CYS:SG	1:C:7:LYS:HE3	2.50	0.52
1:C:106:LEU:O	1:C:109:SER:CB	2.58	0.52
1:D:103:GLN:NE2	1:D:103:GLN:HA	2.25	0.52
1:D:69:SER:O	1:D:73:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HD12	1:C:110:LEU:N	2.24	0.52
1:A:809:ALA:O	1:A:814:ASP:OD2	2.28	0.51
1:C:88:ILE:HB	1:C:89:GLU:OE2	2.09	0.51
1:A:567:LEU:CD2	1:A:604:VAL:HG21	2.40	0.51
1:D:62:GLY:HA2	1:D:65:ILE:HG13	1.92	0.51
1:A:76:ASP:O	1:A:79:LYS:N	2.40	0.51
1:A:553:LEU:HD13	1:A:553:LEU:O	2.10	0.51
1:B:608:THR:HG22	1:B:610:GLU:H	1.74	0.51
1:C:95:LEU:O	1:C:95:LEU:CD1	2.59	0.51
1:B:171:GLY:HA3	1:B:338:LYS:HG2	1.92	0.51
1:B:606:SER:CB	1:B:608:THR:O	2.59	0.51
1:C:95:LEU:HD22	1:C:132:LEU:CD1	2.41	0.51
1:D:52:LEU:HD22	1:D:136:LEU:HB3	1.93	0.51
1:D:88:ILE:HD11	1:D:110:LEU:CB	2.40	0.51
1:D:580:GLY:HA2	1:D:581:GLY:C	2.31	0.51
1:D:682:CYS:SG	1:D:697:TRQ:HB3	2.51	0.51
1:B:70:GLN:O	1:B:73:THR:OG1	2.19	0.51
1:D:87:GLU:HA	1:D:90:THR:OG1	2.10	0.51
1:D:465:ASP:HB3	1:D:468:GLN:CG	2.40	0.51
1:A:727:GLY:N	4:A:1007:HOH:O	2.14	0.51
1:D:504:ASN:HB3	1:D:514:VAL:O	2.10	0.51
1:A:104:GLN:O	1:A:108:ARG:HD2	2.11	0.51
1:A:349:GLN:O	1:A:620:ARG:HD2	2.10	0.51
1:C:582:PHE:HD2	1:C:593:ARG:HH21	1.57	0.51
1:D:153:ILE:CD1	1:D:174:VAL:HG21	2.40	0.51
1:B:45:TYR:HB2	1:B:788:MET:HG2	1.93	0.50
1:D:68:ILE:HG23	1:D:71:ILE:HD11	1.92	0.50
1:A:175:THR:HB	1:A:334:VAL:HG12	1.93	0.50
1:B:124:ILE:HG23	1:B:125:VAL:N	2.26	0.50
1:B:724:GLU:HA	1:B:728:MET:O	2.12	0.50
1:B:154:TYR:CZ	1:B:165:LYS:HG2	2.47	0.50
1:C:26:LEU:HD21	1:C:52:LEU:CD2	2.42	0.50
1:D:368:ILE:HG23	1:D:369:VAL:HG23	1.93	0.50
1:D:635:GLN:HB3	1:D:658:TRP:CZ2	2.47	0.50
1:B:604:VAL:HG23	1:B:605:SER:N	2.26	0.50
1:C:751:GLN:NE2	1:D:750:SER:O	2.44	0.50
1:D:279:ARG:HG3	1:D:279:ARG:HH11	1.77	0.50
1:A:564:ASN:ND2	1:A:567:LEU:HD22	2.26	0.50
1:A:682:CYS:SG	1:A:697:TRQ:HB3	2.52	0.50
1:B:59:ALA:HB1	1:B:95:LEU:HB3	1.94	0.50
1:A:204:GLY:O	1:A:521:PRO:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:TYR:CD2	1:C:790:MET:HG2	2.47	0.50
1:A:26:LEU:O	1:A:145:LYS:HG2	2.12	0.50
1:A:235:LYS:HG2	1:A:634:TYR:CD1	2.46	0.50
1:A:236:GLN:HA	1:A:261:ALA:HB3	1.94	0.50
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.94	0.50
1:A:301:ASN:HB2	1:A:303:ILE:HD12	1.94	0.49
1:B:358:PRO:HB3	1:B:675:TRP:CE3	2.47	0.49
1:C:606:SER:HB3	1:C:612:ASN:HA	1.93	0.49
1:D:67:GLU:HA	1:D:70:GLN:OE1	2.12	0.49
1:B:103:GLN:O	1:B:103:GLN:HG3	2.11	0.49
1:D:62:GLY:C	1:D:65:ILE:HG13	2.33	0.49
1:A:115:LEU:CB	1:A:124:ILE:HD11	2.41	0.49
1:B:121:SER:O	1:B:122:ASP:CB	2.59	0.49
1:D:484:ASP:O	4:D:1011:HOH:O	2.19	0.49
1:A:596:LEU:HD11	1:A:650:ILE:HD12	1.95	0.49
1:C:582:PHE:CD2	1:C:593:ARG:NH2	2.78	0.49
1:B:90:THR:O	1:B:94:LEU:HD12	2.12	0.49
1:B:707:PRO:HB3	1:B:814:ASP:OD1	2.13	0.49
1:C:508:ASP:OD1	1:C:583:HIS:NE2	2.44	0.49
1:C:292:GLU:OE2	1:C:292:GLU:HA	2.12	0.49
1:A:262:ASN:HA	1:A:279:ARG:NH1	2.27	0.49
1:C:236:GLN:HA	1:C:261:ALA:HB3	1.95	0.49
1:A:474:VAL:HG11	1:D:230:THR:HG22	1.94	0.49
1:B:706:LEU:HD21	1:B:714:PHE:CZ	2.48	0.49
1:A:604:VAL:O	1:A:605:SER:HB3	2.12	0.49
1:C:150:ASN:OD1	1:C:296:ARG:HG3	2.13	0.49
1:D:371:MET:O	1:D:374:MET:HB2	2.12	0.49
1:A:60:PHE:CE1	1:A:95:LEU:HD21	2.48	0.49
1:B:14:ILE:HG21	1:B:577:LEU:HD11	1.95	0.49
1:B:84:LYS:C	1:B:86:GLU:H	2.07	0.48
1:B:604:VAL:CG2	1:B:605:SER:N	2.76	0.48
1:C:589:THR:HG23	1:C:591:PRO:CD	2.43	0.48
1:A:23:ILE:HD13	1:A:100:LEU:HD21	1.94	0.48
1:D:250:ASN:HA	1:D:289:CYS:O	2.13	0.48
1:A:60:PHE:CZ	1:A:95:LEU:HD21	2.49	0.48
1:A:367:PRO:O	1:A:401:ARG:HD3	2.13	0.48
1:C:13:GLY:HA3	1:C:151:PHE:CZ	2.49	0.48
1:C:278:GLU:O	1:C:279:ARG:CB	2.61	0.48
1:D:74:LYS:HG3	1:D:74:LYS:O	2.13	0.48
1:C:54:GLN:HA	1:C:54:GLN:NE2	2.28	0.48
1:A:83:PHE:HB2	1:A:88:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:TRQ:O6	3:B:902:GLY:N	2.46	0.48
1:B:64:VAL:O	1:B:68:ILE:HB	2.14	0.48
1:C:107:SER:C	1:C:109:SER:N	2.64	0.48
1:B:26:LEU:HD21	1:B:52:LEU:HD23	1.96	0.48
1:C:110:LEU:O	1:C:113:LEU:HB2	2.13	0.48
1:B:154:TYR:CE1	1:B:165:LYS:HG2	2.49	0.48
1:B:349:GLN:C	1:B:620:ARG:HD2	2.34	0.48
1:C:103:GLN:C	1:C:105:GLN:H	2.17	0.48
1:C:107:SER:O	1:C:109:SER:N	2.44	0.48
1:C:683:GLN:CG	1:C:756:LEU:HD11	2.40	0.48
1:A:16:ARG:O	4:A:1009:HOH:O	2.19	0.48
1:A:110:LEU:CD2	1:A:128:ILE:HG23	2.44	0.48
1:A:454:ASN:OD1	1:A:455:PRO:HD2	2.14	0.48
1:A:662:SER:OG	4:A:1006:HOH:O	2.13	0.48
1:D:177:ARG:NH1	4:D:1032:HOH:O	2.47	0.48
1:D:746:LEU:HD23	1:D:802:ILE:CG1	2.38	0.48
1:A:71:ILE:O	1:A:75:LEU:HB2	2.14	0.47
1:A:767:HIS:NE2	3:A:902:GLY:OXT	2.46	0.47
1:B:101:VAL:CG1	1:B:102:PRO:HD2	2.43	0.47
1:B:154:TYR:CE2	1:B:566:ALA:HB2	2.49	0.47
1:A:51:GLU:OE2	1:A:145:LYS:NZ	2.35	0.47
1:D:395:VAL:HG13	1:D:527:LEU:CD1	2.44	0.47
1:A:567:LEU:HD23	1:A:604:VAL:HG21	1.96	0.47
1:C:58:GLU:OE2	1:C:58:GLU:HA	2.14	0.47
1:D:62:GLY:HA2	1:D:65:ILE:CG1	2.44	0.47
1:B:19:ASN:OD1	1:B:19:ASN:N	2.46	0.47
1:B:60:PHE:CE2	1:B:129:LYS:HG3	2.50	0.47
1:B:95:LEU:CD1	1:B:97:LEU:HG	2.40	0.47
1:B:128:ILE:HG22	1:B:132:LEU:HD22	1.96	0.47
1:B:148:ALA:HB3	1:B:296:ARG:CZ	2.45	0.47
1:B:608:THR:HG23	1:B:609:PRO:CD	2.40	0.47
1:C:128:ILE:HD12	1:C:128:ILE:H	1.78	0.47
1:C:373:ASP:OD1	4:C:1016:HOH:O	2.20	0.47
1:C:608:THR:HG22	1:C:610:GLU:H	1.78	0.47
1:C:690:ASP:OD2	1:D:814:ASP:N	2.48	0.47
1:A:600:GLN:O	1:A:619:PHE:HA	2.15	0.47
1:C:91:ILE:O	1:C:95:LEU:HD11	2.15	0.47
1:D:88:ILE:HA	1:D:91:ILE:HG13	1.96	0.47
1:D:715:LYS:O	4:D:1012:HOH:O	2.20	0.47
1:A:214:ARG:NH1	4:A:1034:HOH:O	2.48	0.47
1:B:358:PRO:HB3	1:B:675:TRP:CZ3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:TYR:CG	1:B:571:ARG:HG3	2.50	0.47
1:B:682:CYS:HB2	1:B:697:TRQ:HZ3	1.33	0.47
1:B:757:HIS:HA	1:B:763:PHE:CZ	2.49	0.47
1:B:787:ALA:HA	1:B:811:SER:HB3	1.95	0.47
1:D:80:ALA:HB1	1:D:81:GLU:CB	2.45	0.47
1:D:789:VAL:HG22	1:D:809:ALA:HB2	1.96	0.47
1:C:95:LEU:O	1:C:97:LEU:HG	2.15	0.47
1:C:347:ASP:OD1	1:C:350:SER:HB2	2.13	0.47
1:D:110:LEU:HD22	1:D:128:ILE:HG12	1.97	0.47
1:D:170:ASP:C	1:D:172:ASP:H	2.18	0.47
1:D:757:HIS:HA	1:D:763:PHE:CZ	2.50	0.47
1:C:505:ASP:OD2	1:C:593:ARG:NH2	2.45	0.47
1:C:760:ASP:OD2	1:D:485:GLU:OE2	2.32	0.47
1:C:258:LYS:CD	1:C:262:ASN:HD21	2.27	0.47
1:C:567:LEU:HD21	1:C:604:VAL:HG21	1.96	0.47
1:D:83:PHE:HZ	1:D:110:LEU:HB3	1.77	0.47
1:A:95:LEU:HD12	1:A:95:LEU:H	1.80	0.46
1:B:79:LYS:HB2	1:B:79:LYS:HE2	1.42	0.46
1:B:250:ASN:HB3	4:B:1096:HOH:O	2.14	0.46
1:B:453:ARG:CG	1:B:518:ALA:HB2	2.44	0.46
1:D:45:TYR:CD2	1:D:790:MET:HG2	2.50	0.46
1:D:279:ARG:HG3	1:D:279:ARG:NH1	2.31	0.46
1:A:682:CYS:SG	1:A:701:LEU:HD12	2.55	0.46
1:D:121:SER:O	1:D:122:ASP:CB	2.63	0.46
1:A:423:ARG:HE	1:A:423:ARG:HB3	1.41	0.46
1:B:45:TYR:CD2	1:B:790:MET:HG2	2.51	0.46
1:B:538:THR:OG1	1:B:540:VAL:HG12	2.16	0.46
1:B:760:ASP:O	1:B:782:GLN:HG3	2.15	0.46
1:C:110:LEU:O	1:C:113:LEU:N	2.47	0.46
1:A:470:SER:HB2	1:D:635:GLN:OE1	2.15	0.46
1:C:90:THR:O	1:C:90:THR:HG22	2.14	0.46
1:A:75:LEU:HD22	1:A:78:ARG:NH2	2.21	0.46
1:A:184:LYS:HE2	1:A:671:MET:HB2	1.98	0.46
1:A:222:LYS:HE3	1:A:222:LYS:HB2	1.61	0.46
1:B:59:ALA:HB1	1:B:95:LEU:HB2	1.96	0.46
1:B:157:ASP:OD1	1:B:161:ASN:HB3	2.16	0.46
1:B:507:ILE:HA	1:B:515:GLN:HG2	1.98	0.46
1:B:608:THR:CG2	1:B:609:PRO:HD2	2.40	0.46
1:B:695:SER:CB	1:B:703:VAL:HG21	2.45	0.46
1:C:559:PHE:CE2	1:C:613:LEU:HD13	2.50	0.46
1:C:707:PRO:HB3	1:C:814:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ALA:HB3	1:A:776:LEU:HD22	1.97	0.46
1:B:57:GLU:OE2	1:B:129:LYS:HD3	2.16	0.46
1:B:61:GLY:HA2	1:B:62:GLY:HA2	1.60	0.46
1:C:124:ILE:HD12	1:C:127:GLN:HB2	1.96	0.46
1:A:580:GLY:HA2	1:A:581:GLY:C	2.35	0.46
1:A:682:CYS:HB3	1:A:701:LEU:HD13	1.98	0.46
1:B:213:HIS:HB2	1:B:215:LEU:HD13	1.97	0.46
1:B:312:LEU:HD11	1:D:312:LEU:HD11	1.97	0.46
1:D:83:PHE:CE1	1:D:88:ILE:CD1	2.99	0.46
1:B:568:LEU:HD23	1:B:616:LEU:HD21	1.98	0.46
1:C:504:ASN:HB2	1:C:516:TRP:C	2.37	0.46
1:D:453:ARG:HG2	1:D:518:ALA:HB2	1.98	0.46
1:D:787:ALA:HB2	1:D:811:SER:HB3	1.96	0.46
1:A:590:TRP:HB2	1:A:593:ARG:HH11	1.81	0.46
1:B:250:ASN:HA	1:B:289:CYS:O	2.15	0.46
1:C:181:ALA:HA	1:C:239:ILE:O	2.16	0.46
1:A:146:LYS:NZ	1:A:300:GLY:O	2.49	0.45
1:A:562:SER:HB3	1:A:568:LEU:HD11	1.98	0.45
1:C:110:LEU:O	1:C:113:LEU:CB	2.64	0.45
1:C:235:LYS:HG2	1:C:634:TYR:CE1	2.51	0.45
1:D:465:ASP:HB3	1:D:468:GLN:HG3	1.97	0.45
1:A:632:ASN:HA	1:A:635:GLN:HG2	1.98	0.45
1:C:109:SER:CA	1:C:112:ASN:HD21	2.22	0.45
1:D:98:SER:HB3	1:D:103:GLN:HE22	1.80	0.45
1:A:45:TYR:CD2	1:A:790:MET:HG2	2.52	0.45
1:A:222:LYS:HG2	1:D:509:TYR:HE1	1.82	0.45
1:C:125:VAL:O	1:C:127:GLN:N	2.49	0.45
1:D:80:ALA:CB	1:D:81:GLU:CB	2.93	0.45
1:C:709:ALA:HB2	1:C:815:LYS:HB2	1.97	0.45
1:D:154:TYR:CE2	1:D:566:ALA:HB2	2.52	0.45
1:D:213:HIS:HB2	1:D:215:LEU:HD13	1.98	0.45
1:A:223:ARG:HD3	1:A:234:ARG:CZ	2.47	0.45
1:B:6:TYR:CE1	1:B:166:LEU:HD13	2.52	0.45
1:B:742:GLU:O	1:B:745:ARG:HB2	2.15	0.45
1:D:69:SER:O	1:D:73:THR:CG2	2.65	0.45
1:D:108:ARG:HA	1:D:111:ASP:HB2	1.99	0.45
1:D:153:ILE:N	4:D:1017:HOH:O	2.32	0.45
1:A:717:SER:HB3	1:A:796:ASN:HB3	1.97	0.45
3:C:902:GLY:O	1:D:767:HIS:CD2	2.70	0.45
1:D:390:THR:HG23	1:D:526:HIS:ND1	2.31	0.45
1:C:673:ILE:HD12	1:C:674:PRO:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:CD2	1:A:78:ARG:HH21	2.22	0.45
1:A:613:LEU:O	1:A:614:LEU:HB2	2.17	0.45
1:B:78:ARG:HH12	1:B:84:LYS:HB2	1.82	0.45
1:C:95:LEU:HD22	1:C:132:LEU:HD12	1.99	0.45
1:C:730:HIS:CD2	1:C:734:GLN:HG3	2.51	0.45
1:D:564:ASN:HD21	1:D:567:LEU:HD13	1.81	0.45
1:A:7:LYS:HG2	1:A:350:SER:HA	1.99	0.45
1:A:13:GLY:HA3	1:A:151:PHE:CZ	2.52	0.45
1:A:72:LYS:HA	1:A:75:LEU:CB	2.47	0.45
1:A:590:TRP:CG	1:A:591:PRO:HD3	2.51	0.45
1:B:101:VAL:HG13	1:B:102:PRO:HD2	1.98	0.45
1:B:596:LEU:HD12	1:B:596:LEU:HA	1.77	0.45
1:B:687:THR:HB	1:B:688:PRO:HD2	1.99	0.45
1:C:580:GLY:HA2	1:C:581:GLY:C	2.37	0.45
1:B:767:HIS:NE2	3:B:902:GLY:O	2.45	0.45
1:C:235:LYS:HE2	1:C:634:TYR:CD2	2.51	0.45
1:D:8:ILE:HG13	1:D:345:ILE:HG21	1.99	0.45
1:D:20:GLY:O	1:D:146:LYS:HE2	2.17	0.45
1:A:476:ASN:OD1	1:A:495:SER:HB3	2.17	0.44
1:B:71:ILE:HD13	1:B:87:GLU:CG	2.47	0.44
1:B:249:ASN:O	1:B:250:ASN:CG	2.55	0.44
1:C:476:ASN:OD1	1:C:495:SER:HB2	2.17	0.44
1:C:279:ARG:HD3	1:C:279:ARG:HA	1.62	0.44
1:C:290:ASP:OD2	4:C:1017:HOH:O	2.21	0.44
1:A:88:ILE:HG23	1:A:110:LEU:HD12	1.99	0.44
1:B:432:ALA:HA	1:B:435:LEU:HD13	1.98	0.44
1:C:632:ASN:HA	1:C:635:GLN:HG2	1.98	0.44
1:D:455:PRO:HG3	1:D:519:ILE:O	2.16	0.44
1:D:608:THR:HG22	1:D:610:GLU:N	2.29	0.44
1:A:83:PHE:O	1:A:84:LYS:HB2	2.17	0.44
1:A:104:GLN:HG2	1:A:108:ARG:NH1	2.33	0.44
1:B:165:LYS:HB2	1:B:165:LYS:HE3	1.90	0.44
1:B:553:LEU:HD23	1:B:553:LEU:HA	1.73	0.44
1:C:455:PRO:HG3	1:C:519:ILE:O	2.17	0.44
1:D:128:ILE:O	1:D:130:GLY:N	2.51	0.44
1:B:74:LYS:O	1:B:78:ARG:HB2	2.16	0.44
1:B:121:SER:O	1:B:122:ASP:HB3	2.17	0.44
1:B:787:ALA:CB	1:B:809:ALA:HB1	2.43	0.44
1:C:19:ASN:ND2	1:C:784:LYS:HD3	2.33	0.44
1:C:105:GLN:O	1:C:109:SER:HB3	2.18	0.44
1:C:705:VAL:HB	1:C:809:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:THR:HB	1:A:611:ILE:HB	1.99	0.44
1:C:106:LEU:O	1:C:110:LEU:HD12	2.18	0.44
1:D:349:GLN:OE1	1:D:600:GLN:OE1	2.36	0.44
1:C:124:ILE:HD11	1:C:127:GLN:CG	2.48	0.44
1:C:129:LYS:O	1:C:129:LYS:CG	2.66	0.44
1:A:746:LEU:HA	1:A:746:LEU:HD23	1.79	0.44
1:C:101:VAL:HG13	1:C:102:PRO:HD2	1.98	0.44
1:C:390:THR:HG22	1:C:391:GLN:O	2.18	0.44
1:D:208:LYS:HE2	1:D:208:LYS:HB2	1.86	0.44
1:A:757:HIS:HA	1:A:763:PHE:CZ	2.53	0.44
1:B:163:VAL:O	1:B:164:GLU:CB	2.64	0.44
1:C:256:ARG:NH1	1:C:283:LEU:HD13	2.32	0.44
1:A:175:THR:O	1:A:333:ALA:HA	2.18	0.43
1:A:698:ALA:HA	1:A:701:LEU:O	2.18	0.43
1:A:124:ILE:O	1:A:128:ILE:HG13	2.18	0.43
1:D:30:THR:HG21	1:D:149:GLN:OE1	2.18	0.43
1:A:75:LEU:C	1:A:75:LEU:HD13	2.38	0.43
1:B:169:THR:OG1	1:B:172:ASP:OD2	2.29	0.43
1:B:258:LYS:HZ1	1:B:279:ARG:HB3	1.80	0.43
1:C:372:TYR:CD1	1:C:571:ARG:HG3	2.54	0.43
1:B:75:LEU:HD13	1:B:75:LEU:HA	1.25	0.43
1:B:204:GLY:O	1:B:520:PRO:HB2	2.19	0.43
1:C:220:THR:HG22	1:C:642:ALA:HB2	2.00	0.43
1:A:330:ARG:HG3	1:A:623:GLN:OE1	2.18	0.43
1:A:435:LEU:HD12	1:A:435:LEU:N	2.34	0.43
1:C:39:TYR:HH	1:C:400:TYR:HH	1.61	0.43
1:C:453:ARG:HG2	1:C:518:ALA:HB2	1.99	0.43
1:B:597:ILE:HG12	1:B:621:LEU:HD22	2.00	0.43
1:D:235:LYS:HG2	1:D:634:TYR:CD1	2.54	0.43
1:A:171:GLY:HA3	1:A:338:LYS:HB3	2.01	0.43
1:B:608:THR:HB	1:B:611:ILE:HB	2.01	0.43
1:C:35:TRP:N	1:C:35:TRP:CD1	2.87	0.43
1:C:628:LEU:CD2	1:C:664:PRO:HG2	2.49	0.43
1:A:12:LEU:HD13	1:A:353:TRP:HB3	2.01	0.43
1:B:307:LEU:HB2	1:B:321:ASN:OD1	2.19	0.43
1:D:10:PRO:HB3	1:D:570:ALA:HA	2.00	0.43
1:D:83:PHE:CZ	1:D:110:LEU:CB	3.01	0.43
1:D:596:LEU:HD12	1:D:596:LEU:HA	1.78	0.43
1:B:509:TYR:CD1	1:C:639:HIS:HB3	2.54	0.43
1:C:567:LEU:HD23	1:C:604:VAL:HG21	1.98	0.43
1:C:635:GLN:HA	1:C:635:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:GLU:HB2	1:D:628:LEU:HG	1.99	0.43
1:D:361:TYR:HA	1:D:788:MET:SD	2.59	0.43
1:A:396:PHE:N	1:A:397:PRO:CD	2.82	0.42
1:A:683:GLN:CD	1:A:756:LEU:HD13	2.38	0.42
1:C:372:TYR:CG	1:C:571:ARG:HG3	2.54	0.42
1:C:710:ARG:HD2	1:C:751:GLN:HB2	2.01	0.42
1:D:62:GLY:C	1:D:65:ILE:CG1	2.88	0.42
1:D:73:THR:OG1	1:D:74:LYS:N	2.52	0.42
1:A:55:LEU:HD21	1:A:100:LEU:CD1	2.49	0.42
1:A:84:LYS:HB3	1:A:87:GLU:HB2	2.01	0.42
1:A:161:ASN:CB	4:A:1008:HOH:O	2.67	0.42
1:B:514:VAL:HG12	1:B:514:VAL:O	2.19	0.42
1:B:709:ALA:HB2	1:B:814:ASP:O	2.20	0.42
1:C:583:HIS:N	1:C:584:PRO:CA	2.81	0.42
1:D:504:ASN:CG	1:D:505:ASP:H	2.22	0.42
1:D:787:ALA:HB1	1:D:809:ALA:HB1	2.01	0.42
1:A:177:ARG:HE	1:A:177:ARG:HB3	1.64	0.42
1:A:498:LYS:HA	1:A:498:LYS:HD3	1.79	0.42
1:B:460:ASP:OD1	4:B:1009:HOH:O	2.22	0.42
1:B:713:LYS:HB3	1:B:748:GLN:HG3	2.01	0.42
1:C:567:LEU:CD2	1:C:604:VAL:CG2	2.92	0.42
1:D:93:GLY:N	1:D:95:LEU:O	2.52	0.42
1:A:101:VAL:CG1	1:A:102:PRO:HD2	2.49	0.42
1:B:172:ASP:OD1	1:B:338:LYS:N	2.53	0.42
1:C:190:TYR:CD2	1:C:584:PRO:HB3	2.54	0.42
1:C:262:ASN:N	1:C:262:ASN:OD1	2.52	0.42
1:C:435:LEU:HD12	1:C:435:LEU:N	2.34	0.42
1:D:396:PHE:N	1:D:397:PRO:CD	2.83	0.42
1:B:590:TRP:N	1:B:591:PRO:CD	2.82	0.42
1:C:183:LYS:HE2	1:C:633:MET:O	2.20	0.42
1:C:354:VAL:HG13	1:C:354:VAL:O	2.19	0.42
1:C:436:ASP:O	1:C:445:ARG:NH1	2.52	0.42
1:C:732:ILE:HD13	1:D:421:GLN:HB2	2.01	0.42
1:A:56:LEU:O	1:A:59:ALA:HB3	2.19	0.42
1:A:76:ASP:C	1:A:79:LYS:H	2.22	0.42
1:A:163:VAL:O	1:A:164:GLU:CB	2.67	0.42
1:C:11:PRO:HG2	1:C:619:PHE:CE2	2.54	0.42
1:D:64:VAL:O	1:D:67:GLU:CB	2.56	0.42
1:A:101:VAL:HG12	1:A:102:PRO:CD	2.49	0.42
1:A:302:GLY:HA3	1:A:783:TRP:CZ2	2.54	0.42
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ASN:HD22	1:B:459:GLN:HE21	1.67	0.42
1:B:75:LEU:HD12	1:B:80:ALA:HB3	2.01	0.42
1:B:75:LEU:N	1:B:75:LEU:HD22	2.35	0.42
1:D:72:LYS:O	1:D:72:LYS:HG2	2.20	0.42
1:D:582:PHE:HD1	1:D:589:THR:HA	1.83	0.42
1:A:624:ASP:CB	1:A:663:THR:HG22	2.50	0.42
1:B:35:TRP:N	1:B:35:TRP:CD1	2.87	0.42
1:B:171:GLY:H	1:B:338:LYS:HG2	1.85	0.42
1:C:752:ARG:HA	1:C:752:ARG:HD3	1.91	0.42
1:D:84:LYS:HD2	1:D:85:GLN:N	2.31	0.42
1:D:353:TRP:NE1	1:D:667:LEU:HD13	2.35	0.42
1:D:589:THR:HG23	1:D:591:PRO:CD	2.50	0.42
1:A:183:LYS:HE3	1:A:664:PRO:O	2.20	0.42
1:D:553:LEU:HD13	1:D:553:LEU:HA	1.64	0.42
1:D:632:ASN:ND2	4:D:1014:HOH:O	2.26	0.42
1:A:75:LEU:O	1:A:78:ARG:HB3	2.20	0.41
1:A:564:ASN:HD21	1:A:567:LEU:HD22	1.84	0.41
1:A:708:LEU:HD23	1:A:815:LYS:HB3	2.01	0.41
1:B:171:GLY:N	1:B:338:LYS:HG2	2.35	0.41
1:C:91:ILE:HA	1:C:94:LEU:CD2	2.50	0.41
1:D:163:VAL:O	1:D:164:GLU:O	2.38	0.41
1:D:564:ASN:ND2	1:D:567:LEU:HD22	2.34	0.41
1:B:56:LEU:HD11	1:B:136:LEU:CD1	2.50	0.41
1:B:454:ASN:HD22	1:B:459:GLN:NE2	2.18	0.41
1:B:666:ASP:HA	1:B:669:LYS:HD3	2.01	0.41
1:A:84:LYS:O	1:A:85:GLN:C	2.58	0.41
1:B:105:GLN:HE21	1:B:135:VAL:HB	1.84	0.41
1:B:453:ARG:HB2	1:B:453:ARG:CZ	2.51	0.41
1:B:500:PRO:HB2	1:B:502:TYR:CE2	2.56	0.41
1:C:504:ASN:HB3	1:C:514:VAL:O	2.19	0.41
1:D:259:PHE:HA	1:D:260:PRO:C	2.41	0.41
1:D:619:PHE:O	1:D:620:ARG:HG3	2.20	0.41
1:A:396:PHE:HE1	1:A:548:ILE:HG13	1.85	0.41
1:A:676:GLN:HG2	1:A:780:VAL:HA	2.03	0.41
1:C:381:LYS:HD2	1:C:381:LYS:HA	1.89	0.41
1:D:71:ILE:HG12	1:D:71:ILE:H	1.76	0.41
1:D:146:LYS:HB3	4:D:1101:HOH:O	2.19	0.41
1:D:364:GLN:HE22	1:D:791:ALA:HB3	1.85	0.41
1:A:77:GLU:O	1:A:78:ARG:HB2	2.20	0.41
1:B:74:LYS:C	1:B:75:LEU:HD22	2.40	0.41
1:C:95:LEU:H	1:C:95:LEU:HG	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLU:O	1:C:279:ARG:HB3	2.20	0.41
1:D:537:VAL:HG13	1:D:542:LYS:HE2	2.02	0.41
1:D:619:PHE:O	1:D:620:ARG:CG	2.69	0.41
1:D:703:VAL:HG12	1:D:704:HIS:CE1	2.55	0.41
1:A:262:ASN:OD1	1:A:262:ASN:N	2.49	0.41
1:B:306:ALA:HA	1:B:321:ASN:O	2.20	0.41
1:B:756:LEU:HD22	4:B:1155:HOH:O	2.20	0.41
1:C:283:LEU:HD12	1:C:283:LEU:HA	1.95	0.41
1:C:567:LEU:HD23	1:C:604:VAL:CG2	2.50	0.41
1:D:62:GLY:O	1:D:65:ILE:HG13	2.20	0.41
1:D:83:PHE:HZ	1:D:110:LEU:CB	2.33	0.41
1:D:709:ALA:HB2	1:D:815:LYS:C	2.41	0.41
1:A:230:THR:HG21	1:D:491:LYS:HE3	2.02	0.41
1:B:75:LEU:HD13	1:B:78:ARG:CB	2.48	0.41
1:B:347:ASP:OD1	1:B:350:SER:HB2	2.21	0.41
1:B:632:ASN:OD1	1:B:635:GLN:HG3	2.21	0.41
1:C:718:GLN:O	1:C:734:GLN:NE2	2.54	0.41
1:D:564:ASN:ND2	1:D:567:LEU:HD13	2.35	0.41
1:A:41:THR:HB	1:A:793:PRO:HD3	2.02	0.41
1:B:183:LYS:NZ	1:B:663:THR:OG1	2.50	0.41
1:B:313:ASN:OD1	1:B:313:ASN:N	2.50	0.41
1:B:348:GLU:HG3	1:B:599:SER:OG	2.21	0.41
1:B:567:LEU:HD12	1:B:604:VAL:HG21	2.03	0.41
1:C:562:SER:HB3	1:C:568:LEU:HD11	2.02	0.41
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.84	0.41
1:D:103:GLN:HE21	1:D:103:GLN:CA	2.31	0.41
1:D:169:THR:OG1	1:D:170:ASP:N	2.53	0.41
1:D:326:ILE:HG22	1:D:327:CYS:N	2.35	0.41
1:B:95:LEU:O	1:B:96:GLY:C	2.59	0.41
1:B:153:ILE:HG13	1:B:176:TRP:CZ2	2.56	0.41
1:B:173:LYS:HB2	1:B:173:LYS:HE3	1.64	0.41
1:B:205:ASN:OD1	1:B:377:GLY:HA3	2.20	0.41
1:B:435:LEU:N	1:B:435:LEU:HD12	2.36	0.41
1:B:455:PRO:HB2	1:B:521:PRO:HD3	2.03	0.41
1:C:6:TYR:HA	1:C:154:TYR:O	2.21	0.41
1:C:178:VAL:HG11	1:C:297:PHE:HE2	1.86	0.41
1:C:193:ALA:HB3	1:C:196:LEU:HG	2.03	0.41
1:D:155:LYS:HG2	1:D:156:CYS:N	2.35	0.41
1:D:182:ASN:HB2	1:D:326:ILE:O	2.21	0.41
1:D:433:GLN:H	1:D:433:GLN:HG3	1.69	0.41
1:A:453:ARG:HB2	1:A:453:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASN:O	1:B:250:ASN:HB3	2.18	0.41
1:B:65:ILE:HD13	1:B:65:ILE:N	2.36	0.40
1:B:114:GLU:C	1:B:115:LEU:HG	2.40	0.40
1:B:695:SER:HB3	1:B:703:VAL:HG21	2.02	0.40
1:B:64:VAL:HG13	1:B:94:LEU:HD13	2.02	0.40
1:C:110:LEU:HD12	1:C:110:LEU:H	1.86	0.40
1:A:230:THR:HG22	1:D:474:VAL:HG11	2.03	0.40
1:B:80:ALA:CB	1:B:81:GLU:HB3	2.51	0.40
1:B:222:LYS:HB2	1:B:222:LYS:HE3	1.94	0.40
1:B:230:THR:HG22	1:C:474:VAL:HG11	2.03	0.40
1:D:394:ASP:O	1:D:397:PRO:HD2	2.21	0.40
1:C:130:GLY:HA2	1:C:133:LEU:HB3	2.04	0.40
1:D:45:TYR:HB2	1:D:788:MET:HG2	2.02	0.40
1:D:182:ASN:C	1:D:182:ASN:OD1	2.60	0.40
1:A:175:THR:HB	1:A:334:VAL:CG1	2.51	0.40
1:B:78:ARG:NH1	1:B:84:LYS:HB2	2.36	0.40
1:B:110:LEU:CB	1:B:113:LEU:HD12	2.51	0.40
1:B:624:ASP:OD2	1:B:630:SER:OG	2.25	0.40
1:C:306:ALA:HB2	1:C:322:TRP:CE2	2.57	0.40
1:C:347:ASP:OD1	1:C:350:SER:CB	2.70	0.40
1:C:551:LEU:HD12	1:C:551:LEU:HA	1.78	0.40

All (1) 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:C:534:ASP:OD1	1:D:383:GLN:NE2[1_545]	2.09	0.11

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	781/816 (96%)	727 (93%)	44 (6%)	10 (1%)	12 21
1	B	781/816 (96%)	731 (94%)	37 (5%)	13 (2%)	9 16
1	C	749/816 (92%)	700 (94%)	37 (5%)	12 (2%)	9 17
1	D	778/816 (95%)	720 (92%)	45 (6%)	13 (2%)	9 16
All	All	3089/3264 (95%)	2878 (93%)	163 (5%)	48 (2%)	9 17

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	78	ARG
1	A	81	GLU
1	A	122	ASP
1	B	84	LYS
1	B	85	GLN
1	B	92	THR
1	C	94	LEU
1	C	96	GLY
1	D	64	VAL
1	D	65	ILE
1	D	81	GLU
1	D	94	LEU
1	D	123	ASP
1	D	169	THR
1	A	123	ASP
1	B	81	GLU
1	B	82	LYS
1	B	96	GLY
1	B	122	ASP
1	C	88	ILE
1	C	104	GLN
1	C	108	ARG
1	D	129	LYS
1	D	164	GLU
1	A	89	GLU
1	A	96	GLY
1	A	654	SER
1	B	250	ASN
1	B	279	ARG
1	C	126	GLN
1	C	164	GLU
1	C	230	THR

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Mol	Chain	Res	Type
1	C	738	GLU
1	D	279	ARG
1	A	84	LYS
1	B	78	ARG
1	B	129	LYS
1	D	82	LYS
1	D	341	ASP
1	A	230	THR
1	B	79	LYS
1	C	170	ASP
1	D	109	SER
1	B	164	GLU
1	D	93	GLY
1	C	128	ILE
1	C	163	VAL

5.3.2 Protein sidechains (i)

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	686/711 (96%)	667 (97%)	19 (3%)	43	70
1	B	686/711 (96%)	672 (98%)	14 (2%)	55	79
1	C	658/711 (92%)	638 (97%)	20 (3%)	41	68
1	D	683/711 (96%)	669 (98%)	14 (2%)	55	79
All	All	2713/2844 (95%)	2646 (98%)	67 (2%)	47	73

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	67	GLU
1	A	82	LYS
1	A	86	GLU
1	A	115	LEU
1	A	123	ASP

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Mol	Chain	Res	Type
1	A	161	ASN
1	A	170	ASP
1	A	173	LYS
1	A	256	ARG
1	A	262	ASN
1	A	381	LYS
1	A	569	CYS
1	A	578	TYR
1	A	593	ARG
1	A	620	ARG
1	A	677	SER
1	A	814	ASP
1	A	815	LYS
1	B	76	ASP
1	B	170	ASP
1	B	208	LYS
1	B	308	SER
1	B	381	LYS
1	B	575	ASP
1	B	578	TYR
1	B	620	ARG
1	B	678	ASN
1	B	681	SER
1	B	721	ASP
1	B	756	LEU
1	B	814	ASP
1	B	816	ASP
1	C	94	LEU
1	C	95	LEU
1	C	103	GLN
1	C	108	ARG
1	C	137	SER
1	C	161	ASN
1	C	250	ASN
1	C	262	ASN
1	C	279	ARG
1	C	386	ASP
1	C	471	ASN
1	C	556	SER
1	C	569	CYS
1	C	575	ASP
1	C	578	TYR

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Mol	Chain	Res	Type
1	C	593	ARG
1	C	620	ARG
1	C	654	SER
1	C	814	ASP
1	C	815	LYS
1	D	83	PHE
1	D	111	ASP
1	D	127	GLN
1	D	173	LYS
1	D	232	SER
1	D	250	ASN
1	D	258	LYS
1	D	308	SER
1	D	311	SER
1	D	569	CYS
1	D	575	ASP
1	D	578	TYR
1	D	724	GLU
1	D	776	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	B	5	GLN
1	B	105	GLN
1	B	250	ASN
1	B	459	GLN
1	B	539	GLN
1	B	678	ASN
1	C	54	GLN
1	C	406	GLN
1	C	730	HIS
1	D	433	GLN
1	D	600	GLN
1	D	796	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
1	TRQ	D	697	1	13,17,18	1.26	1 (7%)	14,24,26	2.26	4 (28%)
1	TRQ	B	697	1	13,17,18	1.43	1 (7%)	14,24,26	2.32	5 (35%)
1	TRQ	A	697	1	13,17,18	1.85	3 (23%)	14,24,26	1.72	3 (21%)
1	TRQ	C	697	1	13,17,18	1.69	2 (15%)	14,24,26	2.02	4 (28%)

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
1	TRQ	D	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	A	697	1	-	1/4/19/21	0/2/2/2
1	TRQ	C	697	1	-	0/4/19/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CE2-CZ2	-4.60	1.44	1.50
1	C	697	TRQ	CE2-CZ2	-4.04	1.44	1.50
1	B	697	TRQ	CE2-CZ2	-3.36	1.45	1.50
1	C	697	TRQ	CB-CG	-3.17	1.47	1.51
1	A	697	TRQ	CB-CG	-2.94	1.47	1.51
1	A	697	TRQ	CH2-CZ2	-2.41	1.51	1.54
1	D	697	TRQ	CE2-CZ2	-2.17	1.47	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	697	TRQ	CZ2-CE2-NE1	5.58	128.85	119.94
1	D	697	TRQ	CZ2-CE2-NE1	5.25	128.32	119.94
1	A	697	TRQ	CZ2-CE2-NE1	4.18	126.61	119.94
1	C	697	TRQ	CZ2-CE2-NE1	3.84	126.07	119.94
1	D	697	TRQ	O7-CZ2-CE2	3.79	125.85	121.84
1	C	697	TRQ	CB-CG-CD1	-3.59	123.53	127.97
1	D	697	TRQ	CE3-CZ3-CH2	3.54	123.76	121.08
1	C	697	TRQ	CE3-CZ3-CH2	3.15	123.47	121.08
1	B	697	TRQ	CB-CG-CD1	-3.10	124.14	127.97
1	B	697	TRQ	O7-CZ2-CH2	3.08	122.62	119.00
1	D	697	TRQ	O6-CH2-CZ2	2.92	120.49	118.51
1	C	697	TRQ	O7-CZ2-CH2	2.72	122.20	119.00
1	B	697	TRQ	O6-CH2-CZ2	2.67	120.32	118.51
1	B	697	TRQ	CD2-CE3-CZ3	2.63	124.26	121.09
1	A	697	TRQ	O7-CZ2-CE2	2.59	124.58	121.84
1	A	697	TRQ	CB-CG-CD1	-2.16	125.29	127.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	697	TRQ	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	697	TRQ	2	0
1	B	697	TRQ	4	0
1	A	697	TRQ	3	0
1	C	697	TRQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	GLY	A	902	-	4,4,4	2.06	2 (50%)	3,4,4	2.67	2 (66%)
3	GLY	B	902	-	4,4,4	1.02	0	3,4,4	1.49	0
3	GLY	C	902	-	4,4,4	0.85	0	3,4,4	1.47	1 (33%)
3	GLY	D	902	-	4,4,4	0.96	0	3,4,4	1.33	0

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
3	GLY	A	902	-	-	0/2/2/2	-
3	GLY	B	902	-	-	0/2/2/2	-
3	GLY	C	902	-	-	0/2/2/2	-
3	GLY	D	902	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	GLY	OXT-C	-3.21	1.19	1.30
3	A	902	GLY	O-C	-2.09	1.15	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	GLY	OXT-C-O	-4.01	113.30	123.30
3	A	902	GLY	OXT-C-CA	2.23	122.34	113.45
3	C	902	GLY	OXT-C-CA	2.03	121.52	113.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	902	GLY	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	D	902	GLY	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GLY	3	0
3	B	902	GLY	3	0
3	C	902	GLY	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	789/816 (96%)	-0.01	44 (5%)	24	25	19, 31, 80, 116	0
1	B	789/816 (96%)	0.06	49 (6%)	20	21	23, 34, 92, 127	0
1	C	759/816 (93%)	-0.08	33 (4%)	35	38	21, 32, 78, 119	0
1	D	786/816 (96%)	0.23	73 (9%)	8	8	23, 37, 99, 131	0
All	All	3123/3264 (95%)	0.05	199 (6%)	19	20	19, 34, 88, 131	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	GLY	10.9
1	C	88	ILE	9.1
1	D	83	PHE	8.1
1	A	80	ALA	7.3
1	A	122	ASP	7.3
1	C	86	GLU	7.2
1	B	81	GLU	7.0
1	D	62	GLY	7.0
1	D	82	LYS	6.9
1	D	113	LEU	6.3
1	B	82	LYS	6.3
1	C	60	PHE	5.9
1	C	94	LEU	5.9
1	C	124	ILE	5.8
1	B	75	LEU	5.7
1	C	112	ASN	5.7
1	D	121	SER	5.6
1	C	91	ILE	5.5
1	B	83	PHE	5.5
1	B	88	ILE	5.5
1	C	111	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	73	THR	5.3
1	B	78	ARG	5.3
1	C	95	LEU	5.2
1	A	77	GLU	5.2
1	D	81	GLU	5.2
1	D	80	ALA	5.1
1	B	112	ASN	5.1
1	C	104	GLN	4.9
1	D	71	ILE	4.6
1	D	97	LEU	4.6
1	C	98	SER	4.6
1	D	75	LEU	4.6
1	D	68	ILE	4.6
1	B	115	LEU	4.5
1	D	69	SER	4.4
1	D	122	ASP	4.4
1	B	80	ALA	4.3
1	D	88	ILE	4.3
1	B	110	LEU	4.3
1	D	79	LYS	4.3
1	B	111	ASP	4.3
1	D	77	GLU	4.2
1	C	102	PRO	4.2
1	D	60	PHE	4.2
1	D	343	PHE	4.0
1	D	337	LEU	4.0
1	C	339	ASN	4.0
1	D	123	ASP	4.0
1	A	85	GLN	4.0
1	A	63	ASN	4.0
1	B	262	ASN	3.8
1	D	76	ASP	3.8
1	B	74	LYS	3.8
1	C	125	VAL	3.7
1	D	85	GLN	3.7
1	A	74	LYS	3.7
1	B	109	SER	3.7
1	D	127	GLN	3.6
1	B	121	SER	3.6
1	A	113	LEU	3.6
1	B	125	VAL	3.5
1	D	4	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	123	ASP	3.5
1	D	66	ASN	3.5
1	D	95	LEU	3.4
1	D	106	LEU	3.4
1	A	82	LYS	3.4
1	B	73	THR	3.4
1	B	86	GLU	3.4
1	B	77	GLU	3.4
1	B	114	GLU	3.3
1	A	4	CYS	3.3
1	D	104	GLN	3.3
1	C	107	SER	3.3
1	A	108	ARG	3.3
1	A	170	ASP	3.3
1	D	70	GLN	3.3
1	B	107	SER	3.2
1	A	73	THR	3.2
1	A	99	HIS	3.2
1	A	116	LYS	3.2
1	D	91	ILE	3.1
1	B	62	GLY	3.1
1	B	71	ILE	3.1
1	A	87	GLU	3.1
1	D	170	ASP	3.0
1	B	124	ILE	3.0
1	D	6	TYR	3.0
1	D	90	THR	3.0
1	D	98	SER	3.0
1	A	61	GLY	3.0
1	C	4	CYS	2.9
1	B	79	LYS	2.9
1	A	111	ASP	2.9
1	D	126	GLN	2.9
1	A	132	LEU	2.9
1	D	110	LEU	2.9
1	A	81	GLU	2.8
1	A	163	VAL	2.8
1	D	162	PRO	2.8
1	C	97	LEU	2.8
1	D	103	GLN	2.8
1	D	262	ASN	2.8
1	B	68	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	342	THR	2.7
1	C	89	GLU	2.7
1	D	133	LEU	2.7
1	D	339	ASN	2.7
1	A	126	GLN	2.7
1	A	115	LEU	2.6
1	C	262	ASN	2.6
1	B	816	ASP	2.6
1	D	342	THR	2.6
1	D	112	ASN	2.6
1	D	87	GLU	2.6
1	D	65	ILE	2.6
1	D	84	LYS	2.6
1	B	122	ASP	2.6
1	A	71	ILE	2.6
1	A	79	LYS	2.6
1	A	262	ASN	2.6
1	D	248	ASP	2.5
1	A	98	SER	2.5
1	C	90	THR	2.5
1	D	86	GLU	2.5
1	C	56	LEU	2.5
1	D	72	LYS	2.5
1	D	93	GLY	2.5
1	D	109	SER	2.5
1	D	344	GLU	2.5
1	A	109	SER	2.4
1	C	128	ILE	2.4
1	B	113	LEU	2.4
1	A	125	VAL	2.4
1	D	107	SER	2.4
1	A	104	GLN	2.4
1	C	105	GLN	2.4
1	A	343	PHE	2.4
1	B	341	ASP	2.4
1	A	75	LEU	2.4
1	A	95	LEU	2.4
1	A	97	LEU	2.4
1	B	72	LYS	2.3
1	D	124	ILE	2.3
1	B	87	GLU	2.3
1	B	343	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	63	ASN	2.3
1	A	86	GLU	2.3
1	D	125	VAL	2.3
1	D	163	VAL	2.3
1	B	128	ILE	2.3
1	A	112	ASN	2.3
1	D	89	GLU	2.3
1	A	279	ARG	2.3
1	C	109	SER	2.3
1	B	721	ASP	2.3
1	B	61	GLY	2.3
1	B	126	GLN	2.3
1	A	164	GLU	2.3
1	C	163	VAL	2.2
1	B	91	ILE	2.2
1	A	338	LYS	2.2
1	D	131	ALA	2.2
1	C	126	GLN	2.2
1	D	111	ASP	2.2
1	B	101	VAL	2.2
1	A	121	SER	2.2
1	A	88	ILE	2.2
1	A	60	PHE	2.2
1	B	169	THR	2.2
1	A	127	GLN	2.2
1	D	54	GLN	2.2
1	A	124	ILE	2.2
1	B	4	CYS	2.2
1	D	130	GLY	2.2
1	B	108	ARG	2.2
1	B	132	LEU	2.2
1	B	106	LEU	2.1
1	B	66	ASN	2.1
1	D	64	VAL	2.1
1	C	93	GLY	2.1
1	C	340	GLY	2.1
1	C	106	LEU	2.1
1	D	94	LEU	2.1
1	C	467	GLY	2.1
1	D	136	LEU	2.1
1	B	170	ASP	2.1
1	C	99	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	HIS	2.1
1	D	108	ARG	2.1
1	C	87	GLU	2.0
1	D	201	GLN	2.0
1	A	62	GLY	2.0
1	D	171	GLY	2.0
1	D	134	LYS	2.0
1	C	113	LEU	2.0
1	D	164	GLU	2.0
1	D	341	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	TRQ	A	697	16/17	0.96	0.15	22,27,31,33	0
1	TRQ	B	697	16/17	0.96	0.14	25,28,32,33	0
1	TRQ	C	697	16/17	0.96	0.15	21,27,33,33	0
1	TRQ	D	697	16/17	0.97	0.14	23,29,34,35	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	MG	A	901	1/1	0.89	0.14	30,30,30,30	0
3	GLY	C	902	5/5	0.91	0.19	31,40,45,45	0
3	GLY	A	902	5/5	0.93	0.29	39,47,59,59	0
3	GLY	D	902	5/5	0.94	0.21	35,44,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	D	901	1/1	0.95	0.12	34,34,34,34	0
2	MG	B	901	1/1	0.95	0.15	32,32,32,32	0
3	GLY	B	902	5/5	0.97	0.14	26,32,43,43	0
2	MG	C	901	1/1	0.98	0.13	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.