WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 12:02 PM EDT

PDB ID	:	4HUN
Title	:	MATE transporter NorM-NG in complex with R6G and monobody
Authors	:	Lu, M.
Deposited on	:	2012-11-02
Resolution	:	3.59 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
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)	:	2.18

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.59 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	Percentile Ranks	Value
Rfree		0.343
Clashscore		94
Ramachandran outliers		17.4%
Sidechain outliers		33.4%
RSRZ outliers		2.5%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
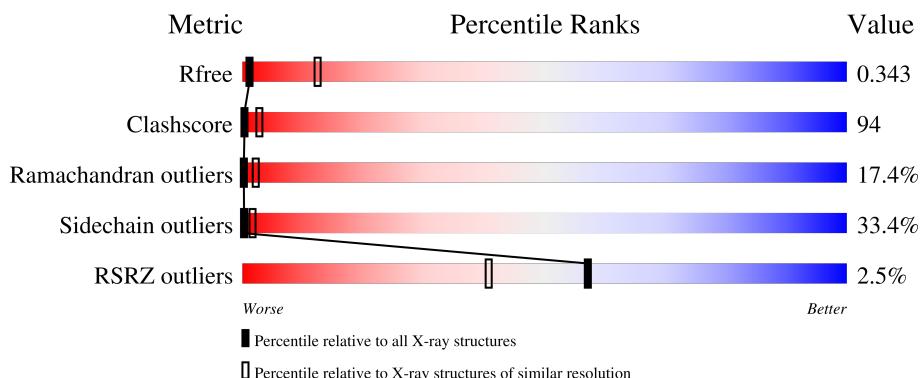
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	2% / 16% / 49% / 28% / 6%
2	B	99	3% / 10% / 43% / 33% / 5% / 8%
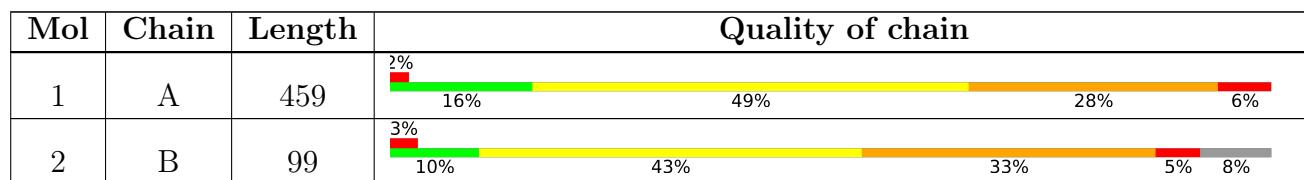
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

W O R L D W I D E
wwPDB
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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RHQ	A	501	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4248 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 Multidrug efflux protein.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total 3508	C 2338	N 558	O 589	S 23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	SER	-	expression tag	UNP E8SM44
A	461	SER	-	expression tag	UNP E8SM44
A	462	GLY	-	expression tag	UNP E8SM44
A	463	LEU	-	expression tag	UNP E8SM44

- Molecule 2 is a protein called protein B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	91	Total 707	C 457	N 110	O 140	0	0	0

- Molecule 3 is RHODAMINE 6G (three-letter code: RHQ) (formula: $C_{28}H_{31}N_2O_3$).

RHQ
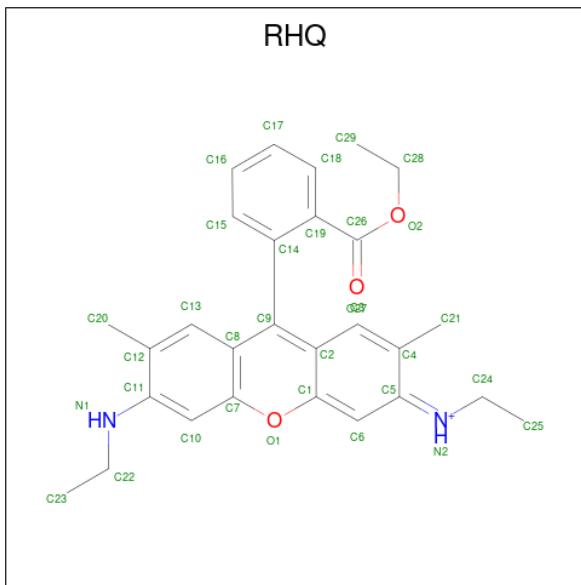
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	28	2	3	0	0

3 Residue-property plots ⓘ

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

- Molecule 2: protein B

T56 A57 T58 I59 S60 G61 L62 S63 P64 G65 V66 D67 Y68 T69 I70 T71 V72 Y73 A74 R75 S76 Y77 Y78 W79 G80 W81 Y82 S83 P84 I85 S86 I87 N88 Y89 R90 T91
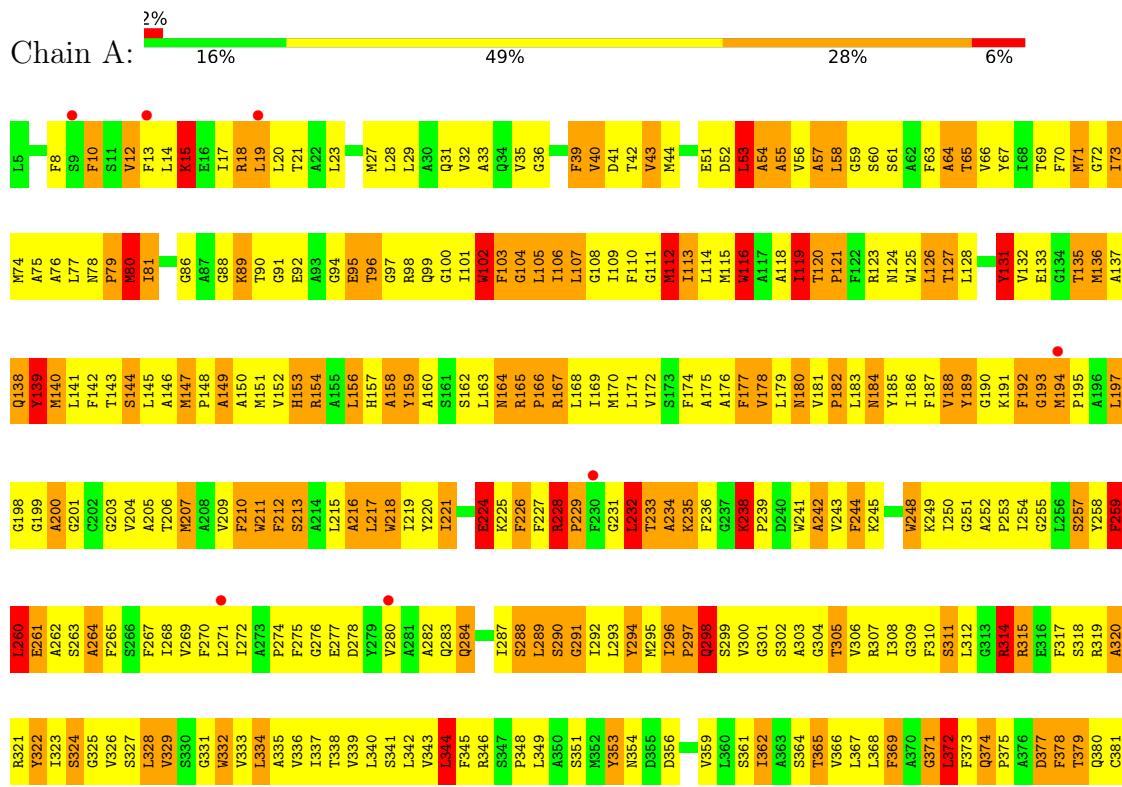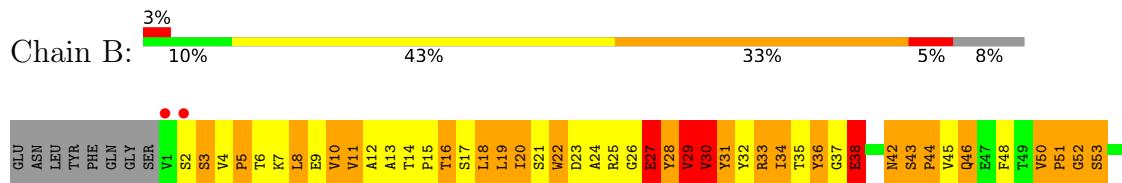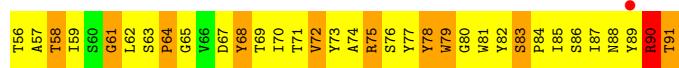
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.23Å 117.23Å 226.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.59 52.04 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.59) 99.7 (52.04-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.306 , 0.327 0.319 , 0.343	Depositor DCC
R_{free} test set	1104 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	123.2	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 123.8	EDS
L-test for twinning[2]	$< |L| > = 0.38, < L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.146 for -h,-k,l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	4248	wwPDB-VP
Average B, all atoms (Å^2)	178.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.82	8/3605 (0.2%)	1.06	11/4898 (0.2%)
2	B	0.93	1/729 (0.1%)	1.18	5/1004 (0.5%)
All	All	0.84	9/4334 (0.2%)	1.08	16/5902 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
2	B	1	2
All	All	1	20

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	ARG	CZ-NH2	9.53	1.45	1.33
1	A	211	TRP	CD2-CE2	5.90	1.48	1.41
1	A	443	TRP	CD2-CE2	5.55	1.48	1.41
1	A	125	TRP	CD2-CE2	5.47	1.48	1.41
1	A	116	TRP	CD2-CE2	5.45	1.47	1.41
2	B	22	TRP	CD2-CE2	5.23	1.47	1.41
1	A	102	TRP	CD2-CE2	5.21	1.47	1.41
1	A	405	TRP	CD2-CE2	5.10	1.47	1.41
1	A	427	TRP	CD2-CE2	5.01	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	LEU	CA-CB-CG	7.84	133.34	115.30
1	A	128	LEU	CA-CB-CG	6.57	130.40	115.30
1	A	372	LEU	CA-CB-CG	6.47	130.19	115.30
1	A	314	ARG	NE-CZ-NH2	-6.39	117.10	120.30
2	B	30	VAL	CB-CA-C	-6.28	99.47	111.40
1	A	441	LEU	CA-CB-CG	6.09	129.32	115.30
1	A	445	LEU	N-CA-C	-5.85	95.20	111.00
1	A	53	LEU	CA-CB-CG	5.47	127.87	115.30
2	B	33	ARG	N-CA-C	-5.41	96.39	111.00
2	B	8	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	328	LEU	CA-CB-CG	5.36	127.62	115.30
2	B	29	VAL	CB-CA-C	5.16	121.20	111.40
1	A	127	THR	N-CA-C	5.16	124.92	111.00
1	A	344	LEU	CA-CB-CG	5.13	127.09	115.30
2	B	27	GLU	C-N-CA	-5.13	108.89	121.70
1	A	55	ALA	N-CA-C	-5.11	97.21	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	28	TYR	CA

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	THR	Peptide
1	A	138	GLN	Peptide
1	A	188	VAL	Peptide
1	A	194	MET	Peptide
1	A	216	ALA	Peptide
1	A	220	TYR	Peptide
1	A	226	PHE	Peptide
1	A	228	ARG	Peptide
1	A	249	LYS	Peptide
1	A	259	PHE	Peptide
1	A	322	TYR	Peptide
1	A	338	THR	Peptide
1	A	387	LEU	Peptide
1	A	395	VAL	Peptide
1	A	396	PRO	Peptide
1	A	410	LEU	Peptide
1	A	446	GLU	Peptide
1	A	54	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	B	27	GLU	Peptide
2	B	29	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3508	0	3587	661	0
2	B	707	0	681	156	0
3	A	33	0	31	9	0
All	All	4248	0	4299	803	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 94.

All (803) 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:A:158:ALA:HB2	1:A:217:LEU:CD1	1.34	1.54
1:A:158:ALA:CB	1:A:217:LEU:HD11	1.60	1.29
1:A:144:SER:CB	1:A:204:VAL:HG12	1.64	1.28
1:A:144:SER:HB3	1:A:204:VAL:CG1	1.63	1.27
1:A:429:ALA:O	1:A:433:SER:HB3	1.11	1.25
1:A:149:ALA:HA	1:A:152:VAL:CG2	1.68	1.22
1:A:98:ARG:HD3	1:A:229:PRO:O	1.39	1.20
1:A:78:ASN:HA	1:A:163:LEU:CD1	1.73	1.17
3:A:501:RHQ:H151	3:A:501:RHQ:H131	1.26	1.15
1:A:248:TRP:HZ3	1:A:252:ALA:HB2	1.06	1.12
1:A:418:ARG:HG2	1:A:422:GLY:HA3	1.16	1.12
1:A:460:SER:O	2:B:8:LEU:CD1	1.98	1.12
2:B:8:LEU:HD13	2:B:87:ILE:HD11	1.16	1.11
1:A:394:LYS:HA	1:A:397:MET:HB2	1.12	1.11
1:A:221:ILE:HD13	1:A:228:ARG:HB2	1.33	1.10
3:A:501:RHQ:H131	3:A:501:RHQ:C15	1.78	1.10
2:B:11:VAL:HG12	2:B:19:LEU:HD12	1.34	1.10
1:A:288:SER:O	1:A:292:ILE:HG23	1.52	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD12	1:A:393:THR:HG22	1.26	1.09
1:A:460:SER:O	2:B:8:LEU:HD12	1.49	1.09
1:A:78:ASN:HA	1:A:163:LEU:HD13	1.12	1.09
2:B:8:LEU:CD1	2:B:87:ILE:HD11	1.82	1.09
1:A:407:CYS:HB3	1:A:433:SER:HB2	1.32	1.08
1:A:248:TRP:CZ3	1:A:252:ALA:HB2	1.89	1.08
1:A:411:PRO:CB	1:A:428:THR:HG23	1.82	1.08
1:A:149:ALA:HA	1:A:152:VAL:HG21	1.34	1.08
1:A:415:LEU:HG	1:A:422:GLY:O	1.53	1.08
1:A:411:PRO:HB3	1:A:428:THR:HG23	1.10	1.07
1:A:218:TRP:HA	1:A:218:TRP:CE3	1.88	1.06
1:A:429:ALA:O	1:A:433:SER:CB	2.03	1.06
1:A:365:THR:HB	1:A:423:ILE:HG21	1.11	1.05
1:A:259:PHE:HA	1:A:262:ALA:HB3	1.41	1.02
1:A:411:PRO:HB3	1:A:428:THR:CG2	1.88	1.02
1:A:73:ILE:O	1:A:76:ALA:HB3	1.60	1.01
1:A:164:ASN:O	1:A:166:PRO:HD3	1.60	1.01
2:B:27:GLU:O	2:B:28:TYR:HD2	1.42	1.01
1:A:224:GLU:HG2	1:A:225:LYS:H	1.23	1.01
2:B:8:LEU:HD13	2:B:87:ILE:CD1	1.92	1.00
1:A:369:PHE:HB3	1:A:372:LEU:HD12	1.45	0.98
1:A:408:GLY:HA3	1:A:430:LEU:HG	1.46	0.98
1:A:149:ALA:HA	1:A:152:VAL:HG22	1.42	0.98
1:A:154:ARG:NH2	1:A:215:LEU:HD21	1.79	0.98
3:A:501:RHQ:H151	3:A:501:RHQ:C13	1.89	0.98
1:A:89:LYS:H	1:A:89:LYS:HD3	1.26	0.98
1:A:387:LEU:HD12	1:A:393:THR:CG2	1.93	0.97
1:A:158:ALA:CB	1:A:217:LEU:CD1	2.30	0.96
1:A:284:GLN:O	1:A:288:SER:HB2	1.63	0.96
1:A:78:ASN:CA	1:A:163:LEU:HD13	1.95	0.96
2:B:30:VAL:O	2:B:31:TYR:HB2	1.66	0.95
1:A:188:VAL:HA	1:A:198:GLY:HA2	1.47	0.95
1:A:141:LEU:CD1	1:A:145:LEU:HD23	1.97	0.95
2:B:38:GLU:HA	2:B:68:TYR:HA	1.46	0.94
1:A:193:GLY:O	1:A:195:PRO:HD3	1.67	0.94
1:A:168:LEU:HA	1:A:171:LEU:HD13	1.49	0.93
1:A:252:ALA:HB3	1:A:253:PRO:HD3	1.48	0.93
1:A:151:MET:SD	1:A:211:TRP:CE3	2.62	0.93
1:A:387:LEU:HD21	1:A:444:CYS:O	1.70	0.92
1:A:102:TRP:O	1:A:106:ILE:HB	1.69	0.92
1:A:154:ARG:HH21	1:A:215:LEU:HD21	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:PRO:HG3	1:A:429:ALA:HB3	1.48	0.92
2:B:9:GLU:O	2:B:22:TRP:NE1	2.01	0.92
1:A:388:ARG:HB3	1:A:394:LYS:HB3	1.50	0.92
1:A:141:LEU:HD11	1:A:145:LEU:HD23	1.51	0.91
1:A:318:SER:HA	1:A:321:ARG:H	1.31	0.91
1:A:339:VAL:HG21	1:A:375:PRO:HD3	1.51	0.91
1:A:89:LYS:HG2	1:A:92:GLU:HB3	1.51	0.90
2:B:67:ASP:HA	2:B:90:ARG:HB3	1.52	0.90
1:A:315:ARG:HG3	1:A:317:PHE:CE1	2.06	0.90
1:A:346:ARG:HD2	1:A:367:LEU:HD11	1.54	0.90
1:A:418:ARG:CG	1:A:422:GLY:HA3	2.01	0.90
1:A:432:ALA:O	1:A:436:ILE:HG23	1.72	0.90
1:A:331:GLY:HA2	1:A:334:LEU:HD22	1.54	0.90
1:A:116:TRP:HH2	1:A:147:MET:HA	1.38	0.89
1:A:418:ARG:HG2	1:A:422:GLY:CA	2.02	0.89
2:B:27:GLU:O	2:B:28:TYR:CD2	2.26	0.89
1:A:375:PRO:HA	1:A:378:PHE:HB2	1.53	0.88
3:A:501:RHQ:H31	3:A:501:RHQ:C26	2.03	0.88
1:A:218:TRP:HA	1:A:218:TRP:HE3	1.37	0.88
1:A:308:ILE:CD1	1:A:386:ALA:HA	2.03	0.88
1:A:387:LEU:CD1	1:A:393:THR:HG22	2.03	0.88
2:B:7:LYS:HB2	2:B:23:ASP:HB2	1.55	0.88
1:A:154:ARG:HH21	1:A:215:LEU:CD2	1.87	0.87
1:A:235:LYS:HB2	1:A:241:TRP:HB3	1.56	0.87
1:A:77:LEU:HA	1:A:80:MET:HG3	1.55	0.87
1:A:105:LEU:O	1:A:109:ILE:HG23	1.74	0.87
2:B:24:ALA:O	2:B:53:SER:OG	1.93	0.87
1:A:242:ALA:HA	1:A:245:LYS:H	1.39	0.86
1:A:384:SER:O	1:A:388:ARG:HG3	1.74	0.86
1:A:102:TRP:CD1	1:A:233:THR:OG1	2.28	0.85
1:A:144:SER:O	1:A:207:MET:HG2	1.76	0.85
1:A:268:ILE:HD12	1:A:287:ILE:HD11	1.57	0.85
1:A:372:LEU:HB3	1:A:431:ILE:HG21	1.58	0.84
1:A:221:ILE:HD13	1:A:228:ARG:CB	2.06	0.84
1:A:151:MET:SD	1:A:211:TRP:CD2	2.71	0.84
2:B:75:ARG:HD2	2:B:79:TRP:O	1.78	0.83
1:A:89:LYS:CG	1:A:92:GLU:HB3	2.08	0.83
1:A:148:PRO:O	1:A:152:VAL:HG13	1.79	0.83
2:B:35:THR:HG23	2:B:73:TYR:HE1	1.43	0.83
1:A:318:SER:C	1:A:320:ALA:H	1.81	0.83
1:A:394:LYS:CA	1:A:397:MET:HB2	2.02	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:SER:HA	2:B:61:GLY:HA3	1.60	0.83
1:A:292:ILE:HG13	1:A:293:LEU:H	1.44	0.82
1:A:379:THR:HA	1:A:382:ILE:HG23	1.61	0.82
1:A:216:ALA:HA	1:A:219:ILE:HG12	1.61	0.82
1:A:289:LEU:HD13	1:A:292:ILE:CD1	2.10	0.82
1:A:441:LEU:O	1:A:443:TRP:N	2.12	0.82
1:A:408:GLY:HA2	1:A:411:PRO:HG2	1.62	0.81
1:A:28:LEU:O	1:A:32:VAL:HG23	1.80	0.81
1:A:238:LYS:HB2	1:A:239:PRO:CD	2.10	0.81
1:A:289:LEU:HA	1:A:292:ILE:HG12	1.63	0.81
2:B:7:LYS:HB3	2:B:23:ASP:H	1.45	0.81
2:B:31:TYR:CD1	2:B:75:ARG:NH1	2.48	0.81
1:A:429:ALA:C	1:A:433:SER:HB3	2.01	0.81
1:A:97:GLY:HA3	1:A:227:PHE:CE2	2.16	0.81
1:A:397:MET:O	1:A:400:HIS:ND1	2.14	0.81
1:A:340:LEU:O	1:A:344:LEU:HB2	1.80	0.80
2:B:10:VAL:HG12	2:B:18:LEU:HD22	1.63	0.80
1:A:403:ALA:O	1:A:407:CYS:HB2	1.82	0.80
1:A:225:LYS:HE2	1:A:226:PHE:CE2	2.17	0.80
1:A:396:PRO:HB3	1:A:399:ILE:HG13	1.62	0.79
1:A:141:LEU:CD2	1:A:203:GLY:HA3	2.12	0.79
1:A:183:LEU:HA	1:A:186:ILE:HD12	1.64	0.79
1:A:224:GLU:CG	1:A:225:LYS:H	1.94	0.79
1:A:95:GLU:HA	1:A:98:ARG:HG2	1.65	0.78
1:A:116:TRP:CH2	1:A:147:MET:HA	2.18	0.78
1:A:411:PRO:HA	1:A:414:LEU:HB2	1.66	0.78
1:A:292:ILE:HG13	1:A:293:LEU:N	1.98	0.78
1:A:253:PRO:HB2	1:A:394:LYS:HD3	1.66	0.78
1:A:372:LEU:HD11	1:A:424:TYR:HB2	1.66	0.78
1:A:332:TRP:CD1	1:A:379:THR:OG1	2.36	0.77
1:A:158:ALA:HB2	1:A:217:LEU:HD12	1.59	0.77
2:B:36:TYR:HA	2:B:70:ILE:HG12	1.67	0.77
1:A:439:VAL:CG2	1:A:440:ALA:H	1.97	0.77
1:A:441:LEU:O	1:A:444:CYS:N	2.17	0.77
1:A:73:ILE:O	1:A:76:ALA:CB	2.31	0.76
1:A:415:LEU:O	1:A:418:ARG:HB2	1.86	0.76
1:A:99:GLN:NE2	1:A:234:ALA:O	2.18	0.76
1:A:263:SER:C	1:A:265:PHE:H	1.88	0.76
1:A:142:PHE:O	1:A:146:ALA:HB3	1.85	0.76
1:A:365:THR:HA	1:A:368:LEU:HG	1.67	0.76
1:A:149:ALA:CA	1:A:152:VAL:HG22	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PHE:O	1:A:181:VAL:HG23	1.84	0.76
1:A:387:LEU:CD1	1:A:393:THR:CG2	2.62	0.75
1:A:394:LYS:HA	1:A:397:MET:CB	2.06	0.75
1:A:351:SER:HB3	1:A:359:VAL:HG11	1.67	0.75
1:A:395:VAL:HG13	1:A:396:PRO:HD3	1.67	0.75
1:A:89:LYS:CG	1:A:92:GLU:CB	2.64	0.75
1:A:439:VAL:HG23	1:A:440:ALA:N	2.02	0.75
1:A:321:ARG:HH22	1:A:391:LYS:HB2	1.51	0.75
1:A:148:PRO:HG3	1:A:207:MET:HB2	1.69	0.75
1:A:365:THR:HG22	1:A:368:LEU:HD11	1.69	0.75
1:A:189:TYR:HA	1:A:195:PRO:O	1.86	0.74
1:A:413:TYR:O	1:A:414:LEU:HD12	1.86	0.74
1:A:73:ILE:HA	1:A:251:GLY:HA2	1.69	0.74
1:A:332:TRP:HD1	1:A:379:THR:OG1	1.69	0.74
1:A:221:ILE:CD1	1:A:228:ARG:HB2	2.16	0.74
1:A:218:TRP:CZ3	1:A:221:ILE:HD11	2.22	0.74
1:A:66:VAL:HA	1:A:69:THR:HG22	1.70	0.74
1:A:441:LEU:C	1:A:443:TRP:H	1.89	0.74
1:A:297:PRO:O	1:A:299:SER:N	2.21	0.73
1:A:424:TYR:HA	1:A:427:TRP:CD1	2.23	0.73
1:A:63:PHE:O	1:A:65:THR:N	2.19	0.73
1:A:73:ILE:HD12	1:A:73:ILE:H	1.53	0.73
2:B:29:VAL:O	2:B:30:VAL:HG12	1.87	0.73
1:A:89:LYS:HG3	1:A:92:GLU:HB2	1.68	0.73
2:B:4:VAL:CG2	2:B:6:THR:CG2	2.66	0.73
1:A:178:VAL:O	1:A:182:PRO:HD2	1.89	0.73
1:A:109:ILE:O	1:A:113:ILE:HB	1.87	0.72
1:A:457:LYS:HZ1	2:B:90:ARG:HH12	1.35	0.72
1:A:259:PHE:HA	1:A:262:ALA:CB	2.18	0.72
1:A:439:VAL:CG2	1:A:440:ALA:N	2.52	0.72
1:A:65:THR:O	1:A:69:THR:HG22	1.89	0.72
1:A:193:GLY:O	1:A:195:PRO:CD	2.37	0.72
1:A:188:VAL:HA	1:A:198:GLY:CA	2.17	0.72
1:A:44:MET:HE3	1:A:180:ASN:HD21	1.52	0.72
1:A:55:ALA:HB1	1:A:58:LEU:HD21	1.71	0.72
1:A:91:GLY:HA3	1:A:226:PHE:CE1	2.24	0.72
1:A:143:THR:HG23	1:A:144:SER:N	2.04	0.72
1:A:364:SER:C	1:A:366:VAL:H	1.90	0.72
1:A:180:ASN:O	1:A:184:ASN:N	2.16	0.71
2:B:19:LEU:HA	2:B:58:THR:HG22	1.71	0.71
1:A:89:LYS:HG2	1:A:92:GLU:CB	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:TYR:C	2:B:80:GLY:H	1.92	0.71
2:B:30:VAL:O	2:B:30:VAL:HG13	1.90	0.70
1:A:89:LYS:HG3	1:A:92:GLU:CB	2.20	0.70
1:A:373:PHE:HB3	1:A:431:ILE:HG22	1.71	0.70
2:B:4:VAL:HG23	2:B:6:THR:CG2	2.19	0.70
1:A:78:ASN:HA	1:A:163:LEU:HD11	1.71	0.70
3:A:501:RHQ:H31	3:A:501:RHQ:O27	1.91	0.70
1:A:308:ILE:HB	1:A:390:TYR:CD1	2.27	0.70
1:A:145:LEU:HD13	1:A:206:THR:HB	1.73	0.70
1:A:63:PHE:C	1:A:65:THR:H	1.93	0.70
1:A:132:VAL:O	1:A:133:GLU:HG3	1.92	0.70
1:A:158:ALA:HB2	1:A:217:LEU:HD11	0.72	0.70
1:A:74:MET:HB2	1:A:156:LEU:HD21	1.74	0.69
1:A:397:MET:O	1:A:400:HIS:N	2.24	0.69
1:A:447:LYS:HD3	1:A:448:TYR:CE1	2.26	0.69
2:B:27:GLU:HG3	2:B:52:GLY:C	2.13	0.69
1:A:56:VAL:HA	1:A:138:GLN:HE22	1.56	0.69
1:A:172:VAL:HG21	1:A:216:ALA:CB	2.22	0.69
1:A:458:ALA:HB1	2:B:8:LEU:CB	2.22	0.69
1:A:461:SER:HA	2:B:8:LEU:HG	1.75	0.69
2:B:71:THR:OG1	2:B:86:SER:HB2	1.93	0.69
1:A:184:ASN:HA	1:A:205:ALA:CB	2.22	0.69
1:A:238:LYS:HB2	1:A:239:PRO:HD2	1.74	0.69
1:A:437:ALA:C	1:A:439:VAL:H	1.95	0.69
2:B:42:ASN:ND2	2:B:43:SER:H	1.89	0.69
1:A:158:ALA:HB2	1:A:217:LEU:CG	2.19	0.69
2:B:69:THR:O	2:B:70:ILE:HG13	1.92	0.69
1:A:141:LEU:HD21	1:A:145:LEU:HD22	1.73	0.69
1:A:116:TRP:HH2	1:A:147:MET:CA	2.05	0.69
1:A:144:SER:CB	1:A:204:VAL:CG1	2.44	0.68
1:A:152:VAL:HG12	1:A:210:PHE:HB3	1.74	0.68
1:A:333:VAL:HG12	1:A:334:LEU:HD13	1.74	0.68
2:B:4:VAL:CG2	2:B:6:THR:HG23	2.24	0.68
1:A:140:MET:HB3	1:A:200:ALA:HB1	1.75	0.68
2:B:50:VAL:HG12	2:B:51:PRO:HD3	1.76	0.68
1:A:318:SER:C	1:A:320:ALA:N	2.47	0.68
1:A:224:GLU:HG2	1:A:225:LYS:N	2.04	0.68
2:B:36:TYR:HD2	2:B:70:ILE:HD13	1.59	0.68
1:A:373:PHE:HB2	1:A:434:LEU:CD2	2.24	0.67
1:A:435:THR:HG22	1:A:438:ALA:HB2	1.76	0.67
2:B:65:GLY:HA2	2:B:91:THR:CB	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ALA:O	1:A:58:LEU:HD11	1.94	0.67
2:B:37:GLY:N	2:B:70:ILE:HD11	2.08	0.67
2:B:69:THR:HA	2:B:88:ASN:HA	1.75	0.67
1:A:76:ALA:O	1:A:250:ILE:HD13	1.95	0.67
2:B:4:VAL:CG2	2:B:6:THR:HG22	2.25	0.67
1:A:58:LEU:HD12	1:A:138:GLN:NE2	2.08	0.67
1:A:241:TRP:NE1	1:A:243:VAL:HG22	2.10	0.67
1:A:254:ILE:HB	1:A:394:LYS:NZ	2.10	0.67
1:A:184:ASN:HA	1:A:205:ALA:HB1	1.77	0.67
2:B:67:ASP:HA	2:B:90:ARG:CB	2.21	0.67
1:A:97:GLY:HA3	1:A:227:PHE:CZ	2.31	0.67
1:A:268:ILE:HD12	1:A:287:ILE:CD1	2.25	0.67
1:A:305:THR:HA	1:A:308:ILE:HD11	1.77	0.67
1:A:148:PRO:CG	1:A:207:MET:HB2	2.25	0.66
1:A:55:ALA:O	1:A:58:LEU:CD1	2.44	0.66
1:A:283:GLN:O	1:A:284:GLN:HG3	1.96	0.66
1:A:331:GLY:HA2	1:A:334:LEU:CD2	2.25	0.66
1:A:458:ALA:HB1	2:B:8:LEU:HB2	1.77	0.66
1:A:225:LYS:HE2	1:A:226:PHE:CD2	2.30	0.66
1:A:408:GLY:HA3	1:A:430:LEU:CG	2.24	0.66
2:B:36:TYR:HA	2:B:70:ILE:CG1	2.25	0.66
2:B:37:GLY:H	2:B:70:ILE:HD11	1.61	0.66
1:A:44:MET:CE	1:A:180:ASN:HD21	2.08	0.66
1:A:458:ALA:CB	2:B:8:LEU:HB2	2.26	0.66
1:A:110:PHE:O	1:A:114:LEU:HG	1.95	0.65
1:A:140:MET:O	1:A:144:SER:HB2	1.97	0.65
1:A:274:PRO:C	1:A:276:GLY:H	1.99	0.65
1:A:373:PHE:HB2	1:A:434:LEU:HD22	1.78	0.65
1:A:306:VAL:O	1:A:308:ILE:N	2.29	0.65
1:A:159:TYR:CB	1:A:169:ILE:HD13	2.27	0.65
1:A:132:VAL:O	1:A:133:GLU:CG	2.45	0.65
2:B:27:GLU:HG3	2:B:52:GLY:O	1.97	0.65
2:B:30:VAL:O	2:B:31:TYR:CB	2.34	0.65
1:A:207:MET:SD	1:A:207:MET:C	2.76	0.64
1:A:183:LEU:HD23	1:A:209:VAL:HG23	1.79	0.64
1:A:241:TRP:CD1	1:A:242:ALA:O	2.50	0.64
1:A:146:ALA:N	1:A:148:PRO:HD2	2.12	0.64
1:A:252:ALA:HB3	1:A:253:PRO:CD	2.25	0.64
1:A:297:PRO:HB3	1:A:378:PHE:CE2	2.33	0.64
1:A:381:CYS:O	1:A:384:SER:N	2.31	0.64
1:A:458:ALA:HB3	2:B:8:LEU:C	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HB	1:A:394:LYS:CE	2.28	0.64
2:B:26:GLY:O	2:B:53:SER:OG	2.16	0.64
1:A:460:SER:O	2:B:8:LEU:HD11	1.92	0.64
3:A:501:RHQ:C24	3:A:501:RHQ:H211	2.27	0.64
1:A:97:GLY:HA3	1:A:227:PHE:HE2	1.61	0.63
1:A:183:LEU:CD1	1:A:187:PHE:HE1	2.12	0.63
1:A:254:ILE:HB	1:A:394:LYS:HE2	1.80	0.63
1:A:321:ARG:HH21	1:A:390:TYR:HB3	1.64	0.63
1:A:251:GLY:O	1:A:254:ILE:HG22	1.99	0.63
1:A:425:GLY:O	1:A:428:THR:HG22	1.97	0.63
1:A:44:MET:HE3	1:A:180:ASN:ND2	2.13	0.63
1:A:148:PRO:O	1:A:152:VAL:CG1	2.46	0.63
1:A:143:THR:HG23	1:A:144:SER:H	1.63	0.63
1:A:221:ILE:HD13	1:A:228:ARG:CG	2.28	0.63
1:A:346:ARG:C	1:A:348:PRO:HD3	2.18	0.63
1:A:458:ALA:CB	2:B:8:LEU:CB	2.77	0.63
1:A:400:HIS:HD2	1:A:404:PHE:HE1	1.46	0.63
2:B:36:TYR:HD2	2:B:70:ILE:CD1	2.11	0.63
1:A:66:VAL:HA	1:A:69:THR:CG2	2.29	0.62
1:A:216:ALA:HA	1:A:219:ILE:CG1	2.27	0.62
1:A:136:MET:O	1:A:136:MET:HG2	1.97	0.62
1:A:224:GLU:CG	1:A:225:LYS:N	2.60	0.62
1:A:261:GLU:HA	1:A:264:ALA:HB3	1.80	0.62
1:A:159:TYR:HB3	1:A:169:ILE:HD13	1.82	0.62
2:B:4:VAL:HG23	2:B:6:THR:HG23	1.79	0.62
1:A:308:ILE:HD11	1:A:386:ALA:HA	1.80	0.62
1:A:183:LEU:CD2	1:A:209:VAL:HG23	2.30	0.62
1:A:365:THR:HA	1:A:368:LEU:CG	2.29	0.62
1:A:147:MET:N	1:A:148:PRO:HD2	2.15	0.62
2:B:4:VAL:HG22	2:B:6:THR:CG2	2.30	0.61
1:A:89:LYS:HD3	1:A:89:LYS:N	2.07	0.61
1:A:388:ARG:HB3	1:A:394:LYS:CB	2.27	0.61
1:A:242:ALA:HA	1:A:245:LYS:N	2.14	0.61
1:A:71:MET:CE	1:A:159:TYR:OH	2.48	0.61
1:A:201:GLY:HA2	1:A:204:VAL:HG22	1.83	0.61
1:A:318:SER:OG	1:A:321:ARG:HB3	2.00	0.61
1:A:36:GLY:HA2	1:A:39:PHE:HE2	1.66	0.61
1:A:372:LEU:CD1	1:A:424:TYR:HB2	2.30	0.61
1:A:408:GLY:CA	1:A:430:LEU:HG	2.28	0.61
1:A:346:ARG:CD	1:A:367:LEU:HD11	2.30	0.60
2:B:35:THR:HG23	2:B:73:TYR:CE1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD13	1:A:292:ILE:HD11	1.83	0.60
1:A:321:ARG:NH2	1:A:391:LYS:HB2	2.16	0.60
1:A:164:ASN:C	1:A:166:PRO:HD3	2.20	0.60
1:A:81:ILE:HG12	1:A:163:LEU:HD12	1.82	0.60
1:A:221:ILE:HG21	1:A:228:ARG:HB2	1.82	0.60
1:A:411:PRO:CB	1:A:428:THR:CG2	2.62	0.60
1:A:447:LYS:HD3	1:A:448:TYR:HE1	1.65	0.60
1:A:387:LEU:CD2	1:A:444:CYS:O	2.48	0.60
1:A:395:VAL:HG13	1:A:396:PRO:CD	2.29	0.60
1:A:287:ILE:HG21	1:A:427:TRP:HH2	1.65	0.60
2:B:31:TYR:HB3	2:B:75:ARG:HB3	1.84	0.60
1:A:145:LEU:HD12	1:A:207:MET:HB3	1.84	0.60
1:A:40:VAL:CG1	1:A:180:ASN:ND2	2.65	0.60
2:B:65:GLY:HA2	2:B:91:THR:HG21	1.82	0.60
1:A:225:LYS:HG2	1:A:226:PHE:H	1.67	0.59
1:A:339:VAL:CG2	1:A:375:PRO:HD3	2.27	0.59
1:A:457:LYS:HZ1	2:B:90:ARG:NH1	2.00	0.59
1:A:12:VAL:HG23	1:A:13:PHE:H	1.66	0.59
1:A:298:GLN:HA	1:A:382:ILE:HG22	1.85	0.59
3:A:501:RHQ:C26	3:A:501:RHQ:C3	2.80	0.59
2:B:13:ALA:HB1	2:B:17:SER:O	2.03	0.59
1:A:300:VAL:O	1:A:304:GLY:N	2.20	0.59
2:B:27:GLU:HG2	2:B:30:VAL:HG23	1.82	0.59
1:A:86:GLY:HA3	1:A:314:ARG:N	2.18	0.59
1:A:318:SER:HA	1:A:321:ARG:N	2.10	0.59
1:A:437:ALA:C	1:A:439:VAL:N	2.56	0.59
1:A:172:VAL:O	1:A:174:PHE:N	2.30	0.58
1:A:369:PHE:HD2	1:A:424:TYR:CB	2.16	0.58
1:A:141:LEU:HD13	1:A:145:LEU:HD23	1.81	0.58
1:A:439:VAL:HG23	1:A:440:ALA:H	1.65	0.58
2:B:27:GLU:HB3	2:B:30:VAL:HG23	1.85	0.58
1:A:267:PHE:CE2	1:A:408:GLY:O	2.56	0.58
2:B:5:PRO:HD3	2:B:74:ALA:HB2	1.86	0.58
1:A:71:MET:HE1	1:A:159:TYR:OH	2.02	0.58
1:A:172:VAL:HG21	1:A:216:ALA:HB1	1.84	0.58
1:A:233:THR:O	1:A:234:ALA:O	2.22	0.58
2:B:78:TYR:C	2:B:80:GLY:N	2.57	0.58
1:A:444:CYS:C	1:A:448:TYR:HB2	2.24	0.58
1:A:260:LEU:C	1:A:262:ALA:H	2.07	0.58
2:B:65:GLY:HA2	2:B:91:THR:CG2	2.34	0.58
1:A:289:LEU:HD13	1:A:292:ILE:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ARG:CZ	1:A:364:SER:HB2	2.34	0.57
1:A:372:LEU:HD13	1:A:427:TRP:HB2	1.85	0.57
1:A:447:LYS:C	1:A:448:TYR:HD1	2.07	0.57
2:B:21:SER:C	2:B:22:TRP:HD1	2.07	0.57
2:B:34:ILE:HG22	2:B:72:VAL:HG23	1.86	0.57
1:A:372:LEU:HD11	1:A:424:TYR:HD1	1.68	0.57
1:A:157:HIS:HA	1:A:160:ALA:HB3	1.86	0.57
2:B:65:GLY:HA2	2:B:91:THR:HB	1.85	0.57
1:A:267:PHE:HZ	1:A:409:LEU:HA	1.70	0.57
1:A:145:LEU:CD1	1:A:206:THR:HB	2.35	0.57
1:A:418:ARG:NH1	1:A:425:GLY:O	2.37	0.57
1:A:458:ALA:HB1	2:B:8:LEU:HB3	1.87	0.57
1:A:461:SER:HA	2:B:8:LEU:CG	2.34	0.57
1:A:43:VAL:HG11	1:A:181:VAL:HG22	1.87	0.57
1:A:385:TYR:HD1	1:A:388:ARG:CZ	2.17	0.57
1:A:31:GLN:HG3	1:A:296:ILE:HA	1.86	0.57
1:A:426:PHE:C	1:A:428:THR:H	2.07	0.57
1:A:143:THR:CG2	1:A:144:SER:N	2.68	0.57
1:A:148:PRO:HB3	1:A:207:MET:HB2	1.87	0.57
1:A:197:LEU:O	1:A:201:GLY:HA3	2.04	0.57
1:A:294:TYR:CZ	1:A:298:GLN:HB2	2.40	0.57
2:B:27:GLU:HG2	2:B:30:VAL:CG2	2.34	0.57
2:B:36:TYR:HA	2:B:70:ILE:CD1	2.35	0.57
2:B:78:TYR:O	2:B:80:GLY:N	2.38	0.57
2:B:9:GLU:O	2:B:22:TRP:CD1	2.57	0.56
3:A:501:RHQ:H211	3:A:501:RHQ:H242	1.86	0.56
1:A:55:ALA:O	1:A:138:GLN:NE2	2.38	0.56
1:A:51:GLU:HB3	1:A:54:ALA:CB	2.35	0.56
1:A:403:ALA:C	1:A:405:TRP:H	2.09	0.56
1:A:40:VAL:O	1:A:43:VAL:N	2.39	0.56
1:A:306:VAL:C	1:A:308:ILE:H	2.06	0.56
1:A:339:VAL:HA	1:A:342:LEU:CD1	2.36	0.56
1:A:369:PHE:HD2	1:A:424:TYR:HB3	1.71	0.56
2:B:82:TYR:O	2:B:83:SER:HB2	2.04	0.56
1:A:131:TYR:O	1:A:133:GLU:HG2	2.05	0.56
1:A:263:SER:HB2	1:A:405:TRP:CD1	2.41	0.56
1:A:398:PHE:HD2	1:A:399:ILE:HG12	1.71	0.56
1:A:143:THR:CG2	1:A:144:SER:H	2.19	0.56
1:A:411:PRO:HB2	1:A:428:THR:HG23	1.85	0.56
2:B:74:ALA:O	2:B:81:TRP:HE3	1.89	0.56
1:A:40:VAL:HG12	1:A:44:MET:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LYS:CD	1:A:448:TYR:CE1	2.89	0.56
1:A:151:MET:HB2	1:A:211:TRP:CE2	2.41	0.55
1:A:183:LEU:HD11	1:A:205:ALA:HA	1.87	0.55
2:B:10:VAL:CG1	2:B:18:LEU:HD22	2.35	0.55
2:B:17:SER:OG	2:B:59:ILE:O	2.24	0.55
2:B:71:THR:HG23	2:B:85:ILE:C	2.26	0.55
1:A:111:GLY:O	1:A:115:MET:HB2	2.06	0.55
1:A:159:TYR:CD1	1:A:159:TYR:C	2.80	0.55
1:A:339:VAL:HG23	1:A:374:GLN:HB3	1.88	0.55
1:A:412:GLY:HA2	1:A:426:PHE:HD1	1.70	0.55
2:B:18:LEU:HB2	2:B:59:ILE:HD11	1.89	0.55
1:A:90:THR:O	1:A:94:GLY:HA3	2.07	0.55
1:A:388:ARG:O	1:A:391:LYS:O	2.25	0.55
1:A:400:HIS:HD2	1:A:404:PHE:CE1	2.25	0.55
1:A:92:GLU:HA	1:A:95:GLU:HG2	1.88	0.55
1:A:149:ALA:C	1:A:152:VAL:HG22	2.27	0.55
1:A:334:LEU:HD12	1:A:337:ILE:HD11	1.89	0.55
2:B:8:LEU:HD13	2:B:87:ILE:CG1	2.36	0.55
1:A:36:GLY:HA2	1:A:39:PHE:CE2	2.41	0.55
1:A:175:ALA:HA	1:A:178:VAL:HG12	1.88	0.55
1:A:260:LEU:O	1:A:262:ALA:N	2.39	0.55
1:A:321:ARG:HA	1:A:324:SER:HB3	1.88	0.55
1:A:388:ARG:N	1:A:393:THR:O	2.40	0.55
2:B:18:LEU:H	2:B:59:ILE:HG13	1.72	0.55
2:B:21:SER:HA	2:B:56:THR:HA	1.89	0.55
1:A:413:TYR:O	1:A:414:LEU:CD1	2.54	0.55
1:A:455:SER:O	2:B:11:VAL:HA	2.07	0.55
2:B:74:ALA:O	2:B:81:TRP:CE3	2.60	0.55
1:A:59:GLY:O	1:A:63:PHE:N	2.38	0.55
1:A:456:HIS:NE2	1:A:459:VAL:HA	2.22	0.55
1:A:332:TRP:HA	1:A:335:ALA:CB	2.37	0.54
1:A:440:ALA:O	1:A:443:TRP:HE3	1.90	0.54
2:B:36:TYR:CD2	2:B:70:ILE:HD13	2.42	0.54
1:A:90:THR:O	1:A:94:GLY:CA	2.56	0.54
1:A:104:GLY:O	1:A:105:LEU:HB2	2.07	0.54
1:A:447:LYS:O	1:A:448:TYR:HD1	1.89	0.54
2:B:33:ARG:O	2:B:73:TYR:HB2	2.07	0.54
1:A:225:LYS:HE2	1:A:226:PHE:HE2	1.71	0.54
1:A:183:LEU:CD1	1:A:187:PHE:CE1	2.91	0.54
1:A:89:LYS:CG	1:A:92:GLU:HB2	2.34	0.54
1:A:263:SER:C	1:A:265:PHE:N	2.58	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TRP:HA	1:A:335:ALA:HB2	1.90	0.54
1:A:439:VAL:HG22	1:A:440:ALA:H	1.69	0.54
2:B:67:ASP:OD2	2:B:68:TYR:N	2.41	0.54
1:A:51:GLU:HB3	1:A:54:ALA:HB2	1.88	0.54
1:A:73:ILE:H	1:A:73:ILE:CD1	2.18	0.54
1:A:81:ILE:CG1	1:A:163:LEU:HD12	2.38	0.54
1:A:141:LEU:HD22	1:A:203:GLY:HA3	1.87	0.54
1:A:253:PRO:O	1:A:257:SER:HB2	2.07	0.54
1:A:372:LEU:HD11	1:A:424:TYR:CD1	2.42	0.54
1:A:89:LYS:H	1:A:89:LYS:CD	2.11	0.54
1:A:132:VAL:C	1:A:133:GLU:HG2	2.27	0.54
1:A:364:SER:HA	1:A:366:VAL:HG22	1.90	0.54
1:A:99:GLN:OE1	1:A:241:TRP:CD1	2.61	0.54
2:B:20:ILE:HG12	2:B:57:ALA:O	2.08	0.54
1:A:132:VAL:C	1:A:133:GLU:CG	2.76	0.53
1:A:172:VAL:C	1:A:174:PHE:H	2.10	0.53
1:A:94:GLY:HA2	1:A:227:PHE:CZ	2.43	0.53
1:A:397:MET:C	1:A:400:HIS:HD1	2.09	0.53
1:A:148:PRO:CB	1:A:207:MET:HB2	2.39	0.53
1:A:212:PHE:C	1:A:212:PHE:CD2	2.81	0.53
1:A:75:ALA:HB2	1:A:156:LEU:HD11	1.90	0.53
2:B:87:ILE:HG22	2:B:89:TYR:H	1.72	0.53
1:A:241:TRP:HE1	1:A:243:VAL:HG22	1.73	0.53
1:A:387:LEU:CD1	1:A:393:THR:HG21	2.39	0.53
1:A:343:VAL:HG13	1:A:367:LEU:O	2.08	0.53
1:A:44:MET:HE1	1:A:184:ASN:HB2	1.89	0.53
1:A:74:MET:HB2	1:A:156:LEU:CD2	2.39	0.53
1:A:119:ILE:HG12	1:A:142:PHE:CD2	2.43	0.53
1:A:250:ILE:O	1:A:394:LYS:HD3	2.09	0.53
1:A:400:HIS:CD2	1:A:404:PHE:HE1	2.26	0.53
1:A:439:VAL:O	1:A:443:TRP:HB3	2.09	0.53
1:A:137:ALA:O	1:A:199:GLY:O	2.26	0.53
1:A:103:PHE:O	1:A:106:ILE:N	2.41	0.52
1:A:340:LEU:O	1:A:344:LEU:CB	2.55	0.52
2:B:71:THR:HG22	2:B:72:VAL:O	2.09	0.52
1:A:71:MET:HG2	1:A:156:LEU:HD22	1.92	0.52
1:A:91:GLY:HA3	1:A:226:PHE:CZ	2.44	0.52
1:A:19:LEU:C	1:A:21:THR:H	2.13	0.52
1:A:35:VAL:O	1:A:39:PHE:HD2	1.91	0.52
1:A:183:LEU:HD13	1:A:187:PHE:HE1	1.74	0.52
2:B:42:ASN:CG	2:B:43:SER:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG13	1:A:423:ILE:HD11	1.92	0.52
1:A:167:ARG:C	1:A:169:ILE:H	2.13	0.52
1:A:221:ILE:HD13	1:A:228:ARG:HG3	1.92	0.52
1:A:79:PRO:O	1:A:80:MET:C	2.48	0.52
1:A:91:GLY:HA2	1:A:94:GLY:HA3	1.91	0.52
1:A:268:ILE:CD1	1:A:287:ILE:CD1	2.88	0.52
1:A:372:LEU:CD1	1:A:427:TRP:HB2	2.40	0.52
1:A:151:MET:SD	1:A:211:TRP:CG	3.02	0.52
1:A:63:PHE:C	1:A:65:THR:N	2.63	0.52
1:A:263:SER:HB2	1:A:405:TRP:HD1	1.73	0.52
1:A:400:HIS:CD2	1:A:404:PHE:CE1	2.98	0.52
2:B:32:TYR:HA	2:B:73:TYR:O	2.10	0.52
1:A:318:SER:OG	1:A:321:ARG:CB	2.58	0.51
1:A:148:PRO:O	1:A:150:ALA:N	2.42	0.51
1:A:70:PHE:HD2	1:A:107:LEU:HG	1.74	0.51
1:A:100:GLY:O	1:A:103:PHE:N	2.43	0.51
1:A:141:LEU:CD2	1:A:145:LEU:HD22	2.40	0.51
1:A:227:PHE:O	1:A:229:PRO:HD3	2.10	0.51
1:A:379:THR:HG22	1:A:382:ILE:HG12	1.92	0.51
1:A:385:TYR:HA	1:A:388:ARG:HE	1.76	0.51
1:A:217:LEU:O	1:A:218:TRP:C	2.47	0.51
1:A:272:ILE:HG22	1:A:280:VAL:O	2.11	0.51
1:A:448:TYR:C	1:A:450:MET:H	2.13	0.51
1:A:95:GLU:O	1:A:99:GLN:CG	2.58	0.51
1:A:140:MET:HG2	1:A:197:LEU:HD11	1.92	0.51
1:A:183:LEU:HD23	1:A:209:VAL:CG2	2.40	0.51
1:A:187:PHE:HB2	1:A:201:GLY:O	2.11	0.51
2:B:22:TRP:O	2:B:56:THR:HG23	2.10	0.51
1:A:115:MET:O	1:A:118:ALA:HB3	2.11	0.51
2:B:32:TYR:HB2	2:B:50:VAL:HG23	1.92	0.51
1:A:267:PHE:CZ	1:A:409:LEU:HA	2.44	0.51
2:B:50:VAL:CB	2:B:51:PRO:CD	2.88	0.51
2:B:68:TYR:O	2:B:88:ASN:O	2.29	0.51
1:A:33:ALA:HB2	1:A:170:MET:HA	1.92	0.51
2:B:8:LEU:HD12	2:B:87:ILE:HD11	1.84	0.51
1:A:64:ALA:HA	1:A:67:TYR:HB3	1.93	0.50
1:A:148:PRO:HG3	1:A:207:MET:CB	2.40	0.50
1:A:172:VAL:O	1:A:176:ALA:N	2.44	0.50
1:A:346:ARG:O	1:A:348:PRO:HD3	2.11	0.50
2:B:27:GLU:CB	2:B:30:VAL:HG23	2.40	0.50
1:A:458:ALA:HB3	2:B:8:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:HA	2:B:70:ILE:HD11	1.92	0.50
1:A:55:ALA:CB	1:A:58:LEU:HD21	2.37	0.50
1:A:100:GLY:HA2	1:A:103:PHE:HB2	1.92	0.50
1:A:253:PRO:HB3	1:A:394:LYS:O	2.10	0.50
1:A:199:GLY:O	1:A:200:ALA:HB2	2.12	0.50
1:A:225:LYS:HD3	1:A:226:PHE:N	2.27	0.50
2:B:35:THR:O	2:B:70:ILE:HG12	2.12	0.50
1:A:115:MET:CG	1:A:146:ALA:HB1	2.42	0.50
1:A:116:TRP:HH2	1:A:147:MET:HB2	1.77	0.50
1:A:141:LEU:HD21	1:A:145:LEU:CD2	2.39	0.50
1:A:335:ALA:HA	1:A:378:PHE:CZ	2.47	0.50
1:A:118:ALA:O	1:A:120:THR:N	2.45	0.50
1:A:144:SER:HB3	1:A:204:VAL:HG12	0.71	0.50
1:A:365:THR:HA	1:A:368:LEU:CD1	2.42	0.50
2:B:79:TRP:O	2:B:79:TRP:CE3	2.65	0.50
1:A:425:GLY:O	1:A:428:THR:CG2	2.60	0.49
1:A:69:THR:HG23	1:A:70:PHE:N	2.27	0.49
1:A:77:LEU:O	1:A:80:MET:HB2	2.12	0.49
1:A:364:SER:C	1:A:366:VAL:N	2.62	0.49
1:A:403:ALA:O	1:A:407:CYS:CB	2.57	0.49
1:A:73:ILE:HD12	1:A:73:ILE:N	2.24	0.49
3:A:501:RHQ:C15	3:A:501:RHQ:C13	2.52	0.49
1:A:343:VAL:HA	1:A:367:LEU:HB3	1.94	0.49
1:A:70:PHE:HB3	1:A:153:HIS:NE2	2.28	0.49
1:A:328:LEU:O	1:A:332:TRP:HB2	2.12	0.49
1:A:369:PHE:C	1:A:371:GLY:H	2.16	0.49
1:A:417:TYR:CG	1:A:417:TYR:O	2.65	0.49
1:A:56:VAL:HA	1:A:138:GLN:NE2	2.27	0.49
2:B:7:LYS:CB	2:B:23:ASP:HB2	2.35	0.49
1:A:33:ALA:HB2	1:A:170:MET:CA	2.43	0.49
1:A:81:ILE:HG13	1:A:163:LEU:HB2	1.94	0.49
1:A:108:GLY:O	1:A:112:MET:HB2	2.12	0.49
1:A:463:LEU:O	2:B:3:SER:CB	2.60	0.49
2:B:59:ILE:HD12	2:B:61:GLY:CA	2.42	0.49
1:A:74:MET:C	1:A:76:ALA:H	2.17	0.49
1:A:78:ASN:C	1:A:163:LEU:HD13	2.33	0.49
1:A:115:MET:HB3	1:A:146:ALA:HB1	1.95	0.49
1:A:140:MET:HB3	1:A:200:ALA:CB	2.42	0.49
1:A:159:TYR:C	1:A:159:TYR:HD1	2.16	0.49
1:A:183:LEU:O	1:A:184:ASN:C	2.51	0.49
1:A:385:TYR:HA	1:A:388:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:O	1:A:248:TRP:HB2	2.14	0.48
2:B:7:LYS:O	2:B:22:TRP:CE3	2.66	0.48
2:B:50:VAL:CG1	2:B:51:PRO:HD3	2.42	0.48
1:A:145:LEU:CD1	1:A:207:MET:HB3	2.43	0.48
1:A:151:MET:HB2	1:A:211:TRP:NE1	2.28	0.48
1:A:182:PRO:O	1:A:186:ILE:HG13	2.13	0.48
2:B:7:LYS:O	2:B:8:LEU:HD23	2.13	0.48
2:B:43:SER:O	2:B:44:PRO:O	2.31	0.48
1:A:156:LEU:HD12	1:A:159:TYR:CE1	2.49	0.48
1:A:339:VAL:HG21	1:A:375:PRO:CD	2.34	0.48
1:A:290:SER:O	1:A:294:TYR:HB3	2.14	0.48
1:A:103:PHE:HA	1:A:106:ILE:HG22	1.95	0.48
1:A:250:ILE:O	1:A:394:LYS:CD	2.62	0.48
1:A:411:PRO:HG3	1:A:429:ALA:CB	2.33	0.48
1:A:463:LEU:O	2:B:3:SER:HB3	2.14	0.48
1:A:102:TRP:HZ3	1:A:235:LYS:CG	2.26	0.48
1:A:372:LEU:HD21	1:A:424:TYR:CD1	2.48	0.48
2:B:75:ARG:CB	2:B:75:ARG:HH11	2.27	0.48
1:A:159:TYR:HB2	1:A:169:ILE:HD13	1.96	0.48
1:A:235:LYS:CB	1:A:241:TRP:HB3	2.36	0.47
1:A:393:THR:HG22	1:A:393:THR:O	2.13	0.47
1:A:398:PHE:CD2	1:A:399:ILE:HG12	2.49	0.47
1:A:90:THR:O	1:A:94:GLY:N	2.46	0.47
2:B:27:GLU:CG	2:B:30:VAL:HG23	2.44	0.47
1:A:116:TRP:CH2	1:A:147:MET:HB2	2.49	0.47
1:A:379:THR:O	1:A:382:ILE:N	2.47	0.47
1:A:396:PRO:CB	1:A:399:ILE:HG13	2.40	0.47
1:A:458:ALA:CB	2:B:8:LEU:HB3	2.43	0.47
2:B:26:GLY:O	2:B:53:SER:HA	2.15	0.47
1:A:141:LEU:CD2	1:A:145:LEU:CD2	2.93	0.47
1:A:387:LEU:CD2	1:A:445:LEU:HB2	2.44	0.47
1:A:457:LYS:HD3	2:B:10:VAL:HB	1.97	0.47
1:A:56:VAL:C	1:A:58:LEU:N	2.68	0.47
1:A:86:GLY:HA3	1:A:314:ARG:H	1.80	0.47
1:A:461:SER:CA	2:B:8:LEU:HG	2.42	0.47
2:B:4:VAL:HG23	2:B:6:THR:HG22	1.90	0.47
2:B:14:THR:C	2:B:16:THR:H	2.17	0.47
2:B:67:ASP:CA	2:B:90:ARG:HB3	2.35	0.47
1:A:58:LEU:HD12	1:A:138:GLN:CD	2.33	0.47
1:A:71:MET:HE2	1:A:159:TYR:OH	2.14	0.47
1:A:339:VAL:HA	1:A:342:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:HD21	1:A:424:TYR:HD1	1.79	0.47
1:A:414:LEU:O	1:A:418:ARG:NH1	2.44	0.47
2:B:9:GLU:N	2:B:22:TRP:NE1	2.58	0.47
1:A:69:THR:HG23	1:A:70:PHE:H	1.79	0.47
1:A:103:PHE:O	1:A:105:LEU:N	2.48	0.47
1:A:119:ILE:HG12	1:A:142:PHE:HB3	1.97	0.47
1:A:231:GLY:O	1:A:232:LEU:C	2.53	0.47
1:A:260:LEU:C	1:A:262:ALA:N	2.68	0.47
1:A:329:VAL:HG23	1:A:332:TRP:CE3	2.50	0.47
2:B:82:TYR:O	2:B:83:SER:CB	2.62	0.47
1:A:185:TYR:C	1:A:187:PHE:H	2.18	0.47
1:A:33:ALA:CB	1:A:170:MET:HA	2.44	0.46
1:A:397:MET:C	1:A:400:HIS:H	2.17	0.46
1:A:412:GLY:HA2	1:A:426:PHE:CD1	2.50	0.46
1:A:18:ARG:O	1:A:18:ARG:HD3	2.15	0.46
1:A:365:THR:CA	1:A:368:LEU:HG	2.42	0.46
2:B:12:ALA:O	2:B:18:LEU:HD23	2.16	0.46
1:A:69:THR:HG23	1:A:70:PHE:HD1	1.80	0.46
1:A:410:LEU:C	1:A:412:GLY:H	2.19	0.46
2:B:22:TRP:HZ3	2:B:85:ILE:HG23	1.79	0.46
2:B:67:ASP:HA	2:B:90:ARG:HG2	1.98	0.46
1:A:65:THR:HG22	1:A:66:VAL:H	1.79	0.46
1:A:148:PRO:HB2	1:A:152:VAL:HG11	1.98	0.46
1:A:416:ALA:O	1:A:417:TYR:HB3	2.15	0.46
1:A:176:ALA:HA	1:A:212:PHE:CE2	2.50	0.46
1:A:260:LEU:HB3	1:A:261:GLU:H	1.55	0.46
1:A:283:GLN:O	1:A:283:GLN:HG2	2.15	0.46
2:B:9:GLU:C	2:B:22:TRP:HE1	2.12	0.46
1:A:162:SER:HB3	1:A:166:PRO:O	2.15	0.46
1:A:169:ILE:HA	1:A:172:VAL:HG12	1.97	0.46
1:A:185:TYR:C	1:A:187:PHE:N	2.68	0.46
1:A:65:THR:CG2	1:A:66:VAL:N	2.79	0.46
1:A:102:TRP:HZ3	1:A:235:LYS:HG3	1.81	0.46
1:A:116:TRP:HH2	1:A:147:MET:CB	2.28	0.46
1:A:297:PRO:O	1:A:298:GLN:C	2.53	0.46
2:B:50:VAL:CB	2:B:51:PRO:HD3	2.43	0.46
1:A:79:PRO:O	1:A:81:ILE:N	2.49	0.46
1:A:119:ILE:HG12	1:A:142:PHE:HD2	1.81	0.46
1:A:126:LEU:HD13	1:A:270:PHE:HZ	1.81	0.46
1:A:397:MET:O	1:A:400:HIS:CG	2.69	0.46
1:A:70:PHE:O	1:A:73:ILE:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:C	1:A:244:PHE:N	2.68	0.46
1:A:243:VAL:HG23	1:A:243:VAL:O	2.16	0.46
2:B:20:ILE:CD1	2:B:59:ILE:HG23	2.45	0.46
1:A:74:MET:CB	1:A:156:LEU:HD21	2.43	0.45
1:A:100:GLY:O	1:A:104:GLY:N	2.42	0.45
1:A:259:PHE:CA	1:A:262:ALA:HB3	2.30	0.45
1:A:334:LEU:HA	1:A:337:ILE:HG13	1.97	0.45
1:A:369:PHE:CD2	1:A:424:TYR:HB3	2.50	0.45
2:B:8:LEU:HB3	2:B:87:ILE:HG13	1.98	0.45
1:A:100:GLY:HA3	1:A:157:HIS:NE2	2.32	0.45
1:A:312:LEU:HB2	1:A:390:TYR:CE2	2.51	0.45
1:A:397:MET:O	1:A:398:PHE:C	2.53	0.45
2:B:67:ASP:HA	2:B:90:ARG:CG	2.45	0.45
1:A:101:ILE:HD11	1:A:217:LEU:HD22	1.98	0.45
1:A:440:ALA:O	1:A:443:TRP:CE3	2.69	0.45
2:B:4:VAL:HA	2:B:83:SER:HB3	1.98	0.45
1:A:29:LEU:HB2	1:A:167:ARG:HG3	1.99	0.45
1:A:102:TRP:CG	1:A:233:THR:HB	2.52	0.45
1:A:167:ARG:HD3	1:A:167:ARG:N	2.31	0.45
1:A:329:VAL:HA	1:A:332:TRP:CB	2.47	0.45
2:B:4:VAL:HB	2:B:85:ILE:HB	1.99	0.45
2:B:19:LEU:HD13	2:B:19:LEU:C	2.36	0.45
1:A:31:GLN:OE1	1:A:299:SER:O	2.35	0.45
1:A:364:SER:OG	1:A:367:LEU:HD12	2.16	0.45
1:A:57:ALA:HA	1:A:60:SER:OG	2.16	0.45
1:A:189:TYR:HD1	1:A:190:GLY:N	2.15	0.45
1:A:325:GLY:C	1:A:327:SER:H	2.19	0.45
2:B:69:THR:OG1	2:B:88:ASN:HB3	2.16	0.45
1:A:311:SER:HB2	1:A:320:ALA:HB2	1.98	0.44
2:B:51:PRO:HB2	2:B:52:GLY:H	1.53	0.44
1:A:331:GLY:O	1:A:335:ALA:N	2.50	0.44
1:A:408:GLY:HA3	1:A:430:LEU:CD2	2.47	0.44
2:B:37:GLY:H	2:B:70:ILE:CD1	2.30	0.44
1:A:136:MET:O	1:A:139:TYR:HB2	2.16	0.44
1:A:372:LEU:HD13	1:A:427:TRP:CB	2.46	0.44
1:A:400:HIS:CG	1:A:401:ALA:N	2.85	0.44
1:A:65:THR:CG2	1:A:66:VAL:HG13	2.48	0.44
1:A:141:LEU:HD21	1:A:203:GLY:HA3	1.95	0.44
1:A:305:THR:OG1	1:A:389:GLY:HA2	2.18	0.44
1:A:396:PRO:HA	1:A:398:PHE:HB3	1.99	0.44
2:B:20:ILE:HD11	2:B:59:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:O	1:A:35:VAL:HG12	2.18	0.44
1:A:74:MET:CB	1:A:156:LEU:CD2	2.95	0.44
2:B:36:TYR:HD1	2:B:46:GLN:HB2	1.83	0.44
1:A:19:LEU:C	1:A:21:THR:N	2.70	0.44
1:A:148:PRO:HA	1:A:211:TRP:HE1	1.82	0.44
1:A:456:HIS:CD2	1:A:459:VAL:HA	2.53	0.44
1:A:460:SER:O	2:B:8:LEU:CG	2.63	0.44
1:A:91:GLY:HA3	1:A:226:PHE:HE1	1.79	0.44
1:A:96:THR:O	1:A:99:GLN:N	2.51	0.44
1:A:186:ILE:O	1:A:186:ILE:HG22	2.17	0.44
1:A:268:ILE:HG13	1:A:269:VAL:HG23	1.98	0.44
1:A:426:PHE:C	1:A:428:THR:N	2.71	0.44
1:A:95:GLU:O	1:A:99:GLN:HG2	2.17	0.43
1:A:321:ARG:HH22	1:A:391:LYS:HD3	1.82	0.43
1:A:329:VAL:HG22	1:A:332:TRP:HE3	1.83	0.43
2:B:13:ALA:HA	2:B:18:LEU:HA	2.00	0.43
2:B:38:GLU:CD	2:B:38:GLU:N	2.71	0.43
1:A:147:MET:SD	1:A:148:PRO:HD3	2.57	0.43
1:A:298:GLN:HA	1:A:382:ILE:CG2	2.47	0.43
2:B:51:PRO:O	2:B:52:GLY:O	2.36	0.43
1:A:15:LYS:HB3	1:A:325:GLY:HA3	2.01	0.43
1:A:119:ILE:H	1:A:119:ILE:HG13	1.25	0.43
1:A:158:ALA:CA	1:A:217:LEU:HD11	2.42	0.43
1:A:424:TYR:O	1:A:427:TRP:HB2	2.18	0.43
1:A:410:LEU:HA	1:A:413:TYR:CE1	2.54	0.43
1:A:411:PRO:C	1:A:426:PHE:HB2	2.39	0.43
1:A:274:PRO:C	1:A:276:GLY:N	2.66	0.43
2:B:34:ILE:HD11	2:B:48:PHE:HB2	1.99	0.43
1:A:28:LEU:HD23	1:A:29:LEU:CD2	2.48	0.43
1:A:221:ILE:HG21	1:A:228:ARG:CB	2.48	0.43
1:A:238:LYS:CB	1:A:239:PRO:CD	2.90	0.43
1:A:315:ARG:HG2	2:B:9:GLU:OE1	2.18	0.43
2:B:21:SER:C	2:B:22:TRP:CD1	2.90	0.43
1:A:15:LYS:NZ	1:A:446:GLU:OE1	2.51	0.43
1:A:76:ALA:C	1:A:250:ILE:HD13	2.39	0.43
1:A:147:MET:N	1:A:148:PRO:CD	2.80	0.43
1:A:15:LYS:HD2	1:A:325:GLY:CA	2.48	0.43
1:A:191:LYS:HB3	1:A:192:PHE:H	1.61	0.43
1:A:254:ILE:O	1:A:258:TYR:N	2.52	0.43
1:A:340:LEU:HD12	1:A:341:SER:N	2.33	0.43
1:A:342:LEU:O	1:A:367:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:CD2	1:A:404:PHE:N	2.86	0.43
1:A:458:ALA:HB3	2:B:8:LEU:HB2	1.99	0.43
2:B:30:VAL:O	2:B:30:VAL:CG1	2.60	0.43
2:B:38:GLU:HB3	2:B:67:ASP:O	2.18	0.43
1:A:103:PHE:O	1:A:107:LEU:N	2.48	0.43
1:A:182:PRO:HB2	1:A:183:LEU:H	1.71	0.43
1:A:227:PHE:C	1:A:229:PRO:HD3	2.40	0.43
1:A:259:PHE:CG	1:A:262:ALA:HB3	2.54	0.43
1:A:263:SER:CB	1:A:405:TRP:CD1	3.02	0.43
1:A:377:ASP:O	1:A:378:PHE:C	2.57	0.43
1:A:455:SER:O	1:A:457:LYS:N	2.52	0.43
1:A:56:VAL:O	1:A:58:LEU:N	2.52	0.42
2:B:7:LYS:HB3	2:B:23:ASP:N	2.22	0.42
1:A:99:GLN:OE1	1:A:241:TRP:NE1	2.52	0.42
1:A:136:MET:C	1:A:138:GLN:H	2.23	0.42
1:A:76:ALA:HB2	1:A:254:ILE:HG21	2.01	0.42
1:A:102:TRP:CH2	1:A:234:ALA:HA	2.55	0.42
1:A:168:LEU:HD23	1:A:171:LEU:HD22	2.01	0.42
1:A:252:ALA:CB	1:A:253:PRO:HD3	2.34	0.42
1:A:329:VAL:CG2	1:A:332:TRP:CE3	3.02	0.42
1:A:448:TYR:CE1	1:A:451:GLU:HG3	2.54	0.42
2:B:38:GLU:CB	2:B:67:ASP:O	2.67	0.42
1:A:72:GLY:O	1:A:73:ILE:C	2.57	0.42
1:A:104:GLY:HA2	1:A:153:HIS:HB3	2.02	0.42
1:A:212:PHE:CD2	1:A:213:SER:N	2.87	0.42
1:A:217:LEU:O	1:A:219:ILE:N	2.53	0.42
1:A:366:VAL:HA	1:A:369:PHE:CZ	2.53	0.42
1:A:387:LEU:HB3	1:A:388:ARG:H	1.59	0.42
1:A:142:PHE:O	1:A:146:ALA:CB	2.61	0.42
1:A:253:PRO:HB2	1:A:394:LYS:CD	2.44	0.42
1:A:346:ARG:NE	1:A:364:SER:HB2	2.34	0.42
1:A:12:VAL:HG23	1:A:13:PHE:N	2.33	0.42
2:B:4:VAL:HG22	2:B:6:THR:HG22	1.96	0.42
1:A:15:LYS:HG2	1:A:322:TYR:HA	2.01	0.42
1:A:396:PRO:HB3	1:A:399:ILE:CG1	2.41	0.42
1:A:448:TYR:C	1:A:450:MET:N	2.70	0.42
1:A:185:TYR:O	1:A:187:PHE:N	2.52	0.42
1:A:120:THR:H	1:A:121:PRO:CD	2.33	0.42
1:A:282:ALA:HB2	1:A:362:ILE:HD12	2.01	0.42
1:A:116:TRP:CH2	1:A:147:MET:CA	2.90	0.42
1:A:321:ARG:HD2	1:A:452:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:HA2	1:A:153:HIS:HD2	1.85	0.41
1:A:241:TRP:O	1:A:244:PHE:HB3	2.20	0.41
1:A:315:ARG:HG3	1:A:317:PHE:HE1	1.72	0.41
1:A:382:ILE:HA	1:A:385:TYR:HD2	1.85	0.41
1:A:53:LEU:HD23	1:A:135:THR:CG2	2.50	0.41
1:A:301:GLY:C	1:A:303:ALA:H	2.22	0.41
1:A:346:ARG:HB2	1:A:348:PRO:HG3	2.01	0.41
1:A:380:GLN:HB3	1:A:437:ALA:HB3	2.02	0.41
1:A:387:LEU:HD21	1:A:445:LEU:HB2	2.01	0.41
2:B:20:ILE:HD11	2:B:59:ILE:N	2.35	0.41
1:A:100:GLY:O	1:A:103:PHE:CB	2.68	0.41
1:A:227:PHE:O	1:A:227:PHE:CD2	2.73	0.41
1:A:227:PHE:O	1:A:227:PHE:HD2	2.01	0.41
1:A:78:ASN:O	1:A:163:LEU:HD13	2.21	0.41
1:A:167:ARG:C	1:A:169:ILE:N	2.73	0.41
1:A:301:GLY:O	1:A:305:THR:N	2.44	0.41
1:A:309:GLY:O	1:A:312:LEU:HB3	2.21	0.41
1:A:426:PHE:HA	1:A:428:THR:HG22	2.02	0.41
1:A:427:TRP:CD1	1:A:427:TRP:N	2.87	0.41
1:A:172:VAL:C	1:A:174:PHE:N	2.72	0.41
1:A:143:THR:C	1:A:145:LEU:N	2.74	0.41
1:A:147:MET:CE	1:A:207:MET:SD	3.09	0.41
1:A:74:MET:HE3	1:A:103:PHE:HB3	2.03	0.41
1:A:218:TRP:CE3	1:A:221:ILE:HD11	2.55	0.41
1:A:254:ILE:HG23	1:A:255:GLY:N	2.36	0.41
1:A:56:VAL:C	1:A:58:LEU:H	2.24	0.41
1:A:78:ASN:N	1:A:79:PRO:CD	2.84	0.41
1:A:100:GLY:C	1:A:102:TRP:N	2.71	0.41
1:A:108:GLY:HA2	1:A:153:HIS:CD2	2.56	0.41
1:A:163:LEU:HB3	1:A:306:VAL:HG22	2.02	0.41
1:A:225:LYS:CG	1:A:226:PHE:N	2.83	0.41
2:B:64:PRO:HB2	2:B:65:GLY:H	1.64	0.41
1:A:35:VAL:HG13	1:A:36:GLY:N	2.36	0.41
1:A:290:SER:O	1:A:291:GLY:C	2.59	0.41
1:A:99:GLN:NE2	1:A:233:THR:O	2.54	0.40
1:A:397:MET:O	1:A:400:HIS:CB	2.70	0.40
2:B:5:PRO:CD	2:B:74:ALA:HB2	2.48	0.40
1:A:344:LEU:HD22	1:A:345:PHE:CD2	2.56	0.40
1:A:369:PHE:HA	1:A:372:LEU:HB2	2.02	0.40
1:A:106:ILE:HD13	1:A:106:ILE:HA	1.86	0.40
1:A:145:LEU:HD13	1:A:203:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD12	1:A:159:TYR:CZ	2.56	0.40
1:A:391:LYS:C	1:A:393:THR:H	2.23	0.40
1:A:410:LEU:O	1:A:414:LEU:HD13	2.21	0.40
2:B:34:ILE:CD1	2:B:48:PHE:HB2	2.51	0.40
1:A:311:SER:HB2	1:A:320:ALA:CB	2.51	0.40
2:B:38:GLU:CD	2:B:38:GLU:H	2.23	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	457/459 (100%)	248 (54%)	133 (29%)	76 (17%)	0	3
2	B	89/99 (90%)	52 (58%)	18 (20%)	19 (21%)	0	1
All	All	546/558 (98%)	300 (55%)	151 (28%)	95 (17%)	0	2

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	41	ASP
1	A	80	MET
1	A	105	LEU
1	A	112	MET
1	A	119	ILE
1	A	127	THR
1	A	139	TYR
1	A	164	ASN
1	A	165	ARG
1	A	194	MET
1	A	229	PRO

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Mol	Chain	Res	Type
1	A	234	ALA
1	A	236	PHE
1	A	238	LYS
1	A	278	ASP
1	A	297	PRO
1	A	298	GLN
1	A	307	ARG
1	A	349	LEU
1	A	386	ALA
1	A	396	PRO
1	A	417	TYR
1	A	442	VAL
1	A	445	LEU
2	B	11	VAL
2	B	15	PRO
2	B	30	VAL
2	B	44	PRO
2	B	51	PRO
2	B	52	GLY
2	B	61	GLY
2	B	62	LEU
2	B	64	PRO
2	B	77	TYR
2	B	79	TRP
2	B	83	SER
2	B	90	ARG
1	A	12	VAL
1	A	15	LYS
1	A	57	ALA
1	A	73	ILE
1	A	131	TYR
1	A	149	ALA
1	A	166	PRO
1	A	193	GLY
1	A	200	ALA
1	A	224	GLU
1	A	260	LEU
1	A	261	GLU
1	A	277	GLU
1	A	291	GLY
1	A	314	ARG
1	A	361	SER

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Mol	Chain	Res	Type
1	A	378	PHE
2	B	31	TYR
2	B	38	GLU
2	B	42	ASN
1	A	14	LEU
1	A	17	ILE
1	A	64	ALA
1	A	79	PRO
1	A	121	PRO
1	A	182	PRO
1	A	233	THR
1	A	242	ALA
1	A	244	PHE
1	A	275	PHE
1	A	284	GLN
1	A	320	ALA
1	A	344	LEU
1	A	372	LEU
2	B	5	PRO
2	B	84	PRO
1	A	104	GLY
1	A	144	SER
1	A	232	LEU
1	A	290	SER
1	A	305	THR
1	A	319	ARG
1	A	354	ASN
1	A	446	GLU
1	A	184	ASN
1	A	192	PHE
1	A	264	ALA
1	A	326	VAL
1	A	365	THR
1	A	398	PHE
1	A	421	MET
2	B	43	SER
1	A	158	ALA
1	A	353	TYR
1	A	371	GLY
1	A	392	VAL
1	A	88	GLY

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	353/353 (100%)	234 (66%)	119 (34%)	0	1
2	B	78/85 (92%)	53 (68%)	25 (32%)	0	2
All	All	431/438 (98%)	287 (67%)	144 (33%)	0	2

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	10	PHE
1	A	15	LYS
1	A	18	ARG
1	A	19	LEU
1	A	20	LEU
1	A	23	LEU
1	A	27	MET
1	A	39	PHE
1	A	40	VAL
1	A	42	THR
1	A	43	VAL
1	A	52	ASP
1	A	53	LEU
1	A	58	LEU
1	A	61	SER
1	A	65	THR
1	A	71	MET
1	A	80	MET
1	A	81	ILE
1	A	89	LYS
1	A	95	GLU
1	A	96	THR
1	A	102	TRP
1	A	103	PHE
1	A	106	ILE
1	A	107	LEU

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Mol	Chain	Res	Type
1	A	112	MET
1	A	113	ILE
1	A	116	TRP
1	A	119	ILE
1	A	123	ARG
1	A	124	ASN
1	A	126	LEU
1	A	131	TYR
1	A	135	THR
1	A	136	MET
1	A	139	TYR
1	A	140	MET
1	A	147	MET
1	A	153	HIS
1	A	154	ARG
1	A	156	LEU
1	A	159	TYR
1	A	165	ARG
1	A	167	ARG
1	A	177	PHE
1	A	178	VAL
1	A	179	LEU
1	A	180	ASN
1	A	189	TYR
1	A	197	LEU
1	A	207	MET
1	A	210	PHE
1	A	212	PHE
1	A	213	SER
1	A	217	LEU
1	A	218	TRP
1	A	221	ILE
1	A	224	GLU
1	A	228	ARG
1	A	232	LEU
1	A	235	LYS
1	A	238	LYS
1	A	248	TRP
1	A	257	SER
1	A	259	PHE
1	A	260	LEU
1	A	271	LEU

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Mol	Chain	Res	Type
1	A	288	SER
1	A	289	LEU
1	A	294	TYR
1	A	295	MET
1	A	296	ILE
1	A	298	GLN
1	A	302	SER
1	A	310	PHE
1	A	311	SER
1	A	314	ARG
1	A	315	ARG
1	A	323	ILE
1	A	324	SER
1	A	329	VAL
1	A	332	TRP
1	A	334	LEU
1	A	336	VAL
1	A	353	TYR
1	A	356	ASP
1	A	362	ILE
1	A	369	PHE
1	A	374	GLN
1	A	377	ASP
1	A	379	THR
1	A	382	ILE
1	A	384	SER
1	A	385	TYR
1	A	387	LEU
1	A	388	ARG
1	A	391	LYS
1	A	397	MET
1	A	407	CYS
1	A	410	LEU
1	A	413	TYR
1	A	417	TYR
1	A	421	MET
1	A	427	TRP
1	A	428	THR
1	A	431	ILE
1	A	433	SER
1	A	434	LEU
1	A	435	THR

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Mol	Chain	Res	Type
1	A	436	ILE
1	A	439	VAL
1	A	441	LEU
1	A	452	LEU
1	A	454	LYS
1	A	457	LYS
1	A	460	SER
1	A	461	SER
2	B	2	SER
2	B	3	SER
2	B	10	VAL
2	B	16	THR
2	B	18	LEU
2	B	19	LEU
2	B	20	ILE
2	B	25	ARG
2	B	28	TYR
2	B	34	ILE
2	B	36	TYR
2	B	38	GLU
2	B	45	VAL
2	B	46	GLN
2	B	50	VAL
2	B	53	SER
2	B	58	THR
2	B	63	SER
2	B	68	TYR
2	B	72	VAL
2	B	75	ARG
2	B	76	SER
2	B	78	TYR
2	B	90	ARG
2	B	91	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	180	ASN
1	A	284	GLN
2	B	42	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	RHQ	A	501	-	33,36,36	2.92	7 (21%)	43,51,51	1.99	12 (27%)

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	RHQ	A	501	-	-	7/15/21/21	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	RHQ	C2-C9	7.89	1.52	1.39
3	A	501	RHQ	C19-C14	7.08	1.51	1.40
3	A	501	RHQ	C8-C7	6.42	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	RHQ	O2-C26	5.48	1.47	1.33
3	A	501	RHQ	C11-C12	5.17	1.50	1.40
3	A	501	RHQ	C5-C4	5.17	1.51	1.43
3	A	501	RHQ	C9-C8	4.05	1.51	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	RHQ	O1-C7-C10	4.58	121.48	116.11
3	A	501	RHQ	C10-C7-C8	-4.25	118.35	123.05
3	A	501	RHQ	O2-C26-C19	3.81	119.75	112.21
3	A	501	RHQ	C2-C9-C8	-3.75	116.44	119.63
3	A	501	RHQ	C5-C6-C1	3.54	122.83	119.46
3	A	501	RHQ	O1-C1-C6	3.13	119.74	116.03
3	A	501	RHQ	C11-C10-C7	2.86	122.18	119.46
3	A	501	RHQ	C13-C8-C7	2.68	119.41	116.39
3	A	501	RHQ	C28-O2-C26	2.52	122.31	116.46
3	A	501	RHQ	C14-C9-C8	-2.31	115.53	119.42
3	A	501	RHQ	C21-C4-C3	-2.28	117.41	120.74
3	A	501	RHQ	C18-C19-C14	-2.12	117.30	119.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	RHQ	C15-C14-C9-C2
3	A	501	RHQ	C19-C14-C9-C2
3	A	501	RHQ	C15-C14-C9-C8
3	A	501	RHQ	C19-C14-C9-C8
3	A	501	RHQ	C12-C11-N1-C22
3	A	501	RHQ	C10-C11-N1-C22
3	A	501	RHQ	C18-C19-C26-O2

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	RHQ	9	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.

Ligand RHQ A 501

Bond lengths

Bond angles

Torsions

Rings
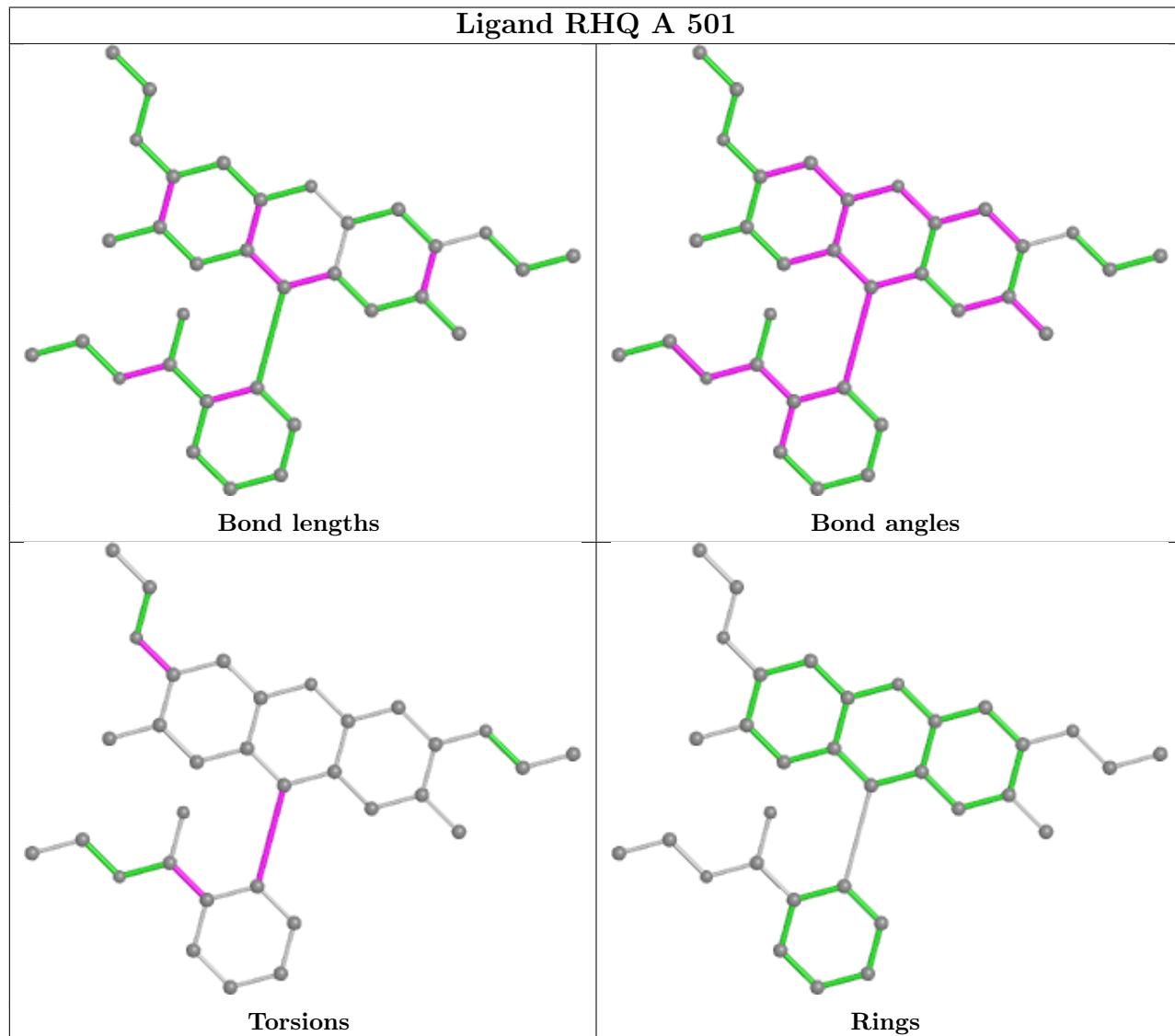
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	459/459 (100%)	-0.25	11 (2%)	59	42	86, 170, 288, 384	0
2	B	91/99 (91%)	-0.02	3 (3%)	46	31	79, 146, 212, 233	0
All	All	550/558 (98%)	-0.21	14 (2%)	57	41	79, 165, 284, 384	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	SER	11.8
2	B	1	VAL	10.7
1	A	9	SER	4.5
1	A	230	PHE	4.0
1	A	420	ASP	3.8
1	A	271	LEU	3.5
2	B	89	TYR	3.5
1	A	421	MET	3.0
1	A	457	LYS	2.9
1	A	280	VAL	2.8
1	A	194	MET	2.8
1	A	416	ALA	2.1
1	A	13	PHE	2.1
1	A	19	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	RHQ	A	501	33/33	0.65	0.49	194,297,346,353	0

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 RHQ A 501:

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 ⓘ

There are no such residues in this entry.