



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:32 pm GMT

PDB ID : 1FPM  
Title : MONOVALENT CATION BINDING SITES IN N10-FORMYLTETRAHYDROFOLATE SYNTHETASE FROM MOORELLA THERMOACETICA  
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Deposited on : 2000-08-31  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

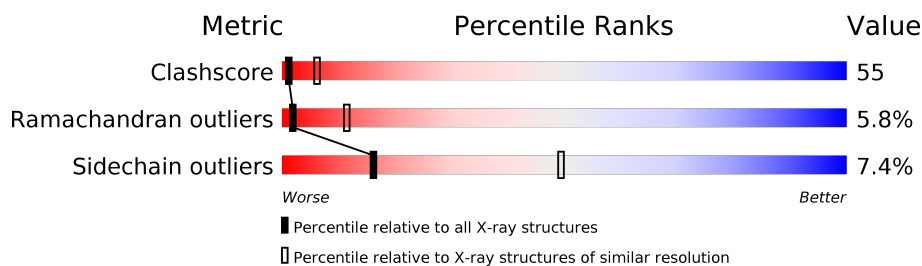
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	561	-	-	X	-
2	SO4	A	565	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8585 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 FORMATE--TETRAHYDROFOLATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4133	2617	715	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4125	2613	714	777	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	DELETION	UNP P21164
A	?	-	VAL	DELETION	UNP P21164
B	?	-	GLU	DELETION	UNP P21164
B	?	-	VAL	DELETION	UNP P21164

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 3 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cs 1 1	0	0
3	A	1	Total Cs 1 1	0	0

- Molecule 4 is water.

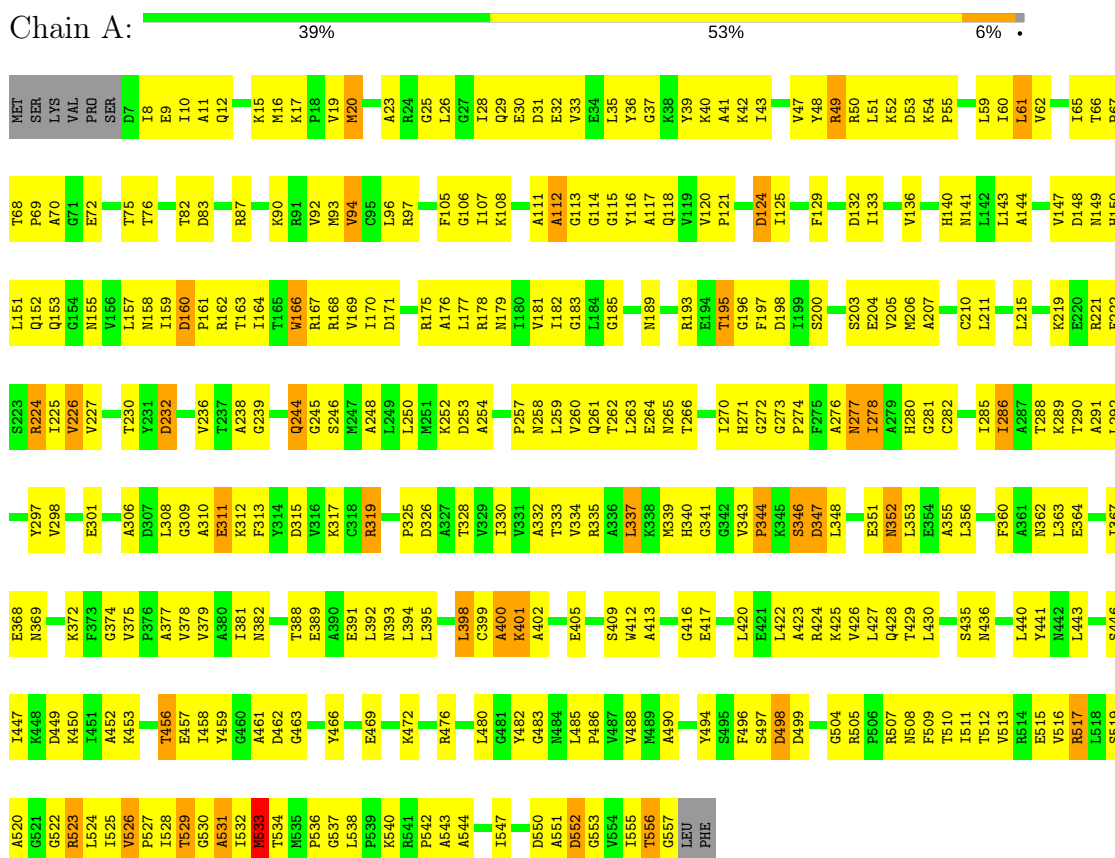
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	70	Total O 70 70	0	0

### 3 Residue-property plots

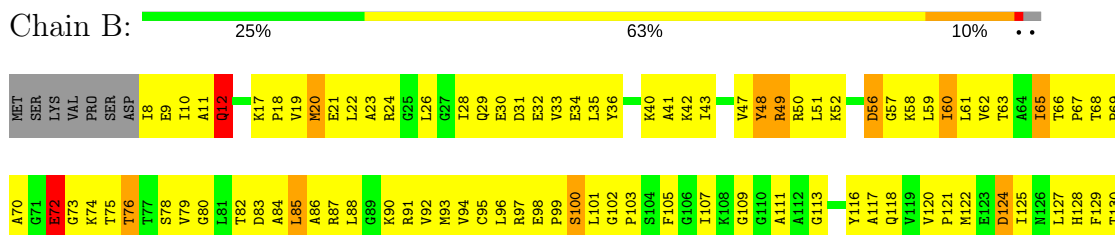
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE



#### • Molecule 1: FORMATE--TETRAHYDROFOLATE LIGASE





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	84.0 (40.00-3.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.266 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8585	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CS, SO4

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	0.52	0/4201	0.72	0/5690
1	B	0.43	0/4193	0.67	0/5679
All	All	0.48	0/8394	0.70	0/11369

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4133	0	4219	382	0
1	B	4125	0	4215	545	1
2	A	35	0	0	10	0
2	B	20	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	200	0	0	27	0
4	B	70	0	0	14	1
All	All	8585	0	8434	927	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.



All (927) 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:166:TRP:CZ3	1:B:225:ILE:HD11	1.30	1.59
1:A:166:TRP:CZ3	1:A:225:ILE:HD11	1.42	1.53
1:B:166:TRP:CH2	1:B:225:ILE:HD11	1.58	1.38
1:B:166:TRP:CH2	1:B:225:ILE:CD1	2.11	1.34
1:B:166:TRP:CZ3	1:B:225:ILE:CD1	2.10	1.33
1:A:166:TRP:CE3	1:A:225:ILE:HD11	1.64	1.31
1:A:166:TRP:CZ3	1:A:225:ILE:CD1	2.20	1.23
1:B:43:ILE:HD11	1:B:259:LEU:HD22	1.29	1.15
1:B:222:PHE:O	1:B:225:ILE:HG22	1.49	1.13
1:B:109:GLY:O	4:B:580:HOH:O	1.65	1.12
1:B:195:THR:HG22	1:B:196:GLY:H	1.02	1.12
1:A:20:MET:HE3	1:A:30:GLU:HG3	1.33	1.09
1:B:376:PRO:HD3	1:B:435:SER:HB3	1.32	1.07
1:B:523:ARG:H	1:B:523:ARG:NE	1.58	1.00
1:B:368:GLU:HG2	1:B:401:LYS:HE2	1.42	0.99
1:A:179:ASN:OD1	4:A:757:HOH:O	1.81	0.98
1:B:166:TRP:CH2	1:B:225:ILE:HD13	1.96	0.98
1:A:25:GLY:O	4:A:677:HOH:O	1.82	0.96
1:B:277:ASN:ND2	1:B:278:ILE:H	1.65	0.95
1:B:166:TRP:HH2	1:B:225:ILE:CD1	1.81	0.93
1:B:195:THR:HG22	1:B:196:GLY:N	1.83	0.92
1:B:93:MET:HG2	1:B:267:PRO:HB2	1.52	0.92
1:B:338:LYS:HG2	1:B:343:VAL:HG21	1.51	0.91
1:B:365:LYS:HE3	1:B:369:ASN:HD21	1.34	0.91
1:A:35:LEU:HD22	1:A:37:GLY:O	1.71	0.91
1:A:140:HIS:HD2	1:A:203:SER:OG	1.53	0.91
1:A:405:GLU:CD	1:A:422:LEU:HA	1.90	0.91
1:A:222:PHE:O	1:A:225:ILE:HG22	1.71	0.90
1:A:169:VAL:HG23	1:A:198:ASP:O	1.70	0.90
1:A:557:GLY:O	4:A:582:HOH:O	1.91	0.88
1:B:21:GLU:HA	1:B:24:ARG:HD2	1.54	0.88
1:A:257:PRO:HD3	1:A:286:ILE:HD11	1.56	0.86
1:B:447:ILE:HD11	1:B:483:GLY:HA2	1.54	0.86
1:B:517:ARG:HH22	1:B:532:ILE:HG13	1.41	0.86
1:B:555:ILE:O	1:B:556:THR:HB	1.74	0.86
1:A:485:LEU:HD13	1:A:523:ARG:HA	1.58	0.85
1:A:9:GLU:HG2	1:A:115:GLY:H	1.42	0.85
1:B:195:THR:CG2	1:B:196:GLY:H	1.85	0.85
1:B:363:LEU:O	1:B:367:ILE:HG12	1.75	0.85
1:B:490:ALA:HB2	1:B:525:ILE:HG22	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLY:HA3	1:B:189:ASN:HD22	1.42	0.84
1:B:265:ASN:HD22	1:B:265:ASN:N	1.76	0.83
1:A:47:VAL:HA	1:A:50:ARG:NH1	1.92	0.83
1:A:136:VAL:HG21	1:A:206:MET:HE2	1.58	0.83
1:B:277:ASN:HD22	1:B:278:ILE:H	1.22	0.83
1:A:277:ASN:HD22	1:A:277:ASN:H	1.26	0.83
1:B:48:TYR:HB2	1:B:290:THR:OG1	1.77	0.83
1:B:394:LEU:O	1:B:398:LEU:HD23	1.78	0.83
1:A:401:LYS:HB2	4:A:748:HOH:O	1.78	0.83
1:B:26:LEU:HD23	1:B:28:ILE:HD11	1.59	0.83
1:A:277:ASN:HD22	1:A:278:ILE:H	1.27	0.82
1:A:169:VAL:HG21	1:A:200:SER:HA	1.61	0.82
1:B:498:ASP:HB3	1:B:528:ILE:HG21	1.61	0.82
1:A:42:LYS:HE3	1:A:258:ASN:OD1	1.80	0.82
1:A:326:ASP:HA	1:A:435:SER:OG	1.80	0.81
1:B:357:ARG:O	1:B:360:PHE:HB3	1.81	0.81
1:A:82:THR:HG21	1:A:94:VAL:HG22	1.62	0.80
1:B:210:CYS:SG	1:B:274:PRO:HD3	2.21	0.80
1:B:33:VAL:HG13	1:B:41:ALA:HB1	1.64	0.80
1:B:40:LYS:HB2	1:B:40:LYS:HZ2	1.44	0.80
1:B:337:LEU:HD21	1:B:363:LEU:HB2	1.61	0.80
1:B:166:TRP:HZ3	1:B:225:ILE:HD11	1.00	0.79
1:B:376:PRO:HG3	1:B:433:ARG:HG2	1.64	0.79
1:A:372:LYS:HE2	4:A:728:HOH:O	1.81	0.79
1:A:447:ILE:HD11	1:A:483:GLY:HA2	1.62	0.79
1:B:557:GLY:HA3	4:B:574:HOH:O	1.81	0.79
1:A:17:LYS:H	1:A:261:GLN:NE2	1.81	0.78
1:A:66:THR:HB	1:A:340:HIS:NE2	1.99	0.78
1:B:550:ASP:C	1:B:552:ASP:H	1.85	0.78
1:A:175:ARG:HD3	2:A:563:SO4:O3	1.84	0.78
1:B:335:ARG:NH2	1:B:349:ALA:HA	1.99	0.77
1:B:286:ILE:HA	1:B:289:LYS:HG2	1.66	0.77
1:A:417:GLU:HA	1:A:420:LEU:HD23	1.66	0.77
1:B:337:LEU:HD23	1:B:360:PHE:HA	1.65	0.77
1:B:215:LEU:HD11	1:B:252:LYS:HA	1.67	0.76
1:B:334:VAL:HG13	1:B:356:LEU:HD21	1.66	0.76
1:A:488:VAL:CG2	1:A:523:ARG:HD3	2.15	0.76
1:B:477:TYR:HE2	1:B:516:VAL:HG12	1.51	0.76
1:B:489:MET:CE	1:B:526:VAL:HG11	2.14	0.76
1:A:210:CYS:SG	1:A:274:PRO:HD3	2.26	0.76
1:B:74:LYS:HB2	1:B:74:LYS:NZ	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PHE:HB3	1:A:544:ALA:HB2	1.66	0.75
1:B:261:GLN:HB2	1:B:265:ASN:HA	1.69	0.75
1:B:488:VAL:CG2	1:B:523:ARG:HD3	2.17	0.75
1:A:92:VAL:HG23	1:A:297:TYR:O	1.86	0.75
1:A:66:THR:HB	1:A:340:HIS:HE2	1.51	0.75
1:B:516:VAL:HA	1:B:527:PRO:HD2	1.67	0.75
1:A:488:VAL:HG21	1:A:523:ARG:HD3	1.68	0.75
1:A:405:GLU:OE1	1:A:425:LYS:HB2	1.87	0.74
1:B:111:ALA:HB2	1:B:122:MET:SD	2.28	0.74
1:B:136:VAL:HG13	1:B:205:VAL:HG12	1.68	0.74
1:B:47:VAL:HG11	1:B:294:LEU:HD11	1.68	0.74
1:B:488:VAL:HG21	1:B:523:ARG:HD3	1.69	0.74
1:A:498:ASP:HB3	1:A:528:ILE:HG21	1.69	0.74
1:A:96:LEU:O	1:A:270:ILE:HA	1.88	0.74
1:A:486:PRO:O	1:A:523:ARG:HB2	1.86	0.74
1:B:43:ILE:CD1	1:B:259:LEU:HD22	2.15	0.74
1:B:451:ILE:HG12	1:B:489:MET:HE1	1.69	0.74
1:B:98:GLU:HG2	1:B:99:PRO:HD2	1.70	0.74
1:B:23:ALA:HA	1:B:28:ILE:HD12	1.69	0.73
1:A:333:THR:HG22	1:A:382:ASN:HB3	1.69	0.73
1:B:12:GLN:NE2	1:B:263:LEU:HD13	2.03	0.73
1:B:417:GLU:HA	1:B:420:LEU:HD23	1.71	0.73
1:B:61:LEU:HD12	1:B:300:THR:O	1.88	0.73
1:A:446:SER:HB3	1:A:449:ASP:HB2	1.71	0.73
1:B:515:GLU:HB3	1:B:527:PRO:HG2	1.69	0.72
1:A:533:MET:HB2	2:A:561:SO4:O2	1.89	0.72
1:A:488:VAL:HG21	1:A:523:ARG:HH11	1.55	0.72
1:A:530:GLY:C	1:A:532:ILE:H	1.92	0.72
1:B:174:ASP:OD1	1:B:177:LEU:HG	1.88	0.72
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.90	0.72
1:B:376:PRO:HD3	1:B:435:SER:CB	2.15	0.72
1:B:405:GLU:OE1	1:B:421:GLU:HG2	1.89	0.72
1:A:17:LYS:H	1:A:261:GLN:HE21	1.37	0.71
1:A:169:VAL:CG2	1:A:200:SER:HA	2.20	0.71
1:B:144:ALA:HB1	1:B:168:ARG:HH21	1.54	0.71
1:B:449:ASP:O	1:B:452:ALA:HB3	1.90	0.71
1:A:382:ASN:OD1	2:A:565:SO4:O1	2.08	0.71
1:B:277:ASN:ND2	1:B:278:ILE:N	2.36	0.71
1:B:292:LEU:HD23	1:B:298:VAL:HG21	1.73	0.71
1:A:160:ASP:OD1	1:A:163:THR:HG23	1.89	0.71
1:B:285:ILE:N	4:B:611:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:VAL:HG22	1:A:526:VAL:HB	1.72	0.71
1:B:169:VAL:HG11	1:B:200:SER:HA	1.72	0.71
1:A:462:ASP:OD2	1:A:508:ASN:HA	1.91	0.70
1:B:136:VAL:HG13	1:B:205:VAL:CG1	2.20	0.70
1:B:169:VAL:CG1	1:B:200:SER:HA	2.21	0.70
1:B:543:ALA:O	1:B:547:ILE:HG13	1.90	0.70
1:A:257:PRO:HD3	1:A:286:ILE:CD1	2.21	0.70
1:B:75:THR:HB	1:B:113:GLY:HA2	1.73	0.70
1:B:472:LYS:HD3	1:B:476:ARG:NH2	2.07	0.70
1:B:173:ASN:HB2	1:B:538:LEU:HD23	1.72	0.70
1:A:405:GLU:OE1	1:A:422:LEU:HA	1.92	0.70
1:A:82:THR:HG21	1:A:94:VAL:CG2	2.22	0.70
1:B:286:ILE:HD12	1:B:287:ALA:N	2.07	0.70
1:A:264:GLU:O	1:A:265:ASN:HB2	1.90	0.70
1:A:412:TRP:CG	2:A:565:SO4:O4	2.45	0.69
1:B:210:CYS:HA	1:B:284:SER:HA	1.74	0.69
1:A:32:GLU:OE2	1:A:50:ARG:NH1	2.25	0.69
1:A:504:GLY:O	4:A:622:HOH:O	2.10	0.69
1:A:92:VAL:HB	1:A:297:TYR:HB2	1.74	0.69
1:B:265:ASN:H	1:B:265:ASN:HD22	1.40	0.69
1:B:334:VAL:HB	1:B:387:ASP:OD1	1.91	0.69
1:B:85:LEU:HD13	1:B:92:VAL:HG11	1.74	0.69
1:B:353:LEU:HD12	1:B:353:LEU:N	2.07	0.69
1:B:242:GLU:HA	1:B:244:GLN:OE1	1.91	0.69
1:A:148:ASP:OD2	1:A:168:ARG:NH2	2.25	0.69
1:B:257:PRO:HA	1:B:271:HIS:ND1	2.08	0.69
1:B:40:LYS:NZ	1:B:130:THR:HG22	2.08	0.69
1:B:148:ASP:OD1	4:B:591:HOH:O	2.11	0.69
1:B:517:ARG:HH12	1:B:532:ILE:HD12	1.57	0.69
1:A:262:THR:HG22	1:A:263:LEU:H	1.57	0.68
1:B:9:GLU:HG3	1:B:118:GLN:HE22	1.57	0.68
1:A:469:GLU:HG3	4:A:700:HOH:O	1.94	0.68
1:B:262:THR:HG22	1:B:263:LEU:H	1.58	0.68
1:B:306:ALA:O	1:B:310:ALA:HB3	1.93	0.68
1:B:219:LYS:O	1:B:222:PHE:HB2	1.92	0.68
1:A:175:ARG:HG2	1:A:178:ARG:NH2	2.09	0.68
1:A:61:LEU:HD13	1:A:313:PHE:CD2	2.29	0.68
1:A:452:ALA:O	1:A:456:THR:HB	1.94	0.68
1:B:167:ARG:HD3	1:B:198:ASP:OD2	1.94	0.68
1:A:159:ILE:O	1:A:161:PRO:HD3	1.93	0.67
1:B:271:HIS:ND1	1:B:286:ILE:HD11	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:367:ILE:HG12	1.94	0.67
1:B:515:GLU:HB3	1:B:527:PRO:CG	2.24	0.67
1:B:83:ASP:O	1:B:87:ARG:HB2	1.92	0.67
1:A:286:ILE:HG23	4:A:627:HOH:O	1.94	0.67
1:B:335:ARG:NH2	1:B:386:THR:HG21	2.10	0.67
1:A:167:ARG:NH2	1:A:178:ARG:O	2.27	0.67
1:A:244:GLN:H	1:A:244:GLN:NE2	1.93	0.67
1:B:166:TRP:HZ3	1:B:225:ILE:CD1	1.79	0.67
1:B:244:GLN:H	1:B:244:GLN:NE2	1.93	0.67
1:B:40:LYS:HB2	1:B:40:LYS:NZ	2.10	0.67
1:A:498:ASP:CB	1:A:528:ILE:HG21	2.25	0.67
1:B:40:LYS:HZ3	1:B:130:THR:HG22	1.59	0.67
1:A:83:ASP:OD1	1:A:262:THR:HG21	1.95	0.67
1:A:532:ILE:O	1:A:532:ILE:HG12	1.95	0.67
1:B:360:PHE:CE2	1:B:364:GLU:HB2	2.30	0.67
1:B:36:TYR:HB2	1:B:40:LYS:HZ2	1.60	0.67
1:B:185:GLY:HA3	1:B:189:ASN:ND2	2.10	0.66
1:B:63:THR:HG22	1:B:329:VAL:O	1.95	0.66
1:B:523:ARG:HH11	1:B:525:ILE:HD11	1.60	0.66
1:A:82:THR:HG22	1:A:266:THR:HG21	1.76	0.66
1:A:262:THR:HG22	1:A:263:LEU:N	2.09	0.66
1:A:125:ILE:HG12	1:A:129:PHE:CE1	2.30	0.66
1:B:277:ASN:HD22	1:B:278:ILE:N	1.93	0.66
1:B:43:ILE:HD11	1:B:259:LEU:CD2	2.17	0.66
1:A:182:ILE:CG2	1:A:183:GLY:N	2.58	0.66
1:A:286:ILE:HA	1:A:289:LYS:HG2	1.78	0.66
1:A:68:THR:HB	1:A:69:PRO:HD2	1.78	0.66
1:B:173:ASN:HB2	1:B:538:LEU:CD2	2.25	0.66
1:A:164:ILE:HG21	1:A:193:ARG:HH22	1.60	0.66
1:B:276:ALA:HA	1:B:281:GLY:HA3	1.77	0.65
1:A:150:HIS:CE1	1:A:157:LEU:H	2.14	0.65
1:A:185:GLY:HA3	1:A:189:ASN:HD22	1.61	0.65
1:B:488:VAL:HG23	1:B:523:ARG:HG2	1.79	0.65
1:B:337:LEU:HD21	1:B:363:LEU:CB	2.27	0.65
1:B:491:LYS:HB3	1:B:528:ILE:CG1	2.27	0.65
1:B:265:ASN:ND2	1:B:265:ASN:N	2.42	0.65
1:B:550:ASP:C	1:B:552:ASP:N	2.50	0.65
1:B:528:ILE:HG22	1:B:529:THR:N	2.12	0.65
1:B:159:ILE:HD11	1:B:236:VAL:HG11	1.79	0.65
1:B:21:GLU:O	1:B:24:ARG:HB2	1.97	0.65
1:B:470:ALA:O	1:B:474:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HB3	1:A:197:PHE:HB2	1.78	0.64
1:B:120:VAL:HB	1:B:121:PRO:HA	1.77	0.64
1:B:476:ARG:O	1:B:480:LEU:HD22	1.97	0.64
1:A:36:TYR:CE1	1:A:42:LYS:HG3	2.32	0.64
1:A:43:ILE:HD12	1:A:43:ILE:N	2.12	0.64
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.32	0.64
1:B:513:VAL:HG21	1:B:526:VAL:HG23	1.79	0.64
1:B:369:ASN:OD1	1:B:458:ILE:HA	1.98	0.64
1:A:166:TRP:CE3	1:A:225:ILE:CD1	2.61	0.64
1:B:244:GLN:HG2	1:B:245:GLY:H	1.63	0.64
1:B:42:LYS:HD2	1:B:256:LYS:HB2	1.79	0.64
1:A:286:ILE:HD12	1:A:286:ILE:C	2.18	0.64
1:B:215:LEU:HG	1:B:255:ILE:HG21	1.78	0.64
1:A:153:GLN:HA	1:A:153:GLN:OE1	1.98	0.64
1:A:166:TRP:CZ3	1:A:225:ILE:HD12	2.27	0.64
1:B:459:TYR:CZ	1:B:491:LYS:HD3	2.33	0.64
1:B:498:ASP:CB	1:B:528:ILE:HG21	2.28	0.64
1:A:405:GLU:OE1	1:A:425:LYS:HD3	1.96	0.63
1:A:490:ALA:HB3	1:A:527:PRO:HA	1.79	0.63
1:B:61:LEU:HD22	1:B:313:PHE:CE2	2.33	0.63
1:A:277:ASN:ND2	1:A:278:ILE:H	1.96	0.63
1:B:278:ILE:O	1:B:525:ILE:HD12	1.97	0.63
1:A:59:LEU:N	1:A:326:ASP:OD2	2.28	0.63
1:A:175:ARG:O	1:A:178:ARG:HG3	1.98	0.63
1:A:16:MET:HB2	1:A:39:TYR:CE2	2.34	0.63
1:A:166:TRP:CH2	1:A:225:ILE:CD1	2.82	0.63
1:A:488:VAL:HG21	1:A:523:ARG:NH1	2.14	0.63
1:B:334:VAL:HG13	1:B:356:LEU:CD2	2.29	0.63
1:A:136:VAL:HG21	1:A:206:MET:CE	2.29	0.62
1:A:82:THR:CG2	1:A:94:VAL:HG22	2.28	0.62
1:B:331:VAL:HG12	1:B:332:ALA:H	1.63	0.62
1:B:374:GLY:O	1:B:435:SER:HB2	1.99	0.62
1:A:381:ILE:HD12	1:A:395:LEU:HD21	1.81	0.62
1:A:140:HIS:CD2	1:A:203:SER:OG	2.44	0.62
1:A:239:GLY:HA2	1:A:244:GLN:HE22	1.64	0.62
1:B:258:ASN:O	1:B:269:PHE:HD1	1.81	0.62
1:B:42:LYS:HZ1	1:B:254:ALA:HA	1.64	0.62
1:B:489:MET:HE1	1:B:526:VAL:HG11	1.81	0.62
1:A:532:ILE:O	1:A:534:THR:HG23	1.99	0.62
1:B:100:SER:HB2	1:B:201:VAL:HG21	1.82	0.62
1:B:350:THR:HG22	1:B:351:GLU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLU:HB3	1:B:42:LYS:HB2	1.82	0.62
1:B:285:ILE:HD13	1:B:321:ALA:HB2	1.82	0.62
1:B:364:GLU:O	1:B:368:GLU:HG3	1.99	0.62
1:B:555:ILE:O	1:B:555:ILE:HG23	2.00	0.62
1:A:261:GLN:HG3	1:A:265:ASN:HA	1.80	0.62
1:A:277:ASN:HD22	1:A:277:ASN:N	1.89	0.61
1:B:206:MET:O	1:B:209:LEU:HB3	2.00	0.61
1:B:65:ILE:HG23	1:B:332:ALA:HB2	1.81	0.61
1:B:116:TYR:HA	1:B:263:LEU:HD12	1.81	0.61
1:B:59:LEU:HD13	1:B:292:LEU:HD21	1.81	0.61
1:A:394:LEU:HG	1:A:398:LEU:HD23	1.81	0.61
1:A:61:LEU:HD13	1:A:313:PHE:CG	2.35	0.61
1:B:338:LYS:CG	1:B:343:VAL:HG21	2.27	0.61
1:A:425:LYS:O	1:A:429:THR:HG23	2.00	0.61
1:B:487:VAL:CG1	1:B:489:MET:HE2	2.30	0.61
1:A:405:GLU:OE2	1:A:422:LEU:HD12	2.00	0.61
1:A:523:ARG:HH11	1:A:525:ILE:CD1	2.14	0.61
1:B:161:PRO:O	4:B:605:HOH:O	2.16	0.61
1:B:166:TRP:O	4:B:632:HOH:O	2.16	0.61
1:B:159:ILE:HG12	1:B:236:VAL:HG21	1.82	0.61
1:B:82:THR:HG22	1:B:266:THR:HG21	1.83	0.61
1:A:168:ARG:O	1:A:197:PHE:HA	1.99	0.61
1:A:532:ILE:O	1:A:534:THR:N	2.34	0.61
1:B:150:HIS:HE1	1:B:156:VAL:N	1.98	0.61
1:A:523:ARG:NH1	1:A:525:ILE:HD11	2.15	0.61
1:A:351:GLU:O	1:A:352:ASN:HB2	2.01	0.61
1:B:286:ILE:O	1:B:290:THR:HB	2.00	0.61
1:A:36:TYR:O	1:A:40:LYS:HB2	2.01	0.60
1:A:257:PRO:CD	1:A:286:ILE:HD11	2.30	0.60
1:A:551:ALA:O	4:A:759:HOH:O	2.17	0.60
1:B:62:VAL:HG13	1:B:301:GLU:HB3	1.82	0.60
1:A:423:ALA:C	1:A:427:LEU:HD12	2.22	0.60
1:B:353:LEU:H	1:B:353:LEU:HD12	1.66	0.60
1:B:523:ARG:H	1:B:523:ARG:CD	2.15	0.60
1:B:490:ALA:HB3	1:B:527:PRO:HA	1.82	0.60
1:A:551:ALA:C	4:A:759:HOH:O	2.38	0.60
1:A:76:THR:HG23	1:A:117:ALA:HB3	1.83	0.60
1:A:547:ILE:HD13	1:A:556:THR:O	2.02	0.60
1:B:321:ALA:HB1	1:B:323:PHE:CE2	2.37	0.60
1:A:210:CYS:O	4:A:620:HOH:O	2.16	0.60
1:B:95:CYS:O	1:B:283:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HD23	1:B:298:VAL:CG2	2.32	0.59
1:A:450:LYS:NZ	1:A:485:LEU:O	2.35	0.59
1:A:476:ARG:CD	4:A:610:HOH:O	2.49	0.59
1:A:87:ARG:HG3	4:A:718:HOH:O	2.02	0.59
1:B:36:TYR:O	1:B:40:LYS:HE3	2.02	0.59
1:B:36:TYR:HB2	1:B:40:LYS:NZ	2.16	0.59
1:B:116:TYR:HB2	1:B:415:GLY:HA2	1.83	0.59
1:A:150:HIS:HE1	1:A:157:LEU:H	1.49	0.59
1:A:450:LYS:NZ	1:A:483:GLY:O	2.33	0.59
1:A:230:THR:C	1:A:232:ASP:H	2.07	0.59
1:A:523:ARG:C	1:A:523:ARG:HD2	2.22	0.59
1:B:204:GLU:O	1:B:207:ALA:HB3	2.03	0.59
1:B:262:THR:HG22	1:B:263:LEU:N	2.18	0.59
1:A:277:ASN:HD22	1:A:278:ILE:N	1.97	0.59
1:A:276:ALA:HB2	1:A:281:GLY:HA3	1.83	0.59
1:B:344:PRO:HD2	1:B:347:ASP:HB2	1.85	0.59
1:A:116:TYR:CD1	1:A:413:ALA:O	2.56	0.58
1:A:476:ARG:HD3	4:A:610:HOH:O	2.01	0.58
1:B:49:ARG:O	1:B:52:LYS:HB2	2.03	0.58
1:B:72:GLU:CD	1:B:73:GLY:H	2.07	0.58
1:A:152:GLN:OE1	1:A:152:GLN:HA	2.04	0.58
1:B:88:LEU:HD21	1:B:420:LEU:CD1	2.34	0.58
1:A:159:ILE:HD11	1:A:236:VAL:HG11	1.84	0.58
1:A:482:TYR:O	1:A:524:LEU:HD11	2.03	0.58
1:A:70:ALA:HB2	1:A:339:MET:SD	2.42	0.58
1:A:422:LEU:O	1:A:426:VAL:HG23	2.04	0.58
1:B:320:TYR:OH	1:B:486:PRO:HG2	2.03	0.58
1:A:19:VAL:HG13	1:A:39:TYR:HA	1.84	0.58
1:B:20:MET:HE3	1:B:30:GLU:HG3	1.86	0.58
1:A:550:ASP:N	1:A:553:GLY:O	2.36	0.58
1:B:276:ALA:HA	1:B:281:GLY:CA	2.34	0.58
1:A:277:ASN:ND2	1:A:277:ASN:N	2.51	0.58
1:A:116:TYR:CZ	2:A:566:SO4:O1	2.57	0.57
1:B:116:TYR:HA	1:B:263:LEU:CD1	2.34	0.57
1:A:360:PHE:CD2	1:A:398:LEU:HD12	2.39	0.57
1:A:486:PRO:HD2	1:A:523:ARG:HB3	1.86	0.57
1:A:544:ALA:HA	1:A:547:ILE:HG13	1.86	0.57
1:B:133:ILE:O	1:B:136:VAL:N	2.37	0.57
1:A:182:ILE:HG23	1:A:183:GLY:H	1.69	0.57
1:A:424:ARG:O	1:A:428:GLN:HB2	2.04	0.57
1:A:540:LYS:O	1:A:542:PRO:HD3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HD13	1:A:524:LEU:HD13	1.86	0.57
1:A:472:LYS:O	1:A:476:ARG:HG3	2.04	0.57
1:B:271:HIS:CE1	1:B:286:ILE:HD11	2.39	0.57
1:A:253:ASP:HB2	4:A:753:HOH:O	2.03	0.57
1:A:498:ASP:OD2	1:A:511:ILE:HA	2.05	0.57
1:B:167:ARG:NH2	1:B:196:GLY:HA3	2.19	0.57
1:B:167:ARG:HA	1:B:195:THR:CG2	2.34	0.57
1:B:166:TRP:CZ3	1:B:225:ILE:CG1	2.86	0.57
1:A:277:ASN:ND2	1:A:277:ASN:H	2.00	0.57
1:B:523:ARG:N	1:B:523:ARG:NE	2.41	0.57
1:A:169:VAL:HG22	1:A:170:ILE:N	2.20	0.57
1:A:347:ASP:N	1:A:347:ASP:OD2	2.36	0.57
1:A:544:ALA:HA	1:A:547:ILE:CG1	2.35	0.57
1:B:288:THR:HG23	1:B:298:VAL:HG11	1.86	0.57
1:A:164:ILE:HG21	1:A:193:ARG:NH2	2.18	0.57
1:B:365:LYS:CE	1:B:369:ASN:HD21	2.12	0.57
1:B:408:LEU:HD13	1:B:414:LYS:CE	2.35	0.57
1:A:20:MET:HE1	1:A:30:GLU:HA	1.86	0.57
1:A:83:ASP:CG	1:A:262:THR:HG21	2.25	0.57
1:A:311:GLU:HG3	1:A:312:LYS:HG3	1.87	0.57
1:A:423:ALA:O	1:A:427:LEU:HD12	2.04	0.57
1:B:353:LEU:HB3	1:B:394:LEU:HD22	1.87	0.57
1:B:405:GLU:HB2	1:B:422:LEU:HD13	1.85	0.57
1:A:120:VAL:HB	1:A:121:PRO:HA	1.86	0.56
1:B:513:VAL:CG2	1:B:526:VAL:HG23	2.34	0.56
1:B:485:LEU:HD22	1:B:522:GLY:O	2.05	0.56
1:B:548:ASP:O	1:B:555:ILE:HG22	2.04	0.56
1:A:167:ARG:NH2	1:A:196:GLY:HA3	2.20	0.56
1:A:523:ARG:NH1	1:A:525:ILE:CD1	2.68	0.56
1:A:533:MET:HG3	1:A:533:MET:O	2.05	0.56
1:A:466:TYR:CD2	1:A:513:VAL:HG22	2.41	0.56
1:B:331:VAL:HG12	1:B:332:ALA:N	2.20	0.56
1:B:74:LYS:HB2	1:B:74:LYS:HZ2	1.69	0.56
1:A:306:ALA:O	1:A:310:ALA:HB3	2.05	0.56
1:A:225:ILE:CG2	1:A:238:ALA:CB	2.84	0.56
1:B:132:ASP:OD2	1:B:254:ALA:HA	2.05	0.56
1:B:426:VAL:O	1:B:430:LEU:HB3	2.04	0.56
1:A:141:ASN:HB3	4:A:598:HOH:O	2.06	0.56
1:B:43:ILE:O	1:B:257:PRO:HD2	2.06	0.56
1:B:199:ILE:HG13	1:B:535:MET:HE1	1.85	0.56
1:B:331:VAL:HA	1:B:380:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:CG	1:A:115:GLY:H	2.17	0.56
1:B:517:ARG:HH22	1:B:532:ILE:CG1	2.16	0.56
1:A:219:LYS:HG3	1:A:248:ALA:HB2	1.89	0.55
1:A:225:ILE:CG2	1:A:238:ALA:HB2	2.36	0.55
1:B:331:VAL:O	1:B:332:ALA:HB2	2.05	0.55
1:B:40:LYS:CB	1:B:40:LYS:NZ	2.69	0.55
1:B:91:ARG:HG2	1:B:295:ALA:HA	1.88	0.55
1:A:8:ILE:CG1	1:A:11:ALA:HB2	2.36	0.55
1:B:83:ASP:HB3	1:B:264:GLU:OE2	2.07	0.55
1:B:455:ALA:HB1	1:B:461:ALA:HB3	1.89	0.55
1:A:167:ARG:HH21	1:A:196:GLY:HA3	1.72	0.55
1:A:195:THR:HG21	4:A:596:HOH:O	2.06	0.55
1:B:182:ILE:O	1:B:192:PRO:HA	2.07	0.55
1:B:313:PHE:CD2	1:B:313:PHE:C	2.78	0.55
1:B:70:ALA:HB2	1:B:339:MET:SD	2.47	0.55
1:A:41:ALA:O	1:A:258:ASN:HA	2.07	0.55
1:B:94:VAL:HG12	1:B:95:CYS:N	2.21	0.55
1:B:339:MET:HA	1:B:343:VAL:HB	1.89	0.55
1:B:446:SER:O	1:B:450:LYS:HG3	2.07	0.55
1:B:86:ALA:C	1:B:88:LEU:H	2.09	0.55
1:A:143:LEU:HD23	1:A:166:TRP:CE2	2.43	0.54
1:A:353:LEU:H	1:A:353:LEU:CD1	2.19	0.54
1:B:212:ALA:O	1:B:286:ILE:HG23	2.06	0.54
1:B:318:CYS:SG	1:B:323:PHE:HB2	2.47	0.54
1:B:335:ARG:HD3	1:B:348:LEU:HB3	1.89	0.54
1:B:516:VAL:HG12	1:B:516:VAL:O	2.07	0.54
1:B:88:LEU:HD21	1:B:420:LEU:HD11	1.90	0.54
1:A:158:ASN:O	1:A:230:THR:HA	2.07	0.54
1:B:149:ASN:O	1:B:153:GLN:HG2	2.08	0.54
1:B:150:HIS:CE1	1:B:157:LEU:H	2.26	0.54
1:B:523:ARG:NH1	1:B:525:ILE:HD11	2.21	0.54
1:B:152:GLN:OE1	1:B:190:GLY:HA2	2.08	0.54
1:B:84:ALA:HB2	1:B:416:GLY:O	2.07	0.54
1:A:36:TYR:HE1	1:A:42:LYS:HG3	1.72	0.54
1:B:509:PHE:HD1	1:B:510:THR:N	2.05	0.54
1:B:61:LEU:HD13	1:B:313:PHE:CE1	2.43	0.54
1:A:143:LEU:CD2	1:A:225:ILE:HD13	2.38	0.54
1:B:220:GLU:OE2	1:B:224:ARG:NH1	2.40	0.54
1:B:277:ASN:HB3	1:B:304:PHE:CE2	2.42	0.54
1:B:326:ASP:O	1:B:376:PRO:HD2	2.08	0.54
1:B:354:GLU:O	1:B:357:ARG:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:TRP:CD2	2:A:565:SO4:O4	2.60	0.54
1:B:219:LYS:HE3	4:B:621:HOH:O	2.05	0.54
1:B:451:ILE:HD12	1:B:466:TYR:OH	2.08	0.54
1:A:125:ILE:HA	1:A:129:PHE:CD1	2.42	0.54
1:A:301:GLU:OE1	4:A:714:HOH:O	2.18	0.54
1:A:341:GLY:HA3	1:A:355:ALA:O	2.07	0.54
1:A:49:ARG:CZ	4:A:692:HOH:O	2.55	0.54
1:B:370:ILE:HG21	1:B:377:ALA:HB2	1.90	0.54
1:B:405:GLU:HB2	1:B:422:LEU:CD1	2.38	0.54
1:B:75:THR:HA	1:B:301:GLU:OE2	2.08	0.53
1:B:488:VAL:HG23	1:B:523:ARG:HD3	1.91	0.53
1:A:488:VAL:HG23	1:A:523:ARG:HD3	1.88	0.53
1:B:121:PRO:HG2	1:B:124:ASP:HB2	1.89	0.53
1:B:459:TYR:HA	1:B:496:PHE:HB3	1.90	0.53
1:B:50:ARG:HG3	1:B:51:LEU:N	2.23	0.53
1:B:375:VAL:HA	1:B:435:SER:CB	2.39	0.53
1:B:8:ILE:HG13	1:B:11:ALA:HB2	1.90	0.53
1:A:47:VAL:HA	1:A:50:ARG:HH12	1.72	0.53
1:A:529:THR:OG1	1:A:530:GLY:N	2.39	0.53
1:B:167:ARG:NH1	1:B:198:ASP:OD1	2.42	0.53
1:B:141:ASN:O	1:B:144:ALA:HB3	2.09	0.53
1:B:22:LEU:HD11	1:B:261:GLN:CD	2.28	0.53
1:B:20:MET:HE1	1:B:30:GLU:HA	1.91	0.53
1:B:23:ALA:CA	1:B:28:ILE:HD12	2.36	0.53
1:A:459:TYR:CD1	1:A:459:TYR:N	2.75	0.53
1:B:408:LEU:HD13	1:B:414:LYS:HE3	1.91	0.53
1:A:169:VAL:CG2	1:A:170:ILE:N	2.71	0.52
1:A:167:ARG:NH1	1:A:198:ASP:OD1	2.42	0.52
1:B:335:ARG:HH21	1:B:349:ALA:HA	1.71	0.52
1:B:515:GLU:HG2	1:B:516:VAL:H	1.74	0.52
1:A:466:TYR:HD2	1:A:513:VAL:HG22	1.74	0.52
1:A:515:GLU:HB3	1:A:527:PRO:HG2	1.92	0.52
1:B:80:GLY:N	1:B:117:ALA:HB1	2.25	0.52
1:A:31:ASP:OD2	1:A:32:GLU:HG3	2.10	0.52
1:B:51:LEU:O	1:B:293:LYS:HG2	2.09	0.52
1:B:325:PRO:HD2	1:B:437:PHE:CD2	2.44	0.52
1:A:378:VAL:HG11	1:A:405:GLU:OE2	2.09	0.52
1:A:49:ARG:NE	4:A:692:HOH:O	2.42	0.52
1:B:143:LEU:HD23	1:B:166:TRP:CZ2	2.45	0.52
1:B:441:TYR:CE2	1:B:454:ILE:HD11	2.44	0.52
1:A:111:ALA:O	1:A:113:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:LEU:HD22	1:A:458:ILE:HD11	1.91	0.52
1:A:530:GLY:C	1:A:532:ILE:N	2.61	0.52
1:B:36:TYR:CE2	1:B:130:THR:HB	2.45	0.52
1:B:315:ASP:O	1:B:319:ARG:HD2	2.10	0.52
1:B:91:ARG:HB3	1:B:296:ASP:CG	2.31	0.52
1:B:58:LYS:HA	1:B:326:ASP:OD2	2.09	0.52
1:B:363:LEU:HD23	1:B:395:LEU:HD11	1.92	0.52
1:B:472:LYS:O	1:B:476:ARG:HG3	2.10	0.52
1:A:66:THR:HB	1:A:340:HIS:CE1	2.45	0.51
1:B:379:VAL:HB	1:B:404:ALA:HA	1.91	0.51
1:B:399:CYS:O	1:B:401:LYS:N	2.43	0.51
1:B:79:VAL:HB	1:B:117:ALA:O	2.10	0.51
1:B:210:CYS:CA	1:B:284:SER:HA	2.40	0.51
1:A:175:ARG:HG2	1:A:178:ARG:CZ	2.40	0.51
1:A:83:ASP:OD2	1:A:262:THR:HG21	2.10	0.51
1:A:533:MET:CE	1:A:536:PRO:HA	2.41	0.51
1:B:9:GLU:OE2	1:B:111:ALA:HB3	2.11	0.51
1:B:150:HIS:CE1	1:B:156:VAL:N	2.78	0.51
1:B:277:ASN:HD22	1:B:277:ASN:N	2.09	0.51
1:B:285:ILE:O	1:B:287:ALA:N	2.43	0.51
1:A:181:VAL:HG13	1:A:193:ARG:O	2.09	0.51
1:A:319:ARG:NH2	1:A:441:TYR:O	2.42	0.51
1:B:275:PHE:HD2	1:B:277:ASN:HD21	1.57	0.51
1:B:550:ASP:O	1:B:552:ASP:N	2.43	0.51
1:A:118:GLN:HG3	1:A:263:LEU:HD21	1.91	0.51
1:A:66:THR:CB	1:A:362:ASN:HD21	2.22	0.51
1:A:389:GLU:HB3	1:A:393:ASN:ND2	2.25	0.51
1:B:75:THR:CB	1:B:113:GLY:HA2	2.41	0.51
1:A:459:TYR:HB3	1:A:496:PHE:O	2.10	0.51
1:B:420:LEU:O	1:B:423:ALA:HB3	2.11	0.51
1:B:487:VAL:HG12	1:B:489:MET:HE2	1.92	0.51
1:B:514:ARG:HD2	1:B:528:ILE:O	2.10	0.51
1:B:303:GLY:HA2	2:B:560:SO4:O1	2.11	0.51
1:A:175:ARG:NH1	1:A:537:GLY:HA3	2.26	0.51
1:A:515:GLU:O	1:A:527:PRO:HD2	2.11	0.51
1:B:10:ILE:HA	1:B:122:MET:CE	2.41	0.51
1:B:221:ARG:HG2	1:B:221:ARG:HH21	1.76	0.51
1:B:323:PHE:CD2	1:B:323:PHE:N	2.77	0.51
1:B:497:SER:HA	1:B:511:ILE:HD11	1.93	0.51
1:B:75:THR:HG23	1:B:301:GLU:OE1	2.11	0.50
1:B:58:LYS:HG2	1:B:297:TYR:HD1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:TYR:OH	4:A:741:HOH:O	2.13	0.50
1:A:540:LYS:C	1:A:542:PRO:HD3	2.31	0.50
1:B:275:PHE:O	1:B:279:ALA:HB3	2.11	0.50
1:B:257:PRO:HD3	1:B:286:ILE:HD13	1.93	0.50
1:B:329:VAL:HG12	1:B:330:ILE:N	2.27	0.50
1:B:448:LYS:HD3	1:B:466:TYR:CZ	2.46	0.50
1:B:150:HIS:HE1	1:B:157:LEU:H	1.57	0.50
1:A:440:LEU:HD11	1:A:457:GLU:OE1	2.11	0.50
1:A:512:THR:O	1:A:528:ILE:HG23	2.11	0.50
1:B:60:ILE:HD12	1:B:299:VAL:HG22	1.92	0.50
1:B:229:TYR:CD1	1:B:229:TYR:N	2.79	0.50
1:B:277:ASN:N	1:B:304:PHE:HE2	2.10	0.50
1:B:443:LEU:HG	1:B:484:ASN:O	2.12	0.50
1:B:42:LYS:NZ	1:B:132:ASP:OD2	2.38	0.50
1:B:159:ILE:HA	1:B:230:THR:HA	1.93	0.50
1:B:451:ILE:HG12	1:B:489:MET:CE	2.38	0.50
1:B:556:THR:O	1:B:556:THR:CG2	2.60	0.50
1:B:350:THR:CG2	1:B:351:GLU:N	2.75	0.50
1:B:398:LEU:C	1:B:400:ALA:H	2.15	0.50
1:B:42:LYS:NZ	1:B:254:ALA:HA	2.26	0.50
1:A:42:LYS:NZ	1:A:132:ASP:OD2	2.44	0.49
1:A:17:LYS:N	1:A:261:GLN:NE2	2.55	0.49
1:B:152:GLN:NE2	1:B:187:LYS:O	2.38	0.49
1:A:530:GLY:O	1:A:532:ILE:N	2.45	0.49
1:A:529:THR:C	1:A:531:ALA:H	2.14	0.49
1:A:92:VAL:HG23	1:A:297:TYR:C	2.33	0.49
1:B:472:LYS:HD3	1:B:476:ARG:HH21	1.74	0.49
1:B:486:PRO:HD2	1:B:523:ARG:HB3	1.94	0.49
1:A:143:LEU:O	1:A:147:VAL:HG23	2.12	0.49
1:A:150:HIS:NE2	1:A:157:LEU:HD12	2.27	0.49
1:A:343:VAL:HG23	1:A:355:ALA:CB	2.42	0.49
1:A:36:TYR:O	1:A:40:LYS:NZ	2.40	0.49
1:B:12:GLN:NE2	1:B:263:LEU:CD1	2.74	0.49
1:B:335:ARG:HB3	1:B:348:LEU:HD22	1.93	0.49
1:B:43:ILE:HD12	1:B:269:PHE:CE1	2.47	0.49
1:B:487:VAL:HG11	1:B:489:MET:HE2	1.93	0.49
1:A:72:GLU:HA	1:A:333:THR:HG23	1.94	0.49
1:B:327:ALA:HB2	1:B:430:LEU:HD13	1.94	0.49
1:A:112:ALA:O	1:A:118:GLN:HA	2.12	0.49
1:A:120:VAL:O	1:A:260:VAL:HB	2.11	0.49
1:A:353:LEU:N	1:A:353:LEU:HD12	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:HIS:HE2	1:B:157:LEU:HG	1.78	0.49
1:B:389:GLU:O	1:B:393:ASN:ND2	2.45	0.49
1:A:461:ALA:HB2	1:A:509:PHE:CE1	2.48	0.49
1:B:125:ILE:HG12	1:B:129:PHE:CE1	2.46	0.49
1:B:258:ASN:O	1:B:269:PHE:CD1	2.64	0.49
1:B:377:ALA:O	1:B:378:VAL:HG23	2.12	0.49
1:B:429:THR:O	1:B:433:ARG:HB3	2.13	0.49
1:A:340:HIS:ND1	1:A:504:GLY:N	2.53	0.49
1:B:133:ILE:O	1:B:134:HIS:C	2.51	0.49
1:B:288:THR:O	1:B:292:LEU:HG	2.13	0.49
1:B:47:VAL:CG1	1:B:294:LEU:HD21	2.43	0.49
1:B:494:TYR:O	1:B:495:SER:HB2	2.13	0.49
1:B:519:SER:C	1:B:521:GLY:H	2.16	0.49
1:A:147:VAL:HG11	1:A:164:ILE:HD13	1.93	0.49
1:A:230:THR:C	1:A:232:ASP:N	2.66	0.49
1:A:344:PRO:O	1:A:348:LEU:HG	2.13	0.49
1:A:401:LYS:CB	4:A:748:HOH:O	2.48	0.49
1:B:276:ALA:CA	1:B:281:GLY:HA3	2.42	0.49
1:B:277:ASN:ND2	1:B:278:ILE:HD13	2.28	0.49
1:B:477:TYR:CE2	1:B:516:VAL:HG12	2.40	0.49
1:B:61:LEU:O	1:B:328:THR:HA	2.13	0.49
1:B:339:MET:C	1:B:341:GLY:H	2.16	0.49
1:A:140:HIS:HE1	1:A:167:ARG:O	1.96	0.48
1:A:277:ASN:ND2	1:A:278:ILE:N	2.60	0.48
1:B:63:THR:O	1:B:331:VAL:HG23	2.13	0.48
1:B:49:ARG:HD3	1:B:49:ARG:C	2.33	0.48
1:A:133:ILE:HG21	1:A:171:ASP:OD1	2.13	0.48
1:A:426:VAL:O	1:A:430:LEU:HB2	2.12	0.48
1:B:8:ILE:HG13	1:B:11:ALA:CB	2.43	0.48
1:B:193:ARG:NH2	1:B:195:THR:OG1	2.45	0.48
1:B:225:ILE:O	1:B:225:ILE:HG23	2.13	0.48
1:B:36:TYR:CB	1:B:40:LYS:NZ	2.76	0.48
1:A:149:ASN:OD1	1:A:153:GLN:HG2	2.13	0.48
1:B:157:LEU:O	1:B:230:THR:CG2	2.61	0.48
1:B:417:GLU:O	1:B:419:GLY:N	2.46	0.48
1:B:65:ILE:HB	1:B:66:THR:H	1.44	0.48
1:A:543:ALA:O	1:A:547:ILE:HG12	2.14	0.48
1:B:304:PHE:CE1	1:B:493:GLN:NE2	2.81	0.48
1:A:182:ILE:HG23	1:A:183:GLY:N	2.26	0.48
1:A:20:MET:CE	1:A:33:VAL:HB	2.43	0.48
1:B:164:ILE:HD12	1:B:193:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASN:HB3	4:B:597:HOH:O	2.14	0.48
1:B:420:LEU:O	1:B:421:GLU:C	2.52	0.48
1:B:94:VAL:HG12	1:B:95:CYS:H	1.79	0.48
1:A:65:ILE:O	1:A:66:THR:C	2.52	0.48
1:B:417:GLU:C	1:B:419:GLY:H	2.17	0.48
1:B:440:LEU:CD2	1:B:458:ILE:HD11	2.43	0.48
1:B:492:THR:O	1:B:492:THR:HG23	2.14	0.48
1:A:35:LEU:HD23	1:A:40:LYS:O	2.13	0.48
1:A:497:SER:C	1:A:499:ASP:H	2.17	0.48
1:A:92:VAL:HG22	1:A:93:MET:N	2.27	0.48
1:B:276:ALA:HB2	1:B:303:GLY:HA3	1.95	0.48
1:B:35:LEU:HD23	1:B:41:ALA:HB2	1.95	0.48
1:B:388:THR:O	1:B:392:LEU:HG	2.13	0.48
1:A:140:HIS:HD2	1:A:203:SER:HG	1.56	0.48
1:A:204:GLU:O	1:A:207:ALA:HB3	2.14	0.48
1:A:211:LEU:HA	1:A:285:ILE:HD12	1.96	0.48
1:A:446:SER:HB3	1:A:449:ASP:CB	2.41	0.48
1:B:461:ALA:HA	1:B:509:PHE:CE1	2.48	0.48
1:A:136:VAL:HG13	1:A:205:VAL:HG12	1.95	0.48
1:A:221:ARG:HA	1:A:224:ARG:HG3	1.94	0.48
1:A:400:ALA:O	1:A:401:LYS:HB2	2.12	0.48
1:B:555:ILE:O	1:B:556:THR:CB	2.55	0.48
1:A:332:ALA:O	1:A:381:ILE:HA	2.13	0.48
1:A:106:GLY:CA	1:A:538:LEU:HD22	2.44	0.48
1:B:414:LYS:O	1:B:417:GLU:HB3	2.14	0.48
1:A:288:THR:O	1:A:291:ALA:N	2.47	0.47
1:A:463:GLY:O	1:A:510:THR:HG23	2.14	0.47
1:A:533:MET:CB	2:A:561:SO4:O2	2.61	0.47
1:B:241:LEU:O	1:B:242:GLU:HB2	2.14	0.47
1:B:244:GLN:CD	1:B:244:GLN:H	2.17	0.47
1:B:20:MET:HE3	1:B:30:GLU:CG	2.44	0.47
1:B:313:PHE:CE2	1:B:318:CYS:SG	3.06	0.47
1:B:351:GLU:OE2	1:B:353:LEU:HD11	2.14	0.47
1:B:247:MET:HA	1:B:250:LEU:HD23	1.96	0.47
1:A:399:CYS:O	1:A:401:LYS:N	2.47	0.47
1:B:144:ALA:HB1	1:B:168:ARG:NH2	2.28	0.47
1:B:466:TYR:HA	1:B:513:VAL:HG13	1.97	0.47
1:A:360:PHE:CE2	1:A:364:GLU:HB2	2.50	0.47
1:B:175:ARG:HG2	1:B:178:ARG:CZ	2.45	0.47
1:A:107:ILE:O	1:A:108:LYS:HB2	2.13	0.47
1:B:169:VAL:HG12	1:B:200:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG23	1:A:238:ALA:HB2	1.96	0.47
1:A:288:THR:HG22	1:A:292:LEU:HD12	1.95	0.47
1:A:61:LEU:HD13	1:A:313:PHE:CE2	2.50	0.47
1:B:450:LYS:O	1:B:454:ILE:HG13	2.14	0.47
1:A:140:HIS:CE1	1:A:166:TRP:CZ2	3.02	0.47
1:B:408:LEU:CD2	1:B:408:LEU:O	2.63	0.47
1:A:87:ARG:NH1	1:A:264:GLU:OE1	2.48	0.47
1:B:459:TYR:HE2	1:B:489:MET:HG3	1.80	0.47
1:B:304:PHE:CD1	1:B:493:GLN:HG3	2.50	0.47
1:B:83:ASP:O	4:B:612:HOH:O	2.21	0.47
1:A:533:MET:HA	2:A:561:SO4:O2	2.15	0.47
1:B:304:PHE:HE1	1:B:493:GLN:HE21	1.60	0.47
1:B:523:ARG:H	1:B:523:ARG:HE	1.51	0.47
1:A:9:GLU:OE1	1:A:114:GLY:HA3	2.14	0.47
1:A:32:GLU:OE1	1:A:47:VAL:HG22	2.15	0.47
1:B:215:LEU:HD21	1:B:255:ILE:HB	1.97	0.47
1:B:303:GLY:O	1:B:309:GLY:HA3	2.14	0.47
1:B:384:PHE:CD1	1:B:385:PRO:HD2	2.50	0.47
1:A:459:TYR:O	1:A:509:PHE:HZ	1.98	0.47
1:A:54:LYS:HB3	1:A:55:PRO:HD2	1.97	0.47
1:A:43:ILE:CD1	1:A:43:ILE:N	2.78	0.46
1:A:550:ASP:C	1:A:552:ASP:H	2.17	0.46
1:B:42:LYS:HE2	1:B:258:ASN:OD1	2.15	0.46
1:B:353:LEU:CD1	1:B:353:LEU:N	2.77	0.46
1:B:375:VAL:HA	1:B:435:SER:HB2	1.97	0.46
1:A:42:LYS:HZ3	1:A:254:ALA:HA	1.80	0.46
1:B:140:HIS:HE1	1:B:167:ARG:O	1.97	0.46
1:B:491:LYS:HB3	1:B:528:ILE:HG13	1.95	0.46
1:A:259:LEU:O	1:A:260:VAL:HG13	2.15	0.46
1:B:338:LYS:O	1:B:341:GLY:N	2.44	0.46
1:B:75:THR:O	1:B:76:THR:C	2.53	0.46
1:A:144:ALA:HB1	1:A:168:ARG:HE	1.81	0.46
1:A:143:LEU:HD23	1:A:166:TRP:CZ2	2.50	0.46
1:A:417:GLU:O	1:A:420:LEU:HD23	2.15	0.46
1:B:333:THR:HB	1:B:382:ASN:HB3	1.97	0.46
1:B:515:GLU:O	1:B:516:VAL:HG23	2.15	0.46
1:B:86:ALA:HA	1:B:90:LYS:HB2	1.96	0.46
1:A:150:HIS:CE1	1:A:157:LEU:HB2	2.51	0.46
1:A:550:ASP:C	1:A:552:ASP:N	2.69	0.46
1:A:97:ARG:HB3	1:A:273:GLY:HA3	1.98	0.46
1:B:12:GLN:HE22	1:B:263:LEU:HD13	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASP:OD2	1:B:32:GLU:HG3	2.16	0.46
1:B:357:ARG:O	1:B:360:PHE:CB	2.61	0.46
1:B:335:ARG:HH21	1:B:386:THR:HG21	1.80	0.46
1:A:526:VAL:O	1:A:526:VAL:HG22	2.15	0.46
1:B:323:PHE:O	1:B:324:LYS:HG3	2.15	0.46
1:B:515:GLU:O	1:B:527:PRO:HD2	2.14	0.46
1:A:394:LEU:O	1:A:398:LEU:HB2	2.16	0.46
1:A:374:GLY:HA3	1:A:436:ASN:O	2.16	0.46
1:A:476:ARG:HD2	4:A:610:HOH:O	2.11	0.46
1:B:323:PHE:N	1:B:323:PHE:HD2	2.14	0.46
1:B:440:LEU:HD22	1:B:458:ILE:HD11	1.96	0.46
1:A:346:SER:HB3	4:A:732:HOH:O	2.16	0.46
1:A:39:TYR:O	1:A:40:LYS:HG3	2.16	0.46
1:A:90:LYS:HD2	1:A:297:TYR:CE2	2.51	0.46
1:B:144:ALA:CB	1:B:168:ARG:HE	2.29	0.46
1:B:146:MET:SD	1:B:243:ALA:HB2	2.55	0.46
1:B:393:ASN:O	1:B:397:GLU:HG2	2.16	0.46
1:B:83:ASP:HB3	1:B:416:GLY:CA	2.45	0.46
1:B:239:GLY:HA2	1:B:244:GLN:NE2	2.30	0.45
1:B:314:TYR:OH	1:B:328:THR:HG21	2.16	0.45
1:B:51:LEU:HD12	1:B:294:LEU:HD23	1.97	0.45
1:B:66:THR:O	1:B:68:THR:HG23	2.15	0.45
1:A:337:LEU:HA	1:A:337:LEU:HD12	1.75	0.45
1:A:51:LEU:O	1:A:53:ASP:N	2.49	0.45
1:B:373:PHE:CE2	1:B:440:LEU:HB2	2.51	0.45
1:A:315:ASP:O	1:A:319:ARG:HD2	2.15	0.45
1:A:353:LEU:H	1:A:353:LEU:HD12	1.82	0.45
1:B:116:TYR:HB2	1:B:415:GLY:CA	2.45	0.45
1:B:69:PRO:HG2	1:B:339:MET:CE	2.46	0.45
1:B:66:THR:HB	1:B:362:ASN:HD21	1.81	0.45
1:B:50:ARG:C	1:B:52:LYS:H	2.18	0.45
1:B:75:THR:CG2	1:B:113:GLY:HA2	2.46	0.45
1:A:215:LEU:HD11	1:A:252:LYS:HA	1.98	0.45
1:A:505:ARG:HG2	1:A:507:ARG:NH2	2.31	0.45
1:B:280:HIS:HA	1:B:312:LYS:HD3	1.97	0.45
1:B:447:ILE:HD12	1:B:478:GLU:HG3	1.98	0.45
1:B:61:LEU:HD22	1:B:313:PHE:CZ	2.52	0.45
1:B:408:LEU:HD23	1:B:408:LEU:O	2.17	0.45
1:B:505:ARG:HG2	1:B:505:ARG:O	2.16	0.45
1:B:463:GLY:O	1:B:510:THR:HG23	2.15	0.45
1:B:95:CYS:HB3	1:B:283:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PHE:CD1	1:A:105:PHE:N	2.84	0.45
1:A:245:GLY:O	1:A:248:ALA:HB3	2.17	0.45
1:A:311:GLU:HG3	1:A:312:LYS:N	2.32	0.45
1:A:353:LEU:N	1:A:353:LEU:CD1	2.79	0.45
1:B:150:HIS:NE2	1:B:157:LEU:HG	2.32	0.45
1:B:40:LYS:HD3	1:B:124:ASP:OD2	2.17	0.45
1:B:127:LEU:HB3	1:B:128:HIS:H	1.55	0.45
1:B:312:LYS:HE2	1:B:488:VAL:HG13	1.99	0.45
1:B:509:PHE:CD1	1:B:510:THR:N	2.84	0.45
1:A:227:VAL:HG22	1:A:236:VAL:O	2.16	0.45
1:A:520:ALA:C	1:A:522:GLY:H	2.21	0.45
1:B:125:ILE:HA	1:B:129:PHE:CD1	2.52	0.45
1:B:22:LEU:HD11	1:B:261:GLN:NE2	2.32	0.45
1:A:20:MET:CE	1:A:30:GLU:HA	2.46	0.45
1:B:175:ARG:O	1:B:178:ARG:HG3	2.17	0.45
1:B:541:ARG:N	1:B:542:PRO:HD3	2.32	0.45
1:B:18:PRO:O	1:B:22:LEU:HG	2.16	0.45
1:B:74:LYS:CB	1:B:74:LYS:NZ	2.76	0.45
1:B:93:MET:HB3	1:B:94:VAL:H	1.55	0.45
1:A:182:ILE:HG22	1:A:183:GLY:N	2.31	0.44
1:B:8:ILE:CG1	1:B:11:ALA:HB2	2.47	0.44
1:B:10:ILE:HG23	1:B:11:ALA:N	2.32	0.44
1:B:160:ASP:HB3	1:B:163:THR:HG23	1.97	0.44
1:A:225:ILE:CG2	1:A:238:ALA:HB3	2.46	0.44
1:A:343:VAL:HG23	1:A:355:ALA:HB1	1.99	0.44
1:A:476:ARG:HG2	1:A:476:ARG:HH11	1.81	0.44
1:B:174:ASP:OD1	1:B:177:LEU:CG	2.63	0.44
1:B:20:MET:CE	1:B:30:GLU:HA	2.46	0.44
1:B:287:ALA:O	1:B:291:ALA:HB2	2.17	0.44
1:B:405:GLU:HG3	1:B:425:LYS:HB2	1.98	0.44
1:B:166:TRP:HZ3	1:B:225:ILE:CG1	2.27	0.44
1:B:12:GLN:HE21	1:B:263:LEU:HD13	1.79	0.44
1:B:285:ILE:O	1:B:286:ILE:C	2.55	0.44
1:B:8:ILE:HB	1:B:10:ILE:HG22	2.00	0.44
1:A:140:HIS:CE1	1:A:166:TRP:CE2	3.04	0.44
1:A:523:ARG:HH11	1:A:525:ILE:HD11	1.79	0.44
1:B:215:LEU:CG	1:B:255:ILE:HG21	2.47	0.44
1:B:329:VAL:HG12	1:B:330:ILE:H	1.82	0.44
1:A:334:VAL:HG21	1:A:392:LEU:HD23	2.00	0.44
1:A:446:SER:CB	1:A:449:ASP:HB2	2.45	0.44
1:B:100:SER:O	1:B:103:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:O	1:B:230:THR:HG21	2.17	0.44
1:B:276:ALA:O	1:B:279:ALA:O	2.36	0.44
1:B:277:ASN:HB3	1:B:304:PHE:HE2	1.82	0.44
1:B:160:ASP:OD1	1:B:162:ARG:HB2	2.18	0.44
1:B:245:GLY:O	1:B:248:ALA:HB3	2.18	0.44
1:B:274:PRO:HG2	1:B:281:GLY:HA2	2.00	0.44
1:B:288:THR:HA	1:B:291:ALA:HB3	2.00	0.44
1:B:339:MET:CG	1:B:348:LEU:HD21	2.47	0.44
1:B:515:GLU:HB3	1:B:527:PRO:HG3	1.99	0.44
1:A:363:LEU:HD11	1:A:379:VAL:HG22	2.00	0.44
1:A:82:THR:CG2	1:A:266:THR:HG21	2.45	0.44
1:B:210:CYS:HA	1:B:284:SER:CA	2.47	0.44
1:B:202:ALA:HB2	1:B:275:PHE:CE1	2.52	0.44
1:B:522:GLY:HA3	1:B:523:ARG:HH21	1.83	0.44
1:B:285:ILE:O	1:B:288:THR:N	2.51	0.44
1:B:367:ILE:O	1:B:370:ILE:HB	2.18	0.44
1:B:417:GLU:C	1:B:419:GLY:N	2.71	0.44
1:B:420:LEU:HD12	1:B:424:ARG:HH12	1.82	0.44
1:A:143:LEU:HD21	1:A:225:ILE:HD13	1.99	0.44
1:A:369:ASN:O	1:A:372:LYS:N	2.48	0.44
1:A:90:LYS:HB3	1:A:297:TYR:CD2	2.53	0.44
1:B:178:ARG:HD3	1:B:535:MET:O	2.17	0.44
1:B:12:GLN:HE21	1:B:263:LEU:CD1	2.31	0.44
1:B:97:ARG:HB3	1:B:273:GLY:HA2	2.00	0.44
1:A:175:ARG:O	1:A:177:LEU:N	2.51	0.43
1:A:556:THR:HG22	1:A:556:THR:O	2.18	0.43
1:B:65:ILE:CG2	1:B:332:ALA:HB2	2.48	0.43
1:B:488:VAL:HG23	1:B:523:ARG:CG	2.47	0.43
1:A:160:ASP:OD2	1:A:162:ARG:NH2	2.43	0.43
1:A:311:GLU:HG2	4:A:741:HOH:O	2.17	0.43
1:A:36:TYR:HB3	1:A:40:LYS:HZ3	1.83	0.43
1:B:29:GLN:HB2	1:B:31:ASP:OD2	2.18	0.43
1:B:493:GLN:CD	1:B:494:TYR:CE1	2.92	0.43
1:B:523:ARG:HB2	1:B:524:LEU:H	1.41	0.43
1:A:262:THR:CG2	1:A:263:LEU:N	2.79	0.43
1:A:555:ILE:O	1:A:556:THR:CB	2.67	0.43
1:B:353:LEU:H	1:B:353:LEU:CD1	2.32	0.43
1:B:42:LYS:HE2	1:B:130:THR:OG1	2.18	0.43
1:B:9:GLU:HG3	1:B:118:GLN:NE2	2.29	0.43
1:A:246:SER:O	1:A:250:LEU:HD23	2.17	0.43
1:B:99:PRO:HD2	1:B:125:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TYR:N	1:B:466:TYR:CD1	2.87	0.43
1:A:226:VAL:HG23	4:A:760:HOH:O	2.18	0.43
1:A:97:ARG:HG2	1:A:273:GLY:HA2	1.99	0.43
1:A:447:ILE:HA	1:A:450:LYS:HD2	2.01	0.43
1:B:150:HIS:O	1:B:151:LEU:C	2.56	0.43
1:B:221:ARG:NH2	1:B:221:ARG:HG2	2.34	0.43
1:B:257:PRO:CA	1:B:271:HIS:ND1	2.81	0.43
1:B:277:ASN:HD22	1:B:277:ASN:H	1.65	0.43
1:B:286:ILE:HD12	1:B:286:ILE:C	2.37	0.43
1:B:320:TYR:CD2	1:B:320:TYR:N	2.86	0.43
1:A:381:ILE:HD12	1:A:395:LEU:CD2	2.47	0.43
1:A:16:MET:HB2	1:A:39:TYR:CD2	2.54	0.43
1:A:48:TYR:O	1:A:51:LEU:N	2.34	0.43
1:B:286:ILE:CA	1:B:289:LYS:HG2	2.44	0.43
1:B:32:GLU:O	1:B:33:VAL:HG23	2.19	0.43
1:B:481:GLY:C	1:B:483:GLY:H	2.21	0.43
1:A:87:ARG:HD2	1:A:416:GLY:HA3	2.00	0.43
1:B:285:ILE:HG22	1:B:286:ILE:N	2.33	0.43
1:B:332:ALA:HB1	1:B:337:LEU:HD11	2.01	0.43
1:B:384:PHE:CG	1:B:385:PRO:HD2	2.54	0.43
1:A:453:LYS:HA	4:A:658:HOH:O	2.18	0.43
1:A:23:ALA:HB1	1:A:28:ILE:HB	2.00	0.43
1:A:246:SER:O	1:A:250:LEU:CD2	2.67	0.43
1:B:358:GLU:O	1:B:359:GLY:C	2.57	0.43
1:A:412:TRP:CB	2:A:565:SO4:O4	2.67	0.42
1:B:215:LEU:HA	1:B:215:LEU:HD23	1.88	0.42
1:B:280:HIS:CD2	1:B:282:CYS:SG	3.12	0.42
1:A:8:ILE:HG13	1:A:11:ALA:HB2	2.01	0.42
1:A:388:THR:HG23	1:A:391:GLU:OE1	2.19	0.42
1:B:111:ALA:HA	1:B:122:MET:HG3	2.00	0.42
1:B:440:LEU:O	1:B:440:LEU:HG	2.18	0.42
1:B:212:ALA:O	1:B:286:ILE:CG2	2.66	0.42
1:B:232:ASP:HB2	4:B:610:HOH:O	2.20	0.42
1:B:333:THR:O	1:B:337:LEU:HD13	2.19	0.42
1:B:488:VAL:HG23	1:B:523:ARG:CD	2.49	0.42
1:B:491:LYS:HB3	1:B:528:ILE:HG12	2.00	0.42
1:B:172:LEU:O	1:B:535:MET:CE	2.68	0.42
1:B:164:ILE:HD12	1:B:193:ARG:CD	2.49	0.42
1:B:332:ALA:O	1:B:381:ILE:HA	2.20	0.42
1:B:335:ARG:HA	1:B:338:LYS:HE3	2.01	0.42
1:B:337:LEU:O	1:B:359:GLY:HA3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASN:OD1	1:B:443:LEU:N	2.51	0.42
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.85	0.42
1:A:151:LEU:HA	1:A:155:ASN:HB2	2.01	0.42
1:B:51:LEU:O	1:B:293:LYS:CG	2.67	0.42
1:B:61:LEU:HD22	1:B:313:PHE:CD2	2.53	0.42
1:A:278:ILE:HG23	1:A:278:ILE:O	2.19	0.42
1:A:75:THR:O	1:A:76:THR:C	2.58	0.42
1:B:207:ALA:O	1:B:208:CYS:C	2.57	0.42
1:B:339:MET:HG2	1:B:348:LEU:HD21	2.02	0.42
1:B:35:LEU:HD23	1:B:41:ALA:CB	2.49	0.42
1:B:83:ASP:HB3	1:B:416:GLY:HA3	2.02	0.42
1:B:555:ILE:O	1:B:555:ILE:CG2	2.67	0.42
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.79	0.42
1:B:150:HIS:O	1:B:153:GLN:N	2.48	0.42
1:B:199:ILE:CD1	4:B:609:HOH:O	2.67	0.42
1:B:47:VAL:HG13	1:B:294:LEU:HD21	2.01	0.42
1:B:507:ARG:C	1:B:509:PHE:H	2.23	0.42
1:A:105:PHE:O	1:A:544:ALA:N	2.52	0.42
1:A:244:GLN:O	1:A:248:ALA:HB2	2.18	0.42
1:A:405:GLU:CD	1:A:425:LYS:HB2	2.40	0.42
1:A:60:ILE:HD13	1:A:426:VAL:HG11	2.01	0.42
1:B:357:ARG:O	1:B:358:GLU:C	2.58	0.42
1:A:20:MET:HE1	1:A:33:VAL:HB	2.02	0.42
1:A:75:THR:HA	1:A:301:GLU:OE2	2.20	0.42
1:B:517:ARG:NH2	1:B:532:ILE:HG13	2.22	0.42
1:B:86:ALA:C	1:B:88:LEU:N	2.72	0.42
1:B:402:ALA:O	1:B:403:GLY:C	2.58	0.42
1:A:297:TYR:HE1	1:A:430:LEU:HD23	1.85	0.41
1:A:343:VAL:HA	1:A:344:PRO:HD3	1.94	0.41
1:A:367:ILE:HG21	1:A:401:LYS:HD3	2.02	0.41
1:B:97:ARG:NH1	1:B:281:GLY:O	2.53	0.41
1:B:459:TYR:OH	1:B:489:MET:CB	2.68	0.41
1:A:280:HIS:CD2	1:A:282:CYS:HB2	2.55	0.41
1:A:440:LEU:O	1:A:453:LYS:HE2	2.20	0.41
1:B:101:LEU:HG	1:B:105:PHE:HE1	1.85	0.41
1:B:19:VAL:HA	1:B:22:LEU:HG	2.02	0.41
1:B:286:ILE:CD1	1:B:287:ALA:N	2.81	0.41
1:B:490:ALA:HB2	1:B:525:ILE:CG2	2.42	0.41
1:B:492:THR:HG21	1:B:498:ASP:O	2.20	0.41
1:A:48:TYR:HB2	1:A:290:THR:OG1	2.19	0.41
1:A:204:GLU:OE1	1:A:519:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:CB	1:B:362:ASN:HD21	2.33	0.41
1:B:532:ILE:HD11	4:B:603:HOH:O	2.21	0.41
1:A:292:LEU:HG	1:A:298:VAL:HG21	2.02	0.41
1:A:29:GLN:HB2	1:A:32:GLU:HG3	2.02	0.41
1:A:308:LEU:O	1:A:309:GLY:C	2.58	0.41
1:A:369:ASN:O	1:A:372:LYS:HB2	2.20	0.41
1:A:377:ALA:O	1:A:402:ALA:HB1	2.21	0.41
1:A:92:VAL:CG2	1:A:93:MET:N	2.83	0.41
1:B:408:LEU:HD13	1:B:414:LYS:NZ	2.35	0.41
1:B:448:LYS:HD3	1:B:466:TYR:CE2	2.54	0.41
1:B:554:VAL:HG12	1:B:555:ILE:N	2.34	0.41
1:B:190:GLY:O	1:B:192:PRO:HD3	2.19	0.41
1:B:193:ARG:NE	4:B:605:HOH:O	2.22	0.41
1:A:225:ILE:HG22	1:A:238:ALA:HB3	2.02	0.41
1:A:335:ARG:HH11	1:A:335:ARG:CB	2.34	0.41
1:A:519:SER:O	1:A:523:ARG:N	2.54	0.41
1:A:488:VAL:HB	1:A:525:ILE:HD12	2.02	0.41
1:B:144:ALA:HB1	1:B:168:ARG:HE	1.84	0.41
1:B:324:LYS:O	1:B:326:ASP:N	2.53	0.41
1:B:352:ASN:O	1:B:356:LEU:HB2	2.21	0.41
1:B:56:ASP:HB3	1:B:57:GLY:H	1.71	0.41
1:A:10:ILE:C	1:A:12:GLN:H	2.23	0.41
1:A:155:ASN:CG	1:A:155:ASN:O	2.59	0.41
1:B:370:ILE:CG2	1:B:377:ALA:HB2	2.50	0.41
1:B:426:VAL:O	1:B:430:LEU:CB	2.69	0.41
1:A:515:GLU:OE2	1:A:517:ARG:HD3	2.21	0.41
1:A:547:ILE:CD1	1:A:556:THR:O	2.68	0.41
1:B:124:ASP:O	1:B:129:PHE:CA	2.69	0.41
1:B:311:GLU:OE1	1:B:315:ASP:OD1	2.39	0.41
1:B:363:LEU:CD2	1:B:395:LEU:HD11	2.50	0.41
1:B:477:TYR:CZ	1:B:518:LEU:HB2	2.56	0.41
1:B:62:VAL:HG21	1:B:78:SER:OG	2.20	0.41
1:B:66:THR:HA	1:B:67:PRO:HD2	1.93	0.41
1:A:170:ILE:HA	1:A:170:ILE:HD12	1.90	0.41
1:B:490:ALA:HB3	1:B:527:PRO:CA	2.49	0.41
1:B:62:VAL:HG11	1:B:78:SER:CB	2.51	0.41
1:B:65:ILE:HG21	1:B:337:LEU:HD11	2.03	0.41
1:A:533:MET:CA	2:A:561:SO4:O2	2.67	0.41
1:B:308:LEU:O	1:B:312:LYS:HG3	2.20	0.41
1:B:367:ILE:HG21	1:B:401:LYS:HD3	2.02	0.41
1:A:360:PHE:CE2	1:A:398:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PRO:O	1:A:494:TYR:HD2	2.03	0.41
1:A:106:GLY:HA3	1:A:538:LEU:HD22	2.03	0.41
1:B:269:PHE:CD2	1:B:291:ALA:HB2	2.57	0.41
1:B:339:MET:C	1:B:341:GLY:N	2.75	0.41
1:B:523:ARG:HH11	1:B:525:ILE:CD1	2.30	0.41
1:A:159:ILE:O	1:A:161:PRO:CD	2.67	0.40
1:A:389:GLU:HB3	1:A:393:ASN:HD21	1.85	0.40
1:A:368:GLU:CG	1:A:401:LYS:HE2	2.51	0.40
1:B:466:TYR:CG	1:B:513:VAL:CG1	3.04	0.40
1:A:149:ASN:O	1:A:153:GLN:HG2	2.21	0.40
1:A:517:ARG:HH12	1:A:532:ILE:HG13	1.86	0.40
1:B:17:LYS:O	1:B:261:GLN:NE2	2.51	0.40
1:B:393:ASN:CB	4:B:597:HOH:O	2.70	0.40
1:B:65:ILE:CD1	1:B:332:ALA:HA	2.51	0.40
1:A:159:ILE:HG12	1:A:236:VAL:HG21	2.04	0.40
1:B:107:ILE:HD12	1:B:107:ILE:O	2.21	0.40
1:B:350:THR:CG2	1:B:351:GLU:H	2.34	0.40
1:A:271:HIS:CD2	1:A:272:GLY:H	2.40	0.40
1:B:319:ARG:HH21	1:B:443:LEU:HB2	1.86	0.40
1:B:539:PRO:O	1:B:542:PRO:HG3	2.22	0.40
1:B:540:LYS:C	1:B:542:PRO:HD3	2.42	0.40
1:A:124:ASP:N	1:A:124:ASP:OD1	2.55	0.40
1:A:311:GLU:OE1	1:A:315:ASP:OD1	2.39	0.40
1:A:33:VAL:HG13	1:A:41:ALA:HB1	2.02	0.40
1:B:203:SER:OG	1:B:205:VAL:HB	2.21	0.40
1:B:96:LEU:C	1:B:97:ARG:HG3	2.41	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:NZ	4:B:572:HOH:O[4_555]	2.02	0.18

## 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	547/557 (98%)	445 (81%)	84 (15%)	18 (3%)	4	25
1	B	546/557 (98%)	392 (72%)	109 (20%)	45 (8%)	1	5
All	All	1093/1114 (98%)	837 (77%)	193 (18%)	63 (6%)	2	11

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	52	LYS
1	A	352	ASN
1	A	556	THR
1	B	65	ILE
1	B	286	ILE
1	B	325	PRO
1	B	400	ALA
1	B	445	LEU
1	A	166	TRP
1	A	176	ALA
1	A	317	LYS
1	A	401	LYS
1	A	531	ALA
1	A	533	MET
1	B	56	ASP
1	B	72	GLU
1	B	187	LYS
1	B	294	LEU
1	B	332	ALA
1	B	388	THR
1	B	401	LYS
1	B	412	TRP
1	B	509	PHE
1	B	556	THR
1	A	49	ARG
1	A	400	ALA
1	B	244	GLN
1	B	317	LYS
1	B	456	THR
1	B	495	SER
1	B	520	ALA
1	A	112	ALA

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Mol	Chain	Res	Type
1	A	498	ASP
1	B	48	TYR
1	B	76	THR
1	B	100	SER
1	B	102	GLY
1	B	176	ALA
1	B	273	GLY
1	B	328	THR
1	B	399	CYS
1	B	403	GLY
1	B	418	GLY
1	B	551	ALA
1	B	554	VAL
1	A	26	LEU
1	B	12	GLN
1	B	49	ARG
1	B	285	ILE
1	B	319	ARG
1	B	334	VAL
1	B	367	ILE
1	A	160	ASP
1	B	376	PRO
1	A	344	PRO
1	B	154	GLY
1	B	385	PRO
1	B	486	PRO
1	B	516	VAL
1	A	325	PRO
1	B	60	ILE
1	B	528	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	432/440 (98%)	399 (92%)	33 (8%)	15 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	431/440 (98%)	400 (93%)	31 (7%)	17	51
All	All	863/880 (98%)	799 (93%)	64 (7%)	16	49

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	61	LEU
1	A	62	VAL
1	A	94	VAL
1	A	124	ASP
1	A	195	THR
1	A	224	ARG
1	A	226	VAL
1	A	232	ASP
1	A	244	GLN
1	A	277	ASN
1	A	278	ILE
1	A	286	ILE
1	A	311	GLU
1	A	319	ARG
1	A	328	THR
1	A	330	ILE
1	A	337	LEU
1	A	346	SER
1	A	347	ASP
1	A	356	LEU
1	A	375	VAL
1	A	398	LEU
1	A	409	SER
1	A	443	LEU
1	A	456	THR
1	A	480	LEU
1	A	517	ARG
1	A	523	ARG
1	A	526	VAL
1	A	529	THR
1	A	533	MET
1	A	552	ASP
1	B	12	GLN
1	B	20	MET
1	B	72	GLU

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Mol	Chain	Res	Type
1	B	85	LEU
1	B	124	ASP
1	B	148	ASP
1	B	193	ARG
1	B	222	PHE
1	B	229	TYR
1	B	244	GLN
1	B	265	ASN
1	B	266	THR
1	B	275	PHE
1	B	277	ASN
1	B	290	THR
1	B	311	GLU
1	B	313	PHE
1	B	333	THR
1	B	375	VAL
1	B	382	ASN
1	B	396	TYR
1	B	462	ASP
1	B	466	TYR
1	B	480	LEU
1	B	503	LEU
1	B	523	ARG
1	B	526	VAL
1	B	529	THR
1	B	535	MET
1	B	549	ILE
1	B	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	126	ASN
1	A	140	HIS
1	A	150	HIS
1	A	189	ASN
1	A	244	GLN
1	A	277	ASN
1	A	362	ASN
1	A	382	ASN
1	A	393	ASN

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Mol	Chain	Res	Type
1	A	465	ASN
1	A	484	ASN
1	A	546	ASN
1	B	12	GLN
1	B	29	GLN
1	B	118	GLN
1	B	140	HIS
1	B	150	HIS
1	B	153	GLN
1	B	189	ASN
1	B	244	GLN
1	B	265	ASN
1	B	277	ASN
1	B	280	HIS
1	B	362	ASN
1	B	369	ASN
1	B	382	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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
2	SO4	A	560	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	A	561	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	A	562	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	A	563	-	4,4,4	0.72	0	6,6,6	0.48	0
2	SO4	A	564	-	4,4,4	0.72	0	6,6,6	0.48	0
2	SO4	A	565	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	A	566	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	B	560	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	B	561	1	4,4,4	0.72	0	6,6,6	0.48	0
2	SO4	B	562	-	4,4,4	0.72	0	6,6,6	0.49	0
2	SO4	B	563	-	4,4,4	0.72	0	6,6,6	0.49	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
2	SO4	A	560	-	-	0/0/0/0	0/0/0/0
2	SO4	A	561	-	-	0/0/0/0	0/0/0/0
2	SO4	A	562	-	-	0/0/0/0	0/0/0/0
2	SO4	A	563	-	-	0/0/0/0	0/0/0/0
2	SO4	A	564	-	-	0/0/0/0	0/0/0/0
2	SO4	A	565	-	-	0/0/0/0	0/0/0/0
2	SO4	A	566	-	-	0/0/0/0	0/0/0/0
2	SO4	B	560	-	-	0/0/0/0	0/0/0/0
2	SO4	B	561	1	-	0/0/0/0	0/0/0/0
2	SO4	B	562	-	-	0/0/0/0	0/0/0/0
2	SO4	B	563	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	SO4	4	0
2	A	563	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	565	SO4	4	0
2	A	566	SO4	1	0
2	B	560	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.