Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2023 – 06:00 PM EDT

PDB ID	:	2GMX
Title	:	Selective Aminopyridine-Based C-Jun N-terminal Kinase inhibitors with cellular activity
Authors	:	Abad-Zapatero, C.
Deposited on	:	2006-04-07
Resolution	:	3.50 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

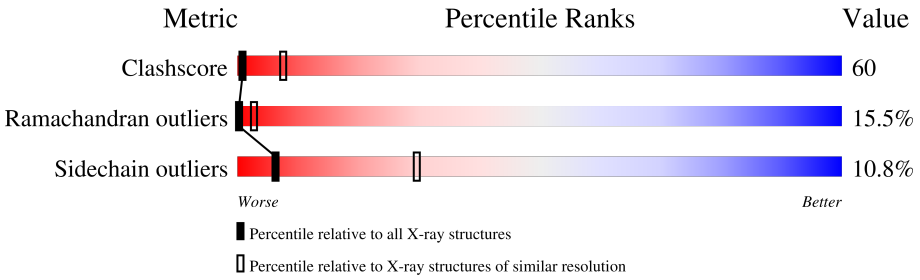
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	22% 54% 18%
1	B	370	25% 55% 15%
2	F	11	36% 45% 9% 9%
2	G	11	55% 27% 9% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5966 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 Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	1
			2868	1839	483	524	22			
1	B	358	Total	C	N	O	S	0	0	1
			2867	1838	483	524	22			

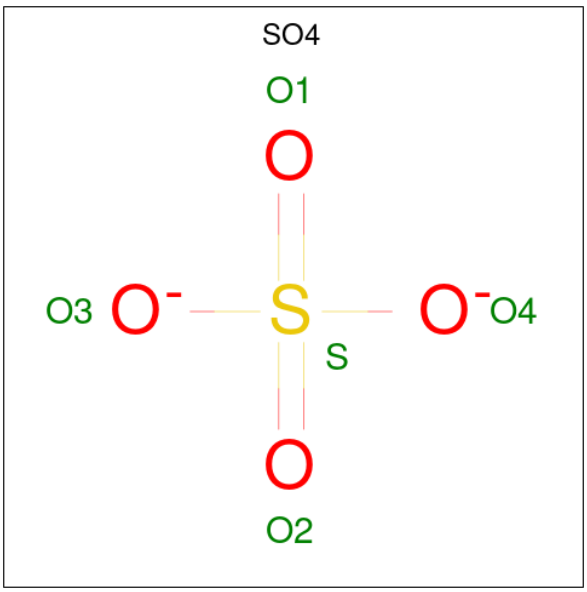
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	THR	engineered mutation	UNP P45983
A	185	GLU	TYR	engineered mutation	UNP P45983
A	365	HIS	-	expression tag	UNP P45983
A	366	HIS	-	expression tag	UNP P45983
A	367	HIS	-	expression tag	UNP P45983
A	368	HIS	-	expression tag	UNP P45983
A	369	HIS	-	expression tag	UNP P45983
A	370	HIS	-	expression tag	UNP P45983
B	183	GLU	THR	engineered mutation	UNP P45983
B	185	GLU	TYR	engineered mutation	UNP P45983
B	365	HIS	-	expression tag	UNP P45983
B	366	HIS	-	expression tag	UNP P45983
B	367	HIS	-	expression tag	UNP P45983
B	368	HIS	-	expression tag	UNP P45983
B	369	HIS	-	expression tag	UNP P45983
B	370	HIS	-	expression tag	UNP P45983

- Molecule 2 is a protein called C-jun-amino-terminal kinase-interacting protein 1.

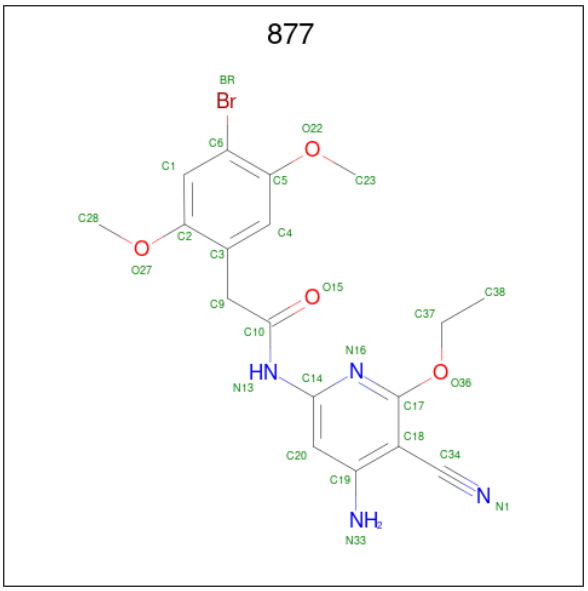
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			84	55	15	14			
2	G	10	Total	C	N	O	0	0	1
			73	46	15	12			

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



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

- Molecule 4 is N-(4-AMINO-5-CYANO-6-ETHOXYPYRIDIN-2-YL)-2-(4-BROMO-2,5-DIMETHOXYPHENYL)ACETAMIDE (three-letter code: 877) (formula: $C_{18}H_{19}BrN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			27	1	18	4	4		
4	B	1	Total	Br	C	N	O	0	0
			27	1	18	4	4		

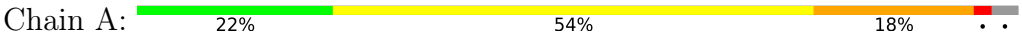
3 Residue-property plots (i)

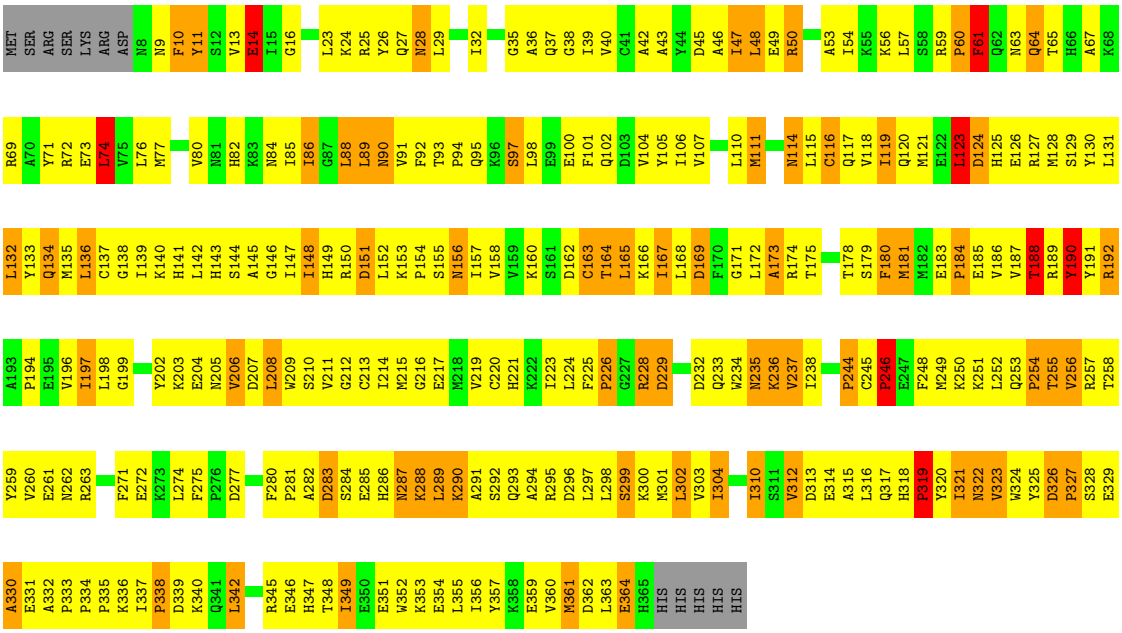
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Mitogen-activated protein kinase 8

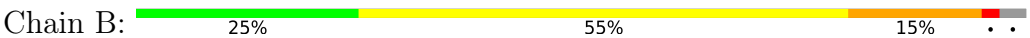
Chain A:

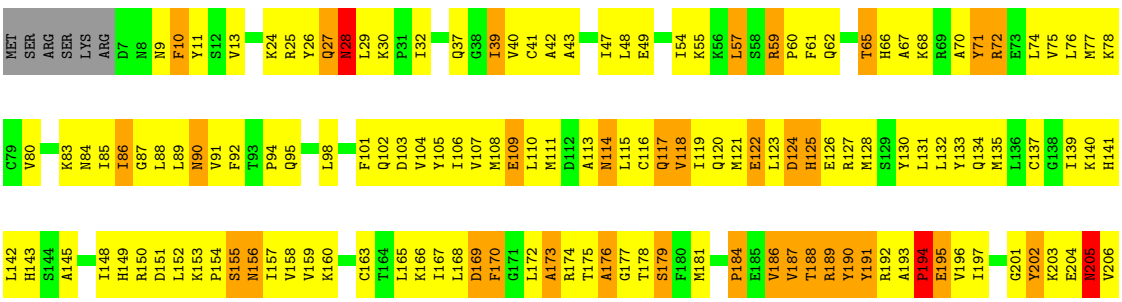


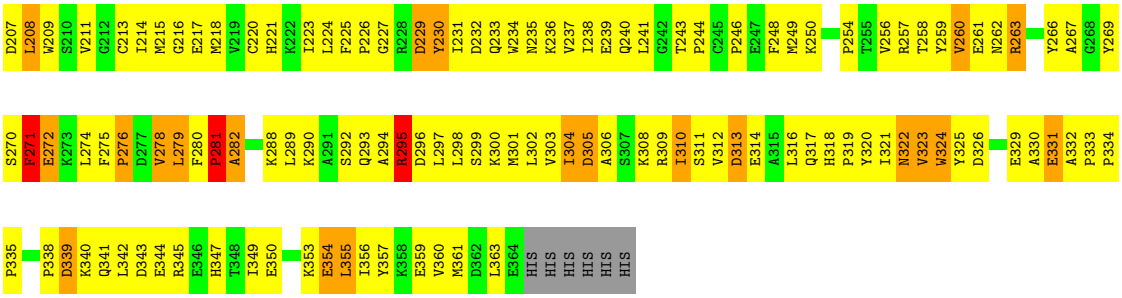


• Molecule 1: Mitogen-activated protein kinase 8

Chain B:







• Molecule 2: C-jun-amino-terminal kinase-interacting protein 1

Chain F:

• Molecule 2: C-jun-amino-terminal kinase-interacting protein 1

Chain G:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.79Å 150.79Å 118.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.91 – 3.50	Depositor
% Data completeness (in resolution range)	83.3 (19.91-3.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.266 , 0.351	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5966	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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: SO4, 877

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	0.40	0/2933	0.69	0/3971
1	B	0.40	0/2932	0.70	0/3970
2	F	0.38	0/86	0.69	0/114
2	G	0.58	0/74	0.81	0/100
All	All	0.40	0/6025	0.70	0/8155

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	ARG	Sidechain

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	2868	0	2868	369	0
1	B	2867	0	2866	340	0
2	F	84	0	91	7	0
2	G	73	0	82	8	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	27	0	19	1	0
4	B	27	0	19	6	0
All	All	5966	0	5945	715	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 60.

All (715) 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:205:ASN:HD21	1:B:309:ARG:HB3	1.20	1.03
1:B:172:LEU:HD21	1:B:186:VAL:HG21	1.40	0.99
1:B:13:VAL:HG21	1:B:29:LEU:HD13	1.45	0.97
1:B:186:VAL:HG13	1:B:187:VAL:H	1.28	0.97
1:A:304:ILE:HD12	1:A:304:ILE:H	1.30	0.97
1:A:132:LEU:O	1:A:136:LEU:HB2	1.67	0.95
1:A:88:LEU:HG	1:A:89:LEU:H	1.31	0.92
1:B:132:LEU:HD21	1:B:215:MET:HB2	1.53	0.91
1:A:190:TYR:H	1:A:190:TYR:HD2	1.00	0.91
1:A:318:HIS:ND1	1:A:319:PRO:HD2	1.86	0.89
1:A:84:ASN:O	1:A:166:LYS:HA	1.72	0.89
1:A:347:HIS:HB3	1:A:351:GLU:OE2	1.72	0.87
1:A:88:LEU:O	1:A:89:LEU:HB2	1.74	0.86
2:G:559:THR:HG22	2:G:560:LEU:H	1.37	0.86
1:A:167:ILE:HG22	1:A:168:LEU:H	1.41	0.86
1:A:244:PRO:HB3	1:A:248:PHE:HD2	1.41	0.85
1:A:208:LEU:HD12	1:A:301:MET:HE3	1.57	0.85
1:A:156:ASN:HD21	1:A:169:ASP:HB3	1.41	0.84
1:B:115:LEU:HD13	1:B:115:LEU:O	1.76	0.84
1:B:275:PHE:HB2	1:B:295:ARG:HD3	1.59	0.84
1:A:116:CYS:SG	1:A:154:PRO:HB2	2.19	0.83
1:A:134:GLN:HE22	1:A:164:THR:HA	1.43	0.82
1:A:60:PRO:HG2	1:A:61:PHE:H	1.44	0.82
1:A:190:TYR:CD2	1:A:190:TYR:N	2.46	0.82
1:A:148:ILE:HD13	1:A:148:ILE:H	1.45	0.82
1:B:39:ILE:HD12	1:B:39:ILE:H	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:HD21	1:B:186:VAL:CG2	2.10	0.81
1:A:164:THR:HG22	1:A:165:LEU:H	1.44	0.81
1:A:114:ASN:HD22	1:A:114:ASN:H	1.28	0.81
1:B:75:VAL:HG21	1:B:340:LYS:HG3	1.62	0.80
1:A:203:LYS:O	1:A:206:VAL:HG12	1.81	0.80
1:B:156:ASN:HD21	1:B:169:ASP:HB2	1.46	0.80
1:B:98:LEU:HD11	1:B:353:LYS:HG2	1.63	0.80
1:B:271:PHE:HZ	1:B:302:LEU:HB2	1.45	0.79
1:A:150:ARG:HH21	1:A:172:LEU:HB3	1.47	0.79
1:B:95:GLN:HG2	1:B:102:GLN:H	1.45	0.79
1:A:74:LEU:HD23	1:A:359:GLU:HG3	1.64	0.78
1:A:210:SER:O	1:A:214:ILE:HG12	1.83	0.78
1:B:208:LEU:HD12	1:B:310:ILE:CG2	2.14	0.78
1:B:208:LEU:HD12	1:B:310:ILE:HG23	1.66	0.78
1:A:48:LEU:HD22	1:A:50:ARG:HE	1.47	0.78
1:A:290:LYS:HE2	1:A:292:SER:HB3	1.66	0.78
1:B:154:PRO:HD3	1:B:191:TYR:CE2	2.18	0.78
1:B:32:ILE:HG12	1:B:42:ALA:HB2	1.65	0.78
1:A:253:GLN:HB3	1:A:254:PRO:HD2	1.67	0.77
1:A:45:ASP:OD2	1:A:48:LEU:HB2	1.84	0.77
1:A:80:VAL:HG11	1:A:85:ILE:HG21	1.66	0.76
1:A:300:LYS:O	1:A:310:ILE:HG22	1.86	0.75
1:A:61:PHE:HE2	1:A:353:LYS:HG3	1.49	0.75
1:A:215:MET:O	1:A:219:VAL:HG23	1.86	0.75
1:B:145:ALA:HB2	1:B:335:PRO:HD2	1.68	0.75
2:G:559:THR:O	2:G:560:LEU:HB2	1.85	0.74
1:A:337:ILE:HG23	1:A:338:PRO:HD2	1.67	0.74
1:B:259:TYR:CZ	1:B:263:ARG:HD3	2.22	0.74
1:B:271:PHE:CE1	1:B:299:SER:HA	2.23	0.74
1:B:275:PHE:HB3	1:B:280:PHE:HE2	1.52	0.74
1:A:53:ALA:HB2	1:A:110:LEU:HD12	1.69	0.73
1:B:305:ASP:CB	1:B:308:LYS:HE2	2.18	0.73
1:B:294:ALA:C	1:B:296:ASP:H	1.93	0.72
1:B:150:ARG:HD3	1:B:202:TYR:HE1	1.53	0.72
1:A:26:TYR:HB3	1:A:54:ILE:HD11	1.71	0.72
1:B:111:MET:HB2	4:B:1001:877:H91	1.71	0.72
1:A:316:LEU:HA	1:A:321:ILE:HG21	1.72	0.71
1:B:177:GLY:HA2	1:B:202:TYR:CE2	2.25	0.71
1:A:163:CYS:HA	2:F:560:LEU:HD12	1.71	0.71
1:B:87:GLY:HA3	1:B:109:GLU:OE2	1.90	0.71
1:A:208:LEU:HD12	1:A:301:MET:CE	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASP:O	1:B:170:PHE:HB2	1.91	0.71
1:B:189:ARG:NH1	1:B:229:ASP:HA	2.06	0.70
1:A:134:GLN:HE22	1:A:164:THR:CA	2.03	0.70
1:A:148:ILE:HG22	1:A:204:GLU:HA	1.73	0.70
1:A:90:ASN:HD22	1:A:91:VAL:H	1.40	0.70
1:B:326:ASP:HB2	2:G:556:ARG:HH22	1.55	0.70
1:A:189:ARG:HB2	1:A:192:ARG:HH21	1.57	0.69
1:A:11:TYR:OH	1:A:27:GLN:HA	1.92	0.69
1:A:181:MET:O	1:A:184:PRO:HD3	1.92	0.69
1:A:310:ILE:HD11	1:A:315:ALA:HA	1.75	0.69
1:A:150:ARG:NH1	1:A:174:ARG:HG2	2.07	0.69
1:B:102:GLN:HG2	1:B:103:ASP:OD1	1.93	0.69
1:B:275:PHE:HB3	1:B:280:PHE:CE2	2.27	0.69
1:B:10:PHE:CE1	1:B:94:PRO:HA	2.28	0.69
1:A:237:VAL:HG13	1:A:238:ILE:HG23	1.75	0.69
1:B:357:TYR:O	1:B:361:MET:HG2	1.92	0.68
1:B:187:VAL:HG22	1:B:192:ARG:HG2	1.74	0.68
1:A:271:PHE:HA	1:A:274:LEU:HB2	1.75	0.68
1:B:360:VAL:HA	1:B:363:LEU:HD11	1.75	0.68
1:B:153:LYS:HE2	1:B:155:SER:OG	1.93	0.68
1:B:275:PHE:CD2	1:B:298:LEU:HD13	2.29	0.68
1:B:114:ASN:ND2	1:B:116:CYS:HB2	2.09	0.68
1:B:115:LEU:HB2	1:B:157:ILE:HB	1.76	0.68
1:A:285:GLU:HB2	1:A:286:HIS:ND1	2.08	0.67
1:A:259:TYR:CZ	1:A:263:ARG:HD3	2.29	0.67
1:B:148:ILE:O	1:B:173:ALA:HA	1.94	0.67
1:B:187:VAL:O	1:B:192:ARG:HD3	1.94	0.67
1:B:61:PHE:HA	1:B:67:ALA:HB2	1.77	0.67
1:B:186:VAL:HG13	1:B:187:VAL:N	2.06	0.67
1:A:32:ILE:HG21	1:A:42:ALA:HB2	1.76	0.67
1:A:288:LYS:HD2	1:A:323:VAL:HG12	1.76	0.67
1:B:30:LYS:HB3	1:B:42:ALA:HB3	1.76	0.66
1:A:117:GLN:HE21	1:A:117:GLN:HA	1.60	0.66
1:A:158:VAL:O	1:A:165:LEU:HA	1.95	0.66
1:B:230:TYR:CE2	1:B:231:ILE:HG13	2.30	0.66
1:A:287:ASN:O	1:A:289:LEU:N	2.28	0.66
1:B:318:HIS:ND1	1:B:319:PRO:HD2	2.10	0.66
1:B:359:GLU:O	1:B:363:LEU:HG	1.95	0.66
1:B:288:LYS:O	1:B:293:GLN:HG2	1.96	0.66
1:A:189:ARG:HA	1:A:192:ARG:HE	1.59	0.66
1:A:257:ARG:O	1:A:261:GLU:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:CE2	1:A:238:ILE:HG21	2.31	0.66
1:A:128:MET:O	1:A:132:LEU:HD22	1.96	0.66
2:F:559:THR:HG22	2:F:560:LEU:H	1.61	0.66
1:A:115:LEU:HB2	1:A:157:ILE:HG22	1.78	0.65
1:B:78:LYS:HD3	1:B:363:LEU:HD22	1.79	0.65
1:A:165:LEU:C	1:A:165:LEU:HD23	2.17	0.65
1:A:220:CYS:O	1:A:221:HIS:HB2	1.97	0.65
1:A:356:ILE:O	1:A:360:VAL:HG23	1.96	0.65
1:B:133:TYR:HB2	1:B:321:ILE:HG23	1.77	0.65
1:A:149:HIS:C	1:A:150:ARG:HG3	2.17	0.65
1:A:101:PHE:HD2	1:A:357:TYR:HB2	1.61	0.65
1:B:303:VAL:HG21	1:B:309:ARG:HA	1.79	0.65
1:B:321:ILE:O	1:B:323:VAL:N	2.29	0.64
1:A:213:CYS:HA	1:A:224:LEU:HD22	1.79	0.64
1:A:315:ALA:O	1:A:318:HIS:HB3	1.98	0.64
1:B:95:GLN:HG2	1:B:102:GLN:N	2.12	0.64
1:B:60:PRO:HG2	1:B:61:PHE:CD2	2.33	0.64
1:A:234:TRP:CZ2	1:A:238:ILE:HG21	2.33	0.64
1:A:244:PRO:HB3	1:A:248:PHE:CD2	2.28	0.64
1:A:289:LEU:O	1:A:293:GLN:HB2	1.98	0.64
1:A:160:LYS:HB3	1:A:162:ASP:OD1	1.98	0.64
1:B:342:LEU:HB2	1:B:345:ARG:HD3	1.80	0.64
1:A:174:ARG:HD3	1:A:175:THR:O	1.98	0.63
1:A:142:LEU:HD11	1:A:147:ILE:HG21	1.81	0.63
1:A:64:GLN:HB3	1:A:346:GLU:CD	2.19	0.63
1:A:114:ASN:HD22	1:A:114:ASN:N	1.94	0.63
1:B:342:LEU:H	1:B:342:LEU:HD23	1.63	0.63
1:B:110:LEU:HD21	4:B:1001:877:H232	1.81	0.63
1:B:128:MET:HG3	1:B:218:MET:HE2	1.80	0.63
1:A:115:LEU:CD1	1:A:119:ILE:HG13	2.29	0.63
1:A:164:THR:O	1:A:165:LEU:HB2	1.99	0.63
1:B:259:TYR:CE1	1:B:263:ARG:HD3	2.34	0.62
1:A:101:PHE:CD2	1:A:357:TYR:HB2	2.34	0.62
1:A:115:LEU:C	1:A:117:GLN:H	2.01	0.62
1:A:235:ASN:HD21	1:A:263:ARG:NE	1.97	0.62
1:B:98:LEU:O	1:B:101:PHE:HB2	1.99	0.62
1:B:290:LYS:HB2	1:B:293:GLN:HB2	1.81	0.62
1:B:148:ILE:HG22	1:B:150:ARG:HG3	1.81	0.61
1:B:152:LEU:O	1:B:214:ILE:HD11	2.00	0.61
1:B:205:ASN:ND2	1:B:309:ARG:HB3	2.04	0.61
1:B:98:LEU:CD1	1:B:353:LYS:HG2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CZ	1:B:299:SER:HA	2.36	0.61
1:A:90:ASN:HD22	1:A:91:VAL:N	1.97	0.61
1:B:215:MET:HE3	1:B:298:LEU:HG	1.81	0.61
1:A:314:GLU:CD	1:A:314:GLU:H	2.04	0.61
1:B:13:VAL:HG21	1:B:29:LEU:CD1	2.28	0.61
1:B:113:ALA:HB1	1:B:117:GLN:OE1	2.00	0.61
1:B:275:PHE:CE2	1:B:298:LEU:HD13	2.36	0.61
1:B:342:LEU:CB	1:B:345:ARG:HD3	2.30	0.61
1:A:143:HIS:C	1:A:145:ALA:H	2.04	0.61
1:B:84:ASN:O	1:B:85:ILE:HD13	2.01	0.61
1:B:77:MET:HB3	1:B:88:LEU:HD22	1.82	0.61
1:A:156:ASN:O	1:A:157:ILE:HD13	2.01	0.61
1:B:163:CYS:HA	2:G:560:LEU:HD22	1.81	0.61
1:B:225:PHE:HE1	1:B:240:GLN:HB2	1.66	0.61
1:A:115:LEU:HD13	1:A:119:ILE:HG13	1.83	0.60
1:A:88:LEU:HG	1:A:89:LEU:N	2.11	0.60
1:B:65:THR:C	1:B:67:ALA:H	2.04	0.60
1:B:125:HIS:ND1	1:B:289:LEU:O	2.34	0.60
1:A:143:HIS:O	1:A:145:ALA:N	2.34	0.60
1:B:78:LYS:NZ	1:B:363:LEU:HB2	2.17	0.60
1:A:94:PRO:HG2	1:A:95:GLN:NE2	2.17	0.60
1:B:128:MET:HG3	1:B:218:MET:CE	2.31	0.60
1:A:86:ILE:HA	1:A:166:LYS:HD3	1.83	0.60
1:B:28:ASN:HD22	1:B:29:LEU:N	1.99	0.60
1:A:64:GLN:HB3	1:A:346:GLU:OE2	2.00	0.60
1:B:165:LEU:HD23	1:B:166:LYS:N	2.17	0.60
1:B:215:MET:CE	1:B:298:LEU:HG	2.31	0.60
1:A:63:ASN:OD1	1:A:65:THR:HB	2.01	0.60
1:B:230:TYR:CD2	1:B:231:ILE:HG13	2.37	0.60
1:A:118:VAL:O	1:A:119:ILE:C	2.40	0.59
1:A:25:ARG:HG2	1:A:47:ILE:HB	1.85	0.59
1:A:136:LEU:HA	1:A:139:ILE:HD12	1.84	0.59
1:A:148:ILE:CG2	1:A:204:GLU:HA	2.32	0.59
1:A:117:GLN:HA	1:A:117:GLN:NE2	2.17	0.59
1:B:194:PRO:HA	1:B:197:ILE:HD12	1.84	0.59
1:A:254:PRO:O	1:A:257:ARG:HB3	2.02	0.59
1:B:193:ALA:HB2	1:B:209:TRP:CG	2.37	0.59
1:A:61:PHE:CE2	1:A:353:LYS:HG3	2.35	0.59
1:A:149:HIS:HA	1:A:173:ALA:CB	2.33	0.59
1:B:59:ARG:CB	1:B:62:GLN:HB2	2.33	0.59
1:A:10:PHE:CE2	1:A:94:PRO:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ASP:HB2	1:B:308:LYS:HE2	1.85	0.59
1:A:74:LEU:HD23	1:A:359:GLU:CG	2.33	0.59
1:A:167:ILE:HG22	1:A:168:LEU:N	2.14	0.59
1:B:354:GLU:O	1:B:355:LEU:C	2.41	0.59
1:B:305:ASP:HB3	1:B:308:LYS:HE2	1.84	0.58
1:A:164:THR:HG22	1:A:165:LEU:N	2.17	0.58
1:A:189:ARG:CA	1:A:192:ARG:HH21	2.15	0.58
1:B:39:ILE:HD12	1:B:39:ILE:N	2.15	0.58
1:A:150:ARG:O	1:A:151:ASP:HB2	2.03	0.58
1:A:165:LEU:HD23	1:A:166:LYS:N	2.19	0.58
1:B:11:TYR:CE1	1:B:24:LYS:HA	2.38	0.58
1:B:250:LYS:HD2	1:B:257:ARG:HH12	1.68	0.58
1:B:272:GLU:HA	1:B:295:ARG:HD2	1.85	0.58
1:A:48:LEU:HD22	1:A:50:ARG:NE	2.17	0.58
1:A:13:VAL:HG11	1:A:29:LEU:HB2	1.86	0.58
1:A:125:HIS:ND1	1:A:320:TYR:OH	2.31	0.58
1:A:300:LYS:C	1:A:310:ILE:HG22	2.24	0.57
1:B:169:ASP:O	1:B:170:PHE:CB	2.52	0.57
1:B:220:CYS:O	1:B:221:HIS:HB2	2.03	0.57
1:A:77:MET:HA	1:A:77:MET:CE	2.34	0.57
1:A:189:ARG:CB	1:A:192:ARG:HH21	2.17	0.57
1:B:216:GLY:HA3	1:B:224:LEU:HD22	1.86	0.57
1:A:244:PRO:HB2	1:A:249:MET:CE	2.35	0.57
1:B:130:TYR:O	1:B:134:GLN:HB2	2.04	0.57
1:A:133:TYR:CE1	1:A:137:CYS:SG	2.97	0.57
1:B:119:ILE:HB	1:B:120:GLN:NE2	2.20	0.57
1:B:349:ILE:HG13	1:B:350:GLU:N	2.20	0.57
1:A:234:TRP:HA	1:A:237:VAL:HG12	1.86	0.56
1:B:193:ALA:HB2	1:B:209:TRP:CD1	2.39	0.56
1:B:270:SER:O	1:B:272:GLU:N	2.38	0.56
1:B:86:ILE:HG13	1:B:168:LEU:HD23	1.87	0.56
1:A:60:PRO:CG	1:A:61:PHE:H	2.17	0.56
1:A:148:ILE:HD13	1:A:148:ILE:N	2.17	0.56
1:A:133:TYR:HB2	1:A:324:TRP:HD1	1.70	0.56
1:A:342:LEU:HB2	1:A:345:ARG:HB3	1.87	0.56
1:B:140:LYS:HA	1:B:312:VAL:HG11	1.88	0.56
1:B:131:LEU:O	1:B:132:LEU:C	2.44	0.55
1:A:190:TYR:HB3	1:A:223:ILE:HG21	1.89	0.55
1:A:234:TRP:NE1	1:A:238:ILE:HD13	2.21	0.55
1:A:297:LEU:HD13	1:A:318:HIS:CD2	2.42	0.55
1:B:39:ILE:O	1:B:55:LYS:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HD12	1:A:128:MET:CA	2.37	0.55
1:B:127:ARG:O	1:B:131:LEU:HG	2.06	0.55
1:A:325:TYR:O	1:A:326:ASP:HB2	2.06	0.55
1:A:361:MET:O	1:A:363:LEU:N	2.39	0.55
1:B:89:LEU:O	1:B:90:ASN:HB2	2.05	0.55
2:F:560:LEU:HD22	2:F:562:LEU:HD21	1.88	0.55
1:B:30:LYS:O	1:B:42:ALA:N	2.35	0.55
1:B:192:ARG:HH22	1:B:230:TYR:HB2	1.72	0.55
1:A:94:PRO:HG3	1:A:105:TYR:HE1	1.71	0.55
1:A:111:MET:HG3	1:A:158:VAL:HB	1.88	0.55
1:A:129:SER:HB3	1:A:320:TYR:CE2	2.41	0.55
1:A:228:ARG:NH2	1:B:262:ASN:OD1	2.40	0.55
1:A:25:ARG:HD3	1:A:45:ASP:OD1	2.07	0.55
1:A:93:THR:O	1:A:93:THR:HG23	2.07	0.55
1:A:192:ARG:HG2	1:A:196:VAL:HG11	1.89	0.55
1:A:197:ILE:HG22	1:A:198:LEU:N	2.20	0.55
1:A:235:ASN:HD21	1:A:263:ARG:HE	1.55	0.55
1:B:115:LEU:CD1	1:B:119:ILE:HD11	2.37	0.55
1:B:321:ILE:O	1:B:322:ASN:C	2.44	0.54
1:A:234:TRP:O	1:A:236:LYS:N	2.40	0.54
1:B:11:TYR:HE1	1:B:24:LYS:HA	1.72	0.54
1:B:325:TYR:HE1	1:B:330:ALA:HB3	1.72	0.54
1:B:65:THR:O	1:B:68:LYS:HG2	2.08	0.54
1:A:216:GLY:O	1:A:220:CYS:HB2	2.08	0.54
1:B:86:ILE:HG13	1:B:168:LEU:CD2	2.38	0.54
1:B:137:CYS:SG	1:B:330:ALA:HB2	2.48	0.54
1:A:105:TYR:O	1:A:106:ILE:HD13	2.07	0.54
1:A:180:PHE:CG	1:A:181:MET:N	2.75	0.53
1:B:257:ARG:O	1:B:259:TYR:N	2.40	0.53
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.22	0.53
1:B:294:ALA:C	1:B:296:ASP:N	2.62	0.53
1:A:39:ILE:HG22	1:A:40:VAL:N	2.23	0.53
1:B:259:TYR:O	1:B:262:ASN:HB2	2.08	0.53
1:B:310:ILE:HG13	1:B:311:SER:H	1.73	0.53
1:A:233:GLN:HA	1:A:233:GLN:NE2	2.23	0.53
1:A:183:GLU:N	1:A:184:PRO:HD3	2.23	0.53
1:A:296:ASP:OD2	1:A:300:LYS:HE2	2.09	0.53
1:A:310:ILE:HG23	1:A:310:ILE:O	2.08	0.53
1:B:239:GLU:HA	1:B:266:TYR:CD1	2.44	0.53
1:A:10:PHE:N	1:A:10:PHE:CD1	2.75	0.53
1:A:101:PHE:CE1	1:A:104:VAL:HG22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PRO:HD3	1:A:209:TRP:CE2	2.44	0.53
1:B:211:VAL:HB	1:B:301:MET:HE1	1.91	0.53
1:B:172:LEU:CD2	1:B:186:VAL:HG21	2.25	0.53
1:A:118:VAL:O	1:A:121:MET:HG2	2.09	0.53
1:B:28:ASN:HD22	1:B:28:ASN:C	2.12	0.53
1:B:149:HIS:O	1:B:150:ARG:HB2	2.09	0.53
1:B:175:THR:O	1:B:176:ALA:O	2.27	0.53
1:B:271:PHE:HA	1:B:274:LEU:HD12	1.91	0.53
1:A:149:HIS:O	1:A:150:ARG:HG3	2.08	0.53
1:A:252:LEU:CD1	1:A:260:VAL:HG11	2.39	0.53
1:A:25:ARG:HE	1:A:47:ILE:HG21	1.74	0.52
1:A:205:ASN:O	1:A:208:LEU:N	2.40	0.52
1:B:139:ILE:HD11	1:B:152:LEU:CD1	2.39	0.52
1:A:197:ILE:HD11	1:A:233:GLN:HG3	1.89	0.52
1:A:154:PRO:C	1:A:156:ASN:H	2.13	0.52
1:A:325:TYR:OH	1:A:331:GLU:HG3	2.10	0.52
1:B:177:GLY:HA2	1:B:202:TYR:HE2	1.72	0.52
1:B:256:VAL:O	1:B:259:TYR:HB3	2.10	0.52
1:B:300:LYS:O	1:B:310:ILE:HB	2.09	0.52
1:A:53:ALA:CB	1:A:110:LEU:HD12	2.37	0.52
1:A:178:THR:HG22	1:A:179:SER:N	2.25	0.52
1:A:137:CYS:O	1:A:138:GLY:C	2.48	0.52
1:A:149:HIS:HA	1:A:173:ALA:HB2	1.92	0.52
1:B:9:ASN:O	1:B:24:LYS:HG3	2.10	0.52
1:A:53:ALA:CA	1:A:110:LEU:HD12	2.40	0.51
1:A:312:VAL:O	1:A:315:ALA:HB3	2.11	0.51
1:B:297:LEU:HG	1:B:301:MET:SD	2.50	0.51
1:A:234:TRP:C	1:A:236:LYS:H	2.14	0.51
1:B:201:GLY:O	1:B:202:TYR:HB3	2.10	0.51
1:B:270:SER:C	1:B:272:GLU:H	2.13	0.51
1:B:293:GLN:NE2	1:B:319:PRO:HG2	2.26	0.51
1:A:164:THR:O	1:A:165:LEU:CB	2.58	0.51
1:B:304:ILE:HD12	1:B:304:ILE:H	1.76	0.51
1:A:131:LEU:HA	1:A:134:GLN:HB2	1.92	0.51
1:B:150:ARG:HH21	1:B:172:LEU:HB3	1.74	0.51
1:B:189:ARG:O	1:B:191:TYR:N	2.43	0.51
1:B:280:PHE:O	1:B:282:ALA:N	2.44	0.51
1:B:356:ILE:O	1:B:360:VAL:HG23	2.10	0.51
1:A:314:GLU:HA	1:A:317:GLN:HB2	1.92	0.51
1:A:293:GLN:HA	1:A:293:GLN:HE21	1.76	0.51
1:B:211:VAL:HB	1:B:301:MET:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PHE:CD1	1:B:299:SER:HA	2.45	0.51
1:A:10:PHE:N	1:A:10:PHE:HD1	2.09	0.51
1:A:123:LEU:HD12	1:A:128:MET:HA	1.92	0.51
1:A:135:MET:O	1:A:139:ILE:HG13	2.10	0.51
1:A:84:ASN:O	1:A:166:LYS:CA	2.52	0.50
1:A:115:LEU:C	1:A:117:GLN:N	2.65	0.50
1:A:163:CYS:HB2	2:F:559:THR:O	2.11	0.50
1:B:40:VAL:HA	1:B:54:ILE:O	2.10	0.50
1:B:294:ALA:HB2	1:B:320:TYR:CE1	2.45	0.50
1:A:90:ASN:HB3	1:A:107:VAL:HB	1.93	0.50
1:A:120:GLN:HG3	1:A:120:GLN:O	2.10	0.50
1:B:107:VAL:O	1:B:108:MET:HB3	2.11	0.50
1:A:152:LEU:N	1:A:152:LEU:HD23	2.26	0.50
1:B:232:ASP:HA	1:B:235:ASN:ND2	2.26	0.50
1:A:48:LEU:HD21	1:A:50:ARG:HH21	1.77	0.50
1:A:88:LEU:CG	1:A:89:LEU:N	2.71	0.50
1:A:94:PRO:HG2	1:A:95:GLN:HE22	1.73	0.50
1:A:212:GLY:C	1:A:214:ILE:H	2.14	0.50
1:B:140:LYS:O	1:B:143:HIS:N	2.44	0.50
1:B:153:LYS:HE2	1:B:155:SER:CB	2.41	0.50
1:A:133:TYR:CB	1:A:324:TRP:HD1	2.24	0.50
1:A:255:THR:O	1:A:256:VAL:C	2.50	0.50
1:B:342:LEU:O	1:B:345:ARG:HB2	2.12	0.50
1:A:111:MET:HE3	1:A:160:LYS:N	2.26	0.50
1:B:217:GLU:CD	1:B:223:ILE:HD13	2.32	0.50
1:B:224:LEU:O	1:B:226:PRO:HD3	2.12	0.50
1:B:32:ILE:HD11	1:B:42:ALA:HA	1.93	0.50
1:B:297:LEU:CD2	1:B:321:ILE:HD11	2.42	0.50
1:A:125:HIS:CE1	1:A:320:TYR:HH	2.22	0.50
1:B:10:PHE:CZ	1:B:94:PRO:HA	2.47	0.50
1:B:122:GLU:O	1:B:123:LEU:HD23	2.11	0.50
1:A:101:PHE:CD1	1:A:102:GLN:N	2.79	0.50
1:B:207:ASP:O	1:B:211:VAL:HG23	2.12	0.50
1:B:281:PRO:O	1:B:282:ALA:O	2.30	0.50
1:A:48:LEU:O	1:A:49:GLU:HB2	2.12	0.49
1:A:61:PHE:HA	1:A:67:ALA:HB2	1.93	0.49
1:A:288:LYS:CD	1:A:323:VAL:HG12	2.42	0.49
1:B:205:ASN:HD21	1:B:309:ARG:CB	2.08	0.49
1:A:128:MET:CE	1:A:132:LEU:HD21	2.41	0.49
1:A:348:THR:HG22	1:A:349:ILE:H	1.77	0.49
1:A:38:GLY:HA3	1:A:56:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:N	1:A:184:PRO:CD	2.75	0.49
1:B:67:ALA:O	1:B:70:ALA:HB3	2.10	0.49
1:B:114:ASN:C	1:B:114:ASN:HD22	2.14	0.49
1:B:154:PRO:HD3	1:B:191:TYR:CZ	2.47	0.49
1:B:174:ARG:HG3	1:B:175:THR:N	2.27	0.49
1:B:215:MET:CE	1:B:297:LEU:HB3	2.42	0.49
1:A:9:ASN:O	1:A:24:LYS:HG3	2.12	0.49
1:A:146:GLY:HA2	1:A:204:GLU:OE2	2.12	0.49
1:A:180:PHE:CD1	1:A:181:MET:N	2.81	0.49
1:A:198:LEU:HD11	1:A:234:TRP:CH2	2.48	0.49
1:B:118:VAL:HA	1:B:121:MET:CG	2.41	0.49
1:B:338:PRO:HG3	1:B:340:LYS:HE2	1.95	0.49
1:B:125:HIS:CE1	1:B:289:LEU:O	2.66	0.49
1:A:334:PRO:HB2	1:A:336:LYS:HE2	1.93	0.49
1:B:172:LEU:O	1:B:173:ALA:C	2.49	0.49
1:A:248:PHE:O	1:A:251:LYS:HG3	2.12	0.49
1:B:303:VAL:HG11	1:B:308:LYS:HB2	1.94	0.49
1:B:313:ASP:O	1:B:317:GLN:HG2	2.13	0.49
1:A:294:ALA:O	1:A:297:LEU:HB3	2.12	0.49
1:B:111:MET:HE3	1:B:160:LYS:HB2	1.94	0.49
1:B:151:ASP:O	1:B:152:LEU:HD23	2.13	0.49
1:B:209:TRP:CD1	1:B:209:TRP:C	2.86	0.49
1:B:27:GLN:HE21	1:B:28:ASN:H	1.59	0.49
1:B:124:ASP:O	1:B:125:HIS:C	2.51	0.49
1:B:189:ARG:NH1	1:B:229:ASP:CA	2.76	0.49
2:G:559:THR:HG22	2:G:560:LEU:N	2.18	0.49
1:A:189:ARG:HG2	1:A:233:GLN:NE2	2.27	0.48
1:A:234:TRP:HA	1:A:237:VAL:CG1	2.43	0.48
1:A:130:TYR:CZ	2:F:556:ARG:HD3	2.48	0.48
2:F:559:THR:O	2:F:560:LEU:HB2	2.13	0.48
1:A:91:VAL:HG21	1:A:363:LEU:CD1	2.44	0.48
1:A:262:ASN:O	1:A:263:ARG:C	2.49	0.48
1:B:111:MET:CE	1:B:160:LYS:HB2	2.44	0.48
1:B:269:TYR:HB2	1:B:274:LEU:CD2	2.43	0.48
1:A:296:ASP:O	1:A:299:SER:HB2	2.13	0.48
1:B:32:ILE:HD11	1:B:41:CYS:O	2.14	0.48
1:A:90:ASN:ND2	1:A:91:VAL:N	2.60	0.48
1:A:229:ASP:OD1	1:A:232:ASP:CB	2.61	0.48
1:B:118:VAL:HA	1:B:121:MET:SD	2.54	0.48
1:B:189:ARG:HH12	1:B:229:ASP:HA	1.76	0.48
1:B:65:THR:O	1:B:67:ALA:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:C	1:A:236:LYS:N	2.67	0.48
1:B:186:VAL:O	1:B:188:THR:N	2.47	0.48
1:A:134:GLN:HE22	1:A:164:THR:C	2.16	0.48
1:A:149:HIS:CG	1:A:152:LEU:HD21	2.49	0.48
1:A:224:LEU:HD23	1:A:225:PHE:CZ	2.49	0.48
1:A:283:ASP:HB2	1:A:291:ALA:HB2	1.95	0.48
1:A:351:GLU:O	1:A:355:LEU:HD13	2.13	0.48
1:B:28:ASN:O	1:B:43:ALA:HA	2.13	0.48
1:B:110:LEU:HD21	4:B:1001:877:C23	2.43	0.48
1:B:117:GLN:O	1:B:120:GLN:N	2.37	0.48
1:B:208:LEU:CD1	1:B:310:ILE:HG23	2.42	0.48
1:B:257:ARG:O	1:B:258:THR:C	2.49	0.48
1:A:233:GLN:HA	1:A:233:GLN:HE21	1.79	0.48
1:B:89:LEU:H	1:B:108:MET:HA	1.79	0.48
1:B:140:LYS:O	1:B:142:LEU:N	2.47	0.48
1:B:303:VAL:HG12	1:B:305:ASP:H	1.79	0.48
1:A:29:LEU:HD12	1:A:43:ALA:CB	2.44	0.47
1:A:32:ILE:CG1	1:A:40:VAL:HG13	2.44	0.47
1:A:189:ARG:HB2	1:A:192:ARG:NH2	2.27	0.47
1:B:27:GLN:NE2	1:B:28:ASN:H	2.12	0.47
1:B:29:LEU:N	1:B:29:LEU:HD12	2.29	0.47
1:B:257:ARG:C	1:B:259:TYR:N	2.64	0.47
1:B:110:LEU:HD23	1:B:111:MET:O	2.14	0.47
1:B:215:MET:O	1:B:215:MET:HG2	2.13	0.47
1:B:355:LEU:O	1:B:359:GLU:N	2.43	0.47
1:A:72:ARG:NH1	1:A:174:ARG:HB3	2.29	0.47
1:A:244:PRO:HB2	1:A:249:MET:HE1	1.94	0.47
1:A:360:VAL:O	1:A:361:MET:C	2.53	0.47
1:B:27:GLN:O	1:B:28:ASN:HB3	2.15	0.47
1:B:169:ASP:HB3	1:B:170:PHE:H	1.37	0.47
1:B:290:LYS:O	1:B:293:GLN:HB3	2.14	0.47
1:A:110:LEU:HD21	4:A:901:877:H232	1.95	0.47
1:A:259:TYR:HB2	1:B:229:ASP:HB2	1.96	0.47
1:B:105:TYR:N	1:B:105:TYR:CD1	2.83	0.47
1:B:165:LEU:HD23	1:B:165:LEU:C	2.35	0.47
1:B:278:VAL:O	1:B:280:PHE:N	2.47	0.47
1:B:338:PRO:HG2	1:B:339:ASP:H	1.80	0.47
1:B:338:PRO:O	1:B:339:ASP:HB3	2.14	0.47
1:A:153:LYS:NZ	1:A:188:THR:HG23	2.30	0.47
1:A:326:ASP:O	1:A:328:SER:N	2.47	0.47
1:A:363:LEU:O	1:A:364:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ILE:CD1	1:B:204:GLU:HA	2.44	0.47
1:B:186:VAL:CG1	1:B:187:VAL:H	2.12	0.47
1:B:244:PRO:HB3	1:B:248:PHE:CD2	2.50	0.47
1:A:285:GLU:HB2	1:A:286:HIS:CE1	2.50	0.47
1:B:293:GLN:HE21	1:B:319:PRO:HG2	1.80	0.47
1:A:69:ARG:HG3	1:A:171:GLY:O	2.15	0.47
1:A:332:ALA:HB1	1:A:333:PRO:HD2	1.97	0.47
1:B:189:ARG:NH2	1:B:227:GLY:O	2.48	0.47
1:A:25:ARG:HG2	1:A:45:ASP:OD1	2.15	0.46
1:A:207:ASP:O	1:A:210:SER:HB2	2.15	0.46
1:B:189:ARG:HH11	1:B:230:TYR:N	2.12	0.46
1:A:29:LEU:HD12	1:A:43:ALA:HB2	1.96	0.46
1:A:39:ILE:HG22	1:A:40:VAL:H	1.80	0.46
1:A:82:HIS:CD2	1:A:84:ASN:H	2.32	0.46
1:A:94:PRO:HD3	1:A:105:TYR:CD1	2.50	0.46
1:B:150:ARG:NH1	1:B:181:MET:SD	2.88	0.46
1:A:118:VAL:O	1:A:121:MET:N	2.47	0.46
1:A:190:TYR:HD1	1:A:223:ILE:HG21	1.80	0.46
1:A:257:ARG:HA	1:A:260:VAL:HG12	1.98	0.46
1:B:132:LEU:O	1:B:135:MET:HB3	2.15	0.46
1:B:133:TYR:HB2	1:B:321:ILE:CG2	2.43	0.46
1:B:133:TYR:CZ	1:B:137:CYS:SG	3.08	0.46
1:B:237:VAL:O	1:B:241:LEU:N	2.47	0.46
1:A:154:PRO:O	1:A:156:ASN:N	2.48	0.46
1:B:190:TYR:HA	1:B:233:GLN:OE1	2.15	0.46
1:A:60:PRO:HG2	1:A:61:PHE:N	2.22	0.46
1:B:123:LEU:CD1	1:B:128:MET:HB2	2.44	0.46
2:G:559:THR:O	2:G:560:LEU:CB	2.58	0.46
1:A:245:CYS:O	1:A:248:PHE:N	2.48	0.46
1:B:72:ARG:NH1	1:B:174:ARG:HB2	2.30	0.46
1:B:95:GLN:HG2	1:B:101:PHE:HA	1.98	0.46
1:A:194:PRO:HD3	1:A:209:TRP:CZ2	2.51	0.46
1:B:192:ARG:O	1:B:197:ILE:HD11	2.16	0.46
1:A:88:LEU:CG	1:A:89:LEU:H	2.03	0.46
1:A:220:CYS:O	1:A:221:HIS:CB	2.61	0.46
1:A:294:ALA:HB2	1:A:320:TYR:CE1	2.51	0.46
1:B:117:GLN:O	1:B:118:VAL:C	2.54	0.46
1:A:14:GLU:H	1:A:14:GLU:HG2	1.46	0.46
1:A:205:ASN:O	1:A:206:VAL:C	2.53	0.46
1:B:193:ALA:O	1:B:195:GLU:N	2.49	0.46
1:B:215:MET:HE1	1:B:297:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLN:NE2	1:B:319:PRO:CG	2.80	0.46
1:B:342:LEU:HD12	1:B:347:HIS:NE2	2.30	0.46
1:A:115:LEU:HB2	1:A:157:ILE:CG2	2.45	0.45
1:A:136:LEU:O	1:A:139:ILE:HB	2.16	0.45
1:A:211:VAL:O	1:A:214:ILE:HB	2.16	0.45
1:A:287:ASN:O	1:A:288:LYS:C	2.55	0.45
1:B:233:GLN:HA	1:B:233:GLN:HE21	1.81	0.45
1:A:252:LEU:HD13	1:A:260:VAL:HG11	1.98	0.45
1:B:111:MET:HE3	1:B:159:VAL:C	2.37	0.45
1:B:131:LEU:O	1:B:134:GLN:N	2.49	0.45
1:A:85:ILE:HD11	1:A:138:GLY:O	2.15	0.45
1:A:125:HIS:O	1:A:126:GLU:C	2.53	0.45
1:A:187:VAL:O	1:A:187:VAL:HG13	2.16	0.45
1:A:190:TYR:CD1	1:A:223:ILE:HG21	2.51	0.45
1:A:198:LEU:O	1:A:199:GLY:C	2.53	0.45
1:A:323:VAL:HG23	1:A:324:TRP:CD2	2.51	0.45
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.84	0.45
1:B:110:LEU:HD11	4:B:1001:877:H232	1.98	0.45
1:B:140:LYS:C	1:B:142:LEU:N	2.70	0.45
1:B:354:GLU:HB3	1:B:355:LEU:H	1.56	0.45
1:B:80:VAL:HG11	1:B:170:PHE:CE1	2.50	0.45
1:B:294:ALA:O	1:B:296:ASP:N	2.49	0.45
1:A:298:LEU:HD22	1:A:302:LEU:CD1	2.47	0.45
1:A:157:ILE:CD1	1:A:167:ILE:HA	2.46	0.45
1:A:184:PRO:O	1:A:187:VAL:HG12	2.16	0.45
1:B:234:TRP:O	1:B:235:ASN:C	2.54	0.45
1:B:295:ARG:HH11	1:B:295:ARG:HG2	1.82	0.45
1:B:338:PRO:O	1:B:339:ASP:CB	2.65	0.45
1:B:360:VAL:HA	1:B:363:LEU:CD1	2.44	0.45
1:A:57:LEU:N	1:A:57:LEU:HD12	2.31	0.45
1:A:63:ASN:C	1:A:65:THR:H	2.20	0.45
1:A:127:ARG:O	1:A:130:TYR:N	2.49	0.45
1:B:11:TYR:OH	1:B:29:LEU:HD11	2.17	0.45
1:B:296:ASP:O	1:B:300:LYS:N	2.46	0.45
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.79	0.45
1:B:90:ASN:O	1:B:107:VAL:N	2.50	0.45
1:B:104:VAL:HG21	1:B:360:VAL:HG21	1.98	0.45
1:B:139:ILE:O	1:B:142:LEU:HB2	2.17	0.45
1:B:214:ILE:O	1:B:217:GLU:N	2.39	0.45
1:B:354:GLU:O	1:B:357:TYR:N	2.50	0.45
1:B:72:ARG:HD2	1:B:173:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:HE1	1:B:240:GLN:CB	2.30	0.44
1:A:134:GLN:NE2	1:A:163:CYS:O	2.50	0.44
1:A:149:HIS:CE1	1:A:151:ASP:HB3	2.52	0.44
1:B:84:ASN:O	1:B:166:LYS:HA	2.17	0.44
1:A:134:GLN:NE2	1:A:164:THR:C	2.71	0.44
1:A:154:PRO:C	1:A:156:ASN:N	2.70	0.44
1:A:257:ARG:O	1:A:260:VAL:HG12	2.17	0.44
1:A:45:ASP:O	1:A:46:ALA:C	2.55	0.44
1:A:118:VAL:HA	1:A:121:MET:HG2	2.00	0.44
1:A:143:HIS:O	1:A:146:GLY:N	2.41	0.44
1:B:25:ARG:NH2	1:B:48:LEU:HD23	2.33	0.44
1:B:233:GLN:HA	1:B:233:GLN:NE2	2.32	0.44
1:A:123:LEU:HD11	1:A:131:LEU:CD1	2.48	0.44
1:B:312:VAL:O	1:B:316:LEU:HD12	2.17	0.44
1:A:212:GLY:C	1:A:214:ILE:N	2.71	0.44
1:A:232:ASP:O	1:A:233:GLN:C	2.56	0.44
1:A:352:TRP:O	1:A:356:ILE:N	2.32	0.44
1:B:318:HIS:CG	1:B:319:PRO:HD2	2.53	0.44
2:G:556:ARG:HA	2:G:557:PRO:HD3	1.56	0.44
1:A:115:LEU:HD22	1:A:118:VAL:HB	1.99	0.44
1:A:295:ARG:O	1:A:296:ASP:C	2.56	0.44
1:B:203:LYS:O	1:B:206:VAL:HG12	2.17	0.44
1:A:27:GLN:O	1:A:28:ASN:HB3	2.17	0.44
1:A:125:HIS:HB3	1:A:289:LEU:HD23	1.98	0.44
1:A:274:LEU:HB3	1:A:275:PHE:CE2	2.52	0.44
1:B:259:TYR:O	1:B:262:ASN:N	2.36	0.44
1:A:140:LYS:HD2	1:A:140:LYS:O	2.18	0.44
1:A:149:HIS:C	1:A:150:ARG:CG	2.86	0.44
1:A:208:LEU:HD13	1:A:208:LEU:HA	1.79	0.44
1:A:286:HIS:O	1:A:287:ASN:C	2.56	0.44
1:B:11:TYR:CE2	1:B:13:VAL:HG23	2.52	0.44
1:A:140:LYS:HA	1:A:312:VAL:HG11	2.00	0.43
1:B:65:THR:C	1:B:67:ALA:N	2.71	0.43
1:B:89:LEU:HB2	1:B:108:MET:HA	2.00	0.43
1:B:123:LEU:HD12	1:B:128:MET:HB2	2.00	0.43
1:B:187:VAL:O	1:B:187:VAL:HG13	2.17	0.43
1:B:360:VAL:O	1:B:363:LEU:HD12	2.18	0.43
1:A:86:ILE:HD13	1:A:168:LEU:CD1	2.48	0.43
1:A:322:ASN:O	1:A:324:TRP:N	2.51	0.43
1:B:324:TRP:CD1	1:B:324:TRP:N	2.84	0.43
1:A:91:VAL:HG12	1:A:106:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:C	1:A:186:VAL:H	2.21	0.43
1:A:298:LEU:HD22	1:A:302:LEU:HD11	2.00	0.43
1:A:29:LEU:CD1	1:A:43:ALA:HB2	2.49	0.43
1:A:92:PHE:CE1	1:A:105:TYR:HB2	2.53	0.43
1:A:283:ASP:OD1	1:A:290:LYS:HA	2.19	0.43
1:B:61:PHE:HA	1:B:67:ALA:CB	2.47	0.43
1:B:92:PHE:CD1	1:B:92:PHE:C	2.91	0.43
1:B:132:LEU:CD2	1:B:215:MET:HB2	2.36	0.43
1:B:167:ILE:HG22	1:B:168:LEU:N	2.33	0.43
1:B:256:VAL:O	1:B:260:VAL:HG23	2.19	0.43
1:A:226:PRO:O	1:A:233:GLN:NE2	2.43	0.43
1:A:293:GLN:HE21	1:A:293:GLN:CA	2.32	0.43
1:A:36:ALA:HB3	1:A:37:GLN:HE22	1.83	0.43
1:B:106:ILE:HG22	1:B:108:MET:HE2	1.99	0.43
1:A:256:VAL:O	1:A:260:VAL:HG12	2.19	0.43
1:A:310:ILE:HD11	1:A:315:ALA:CA	2.48	0.43
1:A:42:ALA:CB	1:A:110:LEU:HD11	2.48	0.43
1:A:244:PRO:HB2	1:A:249:MET:HE2	2.00	0.43
1:A:337:ILE:HG23	1:A:338:PRO:CD	2.42	0.43
1:B:78:LYS:CE	1:B:363:LEU:HB2	2.49	0.43
1:A:77:MET:HA	1:A:77:MET:HE3	2.00	0.43
1:A:143:HIS:C	1:A:145:ALA:N	2.71	0.43
1:B:47:ILE:O	1:B:47:ILE:HG22	2.18	0.43
1:B:78:LYS:HE2	1:B:363:LEU:HB2	2.00	0.43
1:B:104:VAL:CG2	1:B:360:VAL:HG21	2.48	0.43
1:B:111:MET:HE3	1:B:160:LYS:N	2.34	0.43
1:B:332:ALA:HB1	1:B:333:PRO:HD2	2.00	0.43
1:A:190:TYR:HB3	1:A:223:ILE:CG2	2.48	0.43
1:A:244:PRO:CB	1:A:248:PHE:HD2	2.20	0.43
1:B:26:TYR:O	1:B:27:GLN:C	2.55	0.43
1:B:111:MET:HG3	1:B:158:VAL:HG23	2.01	0.43
1:B:115:LEU:CB	1:B:157:ILE:HB	2.48	0.43
1:B:278:VAL:O	1:B:279:LEU:C	2.58	0.43
1:A:163:CYS:SG	2:F:560:LEU:HD12	2.59	0.42
1:B:107:VAL:HG12	1:B:108:MET:N	2.32	0.42
1:B:110:LEU:HA	4:B:1001:877:O15	2.19	0.42
1:B:148:ILE:HG23	1:B:207:ASP:OD2	2.19	0.42
1:B:193:ALA:O	1:B:196:VAL:N	2.48	0.42
1:B:213:CYS:HA	1:B:224:LEU:HD23	2.00	0.42
1:B:233:GLN:HE21	1:B:233:GLN:CA	2.32	0.42
1:A:91:VAL:HG21	1:A:363:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:O	1:A:154:PRO:C	2.57	0.42
1:B:89:LEU:HD12	1:B:108:MET:C	2.39	0.42
1:B:249:MET:CE	1:B:261:GLU:HG2	2.49	0.42
1:A:126:GLU:HG3	1:A:285:GLU:OE2	2.20	0.42
1:A:131:LEU:O	1:A:135:MET:N	2.50	0.42
1:A:255:THR:O	1:A:258:THR:N	2.53	0.42
1:B:28:ASN:C	1:B:28:ASN:ND2	2.71	0.42
1:B:204:GLU:O	1:B:206:VAL:N	2.52	0.42
1:A:42:ALA:HA	1:A:110:LEU:HD11	2.01	0.42
1:A:141:HIS:CE1	1:A:335:PRO:HD3	2.55	0.42
1:A:259:TYR:CD1	1:B:231:ILE:HD12	2.54	0.42
1:A:301:MET:O	1:A:303:VAL:N	2.51	0.42
1:A:342:LEU:O	1:A:342:LEU:HD12	2.19	0.42
1:B:178:THR:O	1:B:179:SER:HB2	2.18	0.42
1:B:271:PHE:CZ	1:B:302:LEU:HB2	2.37	0.42
1:B:128:MET:O	1:B:131:LEU:HB2	2.20	0.42
1:B:244:PRO:CB	1:B:248:PHE:HD2	2.33	0.42
1:B:280:PHE:CE1	1:B:294:ALA:HB3	2.55	0.42
1:A:297:LEU:HD13	1:A:318:HIS:HD2	1.83	0.42
1:A:128:MET:HE3	1:A:132:LEU:HD21	2.01	0.42
1:A:229:ASP:OD1	1:A:232:ASP:N	2.50	0.42
1:B:57:LEU:HA	1:B:57:LEU:HD13	1.67	0.42
1:B:193:ALA:HA	1:B:209:TRP:CE2	2.54	0.42
1:B:297:LEU:HD12	1:B:297:LEU:HA	1.76	0.42
1:A:25:ARG:CG	1:A:47:ILE:HB	2.49	0.42
1:A:214:ILE:O	1:A:217:GLU:N	2.50	0.42
1:A:348:THR:HB	1:A:351:GLU:HG3	2.01	0.42
1:A:61:PHE:N	1:A:61:PHE:CD1	2.86	0.42
1:A:148:ILE:O	1:A:173:ALA:HA	2.20	0.42
1:A:192:ARG:HG2	1:A:196:VAL:CG1	2.50	0.42
1:B:214:ILE:C	1:B:216:GLY:N	2.72	0.42
1:B:326:ASP:HB3	1:B:329:GLU:HB2	2.02	0.42
1:B:343:ASP:OD1	1:B:344:GLU:N	2.52	0.42
1:A:53:ALA:N	1:A:110:LEU:HD12	2.34	0.42
1:A:88:LEU:O	1:A:89:LEU:CB	2.56	0.42
1:A:89:LEU:O	1:A:90:ASN:HB2	2.20	0.42
1:A:98:LEU:HA	1:A:357:TYR:CE2	2.55	0.42
1:A:111:MET:CE	1:A:160:LYS:HB2	2.50	0.42
2:G:559:THR:CG2	2:G:560:LEU:H	2.16	0.42
1:B:275:PHE:N	1:B:276:PRO:HD3	2.35	0.41
1:A:45:ASP:O	1:A:45:ASP:CG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PRO:O	1:A:283:ASP:N	2.53	0.41
1:B:25:ARG:HB2	1:B:47:ILE:HG12	2.02	0.41
1:B:118:VAL:HA	1:B:121:MET:HG2	2.03	0.41
1:B:238:ILE:H	1:B:238:ILE:HG23	1.65	0.41
1:B:361:MET:C	1:B:363:LEU:H	2.22	0.41
1:A:98:LEU:HA	1:A:357:TYR:CZ	2.55	0.41
1:A:114:ASN:N	1:A:114:ASN:ND2	2.65	0.41
1:A:124:ASP:OD2	1:A:127:ARG:HB2	2.19	0.41
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.77	0.41
1:A:257:ARG:HH11	1:A:257:ARG:HD2	1.64	0.41
1:B:153:LYS:O	1:B:154:PRO:C	2.58	0.41
1:B:189:ARG:NH1	1:B:230:TYR:N	2.68	0.41
1:B:269:TYR:HB2	1:B:274:LEU:HD21	2.02	0.41
1:B:330:ALA:O	1:B:331:GLU:HG3	2.20	0.41
1:A:97:SER:HB3	1:A:100:GLU:HB2	2.01	0.41
1:A:115:LEU:O	1:A:117:GLN:N	2.53	0.41
1:A:142:LEU:O	1:A:147:ILE:HB	2.21	0.41
1:B:71:TYR:O	1:B:74:LEU:N	2.53	0.41
1:B:233:GLN:O	1:B:237:VAL:HG23	2.19	0.41
1:A:184:PRO:O	1:A:186:VAL:N	2.53	0.41
1:B:48:LEU:O	1:B:49:GLU:HB2	2.21	0.41
1:B:111:MET:HG3	1:B:158:VAL:CG2	2.51	0.41
1:A:123:LEU:HD12	1:A:128:MET:CB	2.51	0.41
1:A:123:LEU:HD12	1:A:128:MET:HB2	2.02	0.41
1:A:172:LEU:O	1:A:174:ARG:N	2.54	0.41
1:A:211:VAL:CG1	1:A:301:MET:HE1	2.51	0.41
1:B:83:LYS:O	1:B:83:LYS:HG2	2.20	0.41
1:A:11:TYR:HH	1:A:27:GLN:HA	1.83	0.41
1:A:23:LEU:HD12	1:A:26:TYR:HE2	1.85	0.41
1:A:64:GLN:NE2	1:A:346:GLU:OE1	2.54	0.41
1:A:71:TYR:CE1	1:A:355:LEU:HB3	2.55	0.41
1:A:338:PRO:HG3	1:A:340:LYS:NZ	2.35	0.41
1:B:85:ILE:HD12	1:B:167:ILE:HB	2.02	0.41
1:B:186:VAL:HG22	1:B:187:VAL:N	2.36	0.41
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.89	0.41
1:A:288:LYS:CE	1:A:323:VAL:HG12	2.51	0.41
1:B:234:TRP:O	1:B:236:LYS:N	2.54	0.41
1:B:309:ARG:C	1:B:310:ILE:O	2.58	0.41
1:B:334:PRO:HA	1:B:335:PRO:HD3	1.79	0.41
1:A:165:LEU:C	1:A:165:LEU:CD2	2.88	0.41
1:A:198:LEU:HD11	1:A:234:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PRO:HG2	1:A:255:THR:H	1.86	0.41
1:A:262:ASN:O	1:A:263:ARG:O	2.39	0.41
1:A:333:PRO:HA	1:A:334:PRO:HD3	1.86	0.41
1:A:353:LYS:O	1:A:354:GLU:C	2.59	0.41
1:B:9:ASN:HA	1:B:24:LYS:CE	2.50	0.41
1:A:72:ARG:O	1:A:76:LEU:HG	2.21	0.41
1:A:133:TYR:O	1:A:134:GLN:C	2.59	0.41
1:A:329:GLU:O	1:A:329:GLU:HG3	2.21	0.41
1:B:76:LEU:O	1:B:80:VAL:HG12	2.20	0.41
1:B:132:LEU:HD21	1:B:215:MET:CB	2.36	0.41
1:A:215:MET:SD	1:A:297:LEU:HD23	2.61	0.40
1:B:111:MET:O	4:B:1001:877:H4	2.22	0.40
1:B:172:LEU:N	1:B:172:LEU:HD12	2.36	0.40
1:B:193:ALA:HB3	1:B:206:VAL:HG23	2.03	0.40
1:B:214:ILE:C	1:B:216:GLY:H	2.24	0.40
1:B:275:PHE:CB	1:B:280:PHE:HE2	2.28	0.40
1:B:206:VAL:HG13	1:B:207:ASP:N	2.36	0.40
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.83	0.40
1:B:238:ILE:HG13	1:B:266:TYR:CD2	2.56	0.40
1:A:181:MET:C	1:A:183:GLU:H	2.23	0.40
1:A:295:ARG:O	1:A:298:LEU:N	2.55	0.40
1:B:214:ILE:O	1:B:216:GLY:N	2.54	0.40
1:A:65:THR:C	1:A:67:ALA:H	2.24	0.40
1:A:189:ARG:O	1:A:191:TYR:N	2.55	0.40
1:A:245:CYS:HA	1:A:246:PRO:HD3	1.96	0.40
1:A:337:ILE:HD13	1:A:337:ILE:HA	1.95	0.40
1:B:124:ASP:OD2	1:B:127:ARG:HG3	2.22	0.40
1:B:311:SER:H	1:B:314:GLU:HB2	1.87	0.40
1:A:25:ARG:CD	1:A:45:ASP:OD1	2.70	0.40
1:A:330:ALA:C	1:A:332:ALA:H	2.25	0.40
1:B:39:ILE:H	1:B:39:ILE:CD1	2.22	0.40
1:B:123:LEU:HD23	1:B:123:LEU:HA	1.90	0.40
1:B:184:PRO:C	1:B:186:VAL:N	2.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/370 (96%)	219 (62%)	74 (21%)	63 (18%)	0	2
1	B	356/370 (96%)	230 (65%)	80 (22%)	46 (13%)	0	4
2	F	8/11 (73%)	4 (50%)	1 (12%)	3 (38%)	0	0
2	G	8/11 (73%)	3 (38%)	4 (50%)	1 (12%)	0	5
All	All	728/762 (96%)	456 (63%)	159 (22%)	113 (16%)	0	3

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	111	MET
1	A	144	SER
1	A	151	ASP
1	A	165	LEU
1	A	169	ASP
1	A	173	ALA
1	A	226	PRO
1	A	282	ALA
1	A	287	ASN
1	A	288	LYS
1	A	289	LEU
1	A	322	ASN
1	A	327	PRO
1	A	338	PRO
1	A	361	MET
1	A	362	ASP
1	A	364	GLU
2	F	555	LYS
2	F	560	LEU
1	B	176	ALA
1	B	189	ARG

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Mol	Chain	Res	Type
1	B	271	PHE
1	B	278	VAL
1	B	281	PRO
1	B	282	ALA
1	B	322	ASN
1	B	323	VAL
1	B	331	GLU
1	B	339	ASP
1	B	354	GLU
2	G	560	LEU
1	A	14	GLU
1	A	50	ARG
1	A	60	PRO
1	A	61	PHE
1	A	64	GLN
1	A	86	ILE
1	A	88	LEU
1	A	134	GLN
1	A	164	THR
1	A	181	MET
1	A	206	VAL
1	A	283	ASP
1	A	290	LYS
1	A	323	VAL
1	A	330	ALA
1	A	339	ASP
1	B	37	GLN
1	B	66	HIS
1	B	126	GLU
1	B	141	HIS
1	B	155	SER
1	B	170	PHE
1	B	187	VAL
1	B	190	TYR
1	B	205	ASN
1	B	279	LEU
1	B	305	ASP
1	B	306	ALA
1	A	180	PHE
1	A	185	GLU
1	A	188	THR
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	255	THR
1	A	284	SER
1	A	310	ILE
1	A	326	ASP
2	F	561	ASN
1	B	27	GLN
1	B	267	ALA
1	B	310	ILE
1	A	74	LEU
1	A	116	CYS
1	A	155	SER
1	A	246	PRO
1	A	302	LEU
1	B	28	ASN
1	B	71	TYR
1	B	117	GLN
1	B	125	HIS
1	B	194	PRO
1	B	292	SER
1	B	295	ARG
1	B	355	LEU
1	A	47	ILE
1	A	97	SER
1	A	119	ILE
1	A	123	LEU
1	A	167	ILE
1	A	190	TYR
1	A	250	LYS
1	A	299	SER
1	B	72	ARG
1	B	109	GLU
1	B	173	ALA
1	B	260	VAL
1	B	263	ARG
1	A	197	ILE
1	A	254	PRO
1	A	319	PRO
1	B	86	ILE
1	B	179	SER
1	B	186	VAL
1	A	16	GLY
1	A	35	GLY

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Mol	Chain	Res	Type
1	B	254	PRO
1	B	118	VAL
1	B	276	PRO
1	A	59	ARG
1	A	256	VAL
1	A	321	ILE
1	B	59	ARG

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	316/334 (95%)	279 (88%)	37 (12%)	5 26
1	B	316/334 (95%)	284 (90%)	32 (10%)	7 32
2	F	10/11 (91%)	9 (90%)	1 (10%)	7 32
2	G	9/11 (82%)	9 (100%)	0	100 100
All	All	651/690 (94%)	581 (89%)	70 (11%)	6 30

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	11	TYR
1	A	14	GLU
1	A	28	ASN
1	A	48	LEU
1	A	61	PHE
1	A	73	GLU
1	A	74	LEU
1	A	90	ASN
1	A	114	ASN
1	A	123	LEU
1	A	124	ASP
1	A	132	LEU
1	A	136	LEU

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	156	ASN
1	A	163	CYS
1	A	184	PRO
1	A	188	THR
1	A	190	TYR
1	A	192	ARG
1	A	202	TYR
1	A	208	LEU
1	A	229	ASP
1	A	236	LYS
1	A	237	VAL
1	A	244	PRO
1	A	246	PRO
1	A	272	GLU
1	A	277	ASP
1	A	304	ILE
1	A	312	VAL
1	A	313	ASP
1	A	319	PRO
1	A	327	PRO
1	A	342	LEU
1	A	349	ILE
2	F	560	LEU
1	B	10	PHE
1	B	28	ASN
1	B	39	ILE
1	B	57	LEU
1	B	65	THR
1	B	90	ASN
1	B	91	VAL
1	B	114	ASN
1	B	122	GLU
1	B	124	ASP
1	B	156	ASN
1	B	169	ASP
1	B	184	PRO
1	B	188	THR
1	B	191	TYR
1	B	194	PRO
1	B	195	GLU
1	B	202	TYR

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Mol	Chain	Res	Type
1	B	205	ASN
1	B	208	LEU
1	B	229	ASP
1	B	230	TYR
1	B	243	THR
1	B	246	PRO
1	B	271	PHE
1	B	272	GLU
1	B	281	PRO
1	B	295	ARG
1	B	304	ILE
1	B	313	ASP
1	B	324	TRP
1	B	341	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	27	GLN
1	A	28	ASN
1	A	37	GLN
1	A	64	GLN
1	A	66	HIS
1	A	84	ASN
1	A	90	ASN
1	A	102	GLN
1	A	114	ASN
1	A	117	GLN
1	A	134	GLN
1	A	141	HIS
1	A	156	ASN
1	A	233	GLN
1	A	235	ASN
1	A	293	GLN
1	B	27	GLN
1	B	28	ASN
1	B	82	HIS
1	B	114	ASN
1	B	120	GLN
1	B	141	HIS
1	B	156	ASN

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Mol	Chain	Res	Type
1	B	205	ASN
1	B	233	GLN
1	B	235	ASN
1	B	293	GLN

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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	601	-	4,4,4	0.57	0	6,6,6	0.08	0
4	877	B	1001	-	27,28,28	1.84	6 (22%)	33,38,38	1.36	4 (12%)
3	SO4	A	501	-	4,4,4	0.84	0	6,6,6	0.06	0
3	SO4	B	701	-	4,4,4	0.76	0	6,6,6	0.06	0
4	877	A	901	-	27,28,28	2.10	11 (40%)	33,38,38	1.44	6 (18%)
3	SO4	B	801	-	4,4,4	0.53	0	6,6,6	0.12	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
4	877	B	1001	-	-	9/16/17/17	0/2/2/2
4	877	A	901	-	-	7/16/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	877	C17-N16	4.50	1.38	1.32
4	A	901	877	O36-C17	4.08	1.41	1.35
4	A	901	877	C5-C6	3.65	1.46	1.39
4	B	1001	877	C17-N16	3.64	1.37	1.32
4	B	1001	877	O36-C17	3.60	1.40	1.35
4	B	1001	877	C5-C6	3.41	1.46	1.39
4	A	901	877	O27-C2	3.27	1.42	1.37
4	A	901	877	C1-C2	3.19	1.44	1.38
4	B	1001	877	C2-C3	3.15	1.45	1.40
4	B	1001	877	O22-C5	3.11	1.42	1.37
4	A	901	877	C2-C3	2.70	1.44	1.40
4	A	901	877	C1-C6	2.70	1.44	1.38
4	A	901	877	BR-C6	2.30	1.95	1.89
4	A	901	877	C4-C3	2.20	1.43	1.39
4	B	1001	877	O27-C2	2.18	1.40	1.37
4	A	901	877	O22-C5	2.15	1.40	1.37
4	A	901	877	C4-C5	2.10	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	877	C18-C17-N16	-3.39	121.17	124.00
4	B	1001	877	C18-C17-N16	-3.22	121.32	124.00
4	B	1001	877	O22-C5-C6	3.07	121.69	116.83
4	A	901	877	O22-C5-C6	2.90	121.41	116.83
4	A	901	877	C23-O22-C5	-2.59	113.62	117.53
4	A	901	877	O22-C5-C4	-2.45	119.90	124.12
4	A	901	877	BR-C6-C5	2.24	122.42	119.65
4	B	1001	877	O36-C17-C18	2.21	118.95	115.93
4	B	1001	877	O22-C5-C4	-2.14	120.44	124.12
4	A	901	877	O15-C10-N13	2.05	127.37	123.63

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	877	C6-C5-O22-C23
4	A	901	877	N16-C17-O36-C37
4	A	901	877	C18-C17-O36-C37
4	B	1001	877	C6-C5-O22-C23
4	B	1001	877	C18-C17-O36-C37
4	B	1001	877	C19-C18-C34-N1
4	B	1001	877	C38-C37-O36-C17
4	A	901	877	C4-C5-O22-C23
4	A	901	877	C1-C2-O27-C28
4	B	1001	877	C4-C5-O22-C23
4	A	901	877	C3-C2-O27-C28
4	B	1001	877	N16-C17-O36-C37
4	B	1001	877	C1-C2-O27-C28
4	A	901	877	C38-C37-O36-C17
4	B	1001	877	C3-C2-O27-C28
4	B	1001	877	O15-C10-C9-C3

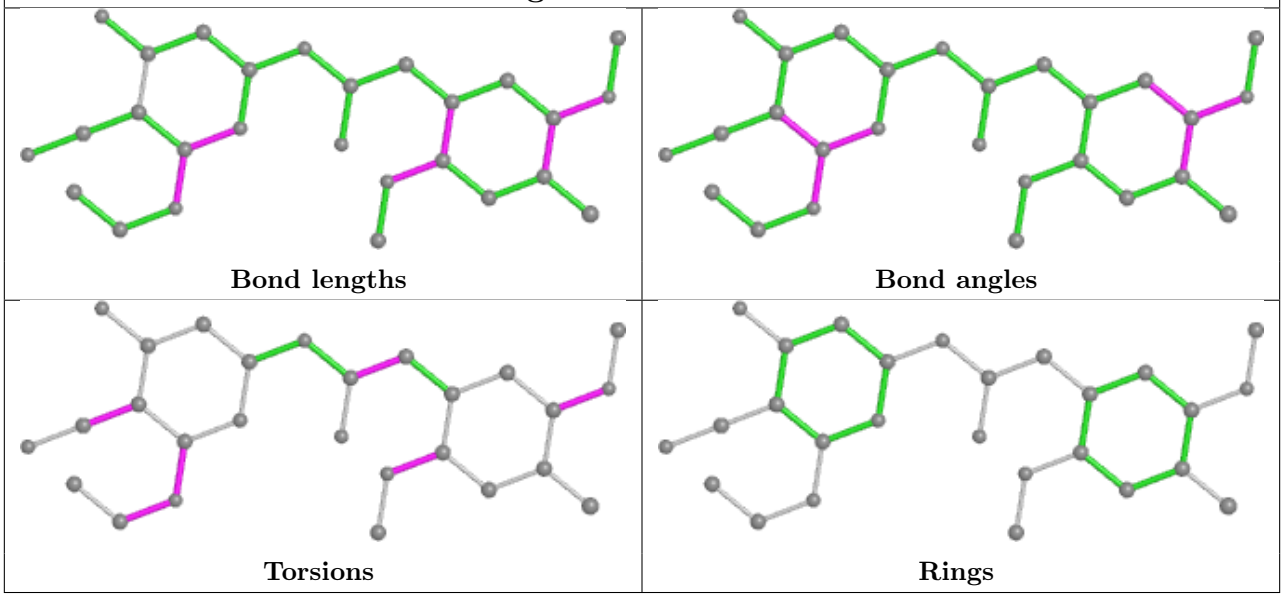
There are no ring outliers.

2 monomers are involved in 7 short contacts:

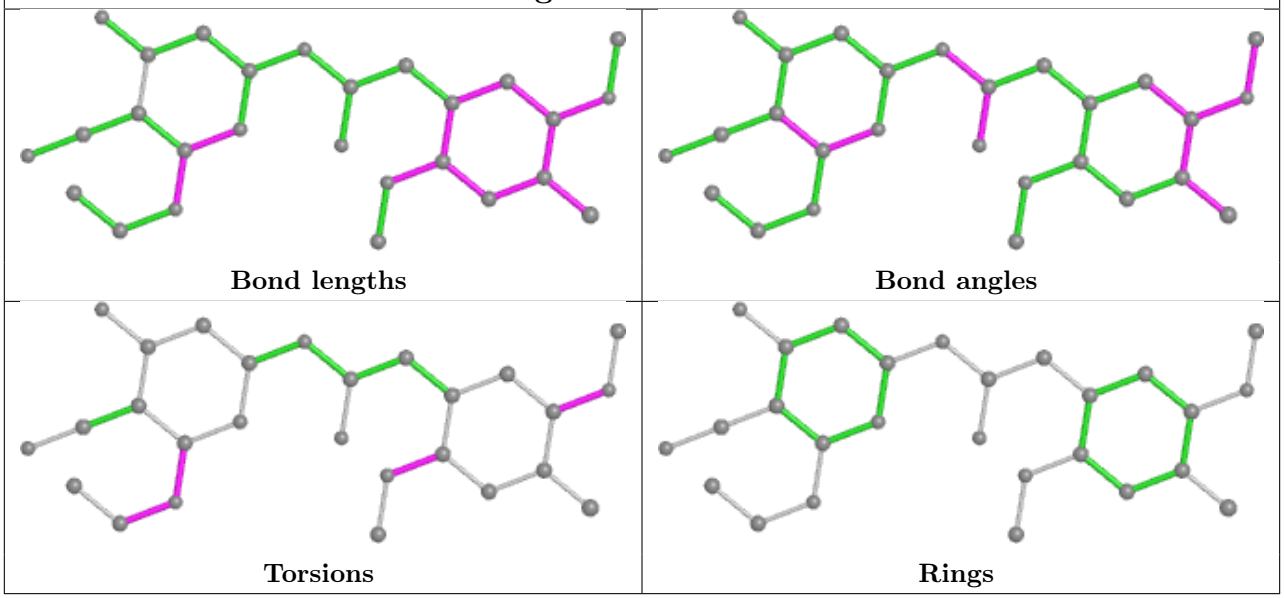
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	877	6	0
4	A	901	877	1	0

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 877 B 1001



Ligand 877 A 901



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.