Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 04:28 pm GMT

PDB ID	:	1GXD
Title	:	proMMP-2/TIMP-2 complex
Authors	:	Morgunova, E.; Tuuttila, A.; Bergmann, U.; Tryggvason, K.
Deposited on	:	2002-04-02
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

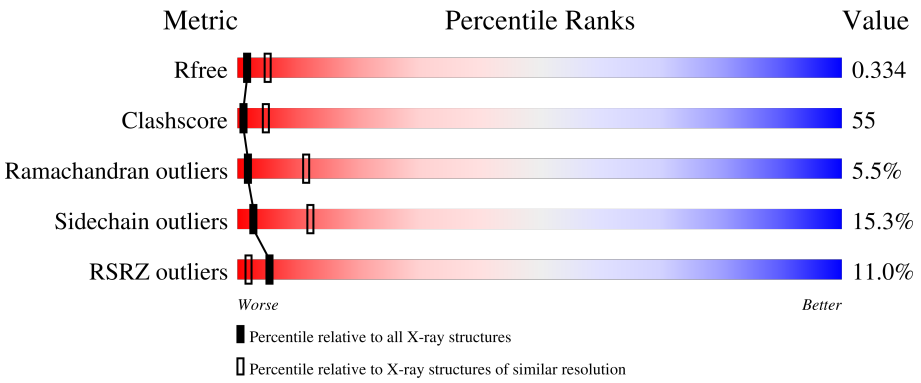
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	631	7%; 41%; 45%; 13%; • •
1	B	631	7%; 38%; 46%; 13%; • •
2	C	194	26%; 24%; 55%; 18%; • •
2	D	194	20%; 31%; 55%; 11%; • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12945 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 72 KDA TYPE IV COLLAGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	624	4963	3186	817	933	27	0	0	0
1	B	623	4958	3183	816	932	27	0	0	0

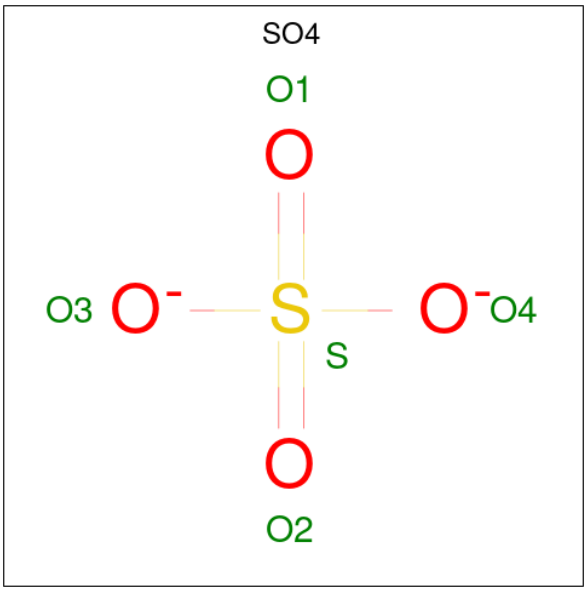
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	ALA	GLU	engineered mutation	UNP P08253
B	375	ALA	GLU	engineered mutation	UNP P08253

- Molecule 2 is a protein called METALLOPROTEINASE INHIBITOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	192	1504	952	254	281	17	0	0	0
2	D	192	1504	952	254	281	17	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

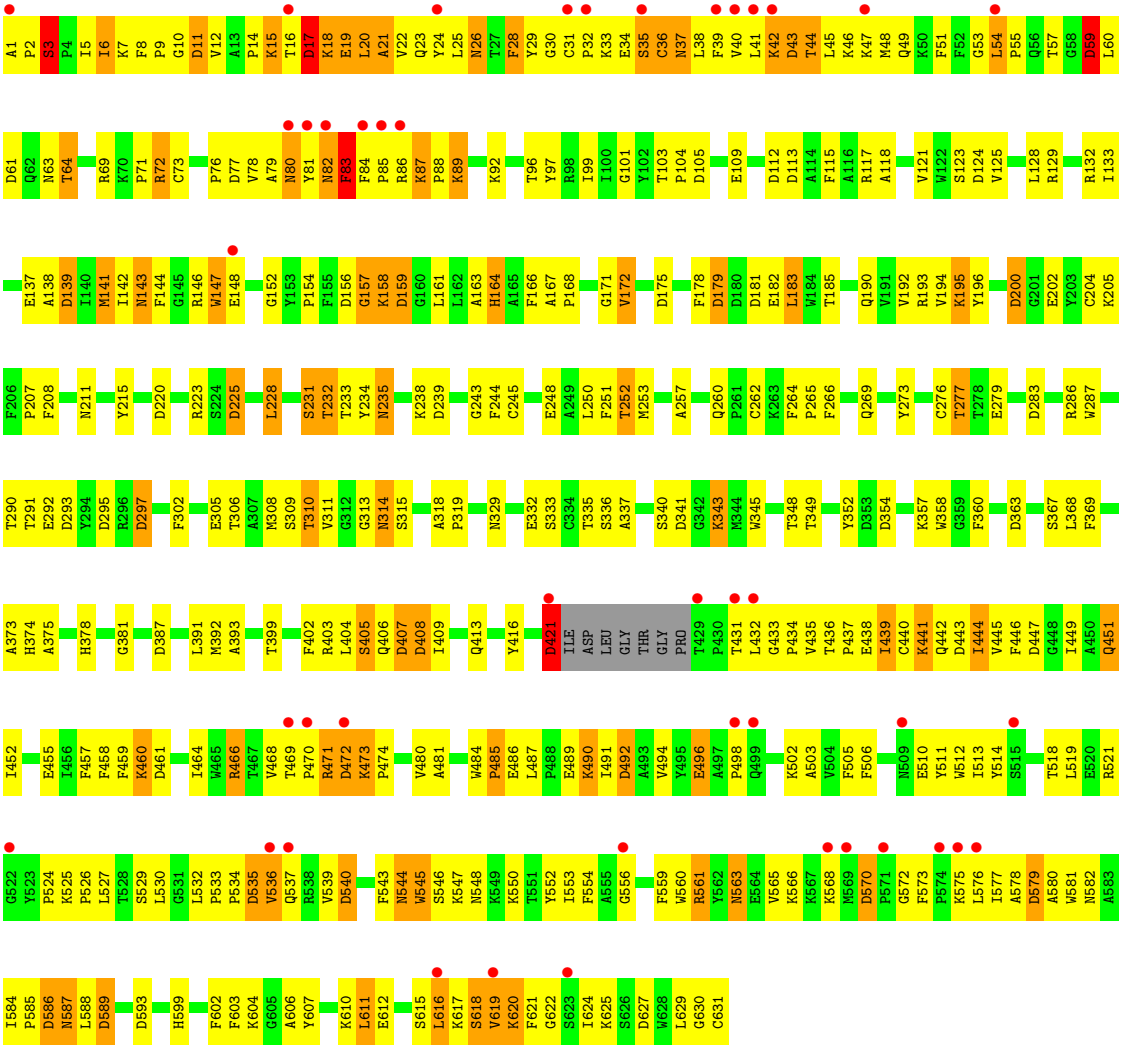
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

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.

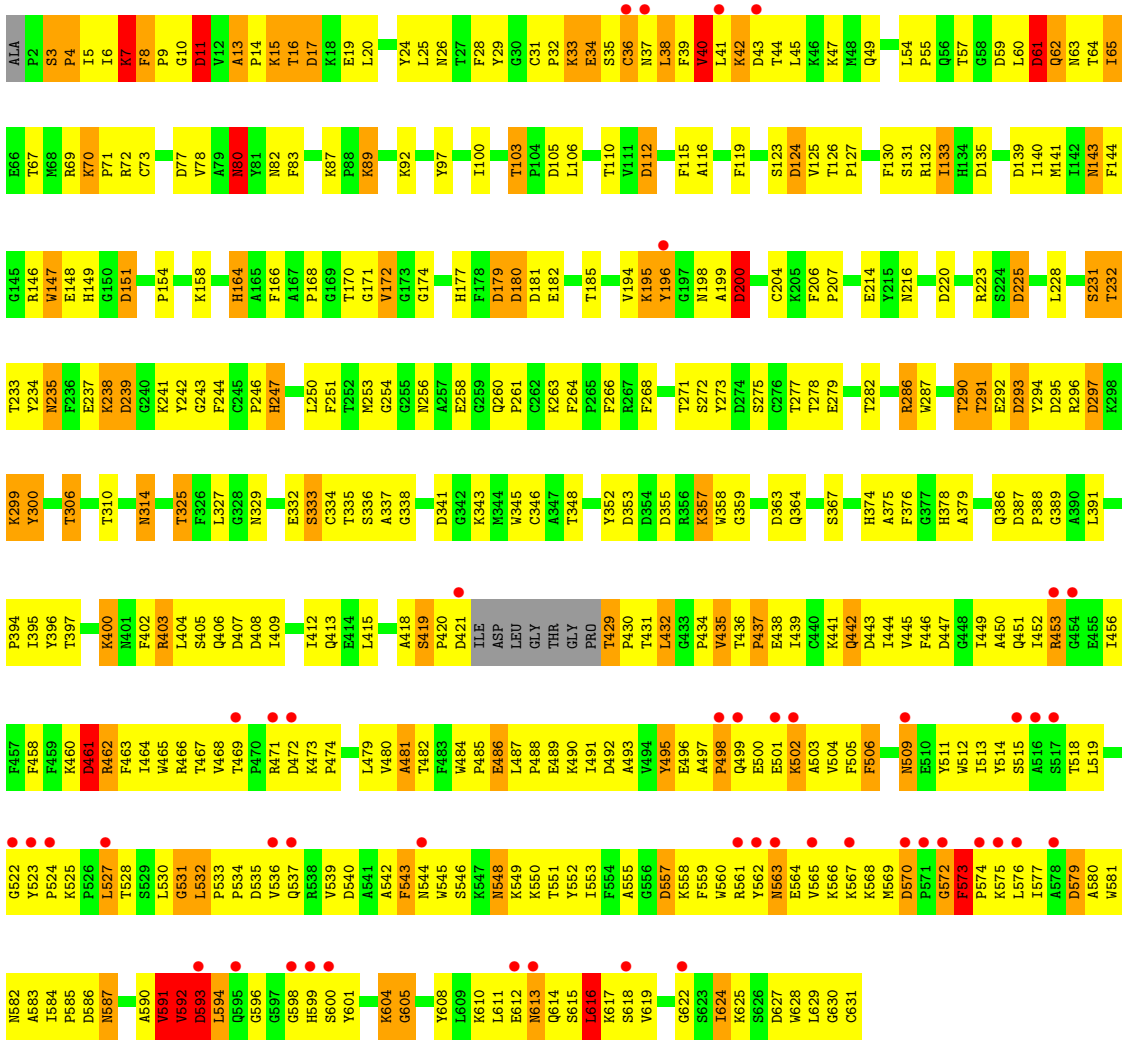
• Molecule 1: 72 KDA TYPE IV COLLAGENASE

Chain A:



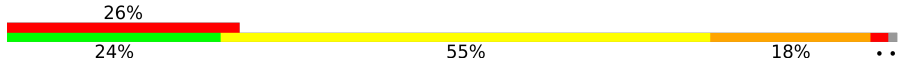
• Molecule 1: 72 KDA TYPE IV COLLAGENASE

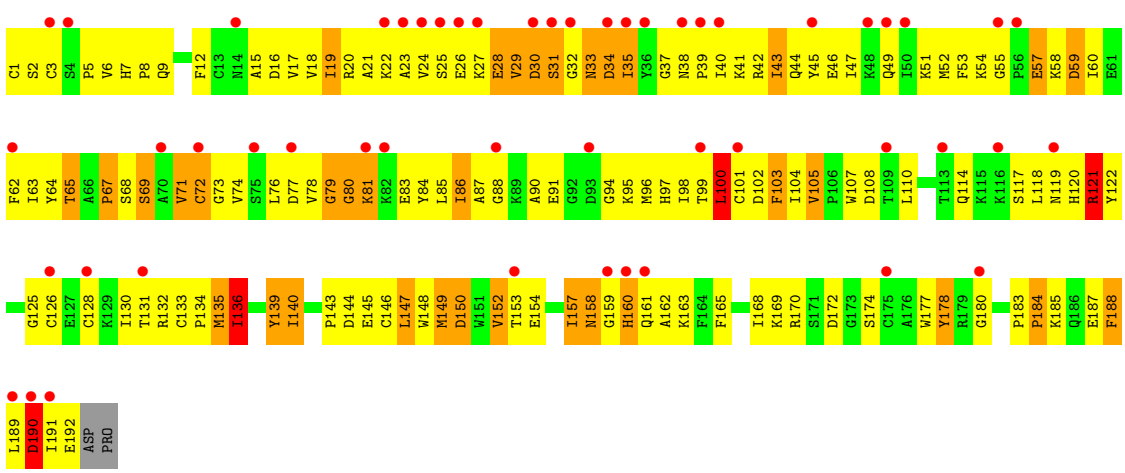
Chain B:



• Molecule 2: METALLOPROTEINASE INHIBITOR 2

Chain C:

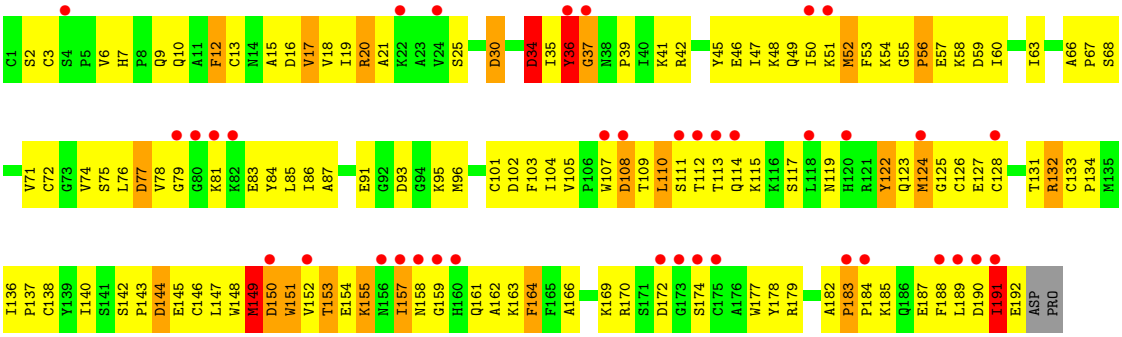




• Molecule 2: METALLOPROTEINASE INHIBITOR 2

Chain D:

20%
31%
55%
11%


C1 S2 C3 S4 P5 V6 H7 P8 Q9 Q10 A11 F12 C13 N14 A15 D16 V17 V18 I19 R20 A21 K22 A23 V24 S25 D30 D34 I35 Y36 G37 N38 P39 I40 K41 R42 Y45 E46 I47 K48 Q49 I50 K51 M52 F53 K54 G55 P56 E57 K58 D59 I60 I63 A66 P67 S68
V71 C72 G73 V74 S75 L76 D77 V78 G79 G80 K81 K82 E83 Y84 L85 I86 A87 E91 G92 D93 G94 K95 M96 C101 D102 F103 I104 V105 P106 W107 D108 T109 L110 S111 T112 T113 Q114 K115 K116 S117 L118 N119 H120 R121 Y122 Q123 M124 G125 C126 E127 C128 T131 R132 C133 P134 M135
I136 P137 C138 Y139 I140 S141 S142 P143 D144 E145 C146 L147 W148 M149 D150 W151 V152 T153 E154 K155 N156 I157 N158 G159 H160 Q161 A162 K163 F164 F165 A166 K169 R170 S171 D172 G173 S174 C175 A176 W177 Y178 R179 A182 P183 P184 K185 Q186 E187 F188 L189 D190 I191 E192 ASP PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	75.70Å 374.57Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10 12.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (8.00-3.10) 94.1 (12.97-3.10)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.275 , 0.333 0.283 , 0.334	Depositor DCC
R_{free} test set	2343 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	84.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12945	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: CA, SO4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.42	0/5118	0.85	34/6939 (0.5%)
1	B	0.48	0/5113	0.89	31/6931 (0.4%)
2	C	0.31	0/1540	0.78	11/2079 (0.5%)
2	D	0.33	1/1540 (0.1%)	0.83	10/2079 (0.5%)
All	All	0.42	1/13311 (0.0%)	0.86	86/18028 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	149	MET	CA-CB	-6.89	1.38	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	149	MET	N-CA-CB	18.16	143.28	110.60
1	B	573	PHE	N-CA-C	-9.62	85.02	111.00
1	A	573	PHE	N-CA-C	-8.03	89.31	111.00
1	B	105	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	179	ASP	CB-CG-OD2	6.56	124.20	118.30
1	B	11	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	200	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	239	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	105	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	113	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	363	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	220	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	11	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	83	PHE	C-N-CA	6.15	137.06	121.70
1	B	181	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	627	ASP	CB-CG-OD2	5.99	123.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	112	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	570	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	220	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	124	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	139	ASP	CB-CG-OD1	5.83	123.54	118.30
1	B	239	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	355	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	363	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	43	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	181	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	200	ASP	CB-CG-OD2	5.75	123.48	118.30
2	D	150	ASP	CB-CG-OD2	5.75	123.47	118.30
2	C	150	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	179	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	61	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	627	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	353	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	492	ASP	CB-CG-OD2	5.63	123.37	118.30
2	C	136	ILE	N-CA-C	-5.61	95.85	111.00
1	A	579	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	586	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	180	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	341	ASP	CB-CG-OD2	5.56	123.30	118.30
2	D	16	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	159	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	408	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	17	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	112	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	573	PHE	CB-CA-C	5.44	121.27	110.40
1	A	472	ASP	CB-CG-OD1	5.43	123.19	118.30
2	C	108	ASP	CB-CG-OD2	5.42	123.18	118.30
2	D	144	ASP	CB-CG-OD1	5.42	123.18	118.30
2	C	190	ASP	CB-CG-OD2	5.38	123.14	118.30
2	D	30	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	297	ASP	CB-CG-OD2	5.35	123.11	118.30
2	D	172	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	589	ASP	CB-CG-OD2	5.33	123.09	118.30
2	C	184	PRO	N-CA-C	5.33	125.95	112.10
2	C	59	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	461	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	540	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	593	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	225	ASP	CB-CG-OD2	5.28	123.05	118.30
2	C	144	ASP	CB-CG-OD2	5.27	123.04	118.30
2	D	34	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	59	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	407	ASP	CB-CG-OD1	5.24	123.02	118.30
2	D	77	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	297	ASP	CB-CG-OD2	5.22	122.99	118.30
1	B	225	ASP	CB-CG-OD2	5.20	122.98	118.30
2	C	172	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	557	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	535	ASP	CB-CG-OD2	5.15	122.93	118.30
2	D	108	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	421	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	586	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	535	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	387	ASP	CB-CG-OD2	5.12	122.91	118.30
2	C	34	ASP	CB-CG-OD2	5.11	122.89	118.30
1	B	540	ASP	CB-CG-OD2	5.09	122.89	118.30
2	C	77	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	492	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	354	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	139	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	293	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	175	ASP	CB-CG-OD2	5.05	122.84	118.30
2	C	30	ASP	CB-CG-OD1	5.04	122.84	118.30
2	D	59	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	407	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4963	0	4674	464	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4958	0	4667	517	0
2	C	1504	0	1470	278	3
2	D	1504	0	1470	176	3
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12945	0	12281	1376	3

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 55.

All (1376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:THR:CG2	1:B:430:PRO:HD2	1.18	1.59
1:A:409:ILE:HG13	1:A:432:LEU:CD1	1.16	1.58
1:A:409:ILE:CD1	1:A:432:LEU:HD21	1.10	1.58
1:A:409:ILE:CG1	1:A:432:LEU:HD11	1.14	1.52
1:B:429:THR:HG23	1:B:430:PRO:CD	1.06	1.49
1:A:409:ILE:HG13	1:A:432:LEU:CG	1.41	1.46
1:A:406:GLN:CA	1:A:432:LEU:HD12	1.41	1.45
2:D:183:PRO:HB2	2:D:184:PRO:CD	1.50	1.38
1:A:406:GLN:HA	1:A:432:LEU:CD1	1.58	1.34
1:B:429:THR:CG2	1:B:430:PRO:CD	1.82	1.33
1:A:409:ILE:CD1	1:A:432:LEU:CD2	2.06	1.31
2:D:36:TYR:O	2:D:36:TYR:CD1	1.84	1.30
1:B:630:GLY:O	1:B:631:CYS:N	1.66	1.29
2:C:86:ILE:CD1	2:C:104:ILE:HG23	1.64	1.27
1:A:618:SER:O	1:A:619:VAL:HG23	1.31	1.26
1:A:53:GLY:O	1:A:55:PRO:HD3	1.24	1.26
1:B:498:PRO:HG2	1:B:564:GLU:CG	1.68	1.23
1:A:618:SER:O	1:A:619:VAL:CG2	1.85	1.23
1:B:196:TYR:CD2	1:B:244:PHE:CD1	2.28	1.21
2:D:149:MET:HB2	2:D:152:VAL:CG1	1.72	1.20
2:C:29:VAL:HG22	2:C:43:ILE:CA	1.72	1.19
2:C:79:GLY:O	2:C:81:LYS:HG3	1.42	1.19
1:B:3:SER:HB2	1:B:4:PRO:CD	1.73	1.19
1:B:60:LEU:O	1:B:60:LEU:HD13	1.43	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:HZ	2:D:188:PHE:CZ	1.62	1.18
1:A:20:LEU:HD23	1:A:21:ALA:H	1.06	1.17
2:D:182:ALA:CB	2:D:185:LYS:HE3	1.73	1.17
1:B:572:GLY:C	1:B:573:PHE:O	1.70	1.16
1:B:497:ALA:HB3	1:B:500:GLU:O	1.44	1.16
2:C:29:VAL:CG2	2:C:43:ILE:HA	1.75	1.15
2:C:86:ILE:HG23	2:C:104:ILE:HG12	1.17	1.15
1:B:61:ASP:HA	1:B:64:THR:HG22	1.27	1.15
1:B:419:SER:CB	1:B:420:PRO:HD3	1.77	1.15
1:A:25:LEU:O	1:A:29:TYR:HB2	1.45	1.14
2:C:27:LYS:HB2	2:C:44:GLN:HG2	1.29	1.14
1:B:37:ASN:HB3	1:B:43:ASP:OD2	1.46	1.13
1:B:622:GLY:HA2	2:D:137:PRO:HB3	1.21	1.13
1:A:580:ALA:HB3	2:C:188:PHE:CE2	1.84	1.12
2:D:149:MET:CB	2:D:152:VAL:CG1	2.26	1.12
1:B:419:SER:CB	1:B:420:PRO:CD	2.27	1.12
2:C:136:ILE:HD11	2:C:152:VAL:CG2	1.79	1.11
1:B:34:GLU:OE1	1:B:34:GLU:HA	1.45	1.11
1:B:453:ARG:O	1:B:453:ARG:HD3	1.49	1.11
1:B:502:LYS:HG3	1:B:515:SER:HB2	1.33	1.10
1:B:530:LEU:O	1:B:532:LEU:N	1.83	1.10
1:A:45:LEU:HD23	1:A:59:ASP:HA	1.21	1.10
1:A:630:GLY:C	1:A:631:CYS:N	2.05	1.10
1:A:409:ILE:CG1	1:A:432:LEU:HD21	1.81	1.10
1:B:473:LYS:HG2	1:B:474:PRO:HD2	1.20	1.10
2:C:86:ILE:HD11	2:C:104:ILE:HG23	1.30	1.10
2:D:149:MET:HB2	2:D:152:VAL:HG13	1.31	1.10
1:A:1:ALA:HB3	1:A:2:PRO:HD3	1.27	1.09
1:A:409:ILE:HG12	1:A:432:LEU:HD11	1.13	1.09
2:C:29:VAL:HG13	2:C:42:ARG:C	1.72	1.09
1:A:36:CYS:HB3	1:A:38:LEU:CD1	1.81	1.09
1:B:612:GLU:HB2	1:B:618:SER:HB3	1.31	1.09
1:B:357:LYS:HB3	1:B:357:LYS:HZ2	1.02	1.09
1:B:429:THR:HG22	1:B:430:PRO:HD2	1.14	1.09
2:D:183:PRO:HB2	2:D:184:PRO:HD3	1.13	1.08
1:A:37:ASN:O	1:A:41:LEU:HB2	1.52	1.08
1:B:357:LYS:HB3	1:B:357:LYS:NZ	1.63	1.08
1:B:559:PHE:CZ	2:D:188:PHE:CZ	2.40	1.08
1:B:419:SER:HB3	1:B:420:PRO:CD	1.81	1.08
1:A:630:GLY:O	1:A:631:CYS:N	1.87	1.08
1:A:409:ILE:HD12	1:A:432:LEU:HD21	1.12	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ILE:HD11	1:A:432:LEU:CD2	1.77	1.06
1:B:196:TYR:HE1	1:B:251:PHE:CZ	1.74	1.06
2:C:60:ILE:HA	2:C:94:GLY:HA2	1.31	1.06
1:A:409:ILE:HD11	1:A:432:LEU:HD21	1.06	1.06
1:A:409:ILE:CG1	1:A:432:LEU:CD1	1.93	1.05
1:B:498:PRO:HG2	1:B:564:GLU:HG2	1.37	1.05
1:B:563:ASN:O	1:B:563:ASN:ND2	1.90	1.04
1:A:45:LEU:CD2	1:A:59:ASP:HA	1.86	1.04
1:B:406:GLN:NE2	1:B:432:LEU:O	1.90	1.04
1:B:497:ALA:CB	1:B:500:GLU:O	2.04	1.04
1:B:438:GLU:OE2	1:B:441:LYS:HD2	1.56	1.04
1:A:630:GLY:O	1:A:631:CYS:CA	2.05	1.04
1:B:403:ARG:HG2	1:B:403:ARG:HH11	1.23	1.04
1:B:5:ILE:HD12	1:B:327:LEU:HD13	1.35	1.03
2:C:29:VAL:HG13	2:C:42:ARG:O	1.56	1.03
1:A:577:ILE:HG23	1:A:581:TRP:HB2	1.40	1.03
1:B:498:PRO:HG2	1:B:564:GLU:HG3	1.34	1.03
1:B:196:TYR:CE1	1:B:251:PHE:CZ	2.47	1.02
1:B:196:TYR:CE1	1:B:251:PHE:CE1	2.46	1.02
1:B:511:TYR:CE2	1:B:523:TYR:HE2	1.78	1.02
1:A:81:TYR:HD2	1:A:86:ARG:CZ	1.71	1.02
2:C:41:LYS:O	2:C:67:PRO:HG3	1.61	1.01
2:D:190:ASP:O	2:D:192:GLU:HG2	1.58	1.01
1:A:545:TRP:HZ3	1:A:547:LYS:HE2	1.23	1.01
1:B:498:PRO:CG	1:B:564:GLU:HG3	1.90	1.00
1:A:409:ILE:CG1	1:A:432:LEU:CD2	2.39	1.00
1:B:511:TYR:CE2	1:B:523:TYR:CE2	2.48	1.00
1:B:143:ASN:HD22	1:B:144:PHE:H	1.02	1.00
1:B:286:ARG:HG3	1:B:286:ARG:HH11	1.20	1.00
1:B:462:ARG:O	1:B:463:PHE:CG	2.15	1.00
1:B:143:ASN:ND2	1:B:144:PHE:H	1.60	0.99
2:D:17:VAL:HA	2:D:54:LYS:O	1.62	0.99
2:D:183:PRO:CB	2:D:184:PRO:CD	2.40	0.99
1:B:196:TYR:CE2	1:B:244:PHE:CG	2.51	0.99
2:C:47:ILE:HG21	2:C:63:ILE:HG12	1.44	0.99
2:C:86:ILE:CG2	2:C:104:ILE:HG12	1.92	0.99
1:B:630:GLY:C	1:B:631:CYS:N	2.14	0.99
1:B:419:SER:HB3	1:B:420:PRO:HD3	0.99	0.98
1:A:409:ILE:HG13	1:A:432:LEU:CD2	1.93	0.97
2:D:146:CYS:HB3	2:D:177:TRP:CZ2	1.99	0.97
1:A:20:LEU:HD23	1:A:21:ALA:N	1.80	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:ILE:CD1	2:C:104:ILE:CG2	2.42	0.97
1:B:5:ILE:HD12	1:B:327:LEU:CD1	1.95	0.97
1:A:527:LEU:HB2	1:A:536:VAL:CG1	1.95	0.96
2:C:27:LYS:HB2	2:C:44:GLN:CG	1.95	0.96
1:A:84:PHE:CE1	1:A:85:PRO:O	2.19	0.96
1:A:406:GLN:CA	1:A:432:LEU:CD1	2.28	0.96
2:D:182:ALA:HB1	2:D:185:LYS:HE3	1.43	0.96
1:A:28:PHE:CE2	1:A:72:ARG:HD2	2.01	0.96
2:C:136:ILE:CD1	2:C:152:VAL:CG2	2.43	0.95
1:A:143:ASN:ND2	1:A:144:PHE:H	1.64	0.95
1:A:630:GLY:O	1:A:631:CYS:HA	1.65	0.95
1:B:622:GLY:CA	2:D:137:PRO:HB3	1.96	0.94
1:A:471:ARG:O	1:A:630:GLY:HA2	1.67	0.94
1:A:53:GLY:O	1:A:55:PRO:CD	2.16	0.94
1:B:3:SER:HB2	1:B:4:PRO:HD2	1.48	0.94
1:B:562:TYR:HE2	1:B:564:GLU:OE2	1.50	0.94
2:C:86:ILE:HG23	2:C:104:ILE:CG1	1.97	0.94
1:A:143:ASN:HD22	1:A:144:PHE:H	1.05	0.93
1:B:194:VAL:CG1	1:B:243:GLY:HA3	1.98	0.93
1:B:559:PHE:CZ	2:D:188:PHE:CE2	2.56	0.93
1:B:61:ASP:HA	1:B:64:THR:CG2	1.97	0.93
1:B:73:CYS:HG	4:B:1634:ZN:ZN	0.69	0.93
2:C:29:VAL:HG21	2:C:43:ILE:HD13	1.49	0.93
1:A:409:ILE:CG1	1:A:432:LEU:CG	2.33	0.93
2:D:183:PRO:HB2	2:D:184:PRO:HD2	1.50	0.92
1:B:429:THR:HG23	1:B:430:PRO:HD3	0.93	0.92
1:B:25:LEU:O	1:B:29:TYR:O	1.88	0.92
1:B:41:LEU:HD12	1:B:43:ASP:OD2	1.70	0.92
1:A:42:LYS:O	1:A:46:LYS:HE3	1.68	0.92
1:B:196:TYR:CZ	1:B:244:PHE:CB	2.52	0.92
1:B:196:TYR:CZ	1:B:244:PHE:HB2	2.05	0.91
1:B:314:ASN:HD21	1:B:358:TRP:H	1.17	0.91
2:C:43:ILE:HB	2:C:65:THR:HG23	1.51	0.91
2:D:36:TYR:O	2:D:36:TYR:HD1	1.36	0.91
1:B:511:TYR:HE2	1:B:523:TYR:HE2	1.08	0.90
2:C:32:GLY:O	2:C:39:PRO:HA	1.71	0.90
2:D:183:PRO:CB	2:D:184:PRO:HD3	1.99	0.90
2:D:102:ASP:O	2:D:104:ILE:HG13	1.72	0.90
2:D:149:MET:HB3	2:D:152:VAL:CG1	2.00	0.90
2:D:68:SER:O	2:D:71:VAL:HG22	1.71	0.90
2:D:149:MET:CB	2:D:152:VAL:HG12	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:HG	1:A:60:LEU:O	1.71	0.90
1:B:357:LYS:NZ	1:B:357:LYS:CB	2.35	0.90
2:D:35:ILE:O	2:D:35:ILE:HG22	1.71	0.90
1:B:473:LYS:HG2	1:B:474:PRO:CD	2.02	0.89
2:D:140:ILE:O	2:D:140:ILE:HG13	1.70	0.89
1:A:36:CYS:HB3	1:A:38:LEU:HD12	1.51	0.89
1:B:61:ASP:CA	1:B:64:THR:HG22	2.02	0.89
1:B:543:PHE:CE2	1:B:545:TRP:HD1	1.89	0.89
1:A:59:ASP:HB2	1:A:61:ASP:OD1	1.73	0.89
1:B:511:TYR:HE2	1:B:523:TYR:CE2	1.89	0.89
2:C:47:ILE:HG21	2:C:63:ILE:CG1	2.03	0.89
1:A:26:ASN:HB2	1:A:31:CYS:H	1.37	0.88
1:B:391:LEU:HD22	1:B:402:PHE:CZ	2.08	0.88
2:C:27:LYS:O	2:C:44:GLN:HB3	1.71	0.88
1:A:403:ARG:HH11	1:A:403:ARG:HG2	1.38	0.88
1:B:196:TYR:CE1	1:B:244:PHE:HB2	2.08	0.88
2:C:34:ASP:OD1	2:C:35:ILE:N	2.06	0.88
1:B:235:ASN:ND2	1:B:238:LYS:H	1.68	0.88
2:D:149:MET:HB2	2:D:152:VAL:HG12	1.54	0.88
1:B:559:PHE:HZ	2:D:188:PHE:CE2	1.90	0.88
1:A:457:PHE:HA	1:A:466:ARG:HB3	1.56	0.88
1:B:194:VAL:HG11	1:B:243:GLY:HA3	1.55	0.88
1:B:580:ALA:HB2	2:D:188:PHE:CZ	2.08	0.88
1:B:57:THR:CG2	1:B:60:LEU:HB2	2.04	0.88
1:B:41:LEU:HB3	1:B:43:ASP:OD1	1.73	0.87
2:D:187:GLU:OE2	2:D:189:LEU:HD13	1.73	0.87
1:A:617:LYS:NZ	2:C:174:SER:HB2	1.90	0.87
2:D:182:ALA:HB3	2:D:185:LYS:HE3	1.56	0.87
1:A:45:LEU:HD23	1:A:59:ASP:CA	2.04	0.87
1:B:473:LYS:CG	1:B:474:PRO:HD2	2.02	0.86
1:A:464:ILE:HG23	1:A:480:VAL:HG12	1.57	0.86
1:A:81:TYR:CD2	1:A:86:ARG:CZ	2.58	0.86
1:B:3:SER:HB2	1:B:4:PRO:HD3	1.57	0.86
1:A:26:ASN:HB3	1:A:31:CYS:O	1.74	0.86
2:D:20:ARG:NH2	2:D:83:GLU:OE2	2.08	0.86
1:B:196:TYR:CZ	1:B:251:PHE:CE1	2.64	0.86
1:A:1:ALA:CB	1:A:2:PRO:HD3	2.06	0.86
2:C:86:ILE:HD11	2:C:104:ILE:CG2	2.05	0.86
2:C:69:SER:HA	2:C:73:GLY:HA3	1.57	0.85
2:D:131:THR:HG22	2:D:132:ARG:H	1.40	0.85
2:C:149:MET:O	2:C:152:VAL:HG12	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PHE:CE2	1:B:545:TRP:CD1	2.65	0.85
2:D:20:ARG:NH2	2:D:83:GLU:CD	2.30	0.85
1:A:10:GLY:HA2	1:B:296:ARG:NH1	1.90	0.85
1:A:38:LEU:O	1:A:41:LEU:O	1.93	0.85
1:A:53:GLY:C	1:A:55:PRO:HD3	1.97	0.85
1:B:123:SER:O	1:B:125:VAL:N	2.09	0.84
1:B:391:LEU:HD22	1:B:402:PHE:HZ	1.39	0.84
1:B:143:ASN:HD22	1:B:144:PHE:N	1.75	0.84
1:A:618:SER:O	1:A:619:VAL:HG22	1.76	0.84
1:A:580:ALA:HB3	2:C:188:PHE:CD2	2.12	0.84
1:B:3:SER:CB	1:B:4:PRO:CD	2.55	0.84
1:B:126:THR:HB	1:B:127:PRO:HD2	1.60	0.84
1:A:54:LEU:H	1:A:54:LEU:HD23	1.42	0.84
1:B:498:PRO:CD	1:B:564:GLU:HG3	2.06	0.84
2:C:18:VAL:HG13	2:C:87:ALA:HB2	1.60	0.84
2:C:27:LYS:CB	2:C:44:GLN:HG2	2.07	0.84
1:B:543:PHE:HE2	1:B:545:TRP:CD1	1.95	0.83
1:A:72:ARG:HD3	1:A:73:CYS:O	1.79	0.83
2:D:149:MET:CB	2:D:152:VAL:HG13	1.99	0.83
1:A:618:SER:C	1:A:619:VAL:HG23	1.99	0.83
2:C:25:SER:OG	2:C:46:GLU:OE1	1.95	0.83
1:B:60:LEU:HD11	1:B:63:ASN:HB3	1.59	0.83
2:C:69:SER:HA	2:C:73:GLY:CA	2.07	0.83
1:A:545:TRP:CZ3	1:A:547:LYS:HE2	2.13	0.83
1:B:462:ARG:O	1:B:463:PHE:CD1	2.31	0.82
2:D:140:ILE:CG2	2:D:147:LEU:HB2	2.09	0.82
1:B:515:SER:O	1:B:518:THR:HG22	1.77	0.82
2:D:131:THR:OG1	2:D:145:GLU:OE1	1.96	0.82
1:A:406:GLN:N	1:A:432:LEU:CD1	2.42	0.82
1:A:439:ILE:HG22	1:A:440:CYS:N	1.94	0.82
1:A:527:LEU:HB2	1:A:536:VAL:HG12	1.59	0.82
1:A:617:LYS:HZ3	2:C:174:SER:HB2	1.45	0.82
1:B:54:LEU:HB3	1:B:55:PRO:CD	2.09	0.82
1:B:453:ARG:O	1:B:453:ARG:CD	2.27	0.82
2:C:133:CYS:HB3	2:C:149:MET:HB3	1.62	0.82
1:A:84:PHE:CD1	1:A:85:PRO:O	2.32	0.82
1:B:54:LEU:HB3	1:B:55:PRO:HD2	1.62	0.82
1:B:196:TYR:OH	1:B:251:PHE:CE1	2.32	0.82
1:B:310:THR:HG21	1:B:359:GLY:HA3	1.62	0.82
2:C:86:ILE:CG1	2:C:104:ILE:HG23	2.10	0.82
2:C:136:ILE:CD1	2:C:152:VAL:HG21	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:THR:O	1:B:306:THR:HG22	1.79	0.81
1:B:469:THR:CG2	1:B:471:ARG:HD3	2.10	0.81
2:D:36:TYR:CD1	2:D:36:TYR:C	2.52	0.81
1:B:493:ALA:HB3	1:B:506:PHE:HB2	1.62	0.81
1:A:409:ILE:CB	1:A:432:LEU:HD11	2.10	0.81
1:B:196:TYR:OH	1:B:251:PHE:HE1	1.63	0.81
2:C:46:GLU:HA	2:C:62:PHE:HD1	1.44	0.81
1:B:34:GLU:OE1	1:B:34:GLU:CA	2.25	0.81
1:A:156:ASP:O	1:A:157:GLY:O	1.98	0.81
2:D:47:ILE:HG12	2:D:63:ILE:HG13	1.62	0.81
2:D:20:ARG:HH22	2:D:83:GLU:CD	1.82	0.80
1:A:25:LEU:HD11	1:A:45:LEU:HD13	1.62	0.80
2:C:143:PRO:O	2:C:174:SER:HB3	1.81	0.80
1:A:471:ARG:O	1:A:630:GLY:CA	2.30	0.80
1:B:196:TYR:CE2	1:B:244:PHE:CB	2.65	0.80
2:C:60:ILE:HA	2:C:94:GLY:CA	2.09	0.80
1:A:143:ASN:HD22	1:A:144:PHE:N	1.79	0.80
1:B:13:ALA:O	1:B:15:LYS:HG3	1.82	0.80
1:B:419:SER:HB2	1:B:420:PRO:CD	2.09	0.80
2:C:165:PHE:CD2	2:C:177:TRP:HB3	2.17	0.80
1:A:128:LEU:O	1:A:129:ARG:HD3	1.81	0.79
1:A:617:LYS:HE2	2:C:170:ARG:HG3	1.65	0.79
2:C:136:ILE:HD11	2:C:152:VAL:HG23	1.63	0.79
2:C:47:ILE:HD11	2:C:60:ILE:O	1.82	0.79
1:B:37:ASN:CB	1:B:43:ASP:OD2	2.28	0.79
1:A:84:PHE:HB2	1:A:167:ALA:HB3	1.64	0.79
1:A:406:GLN:HA	1:A:406:GLN:HE21	1.48	0.79
1:A:223:ARG:NH2	1:A:225:ASP:OD2	2.16	0.79
1:B:562:TYR:CE2	1:B:564:GLU:CD	2.57	0.79
2:C:7:HIS:CE1	2:C:162:ALA:HA	2.17	0.79
2:D:154:GLU:O	2:D:155:LYS:HB2	1.82	0.78
1:B:268:PHE:O	1:B:295:ASP:OD2	2.01	0.78
1:B:573:PHE:CD1	1:B:575:LYS:HE2	2.18	0.78
2:C:136:ILE:HD13	2:C:152:VAL:HG21	1.63	0.78
1:A:409:ILE:HG13	1:A:432:LEU:HG	1.64	0.78
1:B:133:ILE:HG12	1:B:133:ILE:O	1.80	0.78
2:C:29:VAL:CG1	2:C:42:ARG:H	1.96	0.78
1:B:10:GLY:O	1:B:11:ASP:HB3	1.84	0.78
1:B:580:ALA:CB	2:D:188:PHE:CZ	2.67	0.78
2:D:34:ASP:OD1	2:D:34:ASP:N	2.15	0.78
2:D:60:ILE:HG21	2:D:96:MET:HE3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:LEU:HD12	1:B:488:PRO:HD2	1.64	0.77
1:B:591:VAL:O	1:B:592:VAL:HG12	1.84	0.77
1:B:608:TYR:CD1	1:B:622:GLY:O	2.36	0.77
2:C:27:LYS:CB	2:C:44:GLN:CG	2.61	0.77
2:C:161:GLN:O	2:C:165:PHE:HB2	1.82	0.77
2:D:117:SER:O	2:D:122:TYR:CD2	2.38	0.77
2:D:150:ASP:CG	2:D:151:TRP:N	2.36	0.77
1:B:9:PRO:HD2	1:B:352:TYR:OH	1.85	0.77
1:A:15:LYS:HE2	1:A:23:GLN:OE1	1.85	0.77
1:A:286:ARG:HG3	1:A:286:ARG:HH11	1.49	0.77
1:B:151:ASP:OD2	1:B:177:HIS:CE1	2.38	0.77
2:C:53:PHE:CD2	2:C:118:LEU:HB3	2.20	0.77
1:B:450:ALA:HA	1:B:592:VAL:HG21	1.67	0.77
1:B:500:GLU:HG2	1:B:502:LYS:HD3	1.67	0.77
1:B:563:ASN:ND2	1:B:566:LYS:HB2	2.00	0.77
2:C:86:ILE:HD13	2:C:104:ILE:CG2	2.15	0.77
1:B:286:ARG:HG3	1:B:286:ARG:NH1	1.97	0.76
1:A:621:PHE:HE1	2:C:136:ILE:HD13	1.50	0.76
1:B:41:LEU:O	1:B:42:LYS:HB2	1.86	0.76
1:B:462:ARG:C	1:B:463:PHE:CD1	2.58	0.76
1:A:17:ASP:O	1:A:20:LEU:HD22	1.85	0.76
1:A:409:ILE:HD12	1:A:432:LEU:CD2	1.96	0.76
1:B:143:ASN:ND2	1:B:144:PHE:N	2.32	0.76
2:D:150:ASP:CG	2:D:151:TRP:H	1.88	0.76
1:A:84:PHE:CD1	1:A:84:PHE:C	2.59	0.76
1:A:585:PRO:HD2	1:A:588:LEU:HD11	1.68	0.76
1:A:512:TRP:NE1	1:A:524:PRO:HG3	2.01	0.76
2:C:5:PRO:HD2	2:C:132:ARG:NH1	2.01	0.76
1:B:17:ASP:OD2	1:B:65:ILE:HD13	1.85	0.76
1:A:438:GLU:OE1	1:A:441:LYS:HD2	1.86	0.75
1:B:60:LEU:O	1:B:60:LEU:CD1	2.30	0.75
1:B:506:PHE:CE1	1:B:527:LEU:HD11	2.22	0.75
2:C:147:LEU:N	2:C:177:TRP:CH2	2.55	0.75
2:D:140:ILE:HG22	2:D:147:LEU:HB2	1.68	0.75
1:A:621:PHE:HB2	2:C:147:LEU:HD21	1.67	0.75
1:B:563:ASN:HD22	1:B:563:ASN:C	1.89	0.75
1:A:37:ASN:HB2	1:A:41:LEU:HD12	1.69	0.74
1:B:592:VAL:O	1:B:592:VAL:CG2	2.35	0.74
2:C:165:PHE:HD2	2:C:177:TRP:HB3	1.51	0.74
1:A:552:TYR:CE2	2:C:188:PHE:CE1	2.76	0.74
1:A:29:TYR:OH	1:A:48:MET:HA	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:GLU:OE1	1:B:182:GLU:HA	1.88	0.74
1:B:542:ALA:O	1:B:543:PHE:HB3	1.88	0.74
1:A:26:ASN:CB	1:A:31:CYS:O	2.36	0.73
1:B:34:GLU:O	1:B:36:CYS:N	2.19	0.73
1:B:562:TYR:HE2	1:B:564:GLU:CD	1.91	0.73
1:B:57:THR:OG1	1:B:60:LEU:HB2	1.88	0.73
1:A:194:VAL:CG1	1:A:243:GLY:HA3	2.17	0.73
2:C:183:PRO:N	2:C:184:PRO:HD3	2.03	0.73
1:B:39:PHE:O	1:B:40:VAL:HG12	1.89	0.73
1:A:617:LYS:CE	2:C:170:ARG:HG3	2.19	0.73
2:D:17:VAL:CG1	2:D:55:GLY:HA3	2.19	0.73
2:C:27:LYS:HB3	2:C:44:GLN:CD	2.08	0.72
2:D:117:SER:O	2:D:122:TYR:HD2	1.70	0.72
1:A:556:GLY:CA	1:A:587:ASN:OD1	2.37	0.72
1:B:306:THR:O	1:B:306:THR:CG2	2.37	0.72
1:A:277:THR:HB	1:A:279:GLU:H	1.55	0.72
1:B:419:SER:HB2	1:B:420:PRO:HD2	1.68	0.72
2:C:47:ILE:CG2	2:C:63:ILE:HG12	2.16	0.72
1:A:406:GLN:N	1:A:432:LEU:HD13	2.04	0.72
2:D:147:LEU:H	2:D:177:TRP:HH2	1.38	0.72
1:A:621:PHE:HE1	2:C:152:VAL:HG21	1.55	0.72
2:D:182:ALA:CB	2:D:185:LYS:CE	2.62	0.72
2:D:132:ARG:O	2:D:134:PRO:HD3	1.90	0.72
1:B:196:TYR:CE2	1:B:244:PHE:CD1	2.76	0.72
1:B:239:ASP:O	1:B:241:LYS:HE3	1.89	0.72
1:B:310:THR:CG2	1:B:359:GLY:HA3	2.19	0.72
2:C:69:SER:HA	2:C:73:GLY:N	2.05	0.72
1:A:1:ALA:HB3	1:A:2:PRO:CD	2.14	0.71
1:A:85:PRO:HD2	1:A:168:PRO:O	1.89	0.71
1:B:581:TRP:HA	1:B:616:LEU:HD13	1.72	0.71
1:B:33:LYS:HE3	1:B:33:LYS:HA	1.72	0.71
2:C:7:HIS:HE1	2:C:161:GLN:O	1.74	0.71
1:B:449:ILE:O	1:B:592:VAL:HG11	1.89	0.71
1:A:438:GLU:CD	1:A:441:LYS:HD2	2.10	0.71
1:B:497:ALA:HB2	1:B:502:LYS:O	1.90	0.71
1:B:562:TYR:CE2	1:B:564:GLU:OE2	2.40	0.71
2:C:148:TRP:HA	2:C:161:GLN:OE1	1.90	0.71
1:A:10:GLY:CA	1:B:296:ARG:NH1	2.54	0.71
1:B:498:PRO:HD2	1:B:564:GLU:HG3	1.71	0.71
1:B:13:ALA:H	1:B:14:PRO:HD3	1.55	0.71
1:B:80:ASN:C	1:B:80:ASN:ND2	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:GLY:O	2:D:163:LYS:HG3	1.91	0.71
1:A:406:GLN:HA	1:A:406:GLN:NE2	2.06	0.71
1:B:430:PRO:HB3	1:B:435:VAL:HG12	1.72	0.71
1:A:133:ILE:HD11	1:A:138:ALA:HB2	1.72	0.70
2:C:29:VAL:CG1	2:C:42:ARG:O	2.38	0.70
2:D:35:ILE:O	2:D:35:ILE:CG2	2.39	0.70
1:B:119:PHE:HB3	1:B:130:PHE:CD2	2.27	0.70
1:B:611:LEU:HD23	1:B:612:GLU:O	1.92	0.70
2:C:147:LEU:O	2:C:177:TRP:CZ2	2.43	0.70
2:D:111:SER:O	2:D:115:LYS:HG2	1.92	0.70
1:B:503:ALA:N	1:B:514:TYR:O	2.24	0.70
2:C:170:ARG:N	2:C:174:SER:O	2.24	0.70
1:A:84:PHE:HE1	1:A:85:PRO:O	1.72	0.70
2:C:32:GLY:C	2:C:40:ILE:H	1.95	0.70
2:C:46:GLU:HA	2:C:62:PHE:CD1	2.26	0.70
2:C:27:LYS:HE3	2:C:62:PHE:CZ	2.26	0.70
2:C:27:LYS:N	2:C:44:GLN:O	2.25	0.69
2:C:29:VAL:HG13	2:C:42:ARG:N	2.07	0.69
2:C:1:CYS:HB2	2:C:71:VAL:O	1.92	0.69
1:A:413:GLN:O	1:A:416:TYR:O	2.10	0.69
1:B:462:ARG:O	1:B:463:PHE:CD2	2.45	0.69
2:C:29:VAL:HG22	2:C:43:ILE:HA	0.82	0.69
1:A:143:ASN:ND2	1:A:144:PHE:N	2.39	0.69
2:D:15:ALA:O	2:D:54:LYS:HE3	1.92	0.69
1:A:490:LYS:O	1:A:490:LYS:HG2	1.93	0.69
1:B:37:ASN:O	1:B:41:LEU:HB2	1.93	0.69
1:B:235:ASN:HD21	1:B:237:GLU:HB3	1.57	0.69
1:B:563:ASN:HD21	1:B:566:LYS:HB2	1.56	0.69
2:C:147:LEU:N	2:C:177:TRP:CZ2	2.61	0.69
2:D:7:HIS:HB3	2:D:10:GLN:HB2	1.75	0.69
1:A:159:ASP:OD2	1:A:343:LYS:NZ	2.25	0.69
1:A:563:ASN:O	1:A:566:LYS:O	2.11	0.69
2:D:91:GLU:OE1	2:D:91:GLU:HA	1.93	0.69
1:A:405:SER:C	1:A:432:LEU:HD13	2.13	0.69
1:B:195:LYS:O	1:B:200:ASP:HB2	1.93	0.68
1:B:196:TYR:CZ	1:B:244:PHE:HB3	2.27	0.68
1:A:18:LYS:O	1:A:20:LEU:N	2.26	0.68
1:B:397:THR:HG21	1:B:479:LEU:HD12	1.75	0.68
1:A:49:GLN:HE22	1:A:60:LEU:HB3	1.57	0.68
2:C:29:VAL:HG13	2:C:42:ARG:H	1.58	0.68
2:D:36:TYR:HD1	2:D:36:TYR:C	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASN:O	1:B:242:TYR:O	2.11	0.68
1:B:473:LYS:CG	1:B:474:PRO:CD	2.69	0.68
1:A:561:ARG:NH1	1:A:570:ASP:OD2	2.27	0.67
1:A:18:LYS:O	1:A:19:GLU:C	2.33	0.67
1:A:266:PHE:O	1:A:266:PHE:CD1	2.48	0.67
1:A:269:GLN:O	3:A:1632:SO4:O1	2.12	0.67
1:B:464:ILE:HG23	1:B:480:VAL:HG12	1.76	0.67
1:B:572:GLY:O	1:B:573:PHE:O	2.13	0.67
1:B:41:LEU:CB	1:B:43:ASP:OD1	2.41	0.67
1:A:25:LEU:O	1:A:29:TYR:CB	2.35	0.67
1:B:198:ASN:O	1:B:199:ALA:HB3	1.95	0.67
1:B:572:GLY:CA	1:B:573:PHE:O	2.43	0.67
1:A:69:ARG:HH12	1:A:341:ASP:HA	1.60	0.67
1:A:455:GLU:HB2	1:A:457:PHE:CE1	2.30	0.67
1:A:624:ILE:HG23	1:A:625:LYS:N	2.10	0.67
1:A:25:LEU:HD13	1:A:44:THR:HG22	1.76	0.67
1:A:69:ARG:NH1	1:A:341:ASP:HA	2.10	0.67
1:B:44:THR:HG22	1:B:45:LEU:H	1.59	0.67
1:B:80:ASN:C	1:B:80:ASN:HD22	1.98	0.67
1:B:253:MET:HG3	1:B:254:GLY:N	2.09	0.67
2:C:3:CYS:SG	2:C:101:CYS:O	2.53	0.67
2:C:136:ILE:HD11	2:C:152:VAL:HG22	1.72	0.67
2:D:20:ARG:HD2	2:D:107:TRP:CH2	2.30	0.67
1:A:455:GLU:HB2	1:A:457:PHE:HE1	1.60	0.67
1:B:126:THR:HB	1:B:127:PRO:CD	2.25	0.67
1:B:462:ARG:C	1:B:463:PHE:CG	2.69	0.67
1:B:498:PRO:CG	1:B:564:GLU:CG	2.54	0.66
1:B:615:SER:O	1:B:617:LYS:N	2.28	0.66
2:D:170:ARG:N	2:D:174:SER:O	2.26	0.66
1:B:573:PHE:HD1	1:B:575:LYS:HE2	1.60	0.66
1:B:80:ASN:ND2	1:B:80:ASN:O	2.28	0.66
1:A:291:THR:HG21	1:A:297:ASP:HB2	1.77	0.66
1:B:6:ILE:O	1:B:7:LYS:HB2	1.96	0.66
1:B:438:GLU:O	1:B:442:GLN:HG2	1.95	0.66
2:C:147:LEU:H	2:C:177:TRP:HH2	1.42	0.66
2:C:152:VAL:CG1	2:C:153:THR:N	2.59	0.66
2:D:146:CYS:HB3	2:D:177:TRP:CE2	2.30	0.66
2:C:29:VAL:CG1	2:C:42:ARG:N	2.59	0.66
1:A:81:TYR:HD2	1:A:86:ARG:NH1	1.93	0.66
1:A:543:PHE:CE1	1:A:552:TYR:HB2	2.31	0.66
1:B:357:LYS:HA	1:B:357:LYS:HZ3	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:CD2	1:B:244:PHE:HD1	2.11	0.66
1:A:581:TRP:CE2	2:C:188:PHE:HZ	2.14	0.65
2:D:7:HIS:O	2:D:10:GLN:N	2.27	0.65
1:A:194:VAL:HG13	1:A:243:GLY:HA3	1.78	0.65
1:B:291:THR:HG21	1:B:297:ASP:OD2	1.96	0.65
1:A:375:ALA:O	1:A:378:HIS:HB2	1.96	0.65
1:A:487:LEU:HD21	1:A:505:PHE:CD2	2.31	0.65
1:A:556:GLY:O	1:A:587:ASN:OD1	2.14	0.65
1:A:588:LEU:HD22	1:A:604:LYS:HB3	1.76	0.65
1:B:403:ARG:HH11	1:B:403:ARG:CG	2.03	0.65
2:C:131:THR:O	2:C:148:TRP:HB3	1.96	0.65
2:C:29:VAL:HG13	2:C:42:ARG:CA	2.27	0.65
2:D:45:TYR:OH	2:D:74:VAL:O	2.14	0.65
1:B:403:ARG:HG2	1:B:403:ARG:NH1	2.02	0.65
2:C:27:LYS:CE	2:C:62:PHE:CE1	2.80	0.65
1:A:447:ASP:O	1:A:492:ASP:O	2.13	0.65
1:B:41:LEU:CD1	1:B:43:ASP:OD2	2.43	0.65
1:B:290:THR:HG22	1:B:299:LYS:HB3	1.78	0.65
1:B:429:THR:CG2	1:B:430:PRO:HD3	1.87	0.65
1:B:480:VAL:O	1:B:482:THR:N	2.30	0.65
1:B:591:VAL:C	1:B:592:VAL:CG1	2.64	0.65
2:C:83:GLU:HB2	2:C:107:TRP:HB2	1.79	0.65
1:B:59:ASP:OD1	1:B:59:ASP:O	2.14	0.64
1:B:462:ARG:HB2	1:B:463:PHE:CE1	2.32	0.64
1:B:8:PHE:HZ	1:B:345:TRP:CE2	2.15	0.64
1:B:151:ASP:OD2	1:B:177:HIS:ND1	2.30	0.64
1:A:115:PHE:O	1:A:118:ALA:N	2.30	0.64
1:A:539:VAL:HG12	1:A:540:ASP:N	2.12	0.64
1:A:406:GLN:HE21	1:A:432:LEU:HD12	1.63	0.64
1:A:156:ASP:O	1:A:156:ASP:OD1	2.16	0.64
1:B:469:THR:HG21	1:B:471:ARG:HD3	1.79	0.64
1:B:487:LEU:HD12	1:B:488:PRO:CD	2.27	0.64
2:C:43:ILE:HB	2:C:65:THR:CG2	2.26	0.64
1:B:13:ALA:N	1:B:14:PRO:CD	2.61	0.64
2:D:131:THR:HG22	2:D:132:ARG:N	2.12	0.64
2:D:144:ASP:HB3	2:D:174:SER:HA	1.80	0.64
1:A:621:PHE:CE1	2:C:152:VAL:HG21	2.33	0.64
1:B:531:GLY:HA3	1:B:569:MET:HB2	1.78	0.64
1:A:121:VAL:HG13	1:A:404:LEU:HG	1.79	0.64
2:C:33:ASN:ND2	2:C:37:GLY:O	2.31	0.64
2:D:68:SER:OG	2:D:71:VAL:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:THR:HG23	1:A:232:THR:O	1.98	0.63
2:D:20:ARG:HD2	2:D:107:TRP:CZ3	2.33	0.63
2:D:147:LEU:N	2:D:177:TRP:CH2	2.66	0.63
2:D:17:VAL:HG12	2:D:55:GLY:HA3	1.79	0.63
1:A:431:THR:HG22	1:A:432:LEU:H	1.64	0.63
1:B:57:THR:HG23	1:B:60:LEU:HB2	1.78	0.63
2:C:86:ILE:HG12	2:C:104:ILE:HG23	1.80	0.63
1:B:484:TRP:HD1	1:B:514:TYR:CD2	2.16	0.63
2:C:140:ILE:HD13	2:C:145:GLU:HB3	1.81	0.63
1:A:26:ASN:HB2	1:A:31:CYS:N	2.11	0.63
1:B:413:GLN:HG2	1:B:418:ALA:HA	1.80	0.63
2:C:146:CYS:HB3	2:C:177:TRP:CZ2	2.34	0.63
1:A:446:PHE:CZ	1:A:629:LEU:HD22	2.33	0.63
1:A:585:PRO:HD2	1:A:588:LEU:HD21	1.81	0.63
2:C:19:ILE:O	2:C:85:LEU:HA	1.98	0.63
2:C:45:TYR:O	2:C:62:PHE:HA	1.97	0.63
2:C:85:LEU:HD21	2:C:118:LEU:HD21	1.81	0.63
1:A:89:LYS:O	1:A:89:LYS:HG2	1.97	0.62
1:B:480:VAL:HG23	1:B:481:ALA:N	2.13	0.62
1:B:548:ASN:ND2	1:B:552:TYR:HE1	1.97	0.62
2:C:146:CYS:HB3	2:C:177:TRP:CE2	2.34	0.62
1:A:101:GLY:HA3	1:A:143:ASN:ND2	2.15	0.62
1:B:20:LEU:HD22	1:B:69:ARG:NH1	2.15	0.62
1:B:164:HIS:CD2	1:B:177:HIS:HB2	2.33	0.62
1:B:493:ALA:HB3	1:B:506:PHE:CB	2.29	0.62
2:C:63:ILE:HG21	2:C:98:ILE:HD13	1.80	0.62
1:A:29:TYR:CZ	1:A:48:MET:HA	2.34	0.62
1:A:443:ASP:HA	1:A:625:LYS:NZ	2.14	0.62
1:A:26:ASN:HD22	1:A:26:ASN:H	1.45	0.62
2:C:60:ILE:HG13	2:C:96:MET:SD	2.40	0.62
2:C:168:ILE:HG22	2:C:169:LYS:H	1.63	0.62
1:A:533:PRO:HD2	1:A:535:ASP:OD2	2.00	0.62
2:C:74:VAL:HG11	2:C:98:ILE:HD12	1.82	0.62
2:C:130:ILE:HG22	2:C:130:ILE:O	2.00	0.62
1:A:38:LEU:HG	1:A:43:ASP:O	2.00	0.62
1:B:462:ARG:CB	1:B:463:PHE:CE1	2.83	0.62
1:A:166:PHE:CD2	1:A:172:VAL:HG13	2.35	0.61
1:B:24:TYR:O	1:B:24:TYR:CD1	2.53	0.61
1:B:100:ILE:HD11	1:B:141:MET:CE	2.30	0.61
1:B:291:THR:HG23	1:B:292:GLU:N	2.15	0.61
1:A:619:VAL:HG12	1:A:620:LYS:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:VAL:CG2	1:B:481:ALA:N	2.63	0.61
1:B:559:PHE:HB3	1:B:577:ILE:HG12	1.82	0.61
2:C:5:PRO:HD2	2:C:132:ARG:HH12	1.65	0.61
1:B:334:CYS:SG	1:B:346:CYS:HB3	2.41	0.61
2:C:27:LYS:HE2	2:C:62:PHE:CE1	2.35	0.61
2:C:29:VAL:HA	2:C:42:ARG:O	1.99	0.61
2:C:183:PRO:CD	2:C:184:PRO:HD3	2.30	0.61
1:A:539:VAL:CG1	1:A:540:ASP:N	2.63	0.61
2:D:131:THR:C	2:D:132:ARG:HG3	2.18	0.61
1:A:43:ASP:O	1:A:44:THR:CB	2.48	0.61
1:B:196:TYR:CE2	1:B:244:PHE:HB2	2.34	0.61
2:D:66:ALA:HB1	2:D:71:VAL:HG23	1.82	0.61
2:D:9:GLN:HG3	2:D:122:TYR:HD1	1.64	0.61
2:C:27:LYS:CB	2:C:44:GLN:CD	2.69	0.61
2:C:191:ILE:O	2:C:191:ILE:HG13	1.99	0.61
1:B:512:TRP:CE2	1:B:524:PRO:HB3	2.36	0.61
1:A:196:TYR:O	1:A:243:GLY:HA2	2.00	0.60
1:A:511:TYR:CE2	1:A:513:ILE:HD11	2.36	0.60
1:A:315:SER:CB	1:A:348:THR:HG21	2.31	0.60
2:C:34:ASP:CG	2:C:35:ILE:H	2.04	0.60
2:C:83:GLU:OE1	2:C:83:GLU:N	2.33	0.60
2:C:126:CYS:C	2:C:128:CYS:H	2.04	0.60
2:C:133:CYS:CB	2:C:149:MET:HB3	2.30	0.60
1:A:194:VAL:HG11	1:A:243:GLY:HA3	1.82	0.60
2:C:32:GLY:O	2:C:39:PRO:CA	2.47	0.60
1:B:214:GLU:OE2	1:B:234:TYR:OH	2.11	0.60
1:A:235:ASN:HD22	1:A:238:LYS:H	1.49	0.60
1:A:533:PRO:O	1:A:536:VAL:HG13	2.00	0.60
1:A:612:GLU:HG3	1:A:615:SER:H	1.66	0.60
1:B:38:LEU:HG	1:B:39:PHE:N	2.15	0.60
1:A:252:THR:OG1	1:A:260:GLN:O	2.20	0.60
1:A:286:ARG:HG3	1:A:286:ARG:NH1	2.16	0.60
1:B:522:GLY:O	1:B:525:LYS:HG3	2.02	0.60
2:C:44:GLN:HG3	2:C:64:TYR:CZ	2.37	0.60
2:D:20:ARG:HG3	2:D:51:LYS:HB2	1.83	0.60
1:B:314:ASN:ND2	1:B:358:TRP:H	1.95	0.60
2:D:49:GLN:NE2	2:D:52:MET:HB2	2.17	0.60
1:A:228:LEU:HB3	1:A:245:CYS:HB2	1.83	0.59
1:A:405:SER:C	1:A:432:LEU:CD1	2.70	0.59
1:A:550:LYS:NZ	2:C:190:ASP:OD2	2.34	0.59
1:B:166:PHE:CD2	1:B:172:VAL:HG13	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ARG:HH11	1:B:286:ARG:CG	2.02	0.59
2:C:27:LYS:HE3	2:C:62:PHE:CE1	2.36	0.59
1:A:38:LEU:C	1:A:41:LEU:O	2.41	0.59
1:A:99:ILE:HD11	1:A:115:PHE:HD2	1.66	0.59
1:A:543:PHE:CD2	1:A:544:ASN:O	2.55	0.59
1:A:556:GLY:C	1:A:587:ASN:OD1	2.41	0.59
1:B:13:ALA:N	1:B:14:PRO:HD3	2.16	0.59
1:B:452:ILE:O	1:B:452:ILE:CG2	2.50	0.59
1:B:604:LYS:HE3	1:B:605:GLY:N	2.16	0.59
1:B:610:LYS:O	1:B:619:VAL:HA	2.02	0.59
1:B:591:VAL:C	1:B:592:VAL:HG12	2.23	0.59
1:B:6:ILE:HA	1:B:338:GLY:O	2.02	0.59
2:C:99:THR:O	2:C:100:LEU:C	2.41	0.59
2:C:99:THR:O	2:C:102:ASP:N	2.31	0.59
1:A:36:CYS:SG	1:A:44:THR:HG21	2.43	0.59
1:B:495:TYR:HE1	1:B:506:PHE:CD2	2.20	0.59
1:A:36:CYS:CB	1:A:38:LEU:CD1	2.71	0.59
1:A:182:GLU:HA	1:A:182:GLU:OE1	2.02	0.59
1:A:314:ASN:C	1:A:314:ASN:HD22	2.06	0.59
1:B:469:THR:OG1	1:B:471:ARG:HD3	2.03	0.59
1:B:612:GLU:CB	1:B:618:SER:HB3	2.21	0.59
1:B:629:LEU:O	1:B:630:GLY:C	2.40	0.59
2:C:60:ILE:CA	2:C:94:GLY:HA2	2.20	0.59
1:A:60:LEU:HD21	1:A:63:ASN:HB3	1.84	0.59
1:B:486:GLU:HG3	1:B:519:LEU:HD22	1.84	0.59
1:B:592:VAL:O	1:B:592:VAL:HG23	2.01	0.59
1:B:622:GLY:HA2	2:D:137:PRO:CB	2.14	0.59
2:D:148:TRP:NE1	2:D:150:ASP:HB3	2.17	0.59
1:A:25:LEU:HD13	1:A:44:THR:CG2	2.33	0.58
1:A:72:ARG:CD	1:A:73:CYS:O	2.49	0.58
1:B:148:GLU:HA	1:B:148:GLU:OE1	2.01	0.58
2:C:32:GLY:C	2:C:39:PRO:HA	2.23	0.58
1:B:451:GLN:HG2	1:B:456:ILE:HG12	1.84	0.58
1:A:291:THR:HG23	1:A:293:ASP:H	1.66	0.58
1:A:588:LEU:HD13	1:A:602:PHE:HB3	1.85	0.58
1:B:196:TYR:CD1	1:B:244:PHE:HB2	2.39	0.58
2:C:12:PHE:HE1	2:C:53:PHE:HB3	1.67	0.58
2:C:53:PHE:CE2	2:C:118:LEU:HD13	2.38	0.58
2:C:91:GLU:HB2	2:C:95:LYS:HB2	1.84	0.58
1:B:49:GLN:HE22	1:B:60:LEU:HB3	1.69	0.58
2:C:152:VAL:HG13	2:C:153:THR:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:CD1	1:A:138:ALA:HB2	2.33	0.58
1:A:437:PRO:HB3	1:A:444:ILE:HD11	1.85	0.58
1:B:207:PRO:HB3	1:B:216:ASN:OD1	2.04	0.58
1:B:250:LEU:O	1:B:261:PRO:HG3	2.02	0.58
1:B:357:LYS:HZ3	1:B:357:LYS:CA	2.17	0.58
2:C:99:THR:O	2:C:101:CYS:N	2.37	0.58
1:A:535:ASP:O	1:A:537:GLN:N	2.35	0.58
1:A:447:ASP:HB3	1:A:491:ILE:O	2.04	0.58
1:B:487:LEU:HD21	1:B:505:PHE:CD1	2.38	0.58
1:B:566:LYS:C	1:B:568:LYS:H	2.06	0.58
2:C:168:ILE:HG22	2:C:169:LYS:N	2.18	0.58
1:B:445:VAL:O	1:B:445:VAL:HG13	2.04	0.58
2:D:140:ILE:O	2:D:140:ILE:CG1	2.49	0.58
1:A:97:TYR:CZ	1:A:132:ARG:HB2	2.39	0.57
1:A:565:VAL:HG23	1:A:566:LYS:HG3	1.85	0.57
1:B:196:TYR:HH	1:B:251:PHE:HE1	1.33	0.57
2:D:164:PHE:HB3	2:D:179:ARG:HG3	1.85	0.57
1:A:313:GLY:HA2	1:A:358:TRP:CZ2	2.38	0.57
1:A:458:PHE:O	1:A:464:ILE:HA	2.04	0.57
1:A:624:ILE:CG2	1:A:625:LYS:N	2.67	0.57
1:B:562:TYR:OH	1:B:564:GLU:OE1	2.13	0.57
2:D:20:ARG:O	2:D:50:ILE:HG12	2.04	0.57
1:A:57:THR:OG1	1:A:60:LEU:HB2	2.04	0.57
2:D:149:MET:HB3	2:D:152:VAL:HG11	1.86	0.57
2:C:121:ARG:HG2	2:C:121:ARG:HH11	1.68	0.57
1:A:20:LEU:CD2	1:A:21:ALA:N	2.62	0.57
1:A:511:TYR:HE2	1:A:513:ILE:HD11	1.70	0.57
1:A:548:ASN:ND2	1:A:550:LYS:HB2	2.20	0.57
1:A:617:LYS:NZ	2:C:170:ARG:HG3	2.19	0.57
1:B:196:TYR:CD2	1:B:244:PHE:CG	2.75	0.57
2:C:7:HIS:CE1	2:C:161:GLN:O	2.55	0.57
2:C:20:ARG:NH1	2:C:107:TRP:CE2	2.73	0.57
2:C:91:GLU:HB2	2:C:95:LYS:CB	2.34	0.57
2:C:7:HIS:O	2:C:9:GLN:N	2.38	0.57
2:D:56:PRO:C	2:D:58:LYS:H	2.08	0.57
1:A:34:GLU:OE2	1:A:37:ASN:ND2	2.38	0.57
1:A:474:PRO:HG3	1:A:629:LEU:HD12	1.86	0.57
1:B:532:LEU:HB2	1:B:533:PRO:HD2	1.87	0.57
2:D:21:ALA:HB1	2:D:47:ILE:HB	1.86	0.57
2:C:22:LYS:HG2	2:C:23:ALA:N	2.20	0.57
2:D:9:GLN:HG3	2:D:122:TYR:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:THR:N	1:A:470:PRO:CD	2.68	0.57
1:B:431:THR:O	1:B:432:LEU:C	2.41	0.57
1:B:469:THR:O	1:B:472:ASP:OD1	2.23	0.57
2:D:91:GLU:O	2:D:95:LYS:HB2	2.05	0.57
1:A:43:ASP:O	1:A:44:THR:OG1	2.22	0.56
1:A:232:THR:O	1:A:232:THR:CG2	2.53	0.56
1:B:61:ASP:O	1:B:65:ILE:N	2.26	0.56
1:B:452:ILE:O	1:B:452:ILE:HG23	2.04	0.56
2:C:19:ILE:HB	2:C:51:LYS:O	2.05	0.56
2:D:17:VAL:HG13	2:D:55:GLY:HA3	1.86	0.56
1:B:194:VAL:HG13	1:B:243:GLY:HA3	1.84	0.56
1:A:545:TRP:CD1	1:A:552:TYR:CE1	2.94	0.56
1:B:57:THR:HG21	1:B:60:LEU:HB2	1.86	0.56
2:C:32:GLY:HA3	2:C:40:ILE:HB	1.88	0.56
1:B:25:LEU:HD22	1:B:44:THR:CG2	2.36	0.56
1:B:235:ASN:C	1:B:235:ASN:HD22	2.09	0.56
1:A:446:PHE:HZ	1:A:629:LEU:HD22	1.71	0.56
1:A:545:TRP:HZ3	1:A:547:LYS:CE	2.09	0.56
1:A:580:ALA:CB	2:C:188:PHE:CD2	2.88	0.56
1:A:59:ASP:OD1	1:A:59:ASP:N	2.29	0.56
1:A:276:CYS:HB3	1:A:287:TRP:O	2.05	0.56
1:A:443:ASP:HA	1:A:625:LYS:HZ3	1.71	0.56
1:B:147:TRP:CD1	1:B:147:TRP:N	2.72	0.56
1:B:196:TYR:HE1	1:B:251:PHE:HZ	1.46	0.56
2:C:7:HIS:HE1	2:C:162:ALA:HA	1.65	0.56
1:A:311:VAL:O	1:A:360:PHE:HB2	2.06	0.55
1:A:575:LYS:HE3	1:A:579:ASP:HB2	1.88	0.55
2:C:91:GLU:N	2:C:95:LYS:O	2.31	0.55
1:A:527:LEU:O	1:A:530:LEU:HB3	2.07	0.55
1:B:8:PHE:HZ	1:B:345:TRP:CZ2	2.24	0.55
2:C:18:VAL:HG22	2:C:87:ALA:CB	2.37	0.55
1:A:403:ARG:HG2	1:A:403:ARG:NH1	2.09	0.55
1:B:235:ASN:HD22	1:B:238:LYS:H	1.53	0.55
1:A:481:ALA:HA	1:A:484:TRP:O	2.07	0.55
2:D:78:VAL:HG12	2:D:79:GLY:H	1.72	0.55
1:A:115:PHE:CZ	1:A:142:ILE:HG21	2.41	0.55
1:B:133:ILE:O	1:B:133:ILE:CG1	2.51	0.55
2:D:12:PHE:CD1	2:D:12:PHE:C	2.79	0.55
2:C:99:THR:C	2:C:101:CYS:N	2.58	0.55
1:A:527:LEU:HB2	1:A:536:VAL:CB	2.36	0.55
1:A:266:PHE:CD1	1:A:266:PHE:C	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:CD1	1:B:196:TYR:N	2.75	0.55
1:B:266:PHE:CE1	1:B:273:TYR:HB2	2.42	0.55
1:B:506:PHE:CD1	1:B:527:LEU:HD11	2.41	0.55
1:A:519:LEU:H	1:A:519:LEU:HD23	1.72	0.55
1:A:621:PHE:CE1	2:C:136:ILE:HD13	2.38	0.55
1:B:439:ILE:HA	1:B:444:ILE:HD12	1.89	0.55
1:A:405:SER:O	1:A:406:GLN:C	2.44	0.54
1:A:588:LEU:CD1	1:A:602:PHE:HB3	2.37	0.54
1:B:443:ASP:HA	1:B:625:LYS:HE3	1.89	0.54
1:B:497:ALA:HB1	1:B:500:GLU:O	2.03	0.54
2:D:112:THR:HA	2:D:115:LYS:HG3	1.89	0.54
1:A:18:LYS:O	1:A:21:ALA:N	2.40	0.54
2:D:71:VAL:O	2:D:72:CYS:HB2	2.07	0.54
1:A:544:ASN:HA	1:A:550:LYS:O	2.07	0.54
1:A:606:ALA:O	1:A:624:ILE:HG22	2.08	0.54
1:B:387:ASP:OD1	1:B:436:THR:HG21	2.07	0.54
2:C:23:ALA:O	2:C:78:VAL:HG13	2.07	0.54
2:C:25:SER:O	2:C:46:GLU:HB3	2.08	0.54
2:C:140:ILE:HD11	2:C:147:LEU:N	2.23	0.54
1:B:389:GLY:HA2	1:B:479:LEU:HD21	1.90	0.54
2:D:149:MET:HB3	2:D:152:VAL:HG12	1.78	0.54
1:A:439:ILE:CG2	1:A:440:CYS:N	2.66	0.54
2:C:183:PRO:HD2	2:C:184:PRO:HD3	1.88	0.54
1:A:440:CYS:O	1:A:441:LYS:C	2.45	0.54
1:B:100:ILE:HD11	1:B:141:MET:HE1	1.89	0.54
2:D:163:LYS:HB2	2:D:164:PHE:HD1	1.72	0.54
1:B:41:LEU:HB2	1:B:43:ASP:CG	2.28	0.54
1:A:25:LEU:HD23	1:A:29:TYR:CD2	2.43	0.54
1:A:84:PHE:CG	1:A:84:PHE:O	2.59	0.54
1:A:232:THR:O	1:A:233:THR:CG2	2.56	0.54
1:A:559:PHE:HZ	1:A:575:LYS:HE2	1.72	0.54
1:B:16:THR:HB	1:B:19:GLU:HB3	1.90	0.54
1:B:286:ARG:NH1	1:B:286:ARG:CG	2.67	0.54
1:B:527:LEU:HD13	1:B:537:GLN:O	2.07	0.54
2:D:154:GLU:O	2:D:155:LYS:CB	2.54	0.54
1:B:495:TYR:CD2	1:B:551:THR:HG21	2.43	0.54
2:C:34:ASP:OD1	2:C:35:ILE:HG13	2.08	0.54
2:D:54:LYS:O	2:D:54:LYS:HG3	2.07	0.54
1:A:458:PHE:CE2	1:A:629:LEU:HB2	2.43	0.54
2:C:159:GLY:O	2:C:160:HIS:C	2.46	0.54
2:C:79:GLY:O	2:C:80:GLY:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:CYS:O	2:D:127:GLU:C	2.45	0.53
2:D:187:GLU:O	2:D:187:GLU:HG3	2.08	0.53
1:A:49:GLN:NE2	1:A:60:LEU:HB3	2.23	0.53
1:B:532:LEU:C	1:B:532:LEU:HD23	2.28	0.53
1:B:581:TRP:HA	1:B:616:LEU:CD1	2.37	0.53
1:B:593:ASP:OD2	1:B:601:TYR:CE1	2.62	0.53
2:C:20:ARG:NH1	2:C:107:TRP:CZ2	2.75	0.53
1:B:469:THR:HG23	1:B:471:ARG:HD3	1.89	0.53
1:A:406:GLN:N	1:A:432:LEU:HD12	2.03	0.53
2:C:140:ILE:CD1	2:C:147:LEU:N	2.72	0.53
1:B:429:THR:HG22	1:B:430:PRO:CD	1.94	0.53
1:B:458:PHE:HB2	1:B:465:TRP:HB2	1.90	0.53
2:D:12:PHE:CD1	2:D:12:PHE:O	2.61	0.53
2:D:63:ILE:HG12	2:D:96:MET:HG2	1.90	0.53
2:D:153:THR:HG22	2:D:154:GLU:N	2.23	0.53
1:A:584:ILE:HD12	1:A:584:ILE:H	1.73	0.53
1:B:89:LYS:HD2	1:B:415:LEU:O	2.09	0.53
1:B:558:LYS:HD3	1:B:574:PRO:HB3	1.90	0.53
2:D:111:SER:C	2:D:115:LYS:HG2	2.29	0.53
2:D:164:PHE:HD1	2:D:164:PHE:H	1.57	0.53
1:A:544:ASN:H	1:A:544:ASN:HD22	1.55	0.53
1:B:232:THR:O	1:B:232:THR:CG2	2.57	0.53
1:A:71:PRO:HG2	1:A:71:PRO:O	2.09	0.53
1:B:291:THR:CG2	1:B:292:GLU:N	2.72	0.53
1:A:81:TYR:HD2	1:A:86:ARG:NH2	2.05	0.53
1:A:207:PRO:HA	1:A:215:TYR:O	2.08	0.53
1:A:248:GLU:HB2	1:A:262:CYS:SG	2.49	0.53
1:A:406:GLN:HA	1:A:432:LEU:HD12	0.61	0.53
1:B:28:PHE:CE1	1:B:72:ARG:NE	2.76	0.53
1:B:44:THR:HG22	1:B:45:LEU:N	2.24	0.53
1:B:194:VAL:HG11	1:B:243:GLY:CA	2.34	0.53
2:D:7:HIS:NE2	2:D:162:ALA:HA	2.24	0.53
1:A:39:PHE:CD2	1:A:40:VAL:N	2.77	0.53
1:B:550:LYS:NZ	2:D:190:ASP:OD1	2.42	0.53
2:D:37:GLY:O	2:D:39:PRO:HD3	2.09	0.53
1:B:41:LEU:CB	1:B:43:ASP:CG	2.77	0.52
2:D:91:GLU:H	2:D:96:MET:HA	1.73	0.52
1:B:3:SER:CB	1:B:4:PRO:HD3	2.27	0.52
1:B:146:ARG:O	1:B:147:TRP:C	2.45	0.52
1:B:608:TYR:HB3	1:B:624:ILE:HG22	1.91	0.52
1:A:185:THR:O	1:A:367:SER:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ARG:CG	1:B:403:ARG:NH1	2.67	0.52
2:C:22:LYS:O	2:C:47:ILE:HA	2.09	0.52
1:A:60:LEU:HD23	1:A:64:THR:HB	1.90	0.52
1:B:325:THR:HA	1:B:329:ASN:O	2.09	0.52
1:A:585:PRO:HD2	1:A:588:LEU:CD1	2.39	0.52
1:B:38:LEU:N	1:B:43:ASP:HB2	2.25	0.52
1:B:57:THR:HG1	1:B:60:LEU:HB2	1.74	0.52
1:B:67:THR:O	1:B:70:LYS:HG2	2.09	0.52
2:C:25:SER:O	2:C:46:GLU:CB	2.58	0.52
2:D:47:ILE:HG21	2:D:63:ILE:HD12	1.92	0.52
2:D:77:ASP:OD2	2:D:84:TYR:OH	2.28	0.52
1:A:152:GLY:O	1:A:154:PRO:HD3	2.09	0.52
1:A:548:ASN:HD21	1:A:550:LYS:HB2	1.75	0.52
1:B:512:TRP:HB3	1:B:514:TYR:HE1	1.75	0.52
2:C:85:LEU:HD13	2:C:107:TRP:HZ3	1.74	0.52
1:A:618:SER:OG	1:A:619:VAL:N	2.43	0.52
1:B:57:THR:OG1	1:B:60:LEU:N	2.43	0.52
1:B:468:VAL:HG13	1:B:469:THR:HG22	1.92	0.52
1:B:612:GLU:HB2	1:B:618:SER:CB	2.22	0.52
1:A:405:SER:O	1:A:408:ASP:N	2.43	0.52
1:A:552:TYR:CE2	2:C:188:PHE:CD1	2.97	0.52
1:A:556:GLY:HA2	1:A:587:ASN:OD1	2.09	0.52
1:B:429:THR:CG2	1:B:430:PRO:N	2.61	0.52
2:C:139:TYR:N	2:C:139:TYR:CD1	2.77	0.52
2:D:3:CYS:SG	2:D:101:CYS:N	2.82	0.52
2:D:164:PHE:CD1	2:D:164:PHE:N	2.77	0.52
1:B:506:PHE:HE1	1:B:527:LEU:HD11	1.69	0.52
2:D:113:THR:CG2	2:D:164:PHE:HA	2.40	0.52
1:B:196:TYR:CG	1:B:244:PHE:CD1	2.94	0.52
2:C:29:VAL:CG1	2:C:42:ARG:C	2.63	0.52
2:C:60:ILE:HG21	2:C:96:MET:SD	2.50	0.52
2:C:74:VAL:CG1	2:C:98:ILE:HD12	2.38	0.52
1:A:29:TYR:CE2	1:A:48:MET:HG2	2.45	0.51
1:A:440:CYS:O	1:A:442:GLN:N	2.43	0.51
1:A:581:TRP:NE1	2:C:188:PHE:HZ	2.07	0.51
1:B:179:ASP:C	1:B:179:ASP:OD1	2.48	0.51
1:B:467:THR:HB	1:B:474:PRO:HA	1.92	0.51
1:A:39:PHE:CG	1:A:40:VAL:N	2.78	0.51
1:A:87:LYS:O	1:A:87:LYS:HD3	2.10	0.51
1:A:561:ARG:NH1	1:A:570:ASP:CG	2.64	0.51
2:C:51:LYS:HG2	2:C:52:MET:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:LEU:HD22	2:D:114:GLN:OE1	2.09	0.51
1:A:190:GLN:HE22	1:A:308:MET:H	1.57	0.51
1:A:461:ASP:O	1:A:489:GLU:O	2.28	0.51
1:B:7:LYS:O	1:B:8:PHE:CD2	2.63	0.51
1:B:579:ASP:O	2:D:185:LYS:HD3	2.11	0.51
2:C:26:GLU:O	2:C:26:GLU:HG3	2.11	0.51
2:C:33:ASN:O	2:C:40:ILE:HG13	2.10	0.51
2:C:73:GLY:O	2:C:100:LEU:HG	2.10	0.51
1:B:149:HIS:NE2	1:B:151:ASP:OD2	2.43	0.51
1:B:196:TYR:HD2	1:B:244:PHE:CD1	2.18	0.51
1:B:566:LYS:O	1:B:568:LYS:N	2.43	0.51
2:C:27:LYS:HB2	2:C:44:GLN:CB	2.40	0.51
2:D:60:ILE:HG21	2:D:96:MET:CE	2.36	0.51
1:A:86:ARG:O	1:A:88:PRO:HD3	2.10	0.51
1:A:471:ARG:HG3	1:A:472:ASP:N	2.24	0.51
1:B:123:SER:O	1:B:124:ASP:C	2.48	0.51
1:B:194:VAL:HG23	1:B:204:CYS:SG	2.50	0.51
1:B:332:GLU:HG2	1:B:333:SER:OG	2.09	0.51
2:C:17:VAL:HG12	2:C:90:ALA:HB2	1.92	0.51
2:D:18:VAL:HB	2:D:53:PHE:HB2	1.93	0.51
2:D:56:PRO:O	2:D:58:LYS:N	2.44	0.51
1:A:391:LEU:HD22	1:A:402:PHE:HZ	1.76	0.51
1:B:170:THR:HG22	1:B:171:GLY:H	1.75	0.51
1:B:511:TYR:CE2	1:B:523:TYR:CD2	2.97	0.51
2:D:108:ASP:O	2:D:109:THR:OG1	2.09	0.51
1:A:84:PHE:CB	1:A:167:ALA:HB3	2.38	0.51
2:C:53:PHE:HD2	2:C:118:LEU:HB3	1.74	0.51
1:A:147:TRP:CD1	1:A:147:TRP:N	2.78	0.51
1:A:314:ASN:HD21	1:A:358:TRP:H	1.58	0.51
1:A:337:ALA:O	1:A:345:TRP:NE1	2.40	0.51
1:A:582:ASN:OD1	2:C:170:ARG:NH2	2.43	0.51
1:B:72:ARG:NH2	1:B:77:ASP:OD1	2.35	0.51
1:B:82:ASN:OD1	1:B:83:PHE:N	2.44	0.51
2:C:68:SER:O	2:C:71:VAL:HG23	2.11	0.51
1:A:99:ILE:CD1	1:A:115:PHE:HD2	2.24	0.51
1:B:509:ASN:O	1:B:509:ASN:ND2	2.43	0.51
2:C:20:ARG:HB3	2:C:85:LEU:HD12	1.93	0.51
2:C:85:LEU:HD21	2:C:118:LEU:CD2	2.40	0.51
1:A:472:ASP:O	1:A:630:GLY:HA3	2.11	0.50
1:B:9:PRO:CD	1:B:352:TYR:OH	2.58	0.50
1:B:277:THR:O	1:B:287:TRP:CD1	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:O	1:B:434:PRO:HD2	2.12	0.50
1:B:480:VAL:C	1:B:482:THR:N	2.65	0.50
1:B:592:VAL:O	1:B:592:VAL:HG22	2.10	0.50
1:A:202:GLU:OE1	1:A:202:GLU:N	2.43	0.50
2:C:147:LEU:O	2:C:177:TRP:HZ2	1.92	0.50
2:D:123:GLN:O	2:D:126:CYS:N	2.44	0.50
1:A:1:ALA:C	1:A:3:SER:H	2.15	0.50
2:D:152:VAL:HG22	2:D:152:VAL:O	2.11	0.50
1:A:10:GLY:O	1:B:296:ARG:HD2	2.11	0.50
1:A:146:ARG:O	1:A:147:TRP:C	2.48	0.50
1:A:484:TRP:HB3	1:A:514:TYR:CZ	2.47	0.50
1:A:26:ASN:CB	1:A:31:CYS:H	2.18	0.50
1:A:545:TRP:HE3	1:A:548:ASN:H	1.59	0.50
1:B:495:TYR:N	1:B:495:TYR:CD1	2.80	0.50
1:A:391:LEU:HD22	1:A:402:PHE:CZ	2.47	0.50
1:A:585:PRO:HB2	1:A:588:LEU:HD21	1.94	0.50
1:B:5:ILE:CD1	1:B:327:LEU:CD1	2.81	0.50
2:C:12:PHE:CE1	2:C:53:PHE:HB3	2.46	0.50
1:A:431:THR:HG22	1:A:432:LEU:N	2.24	0.50
1:A:584:ILE:HG23	1:A:588:LEU:HD11	1.93	0.50
1:B:194:VAL:CG1	1:B:243:GLY:CA	2.83	0.50
1:B:386:GLN:O	1:B:388:PRO:HD3	2.12	0.50
2:D:163:LYS:HB2	2:D:164:PHE:CD1	2.46	0.50
1:B:38:LEU:HD22	1:B:45:LEU:HB2	1.93	0.50
1:B:624:ILE:HA	1:B:628:TRP:HD1	1.76	0.50
2:C:33:ASN:N	2:C:40:ILE:H	2.10	0.50
2:C:41:LYS:O	2:C:67:PRO:CG	2.47	0.50
2:C:165:PHE:CE2	2:C:177:TRP:HB3	2.47	0.50
2:D:78:VAL:HG12	2:D:79:GLY:N	2.26	0.50
1:A:195:LYS:HG3	1:A:251:PHE:HE2	1.76	0.49
1:A:305:GLU:HG2	1:A:306:THR:N	2.27	0.49
1:A:539:VAL:CG1	1:A:540:ASP:H	2.25	0.49
1:A:15:LYS:HD3	1:A:24:TYR:HE2	1.76	0.49
1:A:137:GLU:HA	1:A:141:MET:HE2	1.94	0.49
1:A:585:PRO:CD	1:A:588:LEU:HD21	2.42	0.49
1:B:73:CYS:SG	1:B:374:HIS:NE2	2.85	0.49
1:B:196:TYR:HE1	1:B:251:PHE:CE1	1.99	0.49
1:B:231:SER:OG	1:B:233:THR:O	2.30	0.49
1:A:47:LYS:NZ	1:A:78:VAL:HG11	2.27	0.49
1:B:548:ASN:ND2	1:B:552:TYR:CE1	2.80	0.49
2:C:80:GLY:O	2:C:81:LYS:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:HD12	1:B:464:ILE:O	2.11	0.49
2:C:27:LYS:CE	2:C:62:PHE:CZ	2.94	0.49
2:C:44:GLN:HG3	2:C:64:TYR:CE2	2.47	0.49
2:C:88:GLY:HA3	2:C:97:HIS:O	2.13	0.49
1:A:20:LEU:O	1:A:23:GLN:N	2.45	0.49
1:A:552:TYR:HE2	2:C:188:PHE:CD1	2.30	0.49
1:B:41:LEU:O	1:B:42:LYS:CB	2.59	0.49
1:B:64:THR:HG23	1:B:65:ILE:N	2.27	0.49
1:B:194:VAL:O	1:B:200:ASP:O	2.30	0.49
1:B:278:THR:O	1:B:279:GLU:C	2.51	0.49
1:B:314:ASN:HD22	1:B:314:ASN:H	1.59	0.49
2:D:20:ARG:HG2	2:D:53:PHE:HE2	1.78	0.49
1:A:313:GLY:HA2	1:A:358:TRP:CH2	2.48	0.49
1:A:510:GLU:HA	1:A:526:PRO:HA	1.94	0.49
1:A:617:LYS:O	1:A:618:SER:HB2	2.13	0.49
1:B:148:GLU:H	1:B:154:PRO:HA	1.77	0.49
1:B:559:PHE:CE2	2:D:188:PHE:CE2	3.00	0.49
1:A:373:ALA:HB1	1:A:391:LEU:HD21	1.94	0.49
1:B:97:TYR:HA	1:B:140:ILE:O	2.13	0.49
2:C:183:PRO:N	2:C:184:PRO:CD	2.75	0.49
2:D:9:GLN:OE1	2:D:166:ALA:HA	2.13	0.49
1:A:406:GLN:NE2	1:A:432:LEU:HD12	2.28	0.49
1:A:409:ILE:HG12	1:A:432:LEU:CD1	2.01	0.49
1:B:35:SER:O	1:B:36:CYS:SG	2.71	0.49
1:B:530:LEU:O	1:B:532:LEU:HD22	2.12	0.49
1:B:576:LEU:O	1:B:579:ASP:HB3	2.12	0.49
1:A:167:ALA:HB1	1:A:168:PRO:HD2	1.95	0.49
1:A:512:TRP:CD1	1:A:524:PRO:HG3	2.47	0.49
1:B:531:GLY:HA3	1:B:569:MET:CB	2.43	0.49
2:C:51:LYS:HG2	2:C:52:MET:N	2.28	0.49
1:B:25:LEU:HD22	1:B:44:THR:HG22	1.94	0.48
1:B:28:PHE:CZ	1:B:72:ARG:HD3	2.48	0.48
1:B:198:ASN:O	1:B:199:ALA:CB	2.61	0.48
1:B:622:GLY:CA	2:D:137:PRO:CB	2.81	0.48
1:B:168:PRO:HG3	1:B:379:ALA:O	2.13	0.48
1:A:545:TRP:CZ3	1:A:547:LYS:CE	2.90	0.48
2:D:78:VAL:O	2:D:81:LYS:HG2	2.13	0.48
1:A:81:TYR:CD2	1:A:86:ARG:NH1	2.77	0.48
1:A:273:TYR:CE2	1:A:277:THR:HG21	2.49	0.48
1:B:8:PHE:CZ	1:B:345:TRP:CE2	2.99	0.48
1:B:61:ASP:O	1:B:62:GLN:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:VAL:O	2:C:53:PHE:N	2.39	0.48
1:A:403:ARG:NH1	1:A:403:ARG:CG	2.76	0.48
1:B:194:VAL:CG1	1:B:195:LYS:N	2.76	0.48
2:C:125:GLY:O	2:C:128:CYS:HB2	2.13	0.48
2:C:189:LEU:HG	2:C:190:ASP:N	2.28	0.48
1:B:405:SER:HA	1:B:434:PRO:HD2	1.95	0.48
1:B:462:ARG:HB3	1:B:463:PHE:CE1	2.48	0.48
1:A:532:LEU:HD21	1:A:553:ILE:HD12	1.96	0.48
1:B:106:LEU:HD22	1:B:110:THR:HG21	1.96	0.48
1:B:532:LEU:HD23	1:B:532:LEU:O	2.13	0.48
1:B:580:ALA:HB2	2:D:188:PHE:CE1	2.48	0.48
1:A:137:GLU:CD	1:A:141:MET:HE2	2.34	0.48
1:A:208:PHE:CD1	1:A:231:SER:HB3	2.47	0.48
2:C:136:ILE:CD1	2:C:152:VAL:HG23	2.28	0.48
2:C:158:ASN:OD1	2:C:163:LYS:HE2	2.13	0.48
1:B:64:THR:CG2	1:B:65:ILE:N	2.77	0.47
1:B:149:HIS:O	1:B:149:HIS:CD2	2.67	0.47
1:B:195:LYS:HB3	1:B:195:LYS:HE2	1.51	0.47
1:B:253:MET:CE	1:B:254:GLY:H	2.27	0.47
1:B:544:ASN:HA	1:B:550:LYS:O	2.14	0.47
2:D:182:ALA:HB3	2:D:185:LYS:CE	2.34	0.47
1:A:87:LYS:O	1:A:87:LYS:CG	2.61	0.47
1:A:118:ALA:O	1:A:121:VAL:HB	2.14	0.47
1:B:38:LEU:HD13	1:B:44:THR:O	2.14	0.47
2:C:86:ILE:HG22	2:C:98:ILE:HG22	1.96	0.47
1:B:17:ASP:CG	1:B:65:ILE:HD13	2.35	0.47
2:C:74:VAL:O	2:C:74:VAL:HG12	2.14	0.47
2:D:68:SER:H	2:D:71:VAL:CG2	2.27	0.47
1:A:409:ILE:HD11	1:A:432:LEU:HD22	1.84	0.47
1:B:60:LEU:HD13	1:B:64:THR:H	1.79	0.47
1:B:223:ARG:NH1	1:B:244:PHE:HE2	2.13	0.47
1:A:42:LYS:H	1:A:42:LYS:CE	2.28	0.47
1:A:223:ARG:HE	1:A:223:ARG:HB3	1.48	0.47
1:B:469:THR:OG1	1:B:471:ARG:CD	2.62	0.47
1:B:561:ARG:CZ	2:D:188:PHE:HB2	2.45	0.47
2:C:78:VAL:O	2:C:80:GLY:N	2.47	0.47
2:D:113:THR:HG22	2:D:113:THR:O	2.14	0.47
2:D:147:LEU:O	2:D:177:TRP:CZ2	2.67	0.47
1:A:84:PHE:CD1	1:A:84:PHE:O	2.67	0.47
1:A:235:ASN:ND2	1:A:238:LYS:H	2.13	0.47
1:A:439:ILE:HG22	1:A:440:CYS:H	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:SER:CB	2:C:177:TRP:HZ3	2.28	0.47
1:A:621:PHE:CB	2:C:147:LEU:HD21	2.42	0.47
1:B:16:THR:CB	1:B:19:GLU:HB3	2.45	0.47
2:D:7:HIS:CE1	2:D:162:ALA:HA	2.50	0.47
1:A:527:LEU:HB2	1:A:536:VAL:HB	1.96	0.47
1:B:196:TYR:CG	1:B:244:PHE:HD1	2.32	0.47
1:B:458:PHE:CE2	1:B:629:LEU:HD21	2.50	0.47
1:B:596:GLY:C	1:B:598:GLY:N	2.68	0.47
1:B:613:ASN:O	1:B:614:GLN:C	2.53	0.47
2:C:86:ILE:HD13	2:C:104:ILE:HG21	1.96	0.47
2:C:114:GLN:O	2:C:117:SER:OG	2.33	0.47
1:A:26:ASN:CB	1:A:31:CYS:C	2.83	0.47
1:A:80:ASN:O	1:A:80:ASN:ND2	2.48	0.47
1:A:314:ASN:C	1:A:314:ASN:ND2	2.68	0.47
1:A:624:ILE:CG2	1:A:625:LYS:H	2.27	0.47
1:B:590:ALA:C	1:B:591:VAL:HG12	2.34	0.47
2:C:19:ILE:HG22	2:C:52:MET:HA	1.97	0.47
2:C:157:ILE:H	2:C:157:ILE:HG13	1.50	0.47
2:D:21:ALA:HB2	2:D:47:ILE:HD13	1.97	0.47
2:D:142:SER:N	2:D:145:GLU:OE2	2.35	0.47
1:A:26:ASN:CB	1:A:31:CYS:N	2.78	0.47
1:A:559:PHE:CZ	2:C:188:PHE:CD2	3.03	0.47
1:B:539:VAL:HG13	1:B:553:ILE:HG23	1.97	0.47
2:C:86:ILE:CG2	2:C:98:ILE:HG22	2.44	0.47
1:A:545:TRP:HB3	1:A:548:ASN:H	1.80	0.47
2:C:102:ASP:OD1	2:C:103:PHE:N	2.48	0.47
1:A:45:LEU:CD2	1:A:59:ASP:CA	2.75	0.46
1:A:581:TRP:CE2	2:C:188:PHE:CZ	3.00	0.46
1:B:495:TYR:CE1	1:B:506:PHE:CD2	3.02	0.46
1:B:570:ASP:OD2	2:D:190:ASP:OD2	2.33	0.46
2:C:5:PRO:O	2:C:6:VAL:HG13	2.16	0.46
2:D:63:ILE:HG12	2:D:96:MET:CG	2.46	0.46
1:A:589:ASP:N	1:A:603:PHE:O	2.49	0.46
1:B:486:GLU:CG	1:B:514:TYR:OH	2.63	0.46
1:A:408:ASP:O	1:A:409:ILE:C	2.51	0.46
1:A:503:ALA:HB1	1:A:505:PHE:HE1	1.80	0.46
1:A:629:LEU:O	1:A:630:GLY:C	2.53	0.46
2:C:18:VAL:HG22	2:C:87:ALA:HB1	1.96	0.46
2:C:78:VAL:HG12	2:C:79:GLY:H	1.81	0.46
2:C:84:TYR:HB3	2:C:86:ILE:HG13	1.96	0.46
2:D:19:ILE:HD12	2:D:21:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LEU:CB	1:A:536:VAL:HG12	2.40	0.46
2:C:53:PHE:CE1	2:C:85:LEU:HD11	2.50	0.46
1:B:437:PRO:HD2	1:B:463:PHE:CD1	2.51	0.46
2:C:80:GLY:O	2:C:81:LYS:HB2	2.16	0.46
2:D:123:GLN:O	2:D:124:MET:C	2.54	0.46
1:A:29:TYR:CZ	1:A:48:MET:HG2	2.50	0.46
1:A:117:ARG:NH2	1:A:369:PHE:HB2	2.31	0.46
1:A:406:GLN:O	1:A:407:ASP:C	2.54	0.46
1:A:446:PHE:CE2	1:A:629:LEU:HD22	2.51	0.46
1:B:57:THR:OG1	1:B:60:LEU:CB	2.62	0.46
1:B:495:TYR:CE2	1:B:504:VAL:HG11	2.51	0.46
1:B:561:ARG:O	1:B:569:MET:HG3	2.15	0.46
2:C:69:SER:CA	2:C:73:GLY:HA3	2.39	0.46
1:A:42:LYS:HZ2	1:A:43:ASP:N	2.13	0.46
1:A:484:TRP:HB3	1:A:514:TYR:CE2	2.49	0.46
1:A:512:TRP:NE1	1:A:524:PRO:CG	2.76	0.46
1:B:206:PHE:HB3	1:B:216:ASN:HA	1.97	0.46
2:C:19:ILE:HG13	2:C:49:GLN:HG3	1.97	0.46
2:C:101:CYS:O	2:C:101:CYS:SG	2.74	0.46
1:A:18:LYS:NZ	1:A:61:ASP:OD1	2.46	0.46
1:A:179:ASP:HB3	1:A:182:GLU:HG2	1.98	0.46
1:B:33:LYS:HE3	1:B:33:LYS:CA	2.44	0.46
1:B:41:LEU:CB	1:B:43:ASP:OD2	2.63	0.46
2:C:135:MET:SD	2:C:135:MET:N	2.88	0.46
1:A:406:GLN:NE2	1:A:432:LEU:HG	2.31	0.46
1:A:485:PRO:C	1:A:487:LEU:H	2.19	0.46
1:B:404:LEU:HD22	1:B:408:ASP:HB2	1.98	0.46
2:D:157:ILE:HG13	2:D:158:ASN:N	2.30	0.46
1:A:109:GLU:OE1	1:A:193:ARG:NH1	2.34	0.46
1:B:29:TYR:N	1:B:29:TYR:CD1	2.84	0.46
1:B:39:PHE:O	1:B:39:PHE:CD1	2.69	0.46
1:B:268:PHE:CD1	1:B:294:TYR:HD2	2.33	0.46
2:C:117:SER:HA	2:C:121:ARG:HB2	1.98	0.46
1:A:42:LYS:C	1:A:46:LYS:HE3	2.36	0.45
1:B:290:THR:CG2	1:B:299:LYS:HB3	2.45	0.45
1:B:587:ASN:N	1:B:587:ASN:HD22	2.14	0.45
1:A:309:SER:HB2	1:A:319:PRO:HA	1.98	0.45
1:A:490:LYS:O	1:A:490:LYS:CG	2.63	0.45
1:A:35:SER:O	1:A:36:CYS:C	2.54	0.45
1:A:81:TYR:CD2	1:A:86:ARG:NH2	2.83	0.45
1:A:87:LYS:O	1:A:87:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LYS:HE2	1:A:547:LYS:HB3	1.88	0.45
1:A:563:ASN:OD1	1:A:563:ASN:N	2.48	0.45
1:B:123:SER:C	1:B:125:VAL:N	2.65	0.45
1:B:499:GLN:OE1	1:B:565:VAL:HG13	2.16	0.45
2:C:146:CYS:C	2:C:177:TRP:CZ2	2.90	0.45
2:D:25:SER:HB2	2:D:46:GLU:HB3	1.98	0.45
2:D:47:ILE:HD11	2:D:60:ILE:O	2.17	0.45
2:D:191:ILE:H	2:D:191:ILE:HG12	1.49	0.45
2:C:19:ILE:O	2:C:85:LEU:O	2.34	0.45
2:C:86:ILE:HG12	2:C:104:ILE:HA	1.97	0.45
1:A:232:THR:C	1:A:233:THR:HG23	2.37	0.45
1:A:534:PRO:C	1:A:536:VAL:H	2.19	0.45
1:B:496:GLU:OE1	1:B:594:LEU:HD22	2.17	0.45
2:C:7:HIS:C	2:C:9:GLN:H	2.20	0.45
2:C:29:VAL:CA	2:C:42:ARG:O	2.64	0.45
1:A:25:LEU:HD22	1:A:44:THR:HG22	1.97	0.45
2:C:105:VAL:HG21	2:C:110:LEU:HD11	1.99	0.45
1:A:147:TRP:O	1:A:148:GLU:HB3	2.17	0.45
1:A:406:GLN:HE21	1:A:432:LEU:CD1	2.27	0.45
1:A:527:LEU:HB2	1:A:536:VAL:HG11	1.93	0.45
1:B:452:ILE:HD11	1:B:503:ALA:HB1	1.99	0.45
2:C:1:CYS:HB2	2:C:71:VAL:C	2.36	0.45
1:A:266:PHE:CZ	1:A:273:TYR:HB2	2.52	0.45
1:A:404:LEU:HD22	1:A:408:ASP:CB	2.46	0.45
1:A:451:GLN:CD	1:A:451:GLN:O	2.55	0.45
1:B:449:ILE:O	1:B:450:ALA:HB2	2.16	0.45
1:B:566:LYS:C	1:B:568:LYS:N	2.70	0.45
2:C:121:ARG:O	2:C:122:TYR:C	2.55	0.45
1:A:6:ILE:CG2	1:A:8:PHE:CE1	2.99	0.45
1:A:45:LEU:HD21	1:A:59:ASP:HA	1.90	0.45
1:A:460:LYS:HD2	1:A:460:LYS:HA	1.51	0.45
1:A:559:PHE:CZ	2:C:188:PHE:CE2	3.05	0.45
1:A:584:ILE:HG23	1:A:588:LEU:CD1	2.47	0.45
1:A:621:PHE:HB2	2:C:147:LEU:CD2	2.40	0.45
1:B:461:ASP:O	1:B:462:ARG:HB2	2.17	0.45
1:B:468:VAL:HG13	1:B:469:THR:N	2.32	0.45
2:D:86:ILE:HG22	2:D:87:ALA:N	2.32	0.45
1:A:315:SER:HB3	1:A:318:ALA:HB3	1.98	0.45
1:A:406:GLN:HE21	1:A:432:LEU:CG	2.30	0.45
1:B:543:PHE:CZ	1:B:545:TRP:HD1	2.34	0.45
1:B:593:ASP:OD2	1:B:601:TYR:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:ILE:HA	2:C:53:PHE:HD1	1.82	0.45
2:C:121:ARG:HH22	2:C:178:TYR:HB3	1.82	0.45
1:B:504:VAL:HG13	1:B:513:ILE:HG12	1.98	0.44
1:B:616:LEU:HG	2:D:170:ARG:HH22	1.82	0.44
2:C:57:GLU:H	2:C:57:GLU:HG2	1.50	0.44
1:A:137:GLU:HA	1:A:141:MET:CE	2.47	0.44
1:B:97:TYR:CG	1:B:119:PHE:HE2	2.35	0.44
1:B:405:SER:O	1:B:409:ILE:HG13	2.17	0.44
1:B:548:ASN:O	1:B:550:LYS:HG3	2.17	0.44
1:B:579:ASP:C	1:B:579:ASP:OD1	2.55	0.44
2:C:1:CYS:CB	2:C:71:VAL:O	2.63	0.44
2:C:16:ASP:O	2:C:55:GLY:HA2	2.18	0.44
2:C:71:VAL:O	2:C:72:CYS:SG	2.76	0.44
2:D:104:ILE:O	2:D:105:VAL:HG13	2.17	0.44
1:A:125:VAL:O	1:A:125:VAL:HG23	2.17	0.44
1:A:459:PHE:CD2	1:A:464:ILE:HG22	2.52	0.44
1:B:41:LEU:HB2	1:B:43:ASP:OD2	2.17	0.44
1:B:61:ASP:OD1	1:B:61:ASP:N	2.50	0.44
1:B:97:TYR:CG	1:B:119:PHE:CE2	3.05	0.44
1:A:26:ASN:HD22	1:A:26:ASN:N	2.15	0.44
1:A:234:TYR:CD2	1:A:521:ARG:HD2	2.52	0.44
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.85	0.44
1:B:446:PHE:CZ	1:B:629:LEU:HD11	2.52	0.44
1:B:484:TRP:CD1	1:B:514:TYR:CD2	3.02	0.44
2:C:126:CYS:C	2:C:128:CYS:N	2.70	0.44
2:D:18:VAL:HG13	2:D:87:ALA:HB2	1.99	0.44
1:A:192:VAL:HB	1:A:204:CYS:SG	2.57	0.44
1:A:343:LYS:HZ2	1:A:343:LYS:HG2	1.44	0.44
1:A:435:VAL:HG12	1:A:436:THR:H	1.81	0.44
1:B:473:LYS:HG3	1:B:630:GLY:HA2	1.99	0.44
1:B:561:ARG:NH2	2:D:190:ASP:OD1	2.51	0.44
2:C:29:VAL:CG2	2:C:43:ILE:HD13	2.33	0.44
1:A:59:ASP:O	1:A:60:LEU:C	2.56	0.44
1:A:459:PHE:CE2	1:A:464:ILE:HG21	2.53	0.44
1:B:25:LEU:HD22	1:B:44:THR:HG21	1.99	0.44
1:B:452:ILE:HD11	1:B:503:ALA:CB	2.47	0.44
1:B:617:LYS:NZ	2:D:174:SER:HB2	2.32	0.44
2:C:20:ARG:HD3	2:C:107:TRP:CZ3	2.53	0.44
2:C:20:ARG:HA	2:C:85:LEU:HA	1.98	0.44
2:D:187:GLU:O	2:D:188:PHE:C	2.54	0.44
1:A:96:THR:O	1:A:139:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TRP:CG	1:A:548:ASN:HB3	2.52	0.44
1:B:37:ASN:C	1:B:43:ASP:OD2	2.56	0.44
1:B:70:LYS:HA	1:B:71:PRO:HD2	1.83	0.44
1:B:437:PRO:HB2	1:B:465:TRP:CH2	2.52	0.44
1:A:576:LEU:C	1:A:578:ALA:H	2.19	0.44
1:B:185:THR:O	1:B:367:SER:HA	2.18	0.44
1:B:260:GLN:HA	1:B:261:PRO:HD3	1.82	0.44
1:B:409:ILE:HA	1:B:412:ILE:HG22	2.00	0.44
1:B:497:ALA:HA	1:B:498:PRO:HD3	1.82	0.44
2:C:147:LEU:C	2:C:177:TRP:HZ2	2.21	0.44
1:A:279:GLU:OE1	1:B:279:GLU:OE1	2.35	0.44
1:B:33:LYS:O	1:B:33:LYS:HG3	2.18	0.44
2:D:52:MET:HG3	2:D:53:PHE:N	2.31	0.44
1:B:336:SER:O	1:B:337:ALA:C	2.54	0.43
2:C:136:ILE:H	2:C:136:ILE:HG12	1.38	0.43
2:D:147:LEU:N	2:D:177:TRP:CZ2	2.86	0.43
1:A:252:THR:HG22	1:A:302:PHE:O	2.18	0.43
1:A:335:THR:OG1	1:A:336:SER:N	2.51	0.43
1:A:552:TYR:HE2	2:C:188:PHE:CE1	2.35	0.43
1:B:486:GLU:HG2	1:B:514:TYR:OH	2.18	0.43
2:C:135:MET:O	2:C:136:ILE:C	2.56	0.43
2:C:150:ASP:OD1	2:C:161:GLN:HB3	2.18	0.43
1:A:42:LYS:H	1:A:42:LYS:HE3	1.83	0.43
1:A:374:HIS:CD2	1:A:378:HIS:CD2	3.06	0.43
1:A:391:LEU:C	1:A:393:ALA:H	2.21	0.43
1:B:140:ILE:HG23	1:B:174:GLY:O	2.17	0.43
1:B:223:ARG:NH2	1:B:225:ASP:OD2	2.50	0.43
2:D:102:ASP:O	2:D:104:ILE:N	2.51	0.43
2:D:148:TRP:CE2	2:D:150:ASP:HB3	2.53	0.43
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.75	0.43
1:A:546:SER:OG	1:A:593:ASP:HB3	2.18	0.43
1:B:293:ASP:OD1	1:B:293:ASP:C	2.57	0.43
2:C:15:ALA:HB1	2:C:87:ALA:HB1	2.01	0.43
2:C:30:ASP:CG	2:C:31:SER:H	2.21	0.43
2:C:74:VAL:HG21	2:C:98:ILE:O	2.18	0.43
2:C:98:ILE:HG13	2:C:98:ILE:O	2.19	0.43
1:A:579:ASP:CG	2:C:185:LYS:NZ	2.70	0.43
1:A:223:ARG:H	1:A:223:ARG:HG2	1.64	0.43
1:A:585:PRO:HD2	1:A:588:LEU:CD2	2.48	0.43
1:B:223:ARG:NH1	1:B:244:PHE:CE2	2.87	0.43
1:B:235:ASN:ND2	1:B:235:ASN:C	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ALA:HA	1:B:592:VAL:CG2	2.44	0.43
2:C:47:ILE:HG21	2:C:63:ILE:HG13	1.95	0.43
2:C:140:ILE:HD11	2:C:146:CYS:C	2.39	0.43
2:C:190:ASP:N	2:C:190:ASP:OD1	2.50	0.43
2:D:147:LEU:N	2:D:177:TRP:HH2	2.06	0.43
1:A:76:PRO:HG2	1:A:82:ASN:OD1	2.18	0.43
1:A:277:THR:HG23	1:B:271:THR:HG21	2.01	0.43
1:B:196:TYR:CD2	1:B:244:PHE:CE1	3.01	0.43
1:B:394:PRO:HG2	1:B:395:ILE:N	2.33	0.43
1:B:584:ILE:HA	1:B:585:PRO:HD3	1.78	0.43
2:C:24:VAL:O	2:C:78:VAL:CG1	2.67	0.43
1:B:97:TYR:CD2	1:B:119:PHE:HE2	2.37	0.43
2:C:85:LEU:CD2	2:C:118:LEU:HD21	2.48	0.43
2:D:21:ALA:HA	2:D:48:LYS:O	2.19	0.43
2:D:127:GLU:OE1	2:D:169:LYS:HD3	2.18	0.43
1:A:459:PHE:CD2	1:A:464:ILE:CG2	3.02	0.43
1:A:506:PHE:HE2	1:A:530:LEU:CD2	2.31	0.43
1:A:585:PRO:CB	1:A:588:LEU:HD21	2.48	0.43
1:A:610:LYS:HB3	1:A:620:LYS:HB3	2.00	0.43
1:B:36:CYS:HB3	1:B:38:LEU:HB3	2.01	0.43
1:B:420:PRO:O	1:B:421:ASP:HB2	2.19	0.43
1:A:80:ASN:ND2	1:A:84:PHE:CE2	2.87	0.43
1:A:310:THR:HB	1:A:318:ALA:O	2.19	0.43
1:A:472:ASP:C	1:A:630:GLY:HA3	2.40	0.43
1:A:511:TYR:HD1	1:A:525:LYS:O	2.01	0.43
1:A:617:LYS:HZ3	2:C:174:SER:CB	2.24	0.43
1:B:103:THR:HG23	1:B:103:THR:O	2.18	0.43
1:B:125:VAL:O	1:B:126:THR:HG23	2.19	0.43
1:B:264:PHE:CZ	1:B:275:SER:HA	2.53	0.43
1:B:430:PRO:HB3	1:B:435:VAL:CG1	2.46	0.43
1:B:491:ILE:HD13	1:B:505:PHE:CE1	2.54	0.43
1:B:582:ASN:O	1:B:583:ALA:HB3	2.18	0.43
2:C:27:LYS:O	2:C:28:GLU:C	2.56	0.43
2:D:138:CYS:SG	2:D:147:LEU:HD11	2.58	0.43
1:A:629:LEU:O	1:A:629:LEU:HG	2.19	0.42
1:B:37:ASN:HB3	1:B:43:ASP:CG	2.32	0.42
1:B:543:PHE:CZ	1:B:545:TRP:CD1	3.07	0.42
1:B:559:PHE:HZ	2:D:188:PHE:CE1	2.27	0.42
1:A:295:ASP:HB2	1:B:146:ARG:NH1	2.34	0.42
1:A:473:LYS:HA	1:A:630:GLY:HA3	2.00	0.42
1:B:397:THR:HG21	1:B:479:LEU:CD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:VAL:C	1:B:482:THR:H	2.20	0.42
1:A:490:LYS:HD3	1:A:490:LYS:N	2.34	0.42
1:A:534:PRO:C	1:A:536:VAL:N	2.73	0.42
2:D:190:ASP:O	2:D:191:ILE:C	2.57	0.42
1:A:54:LEU:H	1:A:54:LEU:CD2	2.20	0.42
1:B:357:LYS:CB	1:B:357:LYS:HZ3	2.18	0.42
1:B:481:ALA:O	1:B:485:PRO:HG3	2.19	0.42
1:B:549:LYS:HA	1:B:549:LYS:HD3	1.80	0.42
1:A:137:GLU:OE2	1:A:141:MET:HE2	2.18	0.42
1:B:179:ASP:OD1	1:B:180:ASP:N	2.53	0.42
1:B:480:VAL:CG2	1:B:481:ALA:H	2.30	0.42
2:D:142:SER:HA	2:D:143:PRO:HD3	1.91	0.42
1:A:156:ASP:OD2	1:A:161:LEU:HG	2.19	0.42
1:A:519:LEU:H	1:A:519:LEU:CD2	2.33	0.42
1:A:589:ASP:OD2	1:A:604:LYS:HA	2.19	0.42
1:B:7:LYS:O	1:B:8:PHE:CG	2.72	0.42
1:B:57:THR:CB	1:B:60:LEU:HB2	2.49	0.42
1:B:123:SER:O	1:B:126:THR:N	2.44	0.42
1:B:450:ALA:HA	1:B:592:VAL:HG11	2.00	0.42
1:B:458:PHE:HZ	1:B:628:TRP:HB3	1.83	0.42
1:B:573:PHE:HB3	1:B:574:PRO:HA	2.01	0.42
1:B:608:TYR:CE1	1:B:622:GLY:O	2.71	0.42
2:C:189:LEU:HG	2:C:190:ASP:H	1.84	0.42
2:D:151:TRP:CD1	2:D:152:VAL:N	2.88	0.42
1:A:17:ASP:HB3	1:A:18:LYS:H	1.38	0.42
1:B:25:LEU:O	1:B:29:TYR:N	2.50	0.42
1:B:123:SER:C	1:B:125:VAL:H	2.23	0.42
1:B:246:PRO:O	1:B:247:HIS:HB2	2.20	0.42
2:C:25:SER:H	2:C:46:GLU:HB3	1.83	0.42
2:C:54:LYS:HG2	2:C:55:GLY:H	1.85	0.42
2:D:85:LEU:HB3	2:D:105:VAL:HG23	2.01	0.42
1:A:264:PHE:HA	1:A:265:PRO:HA	1.76	0.42
1:A:406:GLN:NE2	1:A:432:LEU:CG	2.83	0.42
1:A:446:PHE:HZ	1:A:629:LEU:CD2	2.31	0.42
1:B:17:ASP:CG	1:B:65:ILE:CD1	2.88	0.42
1:B:70:LYS:HG2	1:B:70:LYS:H	1.66	0.42
1:B:335:THR:OG1	1:B:336:SER:N	2.53	0.42
2:C:74:VAL:HG22	2:C:100:LEU:HA	2.02	0.42
2:C:150:ASP:O	2:C:154:GLU:N	2.52	0.42
1:A:34:GLU:O	1:A:34:GLU:HG2	2.20	0.42
1:A:55:PRO:O	1:A:57:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:HA	1:B:33:LYS:CE	2.44	0.42
1:B:587:ASN:N	1:B:587:ASN:ND2	2.67	0.42
2:D:113:THR:HG21	2:D:164:PHE:HA	2.00	0.42
1:A:9:PRO:HD3	1:A:352:TYR:OH	2.19	0.42
1:A:235:ASN:ND2	1:A:238:LYS:N	2.68	0.42
1:A:496:GLU:HA	1:A:502:LYS:O	2.20	0.42
1:A:535:ASP:C	1:A:537:GLN:H	2.22	0.41
1:A:588:LEU:HD12	1:A:602:PHE:CD2	2.55	0.41
2:C:21:ALA:HB1	2:C:47:ILE:HB	2.01	0.41
2:C:28:GLU:O	2:C:29:VAL:C	2.59	0.41
2:D:30:ASP:OD1	2:D:41:LYS:HE3	2.21	0.41
1:A:87:LYS:HA	1:A:88:PRO:HD3	1.83	0.41
1:A:104:PRO:O	1:A:305:GLU:HG3	2.20	0.41
1:A:368:LEU:HD12	1:A:368:LEU:HA	1.80	0.41
1:A:433:GLY:HA3	1:A:434:PRO:HD3	1.74	0.41
1:A:622:GLY:HA2	2:C:136:ILE:HG22	2.02	0.41
1:B:291:THR:CG2	1:B:293:ASP:H	2.32	0.41
2:D:9:GLN:HB2	2:D:122:TYR:HE1	1.83	0.41
1:A:115:PHE:CE2	1:A:142:ILE:HG21	2.55	0.41
1:A:163:ALA:O	1:A:164:HIS:HB3	2.20	0.41
1:A:599:HIS:HA	1:A:611:LEU:O	2.19	0.41
1:B:112:ASP:OD2	1:B:132:ARG:NH2	2.52	0.41
1:B:406:GLN:CB	1:B:434:PRO:O	2.68	0.41
1:B:484:TRP:HB3	1:B:487:LEU:HB2	2.03	0.41
2:C:18:VAL:HG22	2:C:87:ALA:HB2	2.01	0.41
2:C:44:GLN:HA	2:C:63:ILE:O	2.20	0.41
1:A:123:SER:O	1:A:125:VAL:N	2.54	0.41
1:A:223:ARG:NH1	1:A:244:PHE:CZ	2.88	0.41
1:A:577:ILE:CG2	1:A:581:TRP:HB2	2.29	0.41
1:B:460:LYS:O	1:B:461:ASP:C	2.59	0.41
1:B:555:ALA:HB3	1:B:560:TRP:HZ3	1.86	0.41
2:C:9:GLN:HG3	2:C:122:TYR:CD1	2.54	0.41
1:A:10:GLY:HA2	1:B:296:ARG:CZ	2.50	0.41
1:B:404:LEU:HD22	1:B:408:ASP:CB	2.49	0.41
1:B:447:ASP:HB3	1:B:491:ILE:O	2.21	0.41
1:B:581:TRP:HE3	1:B:611:LEU:HD11	1.86	0.41
2:D:140:ILE:HG23	2:D:147:LEU:HB2	2.00	0.41
1:A:18:LYS:HA	1:A:18:LYS:HD2	1.78	0.41
1:A:421:ASP:OD1	1:A:421:ASP:N	2.53	0.41
1:A:543:PHE:CE1	1:A:554:PHE:HE2	2.38	0.41
1:B:273:TYR:CE2	1:B:277:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:TYR:CD1	1:B:396:TYR:C	2.94	0.41
2:C:60:ILE:HD12	2:C:96:MET:HB3	2.02	0.41
2:C:79:GLY:O	2:C:81:LYS:N	2.54	0.41
2:C:85:LEU:O	2:C:86:ILE:C	2.59	0.41
2:C:97:HIS:CE1	2:C:99:THR:HG22	2.56	0.41
1:A:28:PHE:HE2	1:A:72:ARG:HD2	1.70	0.41
1:A:158:LYS:HD3	1:A:343:LYS:HZ1	1.85	0.41
1:B:80:ASN:O	1:B:80:ASN:CG	2.59	0.41
1:B:291:THR:CG2	1:B:297:ASP:OD2	2.67	0.41
2:C:121:ARG:HH11	2:C:121:ARG:CG	2.33	0.41
2:D:7:HIS:HB3	2:D:10:GLN:CB	2.47	0.41
1:A:60:LEU:HD23	1:A:64:THR:CB	2.51	0.41
1:A:205:LYS:O	1:A:208:PHE:HB3	2.20	0.41
1:B:619:VAL:HG21	2:D:177:TRP:CZ3	2.56	0.41
2:C:121:ARG:NH2	2:C:180:GLY:O	2.45	0.41
1:A:257:ALA:O	1:A:260:GLN:HG2	2.21	0.41
1:A:457:PHE:CD1	1:A:457:PHE:N	2.87	0.41
1:A:503:ALA:HB1	1:A:505:PHE:CE1	2.56	0.41
1:A:545:TRP:CD2	1:A:548:ASN:HB3	2.56	0.41
1:B:263:LYS:HB3	1:B:291:THR:O	2.20	0.41
1:B:300:TYR:N	1:B:300:TYR:CD1	2.89	0.41
1:B:314:ASN:ND2	1:B:314:ASN:C	2.74	0.41
1:B:314:ASN:HD22	1:B:314:ASN:C	2.24	0.41
1:B:376:PHE:HA	1:B:379:ALA:HB3	2.03	0.41
1:B:400:LYS:HD2	1:B:485:PRO:O	2.21	0.41
1:B:563:ASN:CG	1:B:566:LYS:HB2	2.41	0.41
1:B:596:GLY:O	1:B:599:HIS:ND1	2.53	0.41
1:B:600:SER:O	1:B:611:LEU:HB3	2.20	0.41
2:C:7:HIS:C	2:C:9:GLN:N	2.74	0.41
2:C:57:GLU:O	2:C:59:ASP:N	2.54	0.41
2:C:86:ILE:HG21	2:C:98:ILE:CG2	2.50	0.41
2:C:190:ASP:OD1	2:C:192:GLU:OE2	2.39	0.41
2:D:75:SER:O	2:D:76:LEU:HD23	2.21	0.41
2:D:123:GLN:O	2:D:125:GLY:N	2.53	0.41
2:D:133:CYS:HB3	2:D:151:TRP:HE1	1.86	0.41
1:A:20:LEU:O	1:A:22:VAL:N	2.54	0.41
1:A:72:ARG:HH22	1:A:77:ASP:CG	2.23	0.41
1:B:256:ASN:O	1:B:258:GLU:HG2	2.21	0.41
1:B:574:PRO:C	1:B:575:LYS:HG2	2.41	0.41
2:C:33:ASN:HA	2:C:39:PRO:HA	2.02	0.41
2:C:44:GLN:CG	2:C:64:TYR:CE2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PHE:HD1	1:A:85:PRO:O	1.98	0.40
1:B:6:ILE:O	1:B:7:LYS:CB	2.66	0.40
1:B:115:PHE:O	1:B:116:ALA:C	2.58	0.40
1:B:314:ASN:HD22	1:B:314:ASN:N	2.16	0.40
1:B:337:ALA:O	1:B:345:TRP:NE1	2.42	0.40
1:B:375:ALA:O	1:B:378:HIS:HB2	2.21	0.40
1:B:497:ALA:HB1	1:B:500:GLU:HB3	2.03	0.40
1:B:572:GLY:O	1:B:573:PHE:C	2.51	0.40
2:C:43:ILE:H	2:C:43:ILE:HG12	1.68	0.40
2:C:152:VAL:HG12	2:C:153:THR:H	1.86	0.40
2:D:36:TYR:O	2:D:36:TYR:CG	2.58	0.40
2:D:56:PRO:C	2:D:58:LYS:N	2.73	0.40
1:A:42:LYS:NZ	1:A:43:ASP:OD2	2.49	0.40
1:A:168:PRO:HD2	1:A:381:GLY:HA2	2.04	0.40
1:A:232:THR:O	1:A:233:THR:HG23	2.21	0.40
1:B:198:ASN:O	1:B:198:ASN:OD1	2.38	0.40
1:B:253:MET:CG	1:B:254:GLY:N	2.83	0.40
2:D:182:ALA:HA	2:D:183:PRO:HD3	1.94	0.40
1:A:42:LYS:NZ	1:A:43:ASP:N	2.68	0.40
1:A:406:GLN:HE21	1:A:432:LEU:HB2	1.86	0.40
1:A:438:GLU:O	1:A:439:ILE:C	2.60	0.40
1:A:581:TRP:HA	1:A:581:TRP:CE3	2.56	0.40
1:B:539:VAL:O	1:B:539:VAL:HG12	2.20	0.40
1:B:558:LYS:HD3	1:B:574:PRO:CB	2.51	0.40
2:C:2:SER:O	2:C:2:SER:OG	2.37	0.40
1:A:144:PHE:HA	1:A:178:PHE:O	2.22	0.40
1:A:156:ASP:O	1:A:157:GLY:C	2.59	0.40
1:A:452:ILE:O	1:A:496:GLU:OE1	2.38	0.40
1:A:570:ASP:OD2	2:C:190:ASP:OD2	2.40	0.40
1:B:232:THR:O	1:B:232:THR:HG22	2.21	0.40
1:B:290:THR:O	1:B:290:THR:HG23	2.20	0.40
2:C:60:ILE:HG23	2:C:94:GLY:O	2.20	0.40
2:D:41:LYS:O	2:D:67:PRO:HG3	2.21	0.40
1:A:183:LEU:HD12	1:A:183:LEU:C	2.42	0.40
1:A:496:GLU:O	1:A:498:PRO:HD3	2.22	0.40
1:A:550:LYS:HD2	1:A:561:ARG:HE	1.85	0.40
1:B:484:TRP:HD1	1:B:514:TYR:CE2	2.40	0.40
1:B:489:GLU:O	1:B:490:LYS:HB3	2.21	0.40
1:B:528:THR:HB	1:B:534:PRO:HB3	2.01	0.40
2:C:45:TYR:O	2:C:62:PHE:CA	2.67	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:LYS:CE	2:D:151:TRP:O[7_645]	1.53	0.67
2:C:135:MET:SD	2:D:42:ARG:NH1[5_545]	1.57	0.63
2:C:41:LYS:NZ	2:D:151:TRP:O[7_645]	1.94	0.26

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	619/631 (98%)	508 (82%)	81 (13%)	30 (5%)	2 14
1	B	618/631 (98%)	513 (83%)	75 (12%)	30 (5%)	2 14
2	C	190/194 (98%)	145 (76%)	27 (14%)	18 (10%)	0 3
2	D	190/194 (98%)	148 (78%)	31 (16%)	11 (6%)	1 10
All	All	1617/1650 (98%)	1314 (81%)	214 (13%)	89 (6%)	2 11

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	44	THR
1	A	54	LEU
1	A	157	GLY
1	A	439	ILE
1	A	441	LYS
1	A	536	VAL
1	A	619	VAL
1	B	40	VAL
1	B	124	ASP
1	B	419	SER
1	B	531	GLY
1	B	546	SER
1	B	573	PHE

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Mol	Chain	Res	Type
1	B	616	LEU
2	C	29	VAL
2	C	31	SER
2	C	72	CYS
2	C	81	LYS
2	C	86	ILE
2	C	121	ARG
2	D	103	PHE
2	D	153	THR
2	D	191	ILE
1	A	14	PRO
1	A	30	GLY
1	A	33	LYS
1	A	36	CYS
1	A	83	PHE
1	A	171	GLY
1	A	572	GLY
1	A	620	LYS
1	B	7	LYS
1	B	11	ASP
1	B	26	ASN
1	B	32	PRO
1	B	432	LEU
1	B	481	ALA
1	B	567	LYS
1	B	605	GLY
2	C	8	PRO
2	C	58	LYS
2	C	80	GLY
2	C	134	PRO
2	C	160	HIS
2	D	57	GLU
2	D	183	PRO
1	A	15	LYS
1	A	79	ALA
1	A	468	VAL
1	A	486	GLU
1	A	568	LYS
1	A	587	ASN
1	A	616	LEU
1	B	80	ASN
1	B	247	HIS

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Mol	Chain	Res	Type
1	B	501	GLU
1	B	543	PHE
1	B	591	VAL
1	B	613	ASN
2	C	28	GLU
2	D	155	LYS
1	A	32	PRO
1	B	4	PRO
1	B	42	LYS
1	B	437	PRO
1	B	587	ASN
2	C	38	ASN
2	C	100	LEU
2	D	56	PRO
2	D	119	ASN
1	A	21	ALA
1	A	392	MET
1	A	460	LYS
1	A	618	SER
2	C	67	PRO
2	C	79	GLY
2	C	103	PHE
2	D	36	TYR
2	D	124	MET
1	B	498	PRO
1	A	3	SER
1	B	3	SER
1	B	13	ALA
2	D	37	GLY
1	B	592	VAL
1	B	572	GLY
2	C	35	ILE
1	A	485	PRO

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	522/527 (99%)	442 (85%)	80 (15%)	2 12
1	B	522/527 (99%)	440 (84%)	82 (16%)	2 11
2	C	166/168 (99%)	140 (84%)	26 (16%)	2 11
2	D	166/168 (99%)	144 (87%)	22 (13%)	4 16
All	All	1376/1390 (99%)	1166 (85%)	210 (15%)	2 12

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5	ILE
1	A	6	ILE
1	A	7	LYS
1	A	11	ASP
1	A	12	VAL
1	A	16	THR
1	A	17	ASP
1	A	18	LYS
1	A	20	LEU
1	A	26	ASN
1	A	28	PHE
1	A	35	SER
1	A	37	ASN
1	A	42	LYS
1	A	51	PHE
1	A	59	ASP
1	A	64	THR
1	A	72	ARG
1	A	80	ASN
1	A	82	ASN
1	A	83	PHE
1	A	87	LYS
1	A	89	LYS
1	A	92	LYS
1	A	103	THR
1	A	141	MET
1	A	143	ASN
1	A	147	TRP
1	A	158	LYS
1	A	164	HIS
1	A	172	VAL
1	A	183	LEU

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Mol	Chain	Res	Type
1	A	195	LYS
1	A	200	ASP
1	A	211	ASN
1	A	228	LEU
1	A	231	SER
1	A	232	THR
1	A	235	ASN
1	A	252	THR
1	A	253	MET
1	A	277	THR
1	A	283	ASP
1	A	290	THR
1	A	292	GLU
1	A	310	THR
1	A	314	ASN
1	A	329	ASN
1	A	332	GLU
1	A	333	SER
1	A	340	SER
1	A	343	LYS
1	A	349	THR
1	A	357	LYS
1	A	399	THR
1	A	405	SER
1	A	421	ASP
1	A	444	ILE
1	A	445	VAL
1	A	449	ILE
1	A	451	GLN
1	A	466	ARG
1	A	471	ARG
1	A	473	LYS
1	A	490	LYS
1	A	494	VAL
1	A	496	GLU
1	A	518	THR
1	A	529	SER
1	A	544	ASN
1	A	545	TRP
1	A	560	TRP
1	A	561	ARG
1	A	563	ASN

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Mol	Chain	Res	Type
1	A	570	ASP
1	A	586	ASP
1	A	607	TYR
1	A	611	LEU
1	A	616	LEU
1	B	7	LYS
1	B	8	PHE
1	B	11	ASP
1	B	15	LYS
1	B	16	THR
1	B	31	CYS
1	B	33	LYS
1	B	34	GLU
1	B	36	CYS
1	B	38	LEU
1	B	40	VAL
1	B	47	LYS
1	B	61	ASP
1	B	62	GLN
1	B	65	ILE
1	B	70	LYS
1	B	78	VAL
1	B	80	ASN
1	B	87	LYS
1	B	89	LYS
1	B	92	LYS
1	B	103	THR
1	B	131	SER
1	B	133	ILE
1	B	135	ASP
1	B	143	ASN
1	B	147	TRP
1	B	151	ASP
1	B	158	LYS
1	B	164	HIS
1	B	172	VAL
1	B	195	LYS
1	B	196	TYR
1	B	200	ASP
1	B	228	LEU
1	B	231	SER
1	B	232	THR

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Mol	Chain	Res	Type
1	B	235	ASN
1	B	238	LYS
1	B	272	SER
1	B	282	THR
1	B	286	ARG
1	B	290	THR
1	B	291	THR
1	B	299	LYS
1	B	300	TYR
1	B	306	THR
1	B	314	ASN
1	B	325	THR
1	B	333	SER
1	B	343	LYS
1	B	348	THR
1	B	357	LYS
1	B	364	GLN
1	B	400	LYS
1	B	403	ARG
1	B	429	THR
1	B	435	VAL
1	B	442	GLN
1	B	453	ARG
1	B	461	ASP
1	B	462	ARG
1	B	466	ARG
1	B	486	GLU
1	B	495	TYR
1	B	502	LYS
1	B	506	PHE
1	B	509	ASN
1	B	527	LEU
1	B	532	LEU
1	B	536	VAL
1	B	548	ASN
1	B	557	ASP
1	B	563	ASN
1	B	579	ASP
1	B	591	VAL
1	B	592	VAL
1	B	593	ASP
1	B	594	LEU

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Mol	Chain	Res	Type
1	B	604	LYS
1	B	616	LEU
1	B	624	ILE
2	C	19	ILE
2	C	33	ASN
2	C	43	ILE
2	C	57	GLU
2	C	65	THR
2	C	69	SER
2	C	71	VAL
2	C	76	LEU
2	C	100	LEU
2	C	105	VAL
2	C	119	ASN
2	C	120	HIS
2	C	121	ARG
2	C	135	MET
2	C	136	ILE
2	C	139	TYR
2	C	140	ILE
2	C	147	LEU
2	C	149	MET
2	C	152	VAL
2	C	157	ILE
2	C	158	ASN
2	C	178	TYR
2	C	187	GLU
2	C	188	PHE
2	C	190	ASP
2	D	2	SER
2	D	6	VAL
2	D	12	PHE
2	D	13	CYS
2	D	17	VAL
2	D	20	ARG
2	D	34	ASP
2	D	36	TYR
2	D	52	MET
2	D	93	ASP
2	D	110	LEU
2	D	122	TYR
2	D	128	CYS

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Mol	Chain	Res	Type
2	D	132	ARG
2	D	136	ILE
2	D	149	MET
2	D	151	TRP
2	D	157	ILE
2	D	161	GLN
2	D	164	PHE
2	D	178	TYR
2	D	191	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	37	ASN
1	A	75	ASN
1	A	80	ASN
1	A	143	ASN
1	A	190	GLN
1	A	235	ASN
1	A	314	ASN
1	A	406	GLN
1	A	544	ASN
1	A	613	ASN
1	B	62	GLN
1	B	80	ASN
1	B	143	ASN
1	B	190	GLN
1	B	235	ASN
1	B	314	ASN
1	B	413	GLN
1	B	442	GLN
1	B	509	ASN
1	B	544	ASN
1	B	548	ASN
1	B	563	ASN
1	B	587	ASN
1	B	595	GLN
1	B	613	ASN
2	C	7	HIS
2	C	33	ASN
2	C	119	ASN

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Mol	Chain	Res	Type
2	C	156	ASN
2	D	44	GLN
2	D	49	GLN
2	D	158	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	SO4	A	1632	-	4,4,4	0.15	0	6,6,6	0.27	0
3	SO4	B	1632	-	4,4,4	0.16	0	6,6,6	0.17	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1632	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	630:GLY	C	631:CYS	N	2.14
1	A	630:GLY	C	631:CYS	N	2.05

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	624/631 (98%)	0.17	43 (6%)	16	7	27, 36, 45, 74	0
1	B	623/631 (98%)	0.13	47 (7%)	14	5	28, 36, 46, 81	0
2	C	192/194 (98%)	1.40	51 (26%)	0	0	35, 37, 76, 106	0
2	D	192/194 (98%)	1.17	38 (19%)	1	0	36, 37, 75, 107	0
All	All	1631/1650 (98%)	0.42	179 (10%)	5	2	27, 37, 47, 107	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	PRO	12.6
2	D	113	THR	11.3
2	C	23	ALA	9.4
2	C	24	VAL	8.0
2	D	156	ASN	7.9
2	D	112	THR	7.7
2	C	31	SER	7.3
1	B	576	LEU	7.0
2	C	36	TYR	6.9
2	C	35	ILE	6.9
2	D	190	ASP	6.3
1	B	536	VAL	6.2
1	B	43	ASP	6.0
1	A	84	PHE	5.9
2	C	55	GLY	5.6
1	A	40	VAL	5.6
2	C	77	ASP	5.3
1	B	618	SER	5.1
1	A	472	ASP	5.0
1	B	571	PRO	5.0
2	C	32	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	196	TYR	4.9
1	A	39	PHE	4.7
2	D	159	GLY	4.7
2	D	37	GLY	4.6
2	C	190	ASP	4.5
1	B	37	ASN	4.5
2	D	189	LEU	4.5
1	B	524	PRO	4.4
2	D	157	ILE	4.4
2	D	107	TRP	4.4
1	A	469	THR	4.4
2	D	160	HIS	4.4
1	B	516	ALA	4.4
1	A	623	SER	4.3
2	D	191	ILE	4.3
2	C	191	ILE	4.3
1	A	569	MET	4.2
2	C	25	SER	4.2
2	C	88	GLY	4.2
2	C	50	ILE	4.2
2	D	150	ASP	4.2
2	D	172	ASP	4.2
2	C	113	THR	4.2
1	B	472	ASP	4.1
2	C	189	LEU	4.1
2	C	119	ASN	4.1
2	D	36	TYR	4.0
2	D	79	GLY	3.9
2	D	184	PRO	3.9
1	B	523	TYR	3.8
1	A	575	LYS	3.8
1	A	574	PRO	3.8
2	C	56	PRO	3.7
2	C	26	GLU	3.7
1	B	572	GLY	3.7
1	A	82	ASN	3.7
1	B	498	PRO	3.7
2	C	153	THR	3.7
1	B	499	GLN	3.6
1	B	563	ASN	3.6
1	A	536	VAL	3.5
2	C	48	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	124	MET	3.5
2	C	39	PRO	3.5
2	C	34	ASP	3.5
2	C	180	GLY	3.5
1	B	41	LEU	3.4
1	B	36	CYS	3.4
1	B	544	ASN	3.4
2	D	173	GLY	3.4
1	B	537	GLN	3.4
2	C	81	LYS	3.3
1	A	54	LEU	3.3
1	B	421	ASP	3.3
1	B	454	GLY	3.3
1	A	42	LYS	3.3
1	B	471	ARG	3.3
1	A	537	GLN	3.2
1	A	470	PRO	3.2
2	C	40	ILE	3.2
1	B	453	ARG	3.2
1	B	613	ASN	3.1
2	C	116	LYS	3.1
2	D	174	SER	3.1
2	D	183	PRO	3.0
1	B	598	GLY	3.0
1	A	31	CYS	3.0
2	C	49	GLN	3.0
2	C	159	GLY	3.0
2	C	160	HIS	3.0
2	C	4	SER	2.9
1	A	421	ASP	2.9
2	C	62	PHE	2.9
2	C	175	CYS	2.9
1	A	568	LYS	2.9
2	C	109	THR	2.9
2	C	14	ASN	2.9
2	D	158	ASN	2.8
1	A	432	LEU	2.8
1	B	622	GLY	2.8
2	D	50	ILE	2.8
1	A	556	GLY	2.8
1	B	575	LYS	2.8
1	A	429	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	517	SER	2.7
1	A	499	GLN	2.7
1	B	612	GLU	2.7
2	D	51	LYS	2.7
1	B	600	SER	2.7
1	A	498	PRO	2.7
1	A	571	PRO	2.7
1	A	1	ALA	2.7
2	D	80	GLY	2.6
2	D	128	CYS	2.6
1	B	593	ASP	2.6
1	B	570	ASP	2.6
2	C	82	LYS	2.6
2	C	70	ALA	2.6
1	A	576	LEU	2.6
1	A	515	SER	2.6
2	D	4	SER	2.6
1	A	616	LEU	2.5
2	C	128	CYS	2.5
1	A	24	TYR	2.5
1	A	41	LEU	2.5
2	C	131	THR	2.5
2	D	24	VAL	2.5
2	C	22	LYS	2.5
2	D	108	ASP	2.5
2	D	188	PHE	2.5
2	C	38	ASN	2.4
1	B	574	PRO	2.4
1	A	522	GLY	2.4
1	B	578	ALA	2.4
1	B	599	HIS	2.4
1	A	81	TYR	2.4
1	B	501	GLU	2.4
2	D	118	LEU	2.4
2	D	81	LYS	2.3
1	B	522	GLY	2.3
2	D	120	HIS	2.3
2	D	111	SER	2.3
2	C	27	LYS	2.3
2	C	72	CYS	2.3
1	A	86	ARG	2.3
1	A	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	148	GLU	2.3
2	C	45	TYR	2.3
2	D	152	VAL	2.3
1	B	515	SER	2.3
1	A	431	THR	2.2
1	B	509	ASN	2.2
1	A	80	ASN	2.2
2	C	3	CYS	2.2
1	B	469	THR	2.2
2	D	22	LYS	2.2
1	B	595	GLN	2.2
1	B	565	VAL	2.2
2	C	93	ASP	2.2
2	D	82	LYS	2.2
1	A	619	VAL	2.1
1	A	16	THR	2.1
1	B	561	ARG	2.1
2	D	175	CYS	2.1
2	C	75	SER	2.1
2	C	99	THR	2.1
1	A	32	PRO	2.1
1	B	562	TYR	2.1
2	C	30	ASP	2.1
2	C	126	CYS	2.1
1	B	502	LYS	2.1
2	C	161	GLN	2.0
2	C	101	CYS	2.0
2	D	114	GLN	2.0
1	A	509	ASN	2.0
1	A	47	LYS	2.0
1	B	567	LYS	2.0
1	B	527	LEU	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 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, 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
5	CA	B	1635	1/1	0.95	0.14	40,40,40,40	0
5	CA	A	1635	1/1	0.97	0.07	58,58,58,58	0
3	SO4	A	1632	5/5	0.97	0.11	63,64,65,66	0
3	SO4	B	1632	5/5	0.98	0.08	74,75,75,75	0
4	ZN	A	1634	1/1	0.98	0.05	72,72,72,72	0
4	ZN	B	1634	1/1	0.99	0.07	55,55,55,55	0
4	ZN	A	1633	1/1	0.99	0.07	61,61,61,61	0
4	ZN	B	1633	1/1	0.99	0.06	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.