Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 01:14 AM EST

PDB ID	:	4D87
Title	:	Crystal Structure of Tyrosinase from Bacillus megaterium in complex with SDS
Authors	:	Adir, N.; Goldfeder, M.; Fishman, A.
Deposited on	:	2012-01-10
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

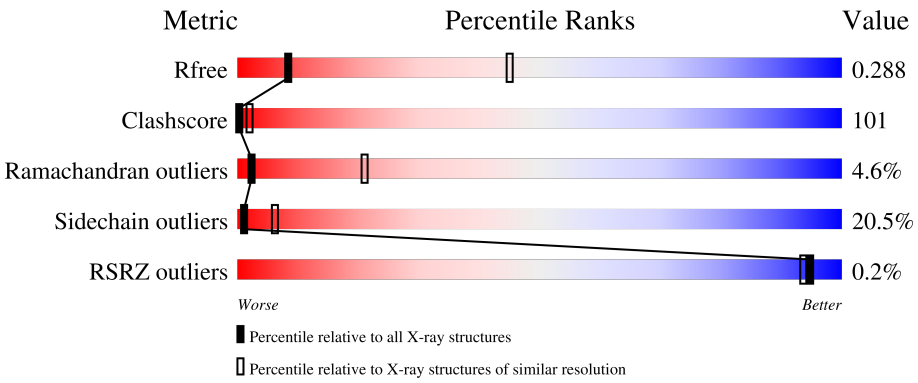
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	303	25% 51% 17% • 6%
1	B	303	21% 50% 21% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4702 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 Tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	286	2346	1492	423	423	8	0	0	0
1	B	285	2337	1487	422	420	8	0	0	0

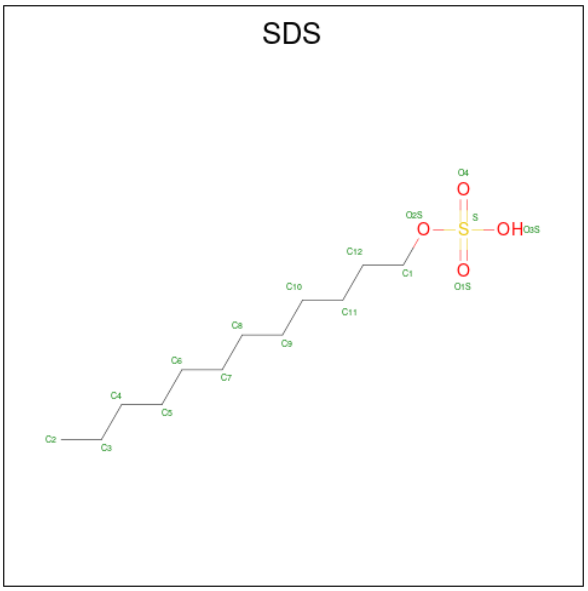
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	HIS	-	expression tag	UNP B2ZB02
A	299	HIS	-	expression tag	UNP B2ZB02
A	300	HIS	-	expression tag	UNP B2ZB02
A	301	HIS	-	expression tag	UNP B2ZB02
A	302	HIS	-	expression tag	UNP B2ZB02
A	303	HIS	-	expression tag	UNP B2ZB02
B	298	HIS	-	expression tag	UNP B2ZB02
B	299	HIS	-	expression tag	UNP B2ZB02
B	300	HIS	-	expression tag	UNP B2ZB02
B	301	HIS	-	expression tag	UNP B2ZB02
B	302	HIS	-	expression tag	UNP B2ZB02
B	303	HIS	-	expression tag	UNP B2ZB02

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is DODECYL SULFATE (three-letter code: SDS) (formula: $C_{12}H_{26}O_4S$).



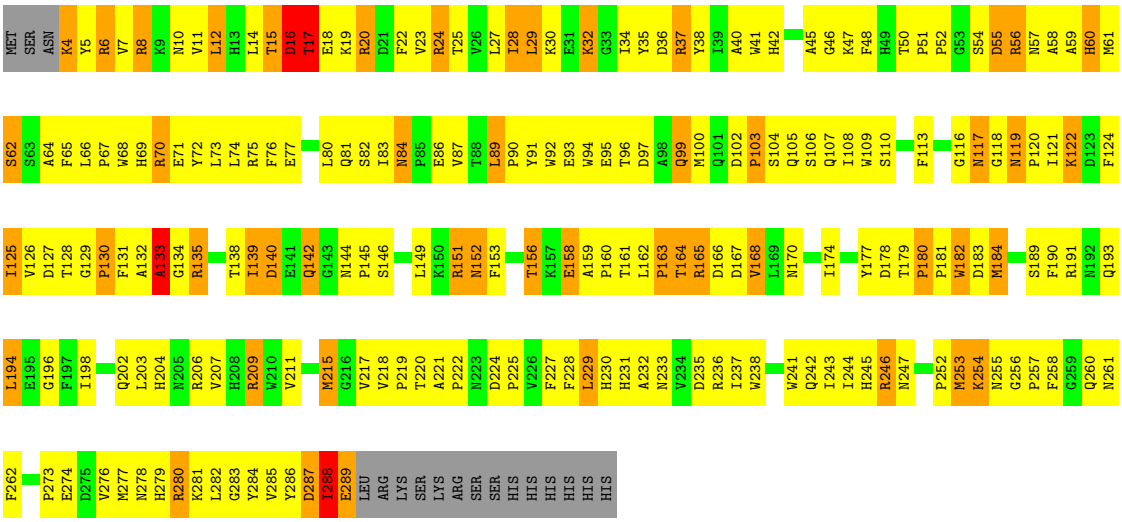
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	17	12	4	1	0	0

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.

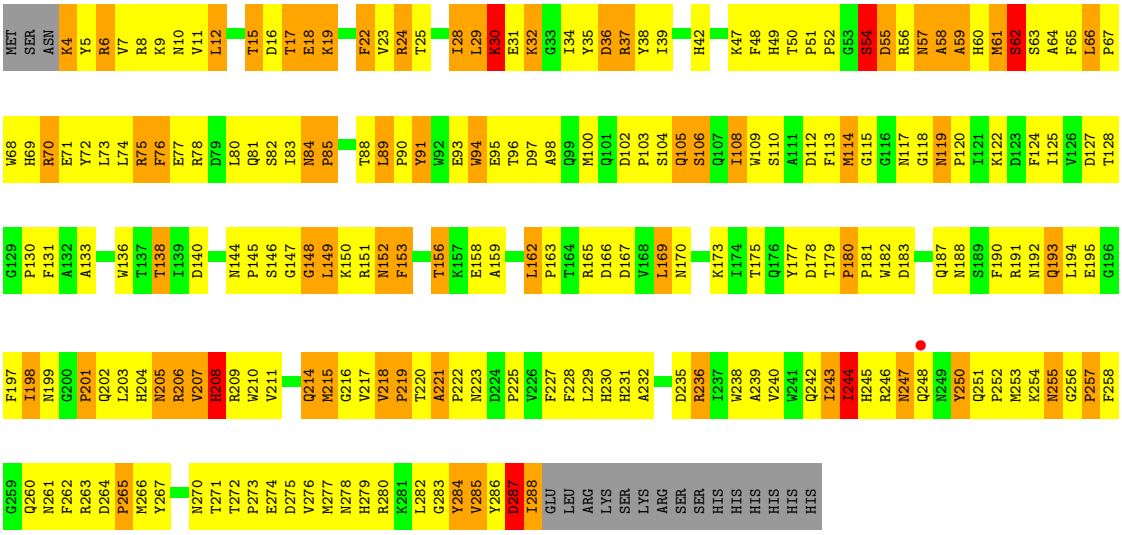
- Molecule 1: Tyrosinase

Chain A: 25% 51% 17% • 6%



- Molecule 1: Tyrosinase

Chain B: 21% 50% 21% • 6%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.84Å 79.14Å 85.93Å 90.00° 103.56° 90.00°	Depositor
Resolution (Å)	83.50 – 3.50 46.51 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.0 (83.50-3.50) 83.0 (46.51-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.22 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.259 , 0.293 0.257 , 0.288	Depositor DCC
R_{free} test set	650 reflections (9.80%)	wwPDB-VP
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 13.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	4702	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: CU, SDS

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	0.74	1/2424 (0.0%)	0.83	6/3303 (0.2%)
1	B	0.73	0/2415	0.99	13/3291 (0.4%)
All	All	0.73	1/4839 (0.0%)	0.91	19/6594 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ARG	C-O	-5.16	1.13	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	HIS	CB-CA-C	-12.40	85.59	110.40
1	B	54	SER	CB-CA-C	-10.09	90.93	110.10
1	B	59	ALA	N-CA-CB	-9.53	96.76	110.10
1	B	207	VAL	CB-CA-C	-9.26	93.81	111.40
1	B	287	ASP	N-CA-C	-8.97	86.77	111.00
1	B	287	ASP	CB-CA-C	8.35	127.09	110.40
1	A	139	ILE	CB-CA-C	-8.32	94.95	111.60
1	B	62	SER	CB-CA-C	8.31	125.88	110.10
1	B	22	PHE	CB-CA-C	-7.78	94.84	110.40
1	B	147	GLY	N-CA-C	-7.57	94.18	113.10
1	B	58	ALA	CB-CA-C	7.48	121.32	110.10
1	B	148	GLY	N-CA-C	7.06	130.75	113.10
1	B	183	ASP	N-CA-CB	-6.73	98.49	110.60
1	B	110	SER	CB-CA-C	-6.05	98.61	110.10
1	A	288	ILE	N-CA-C	-5.81	95.31	111.00
1	A	133	ALA	CB-CA-C	5.44	118.26	110.10
1	A	140	ASP	N-CA-CB	-5.21	101.22	110.60
1	A	16	ASP	C-N-CA	-5.13	108.87	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	CB-CA-C	-5.05	100.30	110.40

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	2346	0	2227	443	0
1	B	2337	0	2220	501	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	17	0	26	8	0
All	All	4702	0	4473	931	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 101.

All (931) 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:254:LYS:CA	1:B:261:ASN:ND2	1.74	1.46
1:B:153:PHE:CD2	1:B:210:TRP:CH2	2.06	1.41
1:A:142:GLN:NE2	1:B:47:LYS:HE2	1.35	1.41
1:B:138:THR:CG2	1:B:223:ASN:OD1	1.74	1.35
1:A:20:ARG:O	1:A:24:ARG:HG2	1.26	1.33
1:A:142:GLN:HE22	1:B:47:LYS:NZ	1.26	1.33
1:B:254:LYS:CA	1:B:261:ASN:HD21	1.35	1.33
1:B:217:VAL:O	1:B:219:PRO:CD	1.75	1.32
1:A:142:GLN:CD	1:B:47:LYS:HE2	1.49	1.31
1:B:138:THR:HG22	1:B:223:ASN:CG	1.49	1.31
1:B:114:MET:CE	1:B:229:LEU:HD21	1.61	1.30
1:A:142:GLN:NE2	1:B:47:LYS:CE	1.97	1.28
1:B:71:GLU:OE1	1:B:271:THR:CG2	1.82	1.28
1:B:215:MET:HE1	1:B:227:PHE:CA	1.64	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLN:HE22	1:B:47:LYS:CE	1.47	1.27
1:B:153:PHE:HD2	1:B:210:TRP:CH2	1.43	1.26
1:A:256:GLY:HA3	1:A:261:ASN:ND2	1.51	1.24
1:B:15:THR:CG2	1:B:18:GLU:OE1	1.84	1.23
1:B:24:ARG:HH11	1:B:24:ARG:CB	1.49	1.23
1:A:4:LYS:HG2	1:A:280:ARG:NH1	1.52	1.22
1:B:15:THR:HG23	1:B:18:GLU:OE1	1.10	1.22
1:B:215:MET:CE	1:B:227:PHE:HA	1.69	1.22
1:A:4:LYS:HD3	1:A:4:LYS:N	1.45	1.21
1:B:76:PHE:CD2	1:B:228:PHE:CE1	2.27	1.21
1:B:215:MET:CE	1:B:227:PHE:CA	2.20	1.20
1:A:8:ARG:NH1	1:A:77:GLU:CD	1.94	1.20
1:A:15:THR:HG22	1:A:18:GLU:OE1	1.43	1.19
1:B:114:MET:HE1	1:B:229:LEU:CD2	1.73	1.18
1:B:113:PHE:HE1	1:B:114:MET:CE	1.56	1.17
1:B:76:PHE:CD2	1:B:228:PHE:CD1	2.32	1.17
1:A:256:GLY:CA	1:A:261:ASN:HD21	1.56	1.17
1:B:113:PHE:CE1	1:B:114:MET:HE2	1.79	1.17
1:A:8:ARG:HH11	1:A:77:GLU:CD	1.48	1.16
1:B:62:SER:OG	1:B:260:GLN:OE1	1.63	1.16
1:B:114:MET:CE	1:B:229:LEU:CD2	2.21	1.16
1:A:15:THR:CG2	1:A:18:GLU:OE1	1.93	1.15
1:A:24:ARG:HG3	1:A:24:ARG:HH11	1.05	1.15
1:B:63:SER:OG	1:B:178:ASP:OD2	1.61	1.15
1:A:253:MET:HE1	1:A:262:PHE:CG	1.81	1.14
1:B:24:ARG:HH11	1:B:24:ARG:CG	1.60	1.13
1:B:77:GLU:HA	1:B:80:LEU:HD12	1.22	1.13
1:B:113:PHE:CE1	1:B:114:MET:CE	2.30	1.13
1:B:29:LEU:HD12	1:B:34:ILE:CG2	1.78	1.12
1:B:70:ARG:NH2	1:B:242:GLN:OE1	1.80	1.12
1:B:24:ARG:HH11	1:B:24:ARG:HB2	1.06	1.11
1:B:29:LEU:CD1	1:B:34:ILE:HG21	1.79	1.11
1:A:8:ARG:NH1	1:A:77:GLU:OE1	1.81	1.11
1:A:126:VAL:O	1:A:132:ALA:HB1	1.51	1.11
1:A:158:GLU:CB	1:A:209:ARG:NH2	2.14	1.11
1:B:254:LYS:HA	1:B:261:ASN:ND2	0.78	1.11
1:B:24:ARG:HB2	1:B:24:ARG:NH1	1.64	1.11
1:A:253:MET:CE	1:A:262:PHE:CB	2.29	1.10
1:B:66:LEU:HD12	1:B:177:TYR:OH	1.51	1.10
1:B:218:VAL:HG12	1:B:219:PRO:N	1.64	1.10
1:B:28:ILE:HG21	1:B:83:ILE:HG21	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:HB3	1:A:209:ARG:HH21	1.15	1.09
1:B:71:GLU:OE1	1:B:271:THR:HG21	0.92	1.09
1:A:209:ARG:HH12	3:A:402:SDS:H121	1.17	1.09
1:A:209:ARG:HH12	3:A:402:SDS:C12	1.64	1.08
1:B:114:MET:HE1	1:B:229:LEU:HD21	1.28	1.08
1:B:71:GLU:OE2	1:B:75:ARG:NH2	1.86	1.08
1:B:238:TRP:O	1:B:242:GLN:HG3	1.53	1.08
1:A:15:THR:HG23	1:A:18:GLU:HB2	1.09	1.07
1:A:280:ARG:HH11	1:A:280:ARG:CG	1.59	1.07
1:B:10:ASN:N	1:B:91:TYR:CE2	2.23	1.07
1:A:280:ARG:NH1	1:A:280:ARG:HG2	1.54	1.07
1:A:8:ARG:HG3	1:A:89:LEU:O	1.53	1.06
1:B:217:VAL:O	1:B:219:PRO:HD2	0.89	1.06
1:B:38:TYR:OH	1:B:75:ARG:O	1.70	1.06
1:B:91:TYR:OH	1:B:287:ASP:OD1	1.72	1.06
1:A:158:GLU:CB	1:A:209:ARG:HH21	1.70	1.05
1:B:8:ARG:NH2	1:B:286:TYR:OH	1.87	1.05
1:B:153:PHE:CD2	1:B:210:TRP:CZ3	2.45	1.04
1:B:217:VAL:C	1:B:219:PRO:HD2	1.76	1.04
1:B:71:GLU:O	1:B:75:ARG:CG	2.04	1.04
1:A:217:VAL:CG2	1:A:220:THR:OG1	2.05	1.03
1:B:194:LEU:HD23	1:B:194:LEU:O	1.56	1.03
1:B:76:PHE:HD2	1:B:228:PHE:CD1	1.70	1.03
1:B:29:LEU:HD11	1:B:34:ILE:HG21	1.38	1.03
1:A:16:ASP:O	1:A:18:GLU:N	1.91	1.02
1:A:8:ARG:CG	1:A:89:LEU:O	2.05	1.02
1:A:28:ILE:HG23	1:A:32:LYS:HD2	1.37	1.02
1:B:70:ARG:NH1	1:B:276:VAL:O	1.93	1.02
1:B:113:PHE:HD1	1:B:114:MET:HG2	1.23	1.02
1:A:253:MET:HE3	1:A:262:PHE:HB2	1.37	1.01
1:B:262:PHE:HE2	1:B:274:GLU:HG3	1.22	1.01
1:A:56:ARG:HG3	1:A:56:ARG:HH11	0.87	1.01
1:B:62:SER:OG	1:B:260:GLN:CD	1.99	1.01
1:B:262:PHE:CE2	1:B:274:GLU:HG3	1.95	1.01
1:A:131:PHE:CE1	1:A:225:PRO:HG2	1.97	0.99
1:A:221:ALA:HB3	1:A:222:PRO:HD3	1.45	0.99
1:B:218:VAL:O	1:B:221:ALA:N	1.94	0.99
1:B:250:TYR:HD2	1:B:251:GLN:N	1.61	0.98
1:B:138:THR:HG22	1:B:223:ASN:OD1	0.81	0.98
1:B:76:PHE:CE2	1:B:228:PHE:CD1	2.51	0.98
1:A:29:LEU:HD22	1:A:80:LEU:CD2	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:HA	1:A:132:ALA:HB1	1.45	0.98
1:A:142:GLN:HA	1:A:142:GLN:HE21	1.28	0.97
1:B:54:SER:OG	1:B:55:ASP:N	1.84	0.97
1:A:253:MET:CE	1:A:262:PHE:HB2	1.91	0.97
1:A:209:ARG:NH1	3:A:402:SDS:C12	2.28	0.97
1:B:29:LEU:CD1	1:B:34:ILE:CG2	2.39	0.97
1:A:209:ARG:NH1	3:A:402:SDS:H121	1.80	0.96
1:B:113:PHE:HE1	1:B:114:MET:HE3	1.28	0.96
1:B:4:LYS:N	1:B:4:LYS:HD2	1.81	0.96
1:B:76:PHE:CE2	1:B:228:PHE:CE1	2.53	0.95
1:B:236:ARG:HH11	1:B:236:ARG:CG	1.78	0.95
1:A:56:ARG:HG3	1:A:56:ARG:NH1	1.67	0.95
1:A:236:ARG:HB2	1:A:286:TYR:CE2	2.01	0.95
1:B:71:GLU:O	1:B:75:ARG:HG3	1.66	0.95
1:A:256:GLY:N	1:A:261:ASN:HD21	1.64	0.94
1:B:88:THR:O	1:B:90:PRO:HD3	1.67	0.94
1:A:12:LEU:N	1:A:12:LEU:HD23	1.82	0.94
1:B:114:MET:HE3	1:B:229:LEU:CD2	1.94	0.94
1:B:182:TRP:CE3	1:B:252:PRO:HD3	2.03	0.94
1:B:243:ILE:HG22	1:B:244:ILE:N	1.82	0.93
1:A:16:ASP:O	1:A:17:THR:C	2.00	0.93
1:B:4:LYS:N	1:B:4:LYS:CD	2.30	0.93
1:A:56:ARG:HH11	1:A:56:ARG:CG	1.78	0.93
1:B:66:LEU:CD1	1:B:177:TYR:OH	2.15	0.93
1:B:114:MET:HE3	1:B:229:LEU:HD21	1.46	0.92
1:B:214:GLN:O	1:B:221:ALA:HA	1.69	0.92
1:B:6:ARG:HE	1:B:284:TYR:HB3	1.32	0.92
1:B:236:ARG:HH11	1:B:236:ARG:HG3	1.34	0.92
1:A:94:TRP:CE3	1:A:163:PRO:CG	2.53	0.92
1:A:4:LYS:CG	1:A:280:ARG:NH1	2.31	0.92
1:A:142:GLN:NE2	1:B:47:LYS:NZ	2.12	0.92
1:A:156:THR:HG23	1:A:158:GLU:H	1.35	0.92
1:A:38:TYR:CE2	1:A:76:PHE:HD1	1.87	0.92
1:A:156:THR:HG22	1:A:159:ALA:H	1.36	0.91
1:A:162:LEU:HB3	1:A:163:PRO:HD2	1.53	0.91
1:A:4:LYS:N	1:A:4:LYS:CD	2.33	0.91
1:A:217:VAL:HG23	1:A:220:THR:OG1	1.70	0.91
1:A:4:LYS:CG	1:A:280:ARG:HG2	2.00	0.91
1:B:51:PRO:HB2	1:B:52:PRO:HD2	1.53	0.90
1:A:20:ARG:NH2	1:A:24:ARG:HH21	1.69	0.90
1:A:29:LEU:HD22	1:A:80:LEU:HD23	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MET:HE1	1:A:262:PHE:CB	1.97	0.90
1:B:153:PHE:HD2	1:B:210:TRP:HH2	0.97	0.90
1:B:215:MET:HE3	1:B:227:PHE:N	1.87	0.90
1:A:24:ARG:HG3	1:A:24:ARG:NH1	1.65	0.90
1:A:89:LEU:HD23	1:A:90:PRO:CD	2.01	0.90
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.36	0.90
1:A:256:GLY:CA	1:A:261:ASN:ND2	2.24	0.90
1:B:15:THR:O	1:B:19:LYS:HG3	1.72	0.89
1:B:38:TYR:O	1:B:72:TYR:OH	1.88	0.89
1:A:158:GLU:HB3	1:A:209:ARG:NH2	1.81	0.89
1:A:158:GLU:HB2	1:A:209:ARG:NH2	1.87	0.89
1:B:54:SER:OG	1:B:56:ARG:N	2.06	0.89
1:B:6:ARG:O	1:B:6:ARG:HG2	1.69	0.89
1:A:4:LYS:HG3	1:A:280:ARG:CG	2.03	0.89
1:A:20:ARG:HH21	1:A:24:ARG:HH21	1.18	0.88
1:A:178:ASP:HA	1:A:189:SER:OG	1.74	0.88
1:B:71:GLU:O	1:B:75:ARG:CD	2.22	0.87
1:A:70:ARG:CD	1:A:235:ASP:OD2	2.21	0.87
1:A:142:GLN:OE1	1:B:47:LYS:HE2	1.73	0.87
1:B:114:MET:HE1	1:B:229:LEU:HD22	1.56	0.87
1:A:126:VAL:O	1:A:132:ALA:CB	2.23	0.87
1:A:12:LEU:N	1:A:12:LEU:CD2	2.38	0.86
1:A:4:LYS:HG2	1:A:280:ARG:HH11	1.39	0.86
1:A:280:ARG:O	1:A:283:GLY:N	2.08	0.86
1:B:57:ASN:HD21	1:B:60:HIS:HB2	1.40	0.86
1:A:4:LYS:CG	1:A:280:ARG:HH11	1.88	0.86
1:A:94:TRP:CE3	1:A:163:PRO:HG3	2.11	0.86
1:A:94:TRP:CE3	1:A:163:PRO:HG2	2.10	0.86
1:A:253:MET:HE1	1:A:262:PHE:CD2	2.11	0.86
1:B:254:LYS:C	1:B:261:ASN:HD21	1.79	0.85
1:B:243:ILE:CG2	1:B:244:ILE:N	2.39	0.85
1:A:95:GLU:HB2	1:A:165:ARG:HA	1.55	0.85
1:B:113:PHE:CE1	1:B:114:MET:HE3	2.04	0.85
1:A:60:HIS:CD2	1:A:69:HIS:HE1	1.95	0.85
1:B:81:GLN:NE2	1:B:85:PRO:O	2.10	0.85
1:A:24:ARG:HH11	1:A:24:ARG:CG	1.85	0.85
1:B:243:ILE:HG22	1:B:244:ILE:H	1.40	0.85
1:A:15:THR:HG23	1:A:18:GLU:CB	2.01	0.85
1:A:70:ARG:HG2	1:A:235:ASP:OD2	1.76	0.85
1:B:10:ASN:N	1:B:91:TYR:HE2	1.73	0.85
1:B:138:THR:O	1:B:146:SER:OG	1.94	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HG2	1:A:280:ARG:HH12	1.39	0.84
1:B:6:ARG:NE	1:B:284:TYR:HB3	1.92	0.84
1:B:48:PHE:CD2	1:B:48:PHE:O	2.30	0.84
1:A:280:ARG:HH11	1:A:280:ARG:HG2	0.70	0.84
1:B:24:ARG:NH1	1:B:24:ARG:HG3	1.92	0.84
1:A:4:LYS:HG3	1:A:280:ARG:HG2	1.60	0.83
1:A:70:ARG:CG	1:A:235:ASP:OD2	2.25	0.83
1:B:125:ILE:HD13	1:B:149:LEU:O	1.77	0.83
1:B:156:THR:HG22	1:B:159:ALA:H	1.44	0.83
1:B:28:ILE:CG2	1:B:83:ILE:HG21	2.09	0.83
1:A:15:THR:CG2	1:A:18:GLU:HB2	2.03	0.83
1:A:89:LEU:HD23	1:A:90:PRO:N	1.93	0.83
1:B:215:MET:CE	1:B:227:PHE:CB	2.56	0.82
1:A:217:VAL:HG21	1:A:220:THR:OG1	1.78	0.82
1:A:130:PRO:O	1:A:131:PHE:HD2	1.63	0.82
1:A:181:PRO:C	1:A:182:TRP:CD1	2.52	0.82
1:A:102:ASP:OD1	1:A:104:SER:OG	1.98	0.82
1:B:29:LEU:HD12	1:B:34:ILE:CB	2.10	0.82
1:B:215:MET:HE2	1:B:227:PHE:HB2	1.61	0.82
1:A:119:ASN:ND2	1:A:121:ILE:H	1.77	0.82
1:B:24:ARG:CG	1:B:24:ARG:NH1	2.30	0.82
1:A:8:ARG:NH1	1:A:77:GLU:OE2	2.11	0.81
1:B:215:MET:HE1	1:B:227:PHE:HA	0.84	0.81
1:A:142:GLN:HE22	1:B:47:LYS:HZ1	1.27	0.81
1:A:130:PRO:C	1:A:131:PHE:CD2	2.54	0.81
1:B:218:VAL:CG1	1:B:219:PRO:N	2.40	0.81
1:B:24:ARG:HH11	1:B:24:ARG:HG3	1.42	0.81
1:A:16:ASP:O	1:A:19:LYS:N	2.13	0.80
1:A:54:SER:O	1:A:56:ARG:N	2.13	0.80
1:B:28:ILE:O	1:B:32:LYS:HG3	1.80	0.80
1:B:108:ILE:HG22	1:B:109:TRP:CD1	2.15	0.80
1:B:23:VAL:CG1	1:B:23:VAL:O	2.30	0.80
1:B:138:THR:CG2	1:B:223:ASN:CG	2.32	0.80
1:A:119:ASN:C	1:A:119:ASN:HD22	1.81	0.80
1:B:31:GLU:O	1:B:31:GLU:HG2	1.79	0.80
1:B:254:LYS:O	1:B:255:ASN:HB2	1.82	0.80
1:A:12:LEU:HD23	1:A:12:LEU:H	1.43	0.80
1:A:286:TYR:O	1:A:288:ILE:N	2.14	0.80
1:B:194:LEU:O	1:B:194:LEU:CD2	2.30	0.80
1:B:288:ILE:O	1:B:288:ILE:HG22	1.80	0.80
1:A:8:ARG:HG2	1:A:89:LEU:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PRO:O	1:A:277:MET:HG2	1.82	0.79
1:B:138:THR:C	1:B:146:SER:OG	2.20	0.79
1:A:20:ARG:NH2	1:A:24:ARG:NH2	2.30	0.79
1:A:256:GLY:HA3	1:A:261:ASN:HD21	1.09	0.79
1:B:208:HIS:O	1:B:216:GLY:HA2	1.82	0.79
1:B:254:LYS:HA	1:B:261:ASN:HD22	0.97	0.79
1:B:288:ILE:O	1:B:288:ILE:CG2	2.30	0.79
1:A:60:HIS:O	1:A:61:MET:HB2	1.81	0.79
1:A:95:GLU:HB2	1:A:165:ARG:CA	2.13	0.79
1:A:217:VAL:CG2	1:A:220:THR:HG1	1.94	0.78
1:B:153:PHE:CD2	1:B:210:TRP:HH2	1.72	0.78
1:A:70:ARG:NH1	1:A:276:VAL:O	2.16	0.78
1:B:8:ARG:HG2	1:B:89:LEU:O	1.84	0.78
1:B:77:GLU:HA	1:B:80:LEU:CD1	2.10	0.78
1:A:253:MET:CE	1:A:262:PHE:HB3	2.12	0.78
1:A:165:ARG:O	1:A:165:ARG:HG3	1.84	0.78
1:B:215:MET:CE	1:B:227:PHE:HB2	2.13	0.78
1:A:209:ARG:HH12	3:A:402:SDS:H122	1.47	0.77
1:B:28:ILE:HG21	1:B:83:ILE:CG2	2.12	0.77
1:B:250:TYR:HB3	1:B:262:PHE:HD1	1.50	0.77
1:B:201:PRO:O	1:B:206:ARG:HB2	1.85	0.77
1:A:288:ILE:C	1:A:289:GLU:HG3	2.04	0.77
1:A:253:MET:HE3	1:A:253:MET:HA	1.65	0.77
1:A:256:GLY:HA3	1:A:261:ASN:CG	2.05	0.77
1:B:250:TYR:CD2	1:B:251:GLN:N	2.50	0.77
1:B:207:VAL:C	1:B:209:ARG:H	1.86	0.76
1:A:29:LEU:HD22	1:A:80:LEU:HD21	1.67	0.76
1:A:38:TYR:O	1:A:72:TYR:OH	2.03	0.76
1:B:31:GLU:O	1:B:31:GLU:CG	2.31	0.76
1:B:77:GLU:CA	1:B:80:LEU:HD12	2.11	0.76
1:B:215:MET:CE	1:B:227:PHE:N	2.45	0.76
1:A:89:LEU:C	1:A:89:LEU:CD2	2.54	0.76
1:B:63:SER:O	1:B:250:TYR:OH	2.03	0.76
1:A:174:ILE:HD11	1:A:193:GLN:HE22	1.51	0.75
1:B:77:GLU:O	1:B:80:LEU:N	2.18	0.75
1:B:71:GLU:O	1:B:75:ARG:HD2	1.85	0.75
1:B:238:TRP:O	1:B:242:GLN:CG	2.34	0.75
1:A:162:LEU:CB	1:A:163:PRO:HD2	2.17	0.75
1:B:156:THR:HG22	1:B:159:ALA:N	2.02	0.75
1:B:265:PRO:HA	1:B:272:THR:HG22	1.68	0.74
1:A:89:LEU:HD23	1:A:90:PRO:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD22	1:A:18:GLU:HB3	1.68	0.74
1:B:5:TYR:O	1:B:284:TYR:HA	1.88	0.74
1:A:29:LEU:CD2	1:A:80:LEU:HD23	2.17	0.74
1:A:94:TRP:HE1	1:A:230:HIS:HD2	1.35	0.74
1:A:127:ASP:CA	1:A:132:ALA:HB1	2.17	0.74
1:A:209:ARG:NH1	3:A:402:SDS:H122	2.02	0.74
1:B:243:ILE:O	1:B:246:ARG:N	2.20	0.74
1:A:132:ALA:O	1:A:133:ALA:C	2.25	0.74
1:A:161:THR:HG23	1:A:206:ARG:NH1	2.03	0.74
1:A:156:THR:HG21	1:A:209:ARG:HH21	1.53	0.73
1:B:218:VAL:CB	1:B:219:PRO:CD	2.65	0.73
1:A:156:THR:HG22	1:A:159:ALA:N	2.02	0.73
1:B:94:TRP:HB2	1:B:162:LEU:HD22	1.71	0.73
1:A:94:TRP:HE3	1:A:163:PRO:HG2	1.54	0.73
1:A:127:ASP:HA	1:A:132:ALA:CB	2.17	0.72
1:B:70:ARG:CZ	1:B:238:TRP:CZ3	2.72	0.72
1:A:59:ALA:O	1:A:65:PHE:HA	1.89	0.72
1:B:287:ASP:O	1:B:288:ILE:HB	1.88	0.72
1:A:215:MET:HE3	1:A:227:PHE:HA	1.72	0.72
1:A:142:GLN:NE2	1:A:142:GLN:HA	2.03	0.72
1:B:29:LEU:HD12	1:B:34:ILE:HB	1.71	0.72
1:B:192:ASN:HD22	1:B:198:ILE:HD11	1.55	0.72
1:B:199:ASN:O	1:B:202:GLN:HG2	1.90	0.72
1:A:8:ARG:HD2	1:A:77:GLU:OE2	1.90	0.72
1:A:280:ARG:NH1	1:A:280:ARG:CG	2.30	0.72
1:A:22:PHE:CE1	1:A:90:PRO:HD3	2.25	0.72
1:B:208:HIS:CA	1:B:215:MET:O	2.37	0.72
1:A:130:PRO:C	1:A:131:PHE:HD2	1.93	0.71
1:B:71:GLU:HG2	1:B:75:ARG:HH21	1.55	0.71
1:A:142:GLN:CD	1:B:47:LYS:CE	2.43	0.71
1:B:4:LYS:HZ1	1:B:280:ARG:NE	1.89	0.71
1:B:114:MET:CE	1:B:229:LEU:HD22	2.13	0.71
1:B:254:LYS:CA	1:B:261:ASN:HD22	1.67	0.71
1:B:76:PHE:HD2	1:B:228:PHE:CE1	1.86	0.71
1:B:250:TYR:HB3	1:B:262:PHE:CD1	2.25	0.71
1:B:30:LYS:HG3	1:B:30:LYS:O	1.89	0.71
1:B:258:PHE:CD1	1:B:264:ASP:OD2	2.43	0.71
1:A:204:HIS:CD2	1:A:230:HIS:HE1	2.09	0.71
1:B:30:LYS:HA	1:B:35:TYR:HB2	1.73	0.70
1:B:217:VAL:O	1:B:219:PRO:CG	2.38	0.70
1:B:218:VAL:O	1:B:220:THR:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HB	1:B:219:PRO:CD	2.22	0.70
1:A:181:PRO:O	1:A:182:TRP:CD1	2.45	0.70
1:A:246:ARG:CZ	1:A:246:ARG:HB2	2.20	0.70
1:A:256:GLY:N	1:A:261:ASN:ND2	2.38	0.70
1:B:254:LYS:O	1:B:255:ASN:CB	2.40	0.70
1:A:174:ILE:HD11	1:A:193:GLN:NE2	2.06	0.70
1:A:287:ASP:CG	1:A:287:ASP:O	2.27	0.70
1:A:38:TYR:CE2	1:A:76:PHE:CD1	2.75	0.70
1:A:246:ARG:HH11	1:A:246:ARG:CG	2.02	0.70
1:B:68:TRP:CH2	1:B:72:TYR:CD1	2.79	0.70
1:B:71:GLU:O	1:B:71:GLU:HG2	1.92	0.69
1:A:164:THR:O	1:A:167:ASP:N	2.25	0.69
1:A:178:ASP:O	1:A:179:THR:HG23	1.91	0.69
1:A:193:GLN:CG	1:A:198:ILE:HG13	2.22	0.69
1:B:29:LEU:HD12	1:B:34:ILE:HG22	1.71	0.69
1:B:113:PHE:O	1:B:130:PRO:HG2	1.91	0.69
1:B:256:GLY:O	1:B:257:PRO:C	2.30	0.69
1:A:139:ILE:CG2	1:A:140:ASP:N	2.53	0.69
1:B:236:ARG:CG	1:B:236:ARG:NH1	2.44	0.69
1:B:71:GLU:CG	1:B:75:ARG:HH21	2.06	0.69
1:B:113:PHE:CD1	1:B:114:MET:HG2	2.16	0.69
1:A:89:LEU:HD23	1:A:89:LEU:C	2.10	0.68
1:B:71:GLU:HB2	1:B:276:VAL:HG11	1.75	0.68
1:A:94:TRP:CZ3	1:A:163:PRO:HG3	2.29	0.68
1:A:279:HIS:HA	1:A:282:LEU:HD12	1.74	0.68
1:B:265:PRO:N	1:B:272:THR:HG22	2.09	0.68
1:A:48:PHE:CE2	1:A:50:THR:CG2	2.77	0.68
1:A:129:GLY:O	1:A:131:PHE:N	2.26	0.68
1:B:279:HIS:HB2	1:B:284:TYR:CE1	2.29	0.68
1:B:15:THR:OG1	1:B:17:THR:HG23	1.94	0.68
1:A:181:PRO:HG2	1:A:183:ASP:OD2	1.93	0.68
1:A:193:GLN:HG3	1:A:198:ILE:HG13	1.75	0.68
1:B:76:PHE:HE2	1:B:228:PHE:CD1	2.10	0.68
1:B:23:VAL:O	1:B:23:VAL:HG12	1.94	0.67
1:B:218:VAL:HG12	1:B:219:PRO:CD	2.22	0.67
1:B:8:ARG:HH21	1:B:286:TYR:HH	1.39	0.67
1:B:51:PRO:HB2	1:B:52:PRO:CD	2.25	0.67
1:A:11:VAL:HG23	1:A:91:TYR:O	1.95	0.67
1:A:28:ILE:O	1:A:32:LYS:HD3	1.94	0.67
1:B:175:THR:O	1:B:248:GLN:HG3	1.95	0.67
1:B:57:ASN:ND2	1:B:60:HIS:H	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LYS:HE2	1:B:127:ASP:HB3	1.77	0.67
1:A:16:ASP:C	1:A:18:GLU:N	2.48	0.67
1:B:265:PRO:CA	1:B:272:THR:HG22	2.25	0.67
1:B:78:ARG:O	1:B:81:GLN:N	2.28	0.67
1:B:113:PHE:CD1	1:B:114:MET:CE	2.78	0.67
1:A:109:TRP:CZ3	1:A:151:ARG:NH1	2.63	0.66
1:B:215:MET:HE2	1:B:227:PHE:CB	2.23	0.66
1:A:262:PHE:CZ	1:A:274:GLU:HG3	2.30	0.66
1:B:66:LEU:HD12	1:B:177:TYR:HH	1.57	0.66
1:B:76:PHE:HE2	1:B:228:PHE:CG	2.13	0.66
1:A:215:MET:CE	1:A:227:PHE:HA	2.26	0.66
1:B:100:MET:HE2	1:B:103:PRO:HA	1.76	0.66
1:A:5:TYR:O	1:A:6:ARG:C	2.33	0.66
1:A:38:TYR:OH	1:A:76:PHE:HA	1.96	0.66
1:A:156:THR:CG2	1:A:158:GLU:H	2.08	0.66
1:B:91:TYR:CD1	1:B:236:ARG:CD	2.78	0.66
1:B:194:LEU:CD2	1:B:194:LEU:C	2.63	0.66
1:A:218:VAL:N	1:A:219:PRO:CD	2.58	0.66
1:A:178:ASP:C	1:A:179:THR:HG23	2.17	0.66
1:B:284:TYR:CD1	1:B:284:TYR:O	2.49	0.66
1:A:70:ARG:HD3	1:A:235:ASP:OD2	1.96	0.66
1:B:91:TYR:H	1:B:91:TYR:HD2	1.43	0.66
1:B:97:ASP:O	1:B:100:MET:HG3	1.96	0.66
1:A:28:ILE:HG23	1:A:32:LYS:CD	2.20	0.65
1:A:130:PRO:O	1:A:131:PHE:CD2	2.48	0.65
1:A:46:GLY:HA2	1:A:57:ASN:HD22	1.61	0.65
1:B:257:PRO:HG2	1:B:260:GLN:HG3	1.77	0.65
1:A:287:ASP:O	1:A:287:ASP:OD1	2.13	0.65
1:A:218:VAL:N	1:A:219:PRO:HD2	2.11	0.65
1:A:164:THR:O	1:A:167:ASP:HB2	1.96	0.65
1:A:253:MET:CE	1:A:253:MET:HA	2.26	0.65
1:A:20:ARG:O	1:A:24:ARG:CG	2.22	0.65
1:B:78:ARG:O	1:B:82:SER:N	2.30	0.65
1:B:6:ARG:HH21	1:B:283:GLY:C	1.99	0.65
1:A:125:ILE:CG2	1:A:126:VAL:N	2.59	0.65
1:A:257:PRO:O	1:A:258:PHE:C	2.33	0.65
1:B:15:THR:OG1	1:B:16:ASP:N	2.30	0.65
1:B:255:ASN:N	1:B:261:ASN:HD21	1.95	0.65
1:B:286:TYR:O	1:B:288:ILE:N	2.29	0.65
1:B:30:LYS:HD2	1:B:136:TRP:CH2	2.32	0.64
1:A:204:HIS:HD2	1:A:230:HIS:CE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:OD1	1:A:11:VAL:N	2.31	0.64
1:B:94:TRP:HE1	1:B:230:HIS:HD2	1.44	0.64
1:A:38:TYR:CD2	1:A:76:PHE:HD1	2.14	0.64
1:B:30:LYS:HD2	1:B:136:TRP:CZ3	2.33	0.64
1:B:112:ASP:OD2	1:B:112:ASP:N	2.29	0.64
1:B:215:MET:HE3	1:B:227:PHE:H	1.62	0.64
1:B:64:ALA:N	1:B:260:GLN:HE22	1.96	0.64
1:A:84:ASN:HD22	1:A:86:GLU:H	1.46	0.64
1:A:254:LYS:O	1:A:255:ASN:HB2	1.98	0.64
1:B:9:LYS:C	1:B:91:TYR:CE2	2.70	0.64
1:B:69:HIS:O	1:B:73:LEU:HG	1.97	0.64
1:B:192:ASN:HD22	1:B:198:ILE:CD1	2.10	0.64
1:B:262:PHE:CE2	1:B:274:GLU:CG	2.77	0.64
1:B:113:PHE:CD1	1:B:114:MET:HE2	2.32	0.64
1:B:9:LYS:C	1:B:91:TYR:HE2	2.02	0.64
1:B:57:ASN:HD22	1:B:60:HIS:H	1.46	0.63
1:A:29:LEU:CD2	1:A:80:LEU:CD2	2.72	0.63
1:B:77:GLU:O	1:B:80:LEU:HB2	1.97	0.63
1:A:127:ASP:CA	1:A:132:ALA:CB	2.75	0.63
1:A:142:GLN:OE1	1:B:47:LYS:CE	2.46	0.63
1:A:254:LYS:C	1:A:256:GLY:H	2.01	0.63
1:A:10:ASN:OD1	1:A:10:ASN:C	2.35	0.63
1:A:161:THR:HG23	1:A:206:ARG:HH12	1.62	0.63
1:B:29:LEU:O	1:B:31:GLU:N	2.32	0.63
1:A:119:ASN:ND2	1:A:119:ASN:C	2.52	0.63
1:B:113:PHE:HE1	1:B:229:LEU:HD21	1.62	0.63
1:A:246:ARG:CG	1:A:246:ARG:NH1	2.60	0.63
1:B:263:ARG:NH1	1:B:274:GLU:OE1	2.31	0.63
1:A:161:THR:O	1:A:206:ARG:HD3	1.99	0.62
1:A:156:THR:CG2	1:A:209:ARG:HH21	2.12	0.62
1:A:256:GLY:H	1:A:261:ASN:ND2	1.97	0.62
1:B:286:TYR:O	1:B:287:ASP:C	2.35	0.62
1:A:4:LYS:HG2	1:A:280:ARG:HG2	1.78	0.62
1:B:54:SER:HG	1:B:56:ARG:N	1.96	0.62
1:B:272:THR:O	1:B:275:ASP:HB2	1.99	0.62
1:A:107:GLN:OE1	1:A:110:SER:HB3	1.98	0.62
1:B:71:GLU:OE1	1:B:271:THR:CB	2.48	0.62
1:A:100:MET:O	1:A:103:PRO:HD3	2.00	0.61
1:B:76:PHE:CD1	1:B:76:PHE:O	2.53	0.61
1:A:181:PRO:O	1:A:182:TRP:HD1	1.83	0.61
1:A:256:GLY:O	1:A:261:ASN:OD1	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASP:OD1	1:A:16:ASP:N	2.30	0.61
1:A:204:HIS:CD2	1:A:230:HIS:CE1	2.89	0.61
1:B:207:VAL:O	1:B:210:TRP:N	2.33	0.61
1:A:81:GLN:OE1	1:A:87:VAL:O	2.18	0.61
1:A:178:ASP:O	1:A:179:THR:CG2	2.49	0.61
1:B:70:ARG:NH1	1:B:238:TRP:CZ3	2.68	0.61
1:A:102:ASP:OD1	1:A:102:ASP:C	2.39	0.61
1:B:51:PRO:CB	1:B:52:PRO:HD2	2.28	0.61
1:B:208:HIS:HA	1:B:215:MET:O	2.01	0.61
1:B:207:VAL:O	1:B:211:VAL:N	2.26	0.60
1:A:119:ASN:HD22	1:A:121:ILE:H	1.50	0.60
1:B:66:LEU:HD11	1:B:191:ARG:CG	2.30	0.60
1:B:181:PRO:O	1:B:182:TRP:CD1	2.54	0.60
1:A:5:TYR:O	1:A:6:ARG:O	2.18	0.60
1:A:131:PHE:CD1	1:A:225:PRO:HG2	2.36	0.60
1:A:221:ALA:HB3	1:A:222:PRO:CD	2.27	0.60
1:B:138:THR:CG2	1:B:223:ASN:CB	2.79	0.60
1:B:182:TRP:CZ3	1:B:252:PRO:HD3	2.37	0.60
1:B:218:VAL:O	1:B:219:PRO:C	2.40	0.60
1:A:97:ASP:O	1:A:103:PRO:HB3	2.01	0.60
1:A:42:HIS:HD2	1:A:68:TRP:CZ3	2.20	0.60
1:A:94:TRP:CZ3	1:A:163:PRO:CG	2.83	0.60
1:A:278:ASN:HD22	1:A:281:LYS:HD3	1.65	0.60
1:B:285:VAL:O	1:B:285:VAL:CG1	2.47	0.60
1:A:28:ILE:O	1:A:32:LYS:CD	2.49	0.60
1:A:125:ILE:HG22	1:A:126:VAL:N	2.17	0.60
1:B:24:ARG:CB	1:B:24:ARG:NH1	2.30	0.60
1:A:15:THR:OG1	1:A:16:ASP:N	2.30	0.59
1:B:256:GLY:CA	1:B:261:ASN:OD1	2.49	0.59
1:B:258:PHE:HD1	1:B:264:ASP:OD2	1.83	0.59
1:B:57:ASN:HD22	1:B:60:HIS:N	2.00	0.59
1:B:15:THR:OG1	1:B:17:THR:N	2.32	0.59
1:A:129:GLY:C	1:A:131:PHE:H	2.05	0.59
1:B:15:THR:OG1	1:B:17:THR:CG2	2.51	0.59
1:A:48:PHE:CE2	1:A:50:THR:HG21	2.38	0.59
1:A:158:GLU:CG	1:A:209:ARG:NH2	2.65	0.59
1:A:6:ARG:HD3	1:A:81:GLN:NE2	2.17	0.59
1:A:161:THR:CG2	1:A:206:ARG:HH12	2.15	0.59
1:A:45:ALA:HB1	1:A:58:ALA:HB3	1.83	0.59
1:B:193:GLN:O	1:B:203:LEU:HD12	2.03	0.59
1:A:25:THR:CG2	1:A:80:LEU:HD22	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HG12	1:A:108:ILE:O	2.02	0.59
1:B:10:ASN:CA	1:B:91:TYR:CE2	2.86	0.59
1:A:93:GLU:OE1	1:A:96:THR:HG21	2.02	0.59
1:A:126:VAL:C	1:A:132:ALA:HB1	2.22	0.59
1:A:278:ASN:ND2	1:A:281:LYS:HD3	2.18	0.59
1:A:4:LYS:CG	1:A:280:ARG:CG	2.70	0.58
1:B:91:TYR:CE1	1:B:236:ARG:HD2	2.38	0.58
1:B:204:HIS:O	1:B:205:ASN:C	2.41	0.58
1:A:117:ASN:ND2	1:A:118:GLY:H	2.01	0.58
1:B:62:SER:HA	1:B:182:TRP:O	2.03	0.58
1:A:20:ARG:HH21	1:A:24:ARG:NH2	1.93	0.58
1:A:89:LEU:CD2	1:A:90:PRO:O	2.51	0.58
1:B:68:TRP:CZ3	1:B:72:TYR:CD1	2.91	0.58
1:B:91:TYR:N	1:B:91:TYR:CD2	2.71	0.58
1:A:64:ALA:H	1:A:260:GLN:HE22	1.51	0.58
1:A:246:ARG:HG2	1:A:246:ARG:NH1	2.14	0.58
1:B:71:GLU:CD	1:B:75:ARG:NH2	2.56	0.58
1:A:180:PRO:HD3	1:A:182:TRP:CH2	2.37	0.58
1:B:94:TRP:HE1	1:B:230:HIS:CD2	2.20	0.58
1:B:119:ASN:HD22	1:B:120:PRO:N	2.00	0.58
1:A:66:LEU:HD12	1:A:177:TYR:CE1	2.39	0.58
1:A:119:ASN:HD22	1:A:120:PRO:N	2.02	0.58
1:B:207:VAL:C	1:B:209:ARG:N	2.53	0.58
1:B:244:ILE:HG22	1:B:245:HIS:N	2.17	0.58
1:A:285:VAL:HG22	1:A:286:TYR:N	2.19	0.58
1:B:63:SER:OG	1:B:178:ASP:CG	2.40	0.58
1:A:124:PHE:CE2	1:A:152:ASN:OD1	2.57	0.58
1:A:142:GLN:HE22	1:B:47:LYS:HZ3	1.38	0.58
1:A:160:PRO:HG2	1:A:161:THR:HG22	1.86	0.58
1:B:49:HIS:HB2	1:B:52:PRO:HA	1.86	0.58
1:A:14:LEU:C	1:A:15:THR:O	2.36	0.57
1:A:254:LYS:C	1:A:256:GLY:N	2.55	0.57
1:A:6:ARG:HB2	1:A:283:GLY:O	2.03	0.57
1:B:153:PHE:CE2	1:B:210:TRP:CZ3	2.91	0.57
1:B:15:THR:HG1	1:B:18:GLU:H	1.52	0.57
1:B:48:PHE:CE2	1:B:50:THR:HG22	2.39	0.57
1:A:167:ASP:O	1:A:168:VAL:C	2.42	0.57
1:B:91:TYR:CD1	1:B:236:ARG:HD3	2.40	0.57
1:A:191:ARG:HD2	1:A:191:ARG:O	2.04	0.57
1:B:208:HIS:CB	1:B:215:MET:O	2.53	0.57
1:A:102:ASP:CG	1:A:104:SER:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HG2	1:B:235:ASP:OD2	2.03	0.57
1:A:70:ARG:HG3	1:A:238:TRP:CZ3	2.40	0.57
1:A:102:ASP:OD1	1:A:104:SER:N	2.32	0.57
1:B:66:LEU:CD1	1:B:177:TYR:CZ	2.87	0.57
1:B:59:ALA:O	1:B:65:PHE:HA	2.04	0.57
1:B:108:ILE:CG2	1:B:109:TRP:CD1	2.86	0.57
1:A:156:THR:HG23	1:A:158:GLU:N	2.13	0.57
1:B:284:TYR:O	1:B:284:TYR:HD1	1.86	0.57
1:A:60:HIS:CD2	1:A:60:HIS:N	2.73	0.56
1:A:84:ASN:HD22	1:A:84:ASN:C	2.08	0.56
1:B:66:LEU:HD11	1:B:191:ARG:HG2	1.87	0.56
1:B:262:PHE:O	1:B:262:PHE:CD2	2.58	0.56
1:B:91:TYR:HA	1:B:232:ALA:HB3	1.87	0.56
1:A:22:PHE:CE1	1:A:90:PRO:CD	2.87	0.56
1:A:94:TRP:NE1	1:A:230:HIS:HD2	2.03	0.56
1:B:8:ARG:NH2	1:B:286:TYR:HH	1.98	0.56
1:B:11:VAL:HG11	1:B:108:ILE:HG13	1.87	0.56
1:B:57:ASN:ND2	1:B:60:HIS:N	2.53	0.56
1:B:67:PRO:HA	1:B:70:ARG:HB2	1.87	0.56
1:B:153:PHE:HB3	1:B:210:TRP:CZ2	2.40	0.56
1:A:182:TRP:CH2	1:A:252:PRO:HB3	2.41	0.56
1:B:103:PRO:C	1:B:105:GLN:N	2.59	0.56
1:A:73:LEU:HD11	1:A:231:HIS:HB3	1.88	0.56
1:A:288:ILE:C	1:A:289:GLU:CG	2.74	0.56
1:B:6:ARG:NH2	1:B:283:GLY:O	2.39	0.56
1:A:253:MET:HE2	1:A:262:PHE:HB3	1.88	0.56
1:A:287:ASP:O	1:A:288:ILE:HG12	2.06	0.56
1:A:70:ARG:HD3	1:A:235:ASP:CG	2.26	0.56
1:A:109:TRP:HZ3	1:A:151:ARG:NH1	2.04	0.56
1:A:145:PRO:HD3	1:B:52:PRO:HB2	1.88	0.56
1:B:49:HIS:C	1:B:51:PRO:O	2.44	0.56
1:A:10:ASN:OD1	1:A:12:LEU:N	2.38	0.56
1:A:30:LYS:HA	1:A:35:TYR:HB3	1.86	0.56
1:A:181:PRO:C	1:A:182:TRP:CG	2.78	0.56
1:A:62:SER:OG	1:A:260:GLN:CD	2.45	0.56
1:A:246:ARG:CZ	1:A:246:ARG:CB	2.84	0.56
1:B:156:THR:CG2	1:B:159:ALA:N	2.69	0.56
1:B:218:VAL:CG1	1:B:219:PRO:CD	2.82	0.56
1:A:127:ASP:OD1	1:A:127:ASP:N	2.37	0.55
1:A:156:THR:HG23	1:A:158:GLU:CB	2.36	0.55
1:A:162:LEU:HD22	1:A:163:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG22	1:A:80:LEU:HD22	1.88	0.55
1:B:100:MET:CE	1:B:103:PRO:HA	2.35	0.55
1:A:99:GLN:O	1:A:100:MET:C	2.45	0.55
1:A:254:LYS:O	1:A:256:GLY:N	2.40	0.55
1:B:119:ASN:HD22	1:B:119:ASN:C	2.07	0.55
1:A:139:ILE:HG22	1:A:140:ASP:N	2.17	0.55
1:B:138:THR:CG2	1:B:223:ASN:HB3	2.36	0.55
1:B:218:VAL:HB	1:B:219:PRO:HD2	1.89	0.55
1:B:113:PHE:HD1	1:B:114:MET:CG	2.09	0.55
1:B:285:VAL:O	1:B:285:VAL:HG12	2.05	0.55
1:A:38:TYR:CD2	1:A:76:PHE:CD1	2.95	0.55
1:A:243:ILE:HG23	1:A:246:ARG:HH21	1.72	0.55
1:B:165:ARG:NH1	1:B:169:LEU:HD21	2.22	0.55
1:B:181:PRO:C	1:B:182:TRP:CD1	2.80	0.55
1:B:280:ARG:O	1:B:283:GLY:N	2.36	0.55
1:A:60:HIS:NE2	1:A:69:HIS:HE1	2.05	0.54
1:B:260:GLN:NE2	1:B:260:GLN:HA	2.21	0.54
1:A:59:ALA:O	1:A:65:PHE:CA	2.55	0.54
1:B:31:GLU:O	1:B:31:GLU:CD	2.46	0.54
1:B:236:ARG:NH1	1:B:236:ARG:HG2	2.20	0.54
1:B:256:GLY:N	1:B:261:ASN:OD1	2.40	0.54
1:A:256:GLY:CA	1:A:261:ASN:OD1	2.56	0.54
1:B:57:ASN:HD21	1:B:60:HIS:CB	2.17	0.54
1:B:77:GLU:O	1:B:80:LEU:CB	2.56	0.54
1:A:158:GLU:HB2	1:A:209:ARG:HH22	1.66	0.54
1:A:28:ILE:HG21	1:A:83:ILE:HD13	1.90	0.54
1:B:8:ARG:HD2	1:B:284:TYR:HD2	1.73	0.54
1:B:37:ARG:HH11	1:B:37:ARG:HB2	1.72	0.54
1:B:217:VAL:HG23	1:B:220:THR:OG1	2.08	0.54
1:A:28:ILE:HG22	1:A:29:LEU:N	2.22	0.53
1:A:34:ILE:O	1:A:34:ILE:CG2	2.57	0.53
1:B:156:THR:CG2	1:B:159:ALA:H	2.17	0.53
1:A:65:PHE:CZ	1:A:204:HIS:CE1	2.96	0.53
1:A:156:THR:CG2	1:A:158:GLU:CB	2.86	0.53
1:B:266:MET:O	1:B:267:TYR:C	2.44	0.53
1:A:96:THR:O	1:A:99:GLN:HG3	2.09	0.53
1:B:194:LEU:HD23	1:B:194:LEU:C	2.11	0.53
1:B:8:ARG:NE	1:B:286:TYR:CZ	2.76	0.53
1:A:7:VAL:HG13	1:A:7:VAL:O	2.09	0.53
1:B:8:ARG:HD2	1:B:284:TYR:CD2	2.43	0.53
1:B:76:PHE:HD2	1:B:228:PHE:HD1	1.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:O	1:B:180:PRO:C	2.47	0.53
1:B:190:PHE:CZ	1:B:194:LEU:HD12	2.43	0.53
1:B:278:ASN:O	1:B:282:LEU:HG	2.09	0.53
1:A:20:ARG:CZ	1:A:24:ARG:NH2	2.72	0.53
1:B:56:ARG:HB3	1:B:62:SER:HB3	1.90	0.53
1:A:28:ILE:HG21	1:A:83:ILE:CD1	2.39	0.53
1:A:94:TRP:HE1	1:A:230:HIS:CD2	2.21	0.53
1:B:254:LYS:N	1:B:261:ASN:ND2	2.49	0.53
1:A:193:GLN:HG2	1:A:198:ILE:HG13	1.91	0.52
1:B:156:THR:HG23	1:B:158:GLU:H	1.73	0.52
1:B:181:PRO:O	1:B:182:TRP:CB	2.58	0.52
1:A:287:ASP:OD1	1:A:287:ASP:C	2.48	0.52
1:B:124:PHE:CE2	1:B:152:ASN:OD1	2.62	0.52
1:B:103:PRO:C	1:B:105:GLN:H	2.13	0.52
1:B:239:ALA:O	1:B:242:GLN:HB2	2.09	0.52
1:A:256:GLY:CA	1:A:261:ASN:CG	2.72	0.52
1:B:204:HIS:CD2	1:B:230:HIS:HE1	2.27	0.52
1:A:4:LYS:HG3	1:A:280:ARG:CB	2.38	0.52
1:A:256:GLY:C	1:A:261:ASN:OD1	2.47	0.52
1:A:38:TYR:OH	1:A:76:PHE:CA	2.57	0.52
1:A:70:ARG:NE	1:A:235:ASP:OD2	2.43	0.52
1:B:76:PHE:CE2	1:B:228:PHE:CZ	2.98	0.52
1:B:119:ASN:HD22	1:B:120:PRO:CD	2.23	0.52
1:A:287:ASP:C	1:A:288:ILE:HG12	2.30	0.52
1:B:56:ARG:HD3	1:B:62:SER:HB2	1.92	0.52
1:B:73:LEU:HD11	1:B:231:HIS:O	2.10	0.52
1:A:40:ALA:HB1	1:B:267:TYR:CZ	2.45	0.52
1:B:117:ASN:HD21	1:B:152:ASN:HA	1.75	0.52
1:B:71:GLU:HA	1:B:74:LEU:HB3	1.91	0.51
1:A:11:VAL:O	1:A:14:LEU:HB2	2.09	0.51
1:B:37:ARG:HH11	1:B:37:ARG:CB	2.22	0.51
1:B:93:GLU:OE1	1:B:96:THR:HG21	2.10	0.51
1:B:207:VAL:O	1:B:209:ARG:N	2.42	0.51
1:B:260:GLN:HA	1:B:260:GLN:HE21	1.74	0.51
1:B:64:ALA:H	1:B:260:GLN:HE22	1.58	0.51
1:B:158:GLU:O	1:B:158:GLU:HG3	2.09	0.51
1:B:227:PHE:O	1:B:230:HIS:HB3	2.10	0.51
1:B:48:PHE:O	1:B:48:PHE:HD2	1.86	0.51
1:B:106:SER:C	1:B:108:ILE:H	2.13	0.51
1:A:100:MET:HE2	1:A:105:GLN:HB2	1.93	0.51
1:A:182:TRP:CZ3	1:A:252:PRO:HB3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:HIS:HB3	1:B:248:GLN:HG2	1.93	0.51
1:B:265:PRO:HA	1:B:272:THR:CG2	2.38	0.51
1:A:132:ALA:O	1:A:133:ALA:O	2.29	0.51
1:B:91:TYR:CE1	1:B:236:ARG:CD	2.94	0.51
1:B:201:PRO:O	1:B:206:ARG:CB	2.58	0.51
1:B:250:TYR:HD2	1:B:250:TYR:C	2.13	0.51
1:B:256:GLY:C	1:B:257:PRO:O	2.49	0.51
1:B:279:HIS:O	1:B:284:TYR:HD1	1.94	0.51
1:A:109:TRP:CE3	1:A:151:ARG:NH1	2.79	0.51
1:A:66:LEU:N	1:A:67:PRO:HD2	2.26	0.51
1:B:25:THR:O	1:B:28:ILE:HG22	2.11	0.51
1:A:229:LEU:O	1:A:232:ALA:HB3	2.11	0.50
1:B:124:PHE:CD2	1:B:152:ASN:OD1	2.64	0.50
1:B:153:PHE:CD1	1:B:153:PHE:N	2.79	0.50
1:B:250:TYR:CE2	1:B:251:GLN:O	2.64	0.50
1:A:34:ILE:O	1:A:34:ILE:HG22	2.11	0.50
1:B:243:ILE:O	1:B:244:ILE:C	2.49	0.50
1:A:25:THR:HG22	1:A:80:LEU:CD2	2.41	0.50
1:A:156:THR:HG23	1:A:158:GLU:HB2	1.94	0.50
1:A:156:THR:CG2	1:A:158:GLU:HB3	2.42	0.50
1:A:91:TYR:HA	1:A:232:ALA:HB3	1.94	0.50
1:B:31:GLU:O	1:B:31:GLU:OE2	2.30	0.50
1:B:138:THR:HG22	1:B:223:ASN:CB	2.36	0.50
1:A:60:HIS:CD2	1:A:69:HIS:CE1	2.86	0.50
1:A:174:ILE:HG21	1:A:190:PHE:N	2.27	0.50
1:B:23:VAL:O	1:B:23:VAL:HG13	2.07	0.50
1:B:119:ASN:HD22	1:B:120:PRO:HD2	1.77	0.50
1:B:153:PHE:N	1:B:153:PHE:HD1	2.09	0.50
1:B:239:ALA:HB1	1:B:279:HIS:NE2	2.26	0.50
1:B:8:ARG:CD	1:B:284:TYR:CD2	2.94	0.49
1:A:5:TYR:C	1:A:6:ARG:O	2.51	0.49
1:A:8:ARG:HH12	1:A:77:GLU:CD	2.02	0.49
1:A:222:PRO:HG3	1:A:227:PHE:CZ	2.47	0.49
1:A:15:THR:CG2	1:A:18:GLU:CD	2.75	0.49
1:A:119:ASN:OD1	1:A:122:LYS:HD2	2.11	0.49
1:A:280:ARG:O	1:A:282:LEU:N	2.46	0.49
1:B:179:THR:O	1:B:180:PRO:O	2.30	0.49
1:B:181:PRO:C	1:B:182:TRP:CG	2.86	0.49
1:A:102:ASP:OD1	1:A:102:ASP:O	2.30	0.49
1:B:217:VAL:CG2	1:B:220:THR:OG1	2.60	0.49
1:B:254:LYS:HA	1:B:261:ASN:HD21	0.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:CG2	1:A:83:ILE:CD1	2.91	0.49
1:B:62:SER:O	1:B:191:ARG:HD3	2.13	0.49
1:B:119:ASN:ND2	1:B:120:PRO:HD2	2.28	0.49
1:B:272:THR:O	1:B:275:ASP:N	2.42	0.49
1:A:243:ILE:HA	1:A:246:ARG:HE	1.76	0.49
1:B:76:PHE:O	1:B:76:PHE:HD1	1.95	0.49
1:B:256:GLY:O	1:B:257:PRO:O	2.30	0.49
1:A:246:ARG:O	1:A:247:ASN:C	2.49	0.49
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.26	0.49
1:B:94:TRP:CB	1:B:162:LEU:HD22	2.41	0.49
1:B:103:PRO:O	1:B:105:GLN:N	2.46	0.49
1:B:117:ASN:ND2	1:B:118:GLY:H	2.11	0.49
1:A:217:VAL:C	1:A:219:PRO:HD2	2.33	0.49
1:A:236:ARG:HB2	1:A:286:TYR:CZ	2.46	0.49
1:B:38:TYR:OH	1:B:76:PHE:HA	2.13	0.49
1:B:42:HIS:HB3	1:B:222:PRO:HG2	1.94	0.49
1:B:71:GLU:CD	1:B:75:ARG:HH21	2.14	0.49
1:B:4:LYS:HZ2	1:B:280:ARG:HG2	1.78	0.48
1:B:61:MET:O	1:B:62:SER:HB3	2.11	0.48
1:A:54:SER:O	1:A:55:ASP:C	2.50	0.48
1:A:66:LEU:HD12	1:A:177:TYR:CZ	2.48	0.48
1:B:8:ARG:CZ	1:B:286:TYR:OH	2.59	0.48
1:B:206:ARG:O	1:B:210:TRP:N	2.46	0.48
1:B:250:TYR:CD2	1:B:250:TYR:C	2.83	0.48
1:A:27:LEU:O	1:A:30:LYS:N	2.47	0.48
1:A:233:ASN:O	1:A:237:ILE:HG12	2.14	0.48
1:B:10:ASN:OD1	1:B:12:LEU:HD12	2.14	0.48
1:A:108:ILE:HG13	1:A:113:PHE:CE1	2.49	0.48
1:A:167:ASP:O	1:A:170:ASN:N	2.47	0.48
1:B:51:PRO:CB	1:B:52:PRO:CD	2.87	0.48
1:B:109:TRP:O	1:B:115:GLY:O	2.30	0.48
1:B:153:PHE:CE2	1:B:210:TRP:CH2	2.88	0.48
1:A:244:ILE:HG22	1:A:245:HIS:N	2.27	0.48
1:B:242:GLN:O	1:B:246:ARG:HA	2.13	0.48
1:A:70:ARG:HG3	1:A:238:TRP:HZ3	1.76	0.48
1:A:162:LEU:CD2	1:A:163:PRO:HD2	2.44	0.48
1:A:32:LYS:CB	1:A:32:LYS:HZ2	2.27	0.48
1:B:76:PHE:CE2	1:B:228:PHE:CG	2.92	0.48
1:A:61:MET:O	1:A:183:ASP:HA	2.14	0.48
3:A:402:SDS:H9C1	3:A:402:SDS:H6C2	1.18	0.48
1:B:253:MET:O	1:B:254:LYS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:C	1:B:31:GLU:N	2.65	0.47
1:B:265:PRO:HB3	1:B:270:ASN:HA	1.94	0.47
1:A:51:PRO:HB2	1:A:52:PRO:HD2	1.95	0.47
1:B:260:GLN:HE21	1:B:260:GLN:CA	2.27	0.47
1:A:278:ASN:ND2	1:A:281:LYS:HB2	2.29	0.47
1:B:35:TYR:O	1:B:37:ARG:N	2.47	0.47
1:B:153:PHE:CG	1:B:210:TRP:CH2	2.91	0.47
1:A:59:ALA:O	1:A:65:PHE:HB2	2.15	0.47
1:A:89:LEU:CD2	1:A:90:PRO:N	2.69	0.47
1:A:278:ASN:HD22	1:A:281:LYS:HB2	1.79	0.47
1:B:66:LEU:HD13	1:B:177:TYR:CE1	2.49	0.47
1:A:22:PHE:HE1	1:A:90:PRO:HD3	1.74	0.47
1:B:109:TRP:CD2	1:B:153:PHE:HZ	2.33	0.47
1:B:198:ILE:N	1:B:198:ILE:HD13	2.29	0.47
1:A:89:LEU:C	1:A:89:LEU:HD22	2.33	0.47
1:A:153:PHE:HE1	1:A:211:VAL:HG13	1.78	0.47
1:B:57:ASN:O	1:B:59:ALA:N	2.47	0.47
1:B:69:HIS:CD2	1:B:231:HIS:CE1	3.03	0.47
1:B:71:GLU:O	1:B:71:GLU:CG	2.61	0.47
1:B:94:TRP:CE3	1:B:163:PRO:HG2	2.49	0.47
1:A:109:TRP:HB3	1:A:116:GLY:HA2	1.96	0.47
1:B:62:SER:OG	1:B:260:GLN:NE2	2.48	0.47
1:B:138:THR:HG21	1:B:223:ASN:HB3	1.95	0.47
1:A:162:LEU:HD22	1:A:163:PRO:CD	2.45	0.47
1:A:38:TYR:OH	1:A:75:ARG:C	2.53	0.46
1:B:102:ASP:OD1	1:B:104:SER:OG	2.29	0.46
1:B:108:ILE:HD11	1:B:229:LEU:HD23	1.97	0.46
1:A:138:THR:O	1:A:138:THR:OG1	2.33	0.46
1:A:156:THR:HG21	1:A:158:GLU:HB3	1.96	0.46
1:A:156:THR:HG21	1:A:209:ARG:NH2	2.24	0.46
1:B:117:ASN:HD21	1:B:152:ASN:CA	2.27	0.46
1:A:69:HIS:CD2	1:A:231:HIS:CE1	3.03	0.46
1:B:140:ASP:OD2	1:B:144:ASN:O	2.33	0.46
1:B:218:VAL:HB	1:B:219:PRO:HD3	1.97	0.46
1:A:139:ILE:HG23	1:A:140:ASP:N	2.29	0.46
1:B:239:ALA:HB1	1:B:279:HIS:CD2	2.50	0.46
1:A:41:TRP:CD1	1:B:267:TYR:CE1	3.03	0.46
1:A:71:GLU:O	1:A:75:ARG:HG3	2.16	0.46
1:B:50:THR:N	1:B:51:PRO:O	2.49	0.46
1:B:206:ARG:O	1:B:209:ARG:HB2	2.16	0.46
1:A:41:TRP:CD1	1:B:267:TYR:HE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:CD2	1:A:178:ASP:HB2	2.50	0.46
1:A:178:ASP:C	1:A:179:THR:CG2	2.84	0.46
1:B:29:LEU:C	1:B:31:GLU:H	2.19	0.46
1:A:10:ASN:HB2	1:A:91:TYR:CZ	2.51	0.46
1:B:11:VAL:HG23	1:B:91:TYR:O	2.16	0.46
1:B:106:SER:C	1:B:108:ILE:N	2.68	0.46
1:B:236:ARG:O	1:B:240:VAL:HG23	2.16	0.46
1:B:250:TYR:CD2	1:B:251:GLN:C	2.89	0.46
1:B:264:ASP:C	1:B:272:THR:HG22	2.37	0.46
1:B:190:PHE:HE2	1:B:238:TRP:HD1	1.64	0.46
1:A:162:LEU:CB	1:A:163:PRO:CD	2.91	0.45
1:B:68:TRP:CH2	1:B:72:TYR:CE1	3.03	0.45
1:B:70:ARG:CG	1:B:235:ASP:OD2	2.64	0.45
1:B:244:ILE:HG22	1:B:245:HIS:CD2	2.51	0.45
1:B:279:HIS:O	1:B:284:TYR:O	2.34	0.45
1:A:56:ARG:NH1	1:A:56:ARG:CG	2.49	0.45
1:A:70:ARG:HD3	1:A:235:ASP:OD1	2.16	0.45
1:B:125:ILE:HG22	1:B:125:ILE:O	2.14	0.45
1:B:287:ASP:O	1:B:288:ILE:CB	2.63	0.45
1:A:32:LYS:HZ2	1:A:32:LYS:HB3	1.81	0.45
1:A:38:TYR:OH	1:A:76:PHE:N	2.49	0.45
1:A:164:THR:C	1:A:166:ASP:N	2.69	0.45
1:A:127:ASP:C	1:A:132:ALA:CB	2.85	0.45
3:A:402:SDS:H101	3:A:402:SDS:O2S	2.15	0.45
1:B:192:ASN:ND2	1:B:198:ILE:CD1	2.78	0.45
1:B:257:PRO:HG2	1:B:260:GLN:CG	2.46	0.45
1:A:221:ALA:CB	1:A:222:PRO:HD3	2.30	0.45
1:B:76:PHE:CD2	1:B:228:PHE:HE1	2.21	0.45
1:B:181:PRO:O	1:B:182:TRP:HB2	2.16	0.45
1:A:134:GLY:C	1:A:135:ARG:HG2	2.35	0.45
1:A:285:VAL:HG22	1:A:286:TYR:H	1.81	0.45
1:B:108:ILE:CG2	1:B:109:TRP:N	2.76	0.45
1:A:177:TYR:CD2	1:A:177:TYR:C	2.90	0.45
1:A:207:VAL:HG11	1:A:230:HIS:CD2	2.52	0.45
1:A:138:THR:O	1:A:146:SER:OG	2.29	0.45
1:B:153:PHE:HA	1:B:210:TRP:O	2.16	0.45
1:A:23:VAL:O	1:A:27:LEU:HG	2.17	0.45
1:A:156:THR:CG2	1:A:158:GLU:N	2.77	0.45
1:A:203:LEU:O	1:A:207:VAL:HG23	2.16	0.45
1:B:91:TYR:HD2	1:B:91:TYR:N	2.11	0.45
1:B:153:PHE:HD1	1:B:153:PHE:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:O	1:B:173:LYS:HB2	2.16	0.45
1:A:246:ARG:NH1	1:A:246:ARG:CB	2.81	0.44
1:B:22:PHE:HE1	1:B:89:LEU:HD23	1.81	0.44
1:B:114:MET:HA	1:B:131:PHE:CD1	2.52	0.44
1:A:119:ASN:HD21	1:A:121:ILE:HG12	1.82	0.44
1:B:166:ASP:O	1:B:167:ASP:C	2.56	0.44
1:B:279:HIS:CB	1:B:284:TYR:HE1	2.31	0.44
1:A:66:LEU:HD12	1:A:177:TYR:OH	2.17	0.44
1:A:66:LEU:HD21	1:A:194:LEU:CD1	2.48	0.44
1:B:6:ARG:CD	1:B:284:TYR:HB3	2.47	0.44
1:B:61:MET:O	1:B:62:SER:CB	2.65	0.44
1:B:114:MET:HA	1:B:131:PHE:CE1	2.52	0.44
1:B:6:ARG:O	1:B:6:ARG:CG	2.48	0.44
1:B:63:SER:O	1:B:250:TYR:CZ	2.70	0.44
1:B:244:ILE:HG22	1:B:245:HIS:CG	2.52	0.44
1:B:262:PHE:HE2	1:B:274:GLU:CG	2.09	0.44
1:A:254:LYS:HD2	1:A:255:ASN:ND2	2.33	0.44
1:A:190:PHE:CD1	1:A:241:TRP:CD1	3.05	0.44
1:B:6:ARG:HE	1:B:284:TYR:CB	2.18	0.44
1:B:59:ALA:O	1:B:65:PHE:CA	2.65	0.44
1:A:15:THR:OG1	1:A:17:THR:HG23	2.18	0.44
1:A:95:GLU:HB2	1:A:165:ARG:CB	2.48	0.44
1:B:273:PRO:O	1:B:274:GLU:C	2.56	0.44
1:B:187:GLN:O	1:B:188:ASN:C	2.55	0.43
1:B:273:PRO:C	1:B:275:ASP:N	2.69	0.43
1:B:7:VAL:HA	1:B:285:VAL:O	2.17	0.43
1:B:78:ARG:C	1:B:80:LEU:N	2.71	0.43
1:B:109:TRP:CE3	1:B:153:PHE:HZ	2.36	0.43
1:A:16:ASP:C	1:A:18:GLU:H	2.21	0.43
1:A:81:GLN:O	1:A:82:SER:C	2.56	0.43
1:A:74:LEU:CD2	1:A:282:LEU:HD22	2.49	0.43
1:B:60:HIS:O	1:B:61:MET:C	2.57	0.43
1:B:124:PHE:HB3	1:B:151:ARG:O	2.18	0.43
1:B:250:TYR:HD2	1:B:251:GLN:CA	2.27	0.43
1:A:40:ALA:O	1:A:41:TRP:C	2.54	0.43
1:A:66:LEU:HB2	1:A:67:PRO:HD3	2.01	0.43
1:A:156:THR:CG2	1:A:159:ALA:N	2.79	0.43
1:A:164:THR:C	1:A:166:ASP:H	2.20	0.43
1:B:84:ASN:O	1:B:85:PRO:C	2.57	0.43
1:A:6:ARG:HB2	1:A:284:TYR:HA	2.01	0.43
1:B:131:PHE:CD2	1:B:225:PRO:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:HIS:O	1:A:73:LEU:HG	2.19	0.43
1:B:65:PHE:CZ	1:B:204:HIS:ND1	2.87	0.43
1:B:95:GLU:O	1:B:98:ALA:HB3	2.19	0.43
1:A:66:LEU:HD21	1:A:194:LEU:HD13	2.00	0.43
1:B:245:HIS:HB2	1:B:248:GLN:HB2	2.00	0.43
1:B:255:ASN:N	1:B:255:ASN:HD22	2.17	0.43
1:B:38:TYR:OH	1:B:75:ARG:C	2.53	0.43
1:B:202:GLN:HA	1:B:202:GLN:NE2	2.34	0.43
1:A:129:GLY:C	1:A:131:PHE:N	2.69	0.42
1:A:174:ILE:CD1	1:A:193:GLN:NE2	2.80	0.42
1:A:288:ILE:N	1:A:289:GLU:HG3	2.34	0.42
1:B:15:THR:HG1	1:B:17:THR:N	2.17	0.42
1:B:109:TRP:CE2	1:B:153:PHE:CZ	3.07	0.42
1:B:115:GLY:HA3	1:B:128:THR:O	2.18	0.42
1:A:72:TYR:CE2	1:A:227:PHE:HE1	2.37	0.42
1:A:202:GLN:O	1:A:203:LEU:C	2.58	0.42
1:B:70:ARG:HG3	1:B:238:TRP:CZ3	2.54	0.42
1:B:108:ILE:HG22	1:B:109:TRP:N	2.34	0.42
1:B:221:ALA:HB3	1:B:222:PRO:HD3	2.01	0.42
1:B:250:TYR:CB	1:B:262:PHE:HD1	2.24	0.42
1:A:32:LYS:CB	1:A:32:LYS:NZ	2.78	0.42
1:A:60:HIS:O	1:A:61:MET:CB	2.59	0.42
1:A:105:GLN:O	1:A:106:SER:C	2.55	0.42
1:B:56:ARG:HB3	1:B:62:SER:CB	2.50	0.42
1:B:81:GLN:HG3	1:B:85:PRO:HA	2.01	0.42
1:B:6:ARG:HD2	1:B:77:GLU:OE2	2.19	0.42
1:B:179:THR:C	1:B:180:PRO:O	2.56	0.42
1:B:266:MET:N	1:B:271:THR:O	2.52	0.42
1:B:35:TYR:O	1:B:36:ASP:C	2.55	0.42
1:B:133:ALA:HB2	1:B:148:GLY:HA3	2.01	0.42
1:A:59:ALA:CB	1:A:60:HIS:CD2	3.03	0.42
1:B:204:HIS:CD2	1:B:204:HIS:C	2.93	0.42
1:A:48:PHE:HD2	1:A:58:ALA:HB2	1.84	0.42
1:B:10:ASN:HA	1:B:91:TYR:CE2	2.55	0.42
1:B:113:PHE:HB3	1:B:114:MET:H	1.55	0.42
1:B:4:LYS:N	1:B:4:LYS:HD3	2.28	0.42
1:B:50:THR:HA	1:B:51:PRO:HA	1.84	0.42
1:B:190:PHE:HE2	1:B:238:TRP:CD1	2.37	0.42
1:A:89:LEU:HD22	1:A:90:PRO:O	2.19	0.41
1:A:196:GLY:HA3	1:A:202:GLN:O	2.20	0.41
1:B:243:ILE:HD12	1:B:243:ILE:HA	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD3	1:A:62:SER:OG	2.19	0.41
1:A:66:LEU:HB2	1:A:67:PRO:CD	2.49	0.41
1:A:138:THR:HG1	1:A:146:SER:HG	1.60	0.41
1:A:164:THR:O	1:A:166:ASP:N	2.53	0.41
1:B:29:LEU:O	1:B:30:LYS:C	2.57	0.41
1:B:35:TYR:OH	1:B:228:PHE:CE2	2.67	0.41
1:A:228:PHE:O	1:A:232:ALA:N	2.48	0.41
1:B:70:ARG:CZ	1:B:238:TRP:CE3	3.02	0.41
1:A:35:TYR:CD2	1:A:35:TYR:C	2.93	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.88	0.41
1:A:102:ASP:O	1:A:104:SER:N	2.52	0.41
1:A:184:MET:HB2	1:A:184:MET:HE2	1.87	0.41
1:A:254:LYS:O	1:A:255:ASN:CB	2.64	0.41
1:B:11:VAL:O	1:B:11:VAL:CG1	2.66	0.41
1:A:92:TRP:HB2	1:A:229:LEU:HB3	2.02	0.41
1:B:36:ASP:O	1:B:39:ILE:HB	2.21	0.41
1:B:245:HIS:C	1:B:247:ASN:N	2.73	0.41
1:A:10:ASN:HB2	1:A:91:TYR:CE1	2.56	0.41
1:B:65:PHE:HZ	1:B:204:HIS:HD1	1.64	0.41
1:B:230:HIS:CD2	1:B:230:HIS:C	2.90	0.41
1:A:279:HIS:O	1:A:280:ARG:C	2.56	0.41
1:B:181:PRO:O	1:B:182:TRP:HD1	2.03	0.41
1:A:6:ARG:HG2	1:A:81:GLN:HE22	1.85	0.41
1:A:156:THR:HG22	1:A:156:THR:O	2.19	0.41
1:A:178:ASP:OD1	1:A:189:SER:OG	2.36	0.41
1:B:254:LYS:N	1:B:261:ASN:HD22	2.13	0.41
1:A:51:PRO:CB	1:A:52:PRO:HD2	2.50	0.41
1:A:84:ASN:HD21	1:A:86:GLU:HB2	1.86	0.41
1:A:84:ASN:ND2	1:A:86:GLU:H	2.15	0.41
1:A:100:MET:CE	1:A:105:GLN:HB2	2.49	0.41
1:A:117:ASN:HD22	1:A:151:ARG:HB3	1.85	0.41
1:B:203:LEU:O	1:B:204:HIS:C	2.58	0.41
1:B:208:HIS:CG	1:B:215:MET:O	2.74	0.41
1:B:279:HIS:CB	1:B:284:TYR:CE1	3.02	0.41
1:A:102:ASP:C	1:A:104:SER:H	2.24	0.41
1:A:280:ARG:C	1:A:282:LEU:N	2.74	0.41
1:B:71:GLU:HG2	1:B:75:ARG:HD2	2.03	0.41
1:B:149:LEU:CD2	1:B:150:LYS:H	2.34	0.41
1:B:158:GLU:O	1:B:201:PRO:HG3	2.21	0.41
1:A:96:THR:O	1:A:99:GLN:CG	2.69	0.40
1:A:126:VAL:C	1:A:132:ALA:CB	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:CD1	1:B:284:TYR:C	2.94	0.40
1:A:11:VAL:HG13	1:A:113:PHE:CE1	2.57	0.40
1:A:95:GLU:CB	1:A:165:ARG:HA	2.40	0.40
1:B:195:GLU:O	1:B:204:HIS:HB3	2.20	0.40
1:A:191:ARG:HD2	1:A:191:ARG:C	2.42	0.40
1:A:224:ASP:O	1:A:225:PRO:C	2.60	0.40
1:A:238:TRP:O	1:A:242:GLN:HG3	2.22	0.40
1:B:11:VAL:O	1:B:11:VAL:HG12	2.22	0.40
1:B:61:MET:CE	1:B:197:PHE:HZ	2.34	0.40
1:A:48:PHE:CE2	1:A:50:THR:HG22	2.54	0.40
1:A:89:LEU:HA	1:A:90:PRO:HD3	1.70	0.40
1:A:183:ASP:OD2	1:A:183:ASP:N	2.53	0.40
1:A:227:PHE:O	1:A:230:HIS:HB3	2.21	0.40
1:A:252:PRO:HD2	1:A:260:GLN:O	2.22	0.40
1:B:76:PHE:CD1	1:B:76:PHE:C	2.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	284/303 (94%)	231 (81%)	42 (15%)	11 (4%)	3 25
1	B	283/303 (93%)	214 (76%)	54 (19%)	15 (5%)	2 17
All	All	567/606 (94%)	445 (78%)	96 (17%)	26 (5%)	2 21

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	55	ASP
1	A	287	ASP

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Mol	Chain	Res	Type
1	B	218	VAL
1	B	219	PRO
1	A	6	ARG
1	A	133	ALA
1	A	180	PRO
1	B	58	ALA
1	B	145	PRO
1	A	168	VAL
1	B	30	LYS
1	B	201	PRO
1	B	214	GLN
1	B	255	ASN
1	A	130	PRO
1	B	36	ASP
1	B	244	ILE
1	B	221	ALA
1	A	103	PRO
1	A	288	ILE
1	B	180	PRO
1	B	257	PRO
1	A	163	PRO
1	B	85	PRO
1	B	265	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	249/266 (94%)	201 (81%)	48 (19%)	1 7
1	B	248/266 (93%)	194 (78%)	54 (22%)	1 5
All	All	497/532 (93%)	395 (80%)	102 (20%)	1 6

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	8	ARG
1	A	12	LEU
1	A	15	THR
1	A	16	ASP
1	A	17	THR
1	A	20	ARG
1	A	24	ARG
1	A	28	ILE
1	A	29	LEU
1	A	32	LYS
1	A	36	ASP
1	A	37	ARG
1	A	47	LYS
1	A	56	ARG
1	A	60	HIS
1	A	62	SER
1	A	70	ARG
1	A	84	ASN
1	A	89	LEU
1	A	99	GLN
1	A	117	ASN
1	A	119	ASN
1	A	122	LYS
1	A	125	ILE
1	A	128	THR
1	A	135	ARG
1	A	142	GLN
1	A	144	ASN
1	A	149	LEU
1	A	151	ARG
1	A	152	ASN
1	A	156	THR
1	A	158	GLU
1	A	164	THR
1	A	165	ARG
1	A	182	TRP
1	A	184	MET
1	A	194	LEU
1	A	209	ARG
1	A	215	MET
1	A	229	LEU
1	A	246	ARG

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Mol	Chain	Res	Type
1	A	253	MET
1	A	254	LYS
1	A	280	ARG
1	A	288	ILE
1	A	289	GLU
1	B	4	LYS
1	B	6	ARG
1	B	12	LEU
1	B	15	THR
1	B	17	THR
1	B	18	GLU
1	B	19	LYS
1	B	24	ARG
1	B	28	ILE
1	B	29	LEU
1	B	30	LYS
1	B	32	LYS
1	B	37	ARG
1	B	54	SER
1	B	55	ASP
1	B	57	ASN
1	B	61	MET
1	B	62	SER
1	B	66	LEU
1	B	70	ARG
1	B	75	ARG
1	B	76	PHE
1	B	84	ASN
1	B	89	LEU
1	B	91	TYR
1	B	94	TRP
1	B	105	GLN
1	B	106	SER
1	B	108	ILE
1	B	114	MET
1	B	119	ASN
1	B	138	THR
1	B	149	LEU
1	B	152	ASN
1	B	153	PHE
1	B	156	THR
1	B	162	LEU

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Mol	Chain	Res	Type
1	B	169	LEU
1	B	193	GLN
1	B	198	ILE
1	B	205	ASN
1	B	206	ARG
1	B	208	HIS
1	B	215	MET
1	B	236	ARG
1	B	243	ILE
1	B	244	ILE
1	B	247	ASN
1	B	250	TYR
1	B	277	MET
1	B	284	TYR
1	B	285	VAL
1	B	287	ASP
1	B	288	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	84	ASN
1	A	101	GLN
1	A	117	ASN
1	A	119	ASN
1	A	142	GLN
1	A	144	ASN
1	A	152	ASN
1	A	176	GLN
1	A	193	GLN
1	A	202	GLN
1	A	204	HIS
1	A	205	ASN
1	A	230	HIS
1	A	231	HIS
1	A	255	ASN
1	A	260	GLN
1	A	261	ASN
1	A	270	ASN
1	A	278	ASN
1	B	57	ASN

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Mol	Chain	Res	Type
1	B	84	ASN
1	B	101	GLN
1	B	117	ASN
1	B	119	ASN
1	B	142	GLN
1	B	152	ASN
1	B	193	GLN
1	B	202	GLN
1	B	205	ASN
1	B	230	HIS
1	B	231	HIS
1	B	247	ASN
1	B	255	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	SDS	A	402	-	16,16,16	0.62	0	16,18,18	0.89	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	SDS	A	402	-	-	10/14/14/14	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

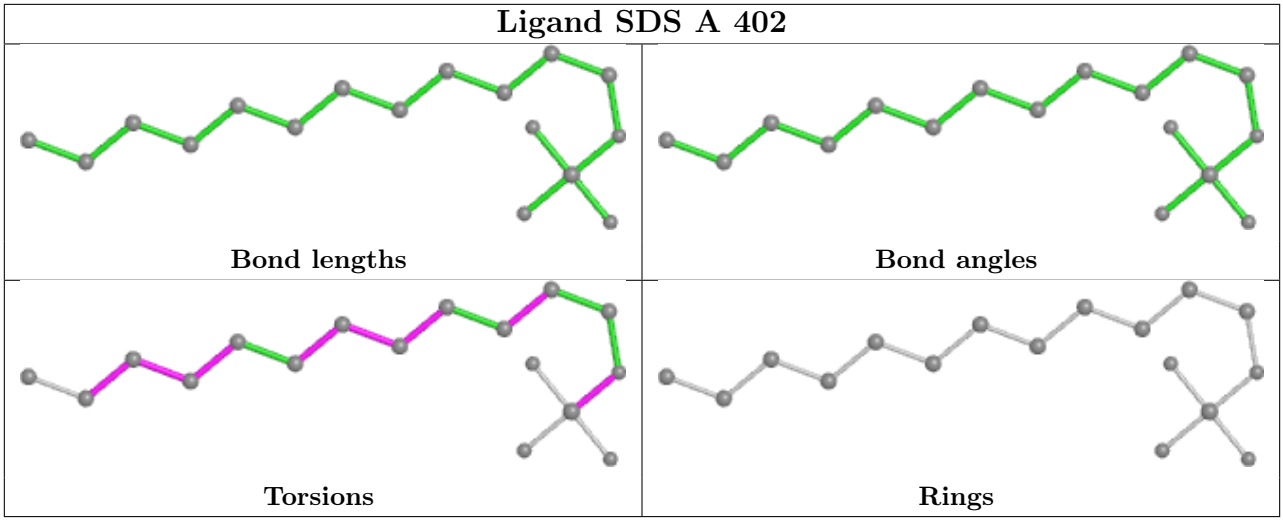
Mol	Chain	Res	Type	Atoms
3	A	402	SDS	C6-C7-C8-C9
3	A	402	SDS	C4-C5-C6-C7
3	A	402	SDS	C7-C8-C9-C10
3	A	402	SDS	C1-O2S-S-O4
3	A	402	SDS	C11-C10-C9-C8
3	A	402	SDS	C1-O2S-S-O1S
3	A	402	SDS	C3-C4-C5-C6
3	A	402	SDS	C2-C3-C4-C5
3	A	402	SDS	C1-O2S-S-O3S
3	A	402	SDS	C10-C11-C12-C1

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SDS	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 (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	286/303 (94%)	-0.49	0	100	100	6, 18, 45, 88	1 (0%)
1	B	285/303 (94%)	-0.28	1 (0%)	92	90	5, 28, 55, 80	1 (0%)
All	All	571/606 (94%)	-0.39	1 (0%)	95	93	5, 23, 52, 88	2 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	GLN	2.2

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)

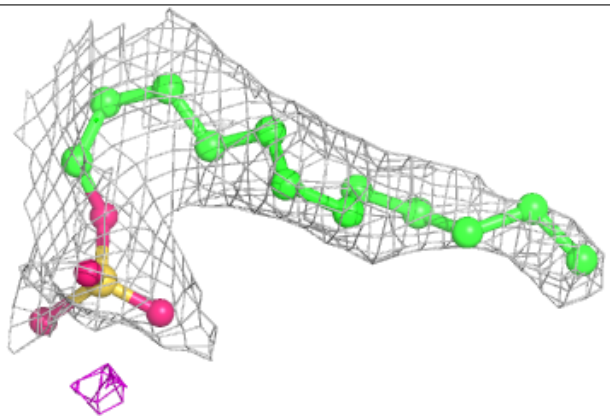
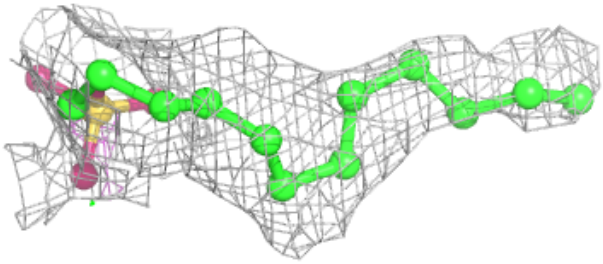
There are no monosaccharides in this entry.

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
3	SDS	A	402	17/17	0.83	0.26	27,51,144,179	0
2	CU	B	401	1/1	0.94	0.37	30,30,30,30	1
2	CU	A	401	1/1	0.98	0.24	22,22,22,22	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SDS A 402: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.