



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:59 AM UTC

PDB ID : 4M2T / pdb_00004m2t
Title : Corrected Structure of Mouse P-glycoprotein bound to QZ59-SSS
Authors : Li, J.; Jaimes, K.F.; Aller, S.G.
Deposited on : 2013-08-05
Resolution : 4.35 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

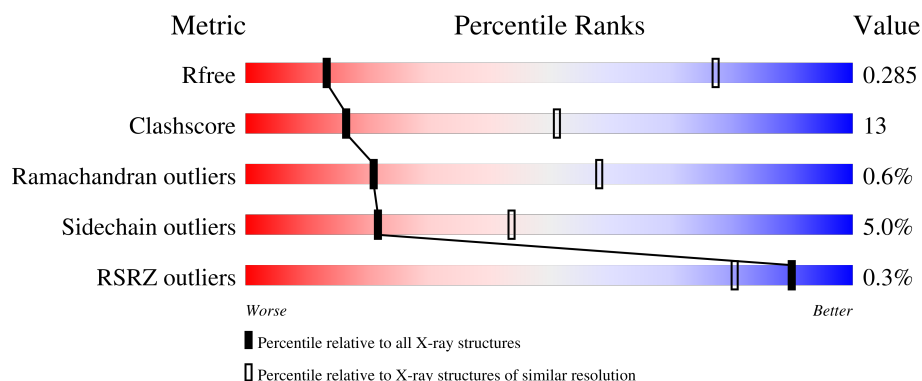
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Ramachandran outliers	187476	1007 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	1282	61% 29% • 7%
1	B	1282	65% 25% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18473 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

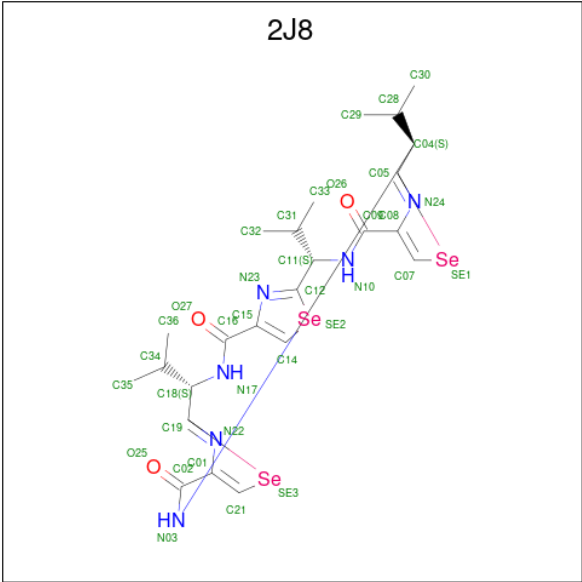
- Molecule 1 is a protein called Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1188	Total	C	N	O	S	0	0	0
			9214	5923	1559	1694	38			
1	B	1180	Total	C	N	O	S	0	0	0
			9153	5887	1550	1678	38			

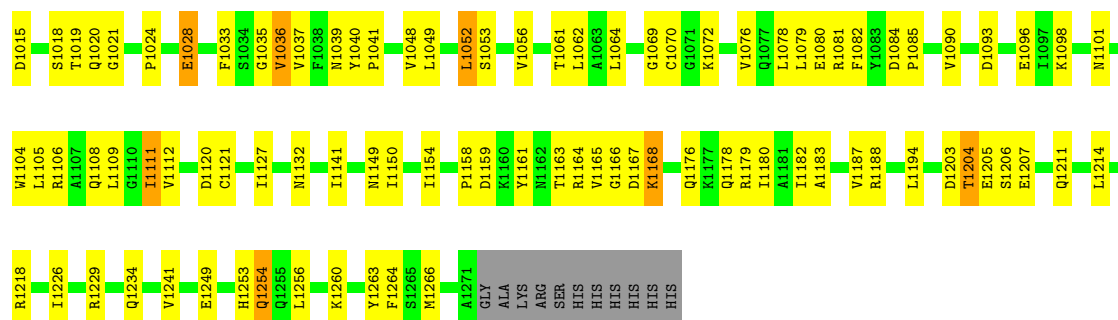
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	conflict	UNP P21447
A	87	GLN	ASN	conflict	UNP P21447
A	90	GLN	ASN	conflict	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	83	GLN	ASN	conflict	UNP P21447
B	87	GLN	ASN	conflict	UNP P21447
B	90	GLN	ASN	conflict	UNP P21447
B	1277	HIS	-	expression tag	UNP P21447
B	1278	HIS	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447

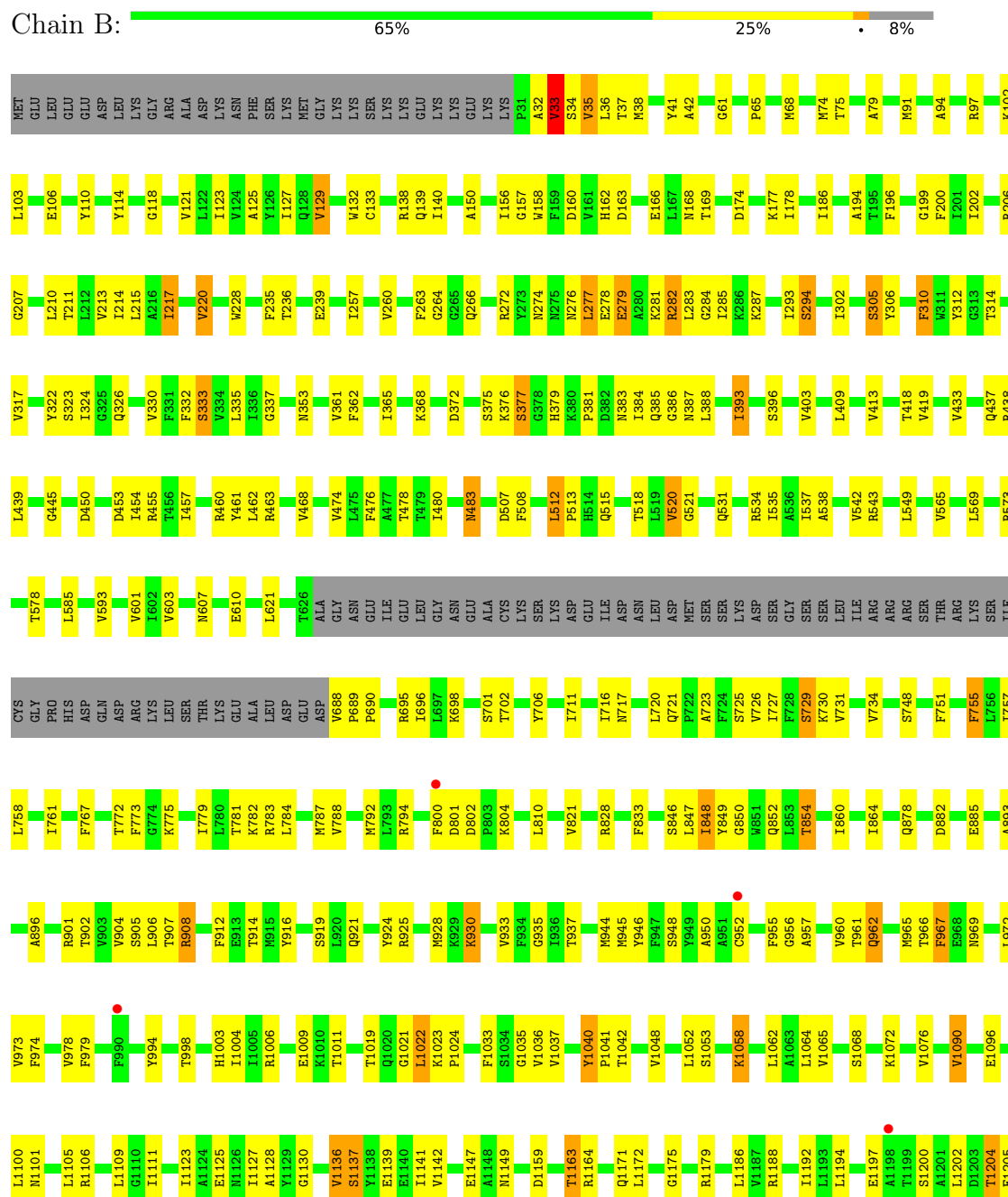
- Molecule 2 is (4S,11S,18S)-4,11,18-tri(propan-2-yl)-6,13,20-triseleno-3,10,17,22,23,24-hexaazatetracyclo[17.2.1.1.5,8.1.12,15]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-tri one (CCD ID: 2J8) (formula: C₂₄H₃₀N₆O₃Se₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	A	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		



• Molecule 1: Multidrug resistance protein 1A



I1226	I1230	I1233	L1238	I1239	V1240	V1241	E1249	L1256	A1271	GLY	ALA	LYS	ARG	SER	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.74Å 114.98Å 375.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 4.35 19.95 – 4.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.95-4.35) 92.1 (19.95-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 4.36Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.221 , 0.283 0.229 , 0.285	Depositor DCC
R_{free} test set	2807 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	196.2	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 94.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18473	wwPDB-VP
Average B, all atoms (Å ²)	201.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2J8

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	0.37	0/9383	0.80	4/12685 (0.0%)
1	B	0.37	0/9322	0.81	9/12602 (0.1%)
All	All	0.37	0/18705	0.81	13/25287 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	LYS	CA-C-N	6.67	126.61	120.21
1	B	368	LYS	C-N-CA	6.67	126.61	120.21
1	B	1040	TYR	CA-C-N	5.92	125.60	119.56
1	B	1040	TYR	C-N-CA	5.92	125.60	119.56
1	A	688	VAL	CA-C-N	-5.90	114.31	120.38
1	A	688	VAL	C-N-CA	-5.90	114.31	120.38
1	B	386	GLY	N-CA-C	-5.38	107.85	115.43
1	B	512	LEU	CA-C-N	5.32	125.38	119.32
1	B	512	LEU	C-N-CA	5.32	125.38	119.32
1	A	30	LYS	CA-C-N	5.13	125.11	120.03
1	A	30	LYS	C-N-CA	5.13	125.11	120.03
1	B	1159	ASP	CB-CA-C	-5.03	110.79	116.63
1	B	515	GLN	CB-CA-C	-5.02	110.81	116.63

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	9214	0	9388	266	0
1	B	9153	0	9338	215	0
2	A	53	0	36	5	0
2	B	53	0	36	6	0
All	All	18473	0	18798	480	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 13.

All (480) 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:1022:LEU:HD11	1:B:1100:LEU:HA	1.56	0.87
1:B:206:ARG:O	1:B:326:GLN:NE2	2.13	0.81
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.63	0.81
1:A:794:ARG:NH1	1:A:1015:ASP:OD2	2.14	0.81
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.64	0.79
1:B:930:LYS:HB2	1:B:930:LYS:HZ2	1.48	0.77
1:B:690:PRO:HD2	1:B:1006:ARG:NH1	2.00	0.75
1:A:966:THR:OG1	1:A:967:PHE:N	2.20	0.74
1:B:228:TRP:HB3	1:B:294:SER:HB2	1.69	0.74
1:A:388:LEU:HB2	1:A:413:VAL:HB	1.70	0.73
1:B:206:ARG:HG3	1:B:326:GLN:HG3	1.69	0.72
1:A:281:LYS:HZ2	1:A:782:LYS:HA	1.54	0.72
1:A:281:LYS:HE2	1:A:785:ARG:NH1	2.06	0.71
1:A:1149:ASN:O	1:A:1179:ARG:NH2	2.24	0.71
1:A:784:LEU:HD22	1:A:821:VAL:HG11	1.73	0.70
1:A:406:LEU:HD13	1:A:409:LEU:HD22	1.73	0.70
1:B:393:ILE:H	1:B:445:GLY:HA3	1.56	0.70
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	1.74	0.70
1:A:794:ARG:HG2	1:A:1012:PRO:HG3	1.74	0.70
1:A:281:LYS:NZ	1:A:782:LYS:HA	2.07	0.68
1:A:559:THR:HG22	1:A:584:ARG:HH12	1.58	0.68
1:A:612:MET:HE1	1:A:622:VAL:HG11	1.74	0.68
1:A:34:SER:OG	1:A:37:THR:OG1	2.11	0.68
1:A:1241:VAL:HB	1:A:1249:GLU:HB2	1.75	0.67
1:B:199:GLY:O	1:B:333:SER:OG	2.11	0.67
1:A:393:ILE:HB	1:A:409:LEU:HB3	1.77	0.67
1:B:846:SER:HB2	1:B:973:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:GLY:HA2	1:A:1072:LYS:HB2	1.77	0.66
1:A:1150:ILE:HG22	1:A:1179:ARG:HB3	1.77	0.65
1:A:1079:LEU:HG	1:A:1109:LEU:HD21	1.79	0.65
1:A:262:ALA:HB1	1:A:1111:ILE:HG21	1.79	0.64
1:A:86:LYS:NZ	1:A:740:PRO:HD3	2.13	0.64
1:B:94:ALA:HB1	1:B:97:ARG:HE	1.63	0.63
1:B:177:LYS:HE2	1:B:353:ASN:HB3	1.81	0.63
1:A:846:SER:O	1:A:854:THR:OG1	2.17	0.62
1:A:930:LYS:HB2	1:A:930:LYS:NZ	2.14	0.62
1:A:318:ILE:HD12	1:A:745:ARG:HE	1.64	0.62
1:B:129:VAL:HG13	1:B:935:GLY:HA2	1.82	0.62
1:A:780:LEU:O	1:A:784:LEU:HB2	2.00	0.61
1:A:424:ASN:H	1:A:429:LYS:NZ	1.97	0.61
1:B:274:ASN:HA	1:B:277:LEU:HB2	1.82	0.61
1:A:730:LYS:HD3	1:A:968:GLU:OE2	2.00	0.61
1:B:689:PRO:HG3	1:B:1003:HIS:CD2	2.35	0.60
1:A:419:VAL:HG22	1:A:593:VAL:HB	1.83	0.60
1:A:916:TYR:O	1:A:919:SER:OG	2.16	0.60
1:B:1136:VAL:HG22	1:B:1137:SER:H	1.67	0.60
1:B:1230:LEU:HD23	1:B:1233:ILE:HD12	1.83	0.60
1:A:698:LYS:O	1:A:701:SER:OG	2.18	0.60
1:A:566:GLN:NE2	1:A:570:ASP:OD1	2.35	0.59
1:B:217:ILE:HG21	1:B:305:SER:HB2	1.84	0.59
1:A:64:LEU:HD12	1:A:336:ILE:HG21	1.84	0.59
1:A:480:ILE:HG23	1:A:535:ILE:HD13	1.84	0.59
1:B:792:MET:HE1	1:B:810:LEU:HB3	1.83	0.59
1:A:70:ILE:HD13	1:A:113:TYR:HB3	1.84	0.59
1:A:695:ARG:NH1	1:A:1009:GLU:OE2	2.36	0.59
1:B:784:LEU:HD22	1:B:821:VAL:HG11	1.84	0.59
1:A:857:LEU:HD12	1:A:973:VAL:HG12	1.85	0.58
2:A:6001:2J8:H36A	2:A:6002:2J8:H30A	1.84	0.58
1:A:122:LEU:HB3	1:A:943:ALA:HB2	1.85	0.58
1:A:471:GLN:HG3	1:A:472:GLU:HG3	1.85	0.58
1:A:852:GLN:CD	1:A:852:GLN:H	2.11	0.58
1:A:1033:PHE:HD1	1:A:1036:VAL:HG11	1.67	0.58
1:A:203:GLY:C	1:A:211:THR:HG21	2.28	0.58
1:A:902:THR:O	1:A:905:SER:OG	2.21	0.58
1:A:1021:GLY:HA3	1:A:1101:ASN:HB2	1.85	0.58
1:B:302:ILE:HD12	2:B:6003:2J8:H35A	1.86	0.57
1:B:1064:LEU:HB2	1:B:1226:ILE:HG13	1.85	0.57
1:A:519:LEU:HD21	1:B:925:ARG:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLY:HA3	1:B:194:ALA:HB3	1.85	0.57
1:B:849:TYR:HB3	1:B:969:ASN:HB3	1.86	0.57
1:A:144:ARG:HB3	1:A:175:VAL:HG11	1.85	0.57
1:A:208:TRP:CE3	1:A:209:LYS:HG2	2.39	0.57
1:B:695:ARG:HA	1:B:698:LYS:NZ	2.19	0.57
1:B:1175:GLY:HA2	1:B:1202:LEU:HD11	1.86	0.57
1:A:382:ASP:OD1	1:A:382:ASP:N	2.36	0.57
1:A:607:ASN:HB3	1:A:610:GLU:OE2	2.04	0.57
1:A:1211:GLN:HA	1:A:1214:LEU:HB2	1.87	0.57
1:B:418:THR:HG23	1:B:578:THR:HB	1.85	0.57
1:A:200:PHE:CE2	1:A:215:LEU:HD12	2.40	0.57
1:A:210:LEU:HD21	1:A:327:VAL:HG13	1.87	0.56
1:A:1234:GLN:HG2	1:A:1253:HIS:CE1	2.40	0.56
1:B:512:LEU:HD13	1:B:518:THR:HG21	1.86	0.56
1:B:534:ARG:HA	1:B:537:ILE:HD12	1.86	0.56
1:B:916:TYR:O	1:B:919:SER:OG	2.19	0.56
1:B:385:GLN:HB2	1:B:450:ASP:OD2	2.04	0.56
1:A:152:MET:HA	1:A:900:PHE:HE2	1.70	0.56
1:A:281:LYS:NZ	1:A:785:ARG:HD2	2.20	0.56
1:A:1064:LEU:HB2	1:A:1226:ILE:HG13	1.88	0.56
1:B:438:ARG:NH1	1:B:455:ARG:HA	2.21	0.56
1:B:902:THR:O	1:B:906:LEU:HD12	2.05	0.56
1:A:1249:GLU:OE2	1:A:1263:TYR:HB2	2.06	0.56
1:A:1106:ARG:O	1:A:1188:ARG:NH1	2.39	0.56
1:A:421:LEU:HB2	1:A:581:ILE:HG12	1.87	0.55
1:A:86:LYS:HD2	1:A:739:GLY:HA2	1.88	0.55
1:A:243:TYR:CD1	1:A:785:ARG:NH1	2.74	0.55
1:B:276:ASN:HA	1:B:279:GLU:HG3	1.87	0.55
1:A:1002:SER:HA	1:A:1005:ILE:HG12	1.89	0.55
1:A:1249:GLU:HB3	1:A:1256:LEU:HD22	1.87	0.55
1:B:696:ILE:HD11	1:B:998:THR:HG23	1.89	0.55
1:A:49:TYR:HA	1:A:131:PHE:HD2	1.71	0.55
1:A:379:HIS:H	1:A:457:ILE:HA	1.71	0.55
1:A:825:THR:OG1	1:A:826:GLY:N	2.39	0.55
1:B:257:ILE:HD12	1:B:260:VAL:HB	1.89	0.55
1:A:371:ILE:O	1:A:373:SER:HB3	2.07	0.54
1:A:699:LEU:HD23	1:A:784:LEU:HD11	1.88	0.54
1:A:208:TRP:HE3	1:A:209:LYS:HG2	1.71	0.54
1:A:1260:LYS:HA	1:A:1264:PHE:HB2	1.90	0.54
1:A:1015:ASP:OD1	1:A:1018:SER:N	2.41	0.54
1:B:1021:GLY:HA2	1:B:1101:ASN:HB2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:HD2	1:A:755:PHE:HE2	1.55	0.54
1:A:453:ASP:HB3	1:A:456:THR:HG23	1.90	0.54
1:B:908:ARG:HE	1:B:908:ARG:HA	1.73	0.54
1:A:534:ARG:NH1	1:A:564:VAL:HG11	2.22	0.54
1:B:846:SER:HA	1:B:973:VAL:HG22	1.90	0.54
1:B:91:MET:SD	1:B:97:ARG:NH2	2.66	0.53
1:A:91:MET:HB3	1:A:94:ALA:HB3	1.88	0.53
1:A:893:ALA:O	1:A:897:ILE:HG12	2.09	0.53
1:B:38:MET:HA	1:B:362:PHE:HE2	1.72	0.53
1:B:585:LEU:HD11	1:B:621:LEU:HB3	1.91	0.53
1:A:286:LYS:O	1:A:290:THR:HG23	2.08	0.53
1:A:979:PHE:HZ	2:A:6002:2J8:C21	2.21	0.53
1:A:66:LEU:HD23	1:A:202:ILE:HD11	1.90	0.53
1:B:317:VAL:HG23	1:B:323:SER:HA	1.91	0.53
1:B:1058:LYS:NZ	1:B:1058:LYS:HB3	2.24	0.53
1:A:406:LEU:HD22	1:A:409:LEU:HD13	1.90	0.53
1:A:512:LEU:HD13	1:A:518:THR:HG21	1.91	0.53
1:A:481:ALA:O	1:A:485:ARG:HG2	2.09	0.52
1:B:102:LYS:HE3	1:B:106:GLU:OE2	2.08	0.52
1:A:621:LEU:HA	1:A:624:THR:HG22	1.91	0.52
1:A:1028:GLU:HB3	1:A:1093:ASP:OD2	2.09	0.52
1:A:46:ASP:OD1	1:A:138:ARG:NH1	2.42	0.52
1:A:833:PHE:HA	1:A:836:ILE:HG22	1.92	0.52
1:A:1096:GLU:OE1	1:A:1098:LYS:N	2.38	0.52
1:B:272:ARG:NH2	1:B:1125:GLU:OE2	2.43	0.52
1:A:79:ALA:HA	1:A:736:THR:HA	1.92	0.52
1:A:1035:GLY:N	1:A:1053:SER:OG	2.42	0.52
1:B:758:LEU:HA	1:B:761:ILE:HD12	1.92	0.52
1:B:979:PHE:CE1	2:B:6004:2J8:H29B	2.44	0.52
1:B:385:GLN:OE1	1:B:387:ASN:ND2	2.43	0.52
1:B:388:LEU:HB2	1:B:413:VAL:HB	1.92	0.52
1:B:507:ASP:OD1	1:B:508:PHE:N	2.41	0.52
1:B:957:ALA:O	1:B:961:THR:HG23	2.10	0.52
1:B:1090:VAL:N	1:B:1096:GLU:OE2	2.35	0.52
1:B:1109:LEU:HD12	1:B:1192:ILE:HB	1.91	0.51
1:A:496:ILE:O	1:A:500:VAL:HG23	2.11	0.51
1:A:1036:VAL:HG23	1:A:1085:PRO:HB3	1.92	0.51
1:B:65:PRO:HB2	1:B:202:ILE:HD12	1.92	0.51
1:A:86:LYS:HZ2	1:A:740:PRO:HD3	1.75	0.51
1:A:299:PHE:HZ	2:A:6001:2J8:C07	2.24	0.51
1:B:437:GLN:HG3	1:B:439:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:THR:H	1:B:967:PHE:HA	1.74	0.51
1:A:604:GLU:OE2	1:A:616:GLY:HA3	2.11	0.51
1:A:1061:THR:HG21	1:A:1218:ARG:HD3	1.91	0.51
1:B:538:ALA:O	1:B:542:VAL:HG23	2.11	0.51
1:A:485:ARG:NH2	1:B:914:THR:OG1	2.41	0.51
1:A:372:ASP:HA	1:A:373:SER:HB3	1.91	0.51
1:B:847:LEU:HG	1:B:854:THR:HG21	1.93	0.51
1:B:956:GLY:O	1:B:960:VAL:HG23	2.11	0.51
1:A:175:VAL:HA	1:A:178:ILE:HG22	1.92	0.51
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.93	0.51
1:B:711:ILE:HG12	1:B:833:PHE:CE2	2.45	0.50
1:A:299:PHE:CE2	2:A:6001:2J8:H33B	2.47	0.50
1:B:160:ASP:OD1	1:B:901:ARG:NH2	2.43	0.50
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.42	0.50
1:B:979:PHE:HZ	2:B:6004:2J8:C01	2.24	0.50
1:A:1049:LEU:HD22	1:A:1052:LEU:HD22	1.93	0.50
1:B:965:MET:HB3	1:B:966:THR:OG1	2.10	0.50
1:B:74:MET:HA	1:B:110:TYR:CE2	2.46	0.50
1:A:1078:LEU:HD22	1:A:1085:PRO:HD3	1.92	0.50
1:B:94:ALA:HB1	1:B:97:ARG:NE	2.27	0.50
1:A:39:PHE:CD1	1:A:50:MET:HE1	2.46	0.50
1:B:460:ARG:HG3	1:B:907:THR:HG21	1.94	0.50
1:B:901:ARG:O	1:B:905:SER:OG	2.19	0.50
1:A:314:THR:OG1	1:A:748:SER:OG	2.25	0.49
1:A:699:LEU:O	1:A:783:ARG:NH2	2.35	0.49
1:A:281:LYS:HZ3	1:A:785:ARG:CD	2.25	0.49
1:B:132:TRP:CZ3	1:B:186:ILE:HD11	2.48	0.49
1:B:285:ILE:HD12	1:B:775:LYS:HG2	1.94	0.49
1:B:960:VAL:HG21	1:B:967:PHE:HB2	1.93	0.49
1:A:257:ILE:HG12	1:A:800:PHE:CE2	2.47	0.49
1:B:322:TYR:O	1:B:326:GLN:HB3	2.13	0.49
1:A:424:ASN:HB2	1:A:621:LEU:HD21	1.95	0.49
1:A:538:ALA:O	1:A:542:VAL:HG23	2.12	0.49
1:B:282:ARG:HH22	1:B:779:ILE:HA	1.77	0.49
1:B:896:ALA:HB2	1:B:912:PHE:CD2	2.48	0.49
1:B:1149:ASN:O	1:B:1179:ARG:NH2	2.46	0.49
1:B:1147:GLU:CD	1:B:1186:LEU:HD21	2.38	0.49
1:A:68:MET:HE3	1:A:332:PHE:HB3	1.94	0.49
1:A:1101:ASN:HB3	1:A:1104:TRP:HB3	1.95	0.49
1:B:695:ARG:NH2	1:B:1009:GLU:OE2	2.46	0.49
1:A:937:THR:O	1:A:941:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:VAL:HG13	1:A:1194:LEU:HB3	1.93	0.48
1:B:381:PRO:O	1:B:461:TYR:OH	2.24	0.48
1:B:772:THR:OG1	1:B:773:PHE:N	2.46	0.48
1:A:281:LYS:NZ	1:A:781:THR:HG22	2.28	0.48
1:B:1123:ILE:HG12	1:B:1163:THR:HG23	1.95	0.48
1:A:692:SER:OG	1:A:695:ARG:HB3	2.13	0.48
1:A:741:PRO:HA	1:A:744:GLN:HG3	1.95	0.48
1:A:129:VAL:HG13	1:A:935:GLY:HA2	1.95	0.48
1:A:158:TRP:HZ2	1:A:364:ILE:HD12	1.77	0.48
1:B:123:ILE:O	1:B:127:ILE:HG12	2.13	0.48
1:B:960:VAL:HG21	1:B:967:PHE:CB	2.43	0.48
1:A:396:SER:HB3	1:A:404:GLN:HA	1.95	0.48
1:B:1106:ARG:O	1:B:1188:ARG:NH1	2.47	0.48
1:B:42:ALA:HB2	1:B:139:GLN:NE2	2.28	0.48
1:B:848:ILE:HG22	1:B:849:TYR:CD2	2.48	0.48
1:A:1024:PRO:HD2	1:A:1104:TRP:CH2	2.49	0.48
1:B:1065:VAL:HG23	1:B:1241:VAL:HA	1.94	0.48
1:A:42:ALA:HB2	1:A:139:GLN:OE1	2.12	0.48
1:A:900:PHE:HA	1:A:903:VAL:HG12	1.96	0.48
1:B:1233:ILE:HG22	1:B:1239:ILE:HG12	1.94	0.48
1:A:75:THR:HG22	1:A:967:PHE:HZ	1.79	0.48
1:B:379:HIS:HB2	1:B:457:ILE:HG22	1.95	0.48
1:A:323:SER:HB3	1:A:326:GLN:HG3	1.96	0.48
1:B:930:LYS:HZ2	1:B:930:LYS:CB	2.22	0.48
1:B:730:LYS:HB3	1:B:751:PHE:CE2	2.48	0.47
1:A:100:PHE:CD1	1:A:961:THR:HB	2.49	0.47
1:A:797:VAL:HG21	1:A:1082:PHE:CG	2.49	0.47
1:B:68:MET:HE3	1:B:332:PHE:HB3	1.96	0.47
1:B:376:LYS:HA	1:B:377:SER:HA	1.65	0.47
1:A:213:VAL:O	1:A:217:ILE:HG12	2.14	0.47
1:A:704:TRP:CG	1:A:705:PRO:HD3	2.49	0.47
1:A:1056:VAL:HG21	1:A:1062:LEU:HB2	1.96	0.47
1:B:784:LEU:HD21	1:B:1004:ILE:HG21	1.96	0.47
1:B:908:ARG:HA	1:B:908:ARG:NE	2.28	0.47
1:B:952:CYS:SG	1:B:974:PHE:HD1	2.38	0.47
1:A:273:TYR:CE2	1:A:277:LEU:HD11	2.49	0.47
1:A:691:ALA:HB1	1:A:692:SER:HB2	1.97	0.47
2:A:6002:2J8:SE1	2:A:6002:2J8:H30B	2.64	0.47
1:B:1033:PHE:HD1	1:B:1036:VAL:HG21	1.79	0.47
1:A:1203:ASP:O	1:A:1206:SER:OG	2.32	0.47
1:B:306:TYR:HE1	2:B:6003:2J8:H35B	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASP:O	1:B:925:ARG:NH1	2.40	0.47
1:B:125:ALA:O	1:B:129:VAL:HG12	2.14	0.47
1:A:114:TYR:CE1	1:A:949:TYR:HB3	2.49	0.47
1:A:239:GLU:HB2	1:A:287:LYS:NZ	2.28	0.47
1:A:268:LYS:HZ1	1:A:1132:ASN:HA	1.79	0.47
1:A:425:SER:OG	1:A:426:GLY:N	2.48	0.47
1:B:200:PHE:CE2	1:B:215:LEU:HD12	2.49	0.47
1:A:965:MET:HA	1:A:966:THR:HA	1.70	0.47
1:A:424:ASN:H	1:A:429:LYS:HZ3	1.63	0.47
1:A:155:GLU:OE1	1:A:370:SER:OG	2.32	0.47
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.97	0.47
1:B:1127:ILE:HG21	1:B:1141:ILE:HG23	1.97	0.47
1:B:1197:GLU:HB3	1:B:1200:SER:HB3	1.97	0.47
1:B:607:ASN:HB3	1:B:610:GLU:OE1	2.15	0.46
1:A:136:ALA:HB2	1:A:182:ILE:O	2.16	0.46
1:B:933:VAL:O	1:B:937:THR:HG22	2.15	0.46
1:A:170:ARG:HG3	1:A:174:ASP:HB2	1.96	0.46
1:B:453:ASP:OD2	1:B:455:ARG:NH2	2.48	0.46
1:A:43:GLY:H	1:A:46:ASP:HB2	1.80	0.46
1:A:714:ALA:HB1	1:A:834:GLN:HG3	1.97	0.46
1:A:723:ALA:O	1:A:727:ILE:HG12	2.16	0.46
1:A:860:ILE:O	1:A:864:ILE:HG13	2.14	0.46
1:A:1158:PRO:HA	1:A:1159:ASP:HA	1.42	0.46
1:A:850:GLY:O	1:A:854:THR:OG1	2.34	0.46
1:B:726:VAL:HA	1:B:972:LEU:HD23	1.97	0.46
1:A:510:MET:HA	1:A:515:GLN:HE22	1.80	0.46
1:B:196:PHE:HD1	1:B:337:GLY:O	1.99	0.46
1:B:278:GLU:HB2	1:B:782:LYS:NZ	2.31	0.46
1:A:61:GLY:HA3	1:A:194:ALA:HB3	1.97	0.46
1:B:850:GLY:O	1:B:854:THR:OG1	2.23	0.46
1:A:156:ILE:HD12	1:A:157:GLY:N	2.31	0.46
1:A:506:TYR:CZ	1:A:510:MET:HE3	2.50	0.46
1:A:802:ASP:OD1	1:A:804:LYS:HG2	2.16	0.46
1:B:257:ILE:HG12	1:B:800:PHE:CE2	2.51	0.46
1:A:422:VAL:C	1:A:429:LYS:NZ	2.74	0.46
1:A:1154:ILE:HD13	1:A:1161:TYR:CE2	2.50	0.46
1:B:314:THR:HA	1:B:317:VAL:HG12	1.98	0.46
1:B:361:VAL:O	1:B:365:ILE:HG13	2.16	0.46
1:A:71:PHE:HE1	1:A:328:LEU:HD13	1.81	0.45
1:B:33:VAL:HB	1:B:34:SER:H	1.46	0.45
1:B:264:GLY:C	1:B:266:GLN:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:HD2	1:B:781:THR:HB	1.98	0.45
1:B:788:VAL:O	1:B:792:MET:HG3	2.16	0.45
1:B:893:ALA:HB2	1:B:916:TYR:CE1	2.51	0.45
1:B:1164:ARG:O	1:B:1171:GLN:NE2	2.49	0.45
1:A:210:LEU:HB2	1:A:322:TYR:HE1	1.80	0.45
1:B:1100:LEU:HD13	1:B:1105:LEU:HD13	1.98	0.45
1:A:147:PHE:O	1:A:151:ILE:HG13	2.16	0.45
1:B:281:LYS:O	1:B:285:ILE:HG12	2.17	0.45
1:B:1023:LYS:HA	1:B:1024:PRO:HD3	1.74	0.45
1:A:838:ASN:ND2	1:A:983:ALA:HB3	2.30	0.45
1:A:981:ALA:O	1:A:984:VAL:HG22	2.16	0.45
1:A:1178:GLN:O	1:A:1182:ILE:HG12	2.16	0.45
1:A:156:ILE:HD11	1:A:439:LEU:C	2.41	0.45
1:A:281:LYS:HZ3	1:A:785:ARG:HD2	1.81	0.45
1:A:707:PHE:O	1:A:711:ILE:HG12	2.16	0.45
1:A:1081:ARG:HG2	1:A:1081:ARG:HH11	1.81	0.45
1:B:34:SER:OG	1:B:37:THR:OG1	2.32	0.45
1:A:156:ILE:HG12	1:A:439:LEU:HB3	1.98	0.45
1:A:906:LEU:O	1:A:907:THR:OG1	2.35	0.45
1:B:236:THR:O	1:B:239:GLU:HB3	2.17	0.45
1:A:471:GLN:HB3	1:A:552:GLU:HB2	1.98	0.45
1:A:513:PRO:HB2	1:A:514:HIS:CD2	2.51	0.45
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.17	0.45
1:B:726:VAL:HG22	1:B:972:LEU:HD21	1.97	0.45
1:B:921:GLN:HB3	1:B:925:ARG:NH2	2.32	0.45
1:A:163:ASP:HB3	1:A:166:GLU:HG2	1.99	0.45
1:A:281:LYS:HZ2	1:A:782:LYS:CA	2.26	0.45
1:B:852:GLN:HG2	1:B:955:PHE:HZ	1.82	0.45
1:A:30:LYS:HA	1:A:31:PRO:HD3	1.72	0.45
1:A:76:ASP:OD1	1:A:323:SER:OG	2.25	0.45
1:B:114:TYR:HB3	1:B:950:ALA:HB2	1.97	0.45
1:B:1022:LEU:HD11	1:B:1100:LEU:HD23	1.98	0.45
1:A:731:VAL:O	1:A:734:VAL:HG12	2.16	0.45
1:A:1040:TYR:HA	1:A:1041:PRO:HD3	1.72	0.45
1:B:235:PHE:HB3	1:B:287:LYS:HB2	1.99	0.45
1:B:848:ILE:HD12	1:B:848:ILE:HA	1.83	0.45
1:A:980:GLY:O	1:A:984:VAL:HG13	2.17	0.44
1:A:1260:LYS:HA	1:A:1264:PHE:CB	2.46	0.44
1:B:121:VAL:HG21	1:B:946:TYR:CE1	2.52	0.44
1:B:284:GLY:O	1:B:287:LYS:HB3	2.16	0.44
1:B:711:ILE:HG12	1:B:833:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:ASP:OD2	1:B:804:LYS:HG2	2.17	0.44
1:A:39:PHE:HD1	1:A:50:MET:HE1	1.81	0.44
1:A:256:ALA:O	1:A:260:VAL:HG23	2.17	0.44
1:A:372:ASP:CA	1:A:373:SER:HB3	2.47	0.44
1:A:773:PHE:CE2	1:A:830:ALA:HB2	2.52	0.44
1:B:210:LEU:O	1:B:214:ILE:HG13	2.17	0.44
1:B:794:ARG:HH12	1:B:1011:THR:HA	1.83	0.44
1:B:156:ILE:HD11	1:B:439:LEU:C	2.43	0.44
1:B:1035:GLY:N	1:B:1053:SER:OG	2.27	0.44
1:A:784:LEU:CD2	1:A:821:VAL:HG11	2.46	0.44
1:A:81:VAL:HG21	1:A:103:LEU:HD11	1.99	0.44
1:A:149:HIS:HA	1:A:913:GLU:OE2	2.18	0.44
1:A:784:LEU:HD21	1:A:1004:ILE:HG21	1.99	0.44
1:A:1165:VAL:HA	1:A:1166:GLY:HA2	1.62	0.44
1:A:828:ARG:HG2	1:A:994:TYR:CE2	2.53	0.44
1:B:207:GLY:HA3	1:B:330:VAL:HG21	2.00	0.44
1:B:792:MET:CE	1:B:810:LEU:HB3	2.48	0.44
1:B:930:LYS:HB2	1:B:930:LYS:NZ	2.26	0.44
1:B:1062:LEU:HD12	1:B:1238:LEU:O	2.16	0.44
1:B:1139:GLU:HA	1:B:1142:VAL:HG12	2.00	0.44
1:B:928:MET:HE2	1:B:928:MET:HB2	1.84	0.44
1:A:870:VAL:HA	1:A:873:LYS:HB3	1.98	0.44
1:A:1080:GLU:HG3	1:A:1106:ARG:HD3	1.99	0.44
1:B:520:VAL:HG22	1:B:521:GLY:H	1.82	0.44
1:B:543:ARG:NH1	1:B:906:LEU:HD23	2.33	0.44
1:B:79:ALA:HB2	1:B:324:ILE:HG21	2.00	0.44
1:A:1266:MET:HE2	1:A:1266:MET:HB3	1.82	0.43
1:A:228:TRP:HB3	1:A:294:SER:HB2	1.98	0.43
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.99	0.43
1:B:512:LEU:HA	1:B:513:PRO:HD3	1.87	0.43
1:A:696:ILE:H	1:A:696:ILE:HG13	1.60	0.43
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	2.00	0.43
1:B:978:VAL:HG12	1:B:979:PHE:CD1	2.53	0.43
1:B:476:PHE:H	1:B:483:ASN:HD21	1.67	0.43
1:A:533:GLN:O	1:A:537:ILE:HG13	2.17	0.43
1:A:696:ILE:HA	1:A:699:LEU:HD13	1.99	0.43
1:A:857:LEU:C	1:A:859:ALA:H	2.25	0.43
1:A:1121:CYS:O	1:A:1164:ARG:NH1	2.52	0.43
1:A:1254:GLN:H	1:A:1254:GLN:NE2	2.17	0.43
1:A:1207:GLU:HB2	1:A:1229:ARG:HH22	1.84	0.43
1:B:168:ASN:OD1	1:B:169:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:CD2	1:A:913:GLU:OE2	2.72	0.43
1:A:1149:ASN:C	1:A:1179:ARG:HH21	2.22	0.43
1:A:565:VAL:O	1:A:569:LEU:HG	2.19	0.43
1:B:293:ILE:HD12	1:B:767:PHE:HD1	1.84	0.43
1:B:882:ASP:HA	1:B:885:GLU:HG2	2.01	0.43
1:A:285:ILE:HD12	1:A:775:LYS:HG2	2.00	0.43
1:A:488:ARG:NH2	1:A:491:VAL:HG12	2.34	0.43
1:A:930:LYS:HB2	1:A:930:LYS:HZ2	1.83	0.42
1:B:480:ILE:HD12	1:B:535:ILE:HD13	2.00	0.42
1:B:731:VAL:O	1:B:734:VAL:HG22	2.19	0.42
1:A:287:LYS:HB3	1:A:287:LYS:HE2	1.69	0.42
1:B:35:VAL:HG13	1:B:36:LEU:H	1.84	0.42
1:B:372:ASP:HB3	1:B:375:SER:HB3	2.00	0.42
1:A:337:GLY:O	1:A:340:SER:OG	2.36	0.42
1:A:706:TYR:HE1	1:A:775:LYS:HD2	1.85	0.42
1:A:1112:VAL:HG21	1:A:1182:ILE:HD13	2.01	0.42
1:A:1159:ASP:N	1:A:1159:ASP:OD1	2.52	0.42
1:B:463:ARG:NH1	1:B:904:VAL:HG22	2.34	0.42
1:B:690:PRO:HD2	1:B:1006:ARG:HH11	1.82	0.42
1:B:757:ILE:O	1:B:761:ILE:HG13	2.20	0.42
1:A:150:ALA:O	1:A:154:GLN:HG2	2.18	0.42
1:A:926:ASN:O	1:A:930:LYS:NZ	2.52	0.42
1:A:1176:GLN:O	1:A:1180:ILE:HG13	2.19	0.42
1:B:846:SER:O	1:B:854:THR:OG1	2.37	0.42
1:A:132:TRP:CZ3	1:A:186:ILE:HD11	2.55	0.42
1:A:699:LEU:HD21	1:A:1005:ILE:HG22	2.01	0.42
1:A:838:ASN:HD21	1:A:983:ALA:HB3	1.85	0.42
1:B:210:LEU:HB2	1:B:322:TYR:HE2	1.83	0.42
1:B:543:ARG:HH11	1:B:906:LEU:HD23	1.84	0.42
1:B:1249:GLU:HG2	1:B:1256:LEU:HG	2.02	0.42
1:A:453:ASP:OD1	1:A:454:ILE:N	2.52	0.42
1:A:719:GLY:C	1:A:722:PRO:HD2	2.45	0.42
1:A:848:ILE:HG13	1:A:849:TYR:CD1	2.55	0.42
1:B:213:VAL:HG21	1:B:312:TYR:CE2	2.54	0.42
1:A:314:THR:O	1:A:318:ILE:HG13	2.19	0.42
1:A:520:VAL:HB	1:A:521:GLY:H	1.65	0.42
1:A:792:MET:HE3	1:A:810:LEU:HD22	2.01	0.42
1:B:140:ILE:HD13	1:B:140:ILE:HA	1.92	0.42
1:B:1202:LEU:HD12	1:B:1202:LEU:HA	1.84	0.42
1:A:429:LYS:HB3	1:A:581:ILE:HD13	2.02	0.42
1:A:908:ARG:HA	1:A:908:ARG:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:ASP:HA	1:A:1085:PRO:HD2	1.88	0.42
1:B:960:VAL:HG22	1:B:966:THR:N	2.34	0.42
1:B:965:MET:HA	1:B:966:THR:HA	1.94	0.42
1:B:1040:TYR:HA	1:B:1041:PRO:HD3	1.81	0.42
1:A:704:TRP:O	1:A:708:VAL:HG23	2.20	0.42
1:A:1104:TRP:NE1	1:A:1108:GLN:HE22	2.18	0.42
1:A:1166:GLY:C	1:A:1168:LYS:H	2.27	0.42
1:B:758:LEU:HD12	1:B:761:ILE:HD12	2.01	0.42
1:A:61:GLY:O	1:A:195:THR:OG1	2.32	0.42
1:A:510:MET:SD	1:A:515:GLN:NE2	2.93	0.42
1:A:519:LEU:HD22	1:A:519:LEU:H	1.84	0.42
1:B:418:THR:HG21	1:B:573:ARG:HD2	2.02	0.42
1:B:706:TYR:O	1:B:772:THR:HB	2.20	0.42
2:B:6004:2J8:H30B	2:B:6004:2J8:SE1	2.70	0.42
1:A:38:MET:HE2	1:A:178:ILE:HG13	2.01	0.41
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.43	0.41
1:B:156:ILE:HD12	1:B:157:GLY:N	2.35	0.41
1:B:878:GLN:HE22	1:B:930:LYS:HA	1.84	0.41
1:B:1076:VAL:HG13	1:B:1194:LEU:CD1	2.47	0.41
1:A:388:LEU:HD13	1:A:577:THR:HG21	2.01	0.41
1:A:707:PHE:HD2	1:A:829:LEU:HD12	1.84	0.41
1:A:720:LEU:O	1:A:723:ALA:HB3	2.20	0.41
1:A:1105:LEU:O	1:A:1109:LEU:HD13	2.20	0.41
1:B:310:PHE:HD2	1:B:755:PHE:HZ	1.68	0.41
1:B:565:VAL:O	1:B:569:LEU:HG	2.20	0.41
1:B:721:GLN:HB2	2:B:6003:2J8:H32A	2.02	0.41
1:A:784:LEU:CD2	1:A:1004:ILE:HG21	2.50	0.41
1:A:944:MET:H	1:A:944:MET:HG3	1.50	0.41
1:B:531:GLN:O	1:B:535:ILE:HG13	2.20	0.41
1:B:716:ILE:HG13	1:B:717:ASN:N	2.35	0.41
1:A:289:ILE:O	1:A:293:ILE:HG12	2.20	0.41
1:A:384:ILE:HD11	1:A:546:LYS:HB2	2.02	0.41
1:A:944:MET:HE3	1:A:944:MET:HB2	1.62	0.41
1:A:1154:ILE:HD13	1:A:1161:TYR:CZ	2.56	0.41
1:B:41:TYR:OH	1:B:365:ILE:HG21	2.19	0.41
1:B:381:PRO:O	1:B:384:ILE:HD11	2.20	0.41
1:A:97:ARG:O	1:A:101:ALA:HB3	2.20	0.41
1:B:138:ARG:HA	1:B:924:TYR:HE1	1.86	0.41
1:B:158:TRP:CE2	1:B:162:HIS:CE1	3.08	0.41
1:B:174:ASP:O	1:B:178:ILE:HG13	2.21	0.41
1:B:217:ILE:O	1:B:220:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:CD1	1:B:1130:GLY:HA2	2.56	0.41
1:B:828:ARG:HG3	1:B:994:TYR:CD2	2.56	0.41
1:A:286:LYS:HA	1:A:289:ILE:HD12	2.03	0.41
1:A:1019:THR:O	1:A:1019:THR:OG1	2.37	0.41
1:A:1127:ILE:HG21	1:A:1141:ILE:HG23	2.02	0.41
1:B:103:LEU:HB2	1:B:961:THR:HG22	2.02	0.41
1:B:396:SER:OG	1:B:403:VAL:O	2.38	0.41
1:A:46:ASP:O	1:A:50:MET:HG3	2.21	0.41
1:A:331:PHE:O	1:A:335:LEU:HB2	2.21	0.41
1:B:163:ASP:O	1:B:166:GLU:HG2	2.21	0.41
1:B:453:ASP:OD1	1:B:454:ILE:N	2.54	0.41
1:B:1068:SER:O	1:B:1072:LYS:HD2	2.20	0.41
1:A:711:ILE:O	1:A:715:ILE:HG13	2.21	0.41
1:B:281:LYS:HG3	1:B:782:LYS:HB2	2.02	0.41
1:B:1175:GLY:CA	1:B:1202:LEU:HD11	2.51	0.41
1:A:510:MET:HA	1:A:515:GLN:NE2	2.36	0.41
1:A:792:MET:HE1	1:A:810:LEU:HB3	2.02	0.41
1:B:91:MET:HB3	1:B:94:ALA:HB3	2.03	0.41
1:B:689:PRO:HA	1:B:690:PRO:HD2	1.93	0.41
1:B:723:ALA:O	1:B:727:ILE:HG12	2.21	0.41
1:B:729:SER:OG	1:B:972:LEU:HD23	2.20	0.41
1:B:801:ASP:O	1:B:1042:THR:HG21	2.21	0.41
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.87	0.41
1:B:1128:ALA:HB1	1:B:1136:VAL:HG11	2.03	0.41
1:A:428:GLY:O	1:A:431:THR:HB	2.21	0.40
1:A:713:CYS:HB2	1:A:768:LEU:HD23	2.02	0.40
1:A:979:PHE:N	1:A:979:PHE:CD1	2.90	0.40
1:B:150:ALA:CB	1:B:365:ILE:HA	2.52	0.40
1:B:698:LYS:O	1:B:701:SER:OG	2.32	0.40
1:A:224:SER:O	1:A:228:TRP:HD1	2.04	0.40
1:A:390:PHE:O	1:A:410:ASN:HA	2.21	0.40
1:A:478:THR:HB	1:A:479:THR:H	1.65	0.40
1:B:118:GLY:O	1:B:121:VAL:HB	2.20	0.40
1:B:860:ILE:O	1:B:864:ILE:HG13	2.21	0.40
1:A:604:GLU:OE1	1:A:617:ILE:N	2.51	0.40
1:A:1120:ASP:HB3	1:A:1168:LYS:HD2	2.03	0.40
1:A:480:ILE:H	1:A:480:ILE:HG12	1.70	0.40
1:A:506:TYR:OH	1:A:510:MET:HE3	2.22	0.40
1:A:957:ALA:HA	1:A:960:VAL:HG12	2.04	0.40
1:B:783:ARG:HG2	1:B:787:MET:HE3	2.03	0.40
1:B:961:THR:OG1	1:B:962:GLN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:PRO:HB3	1:B:928:MET:HE3	2.03	0.40
1:A:945:MET:HE3	1:A:945:MET:HB2	1.97	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	1184/1282 (92%)	1096 (93%)	82 (7%)	6 (0%)	24	62
1	B	1176/1282 (92%)	1077 (92%)	91 (8%)	8 (1%)	18	55
All	All	2360/2564 (92%)	2173 (92%)	173 (7%)	14 (1%)	21	58

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	962	GLN
1	A	1028	GLU
1	A	1036	VAL
1	A	1204	THR
1	B	33	VAL
1	B	1136	VAL
1	B	32	ALA
1	A	838	ASN
1	A	1070	CYS
1	B	1172	LEU
1	B	1204	THR
1	A	429	LYS
1	B	393	ILE
1	B	520	VAL

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	979/1063 (92%)	935 (96%)	44 (4%)	24	46
1	B	973/1063 (92%)	920 (95%)	53 (5%)	20	42
All	All	1952/2126 (92%)	1855 (95%)	97 (5%)	22	44

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	48	LEU
1	A	54	THR
1	A	64	LEU
1	A	129	VAL
1	A	156	ILE
1	A	178	ILE
1	A	266	GLN
1	A	294	SER
1	A	295	MET
1	A	305	SER
1	A	374	PHE
1	A	375	SER
1	A	383	ASN
1	A	396	SER
1	A	403	VAL
1	A	450	ASP
1	A	474	VAL
1	A	478	THR
1	A	520	VAL
1	A	601	VAL
1	A	681	LYS
1	A	695	ARG
1	A	720	LEU
1	A	771	PHE
1	A	778	GLU
1	A	852	GLN

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Mol	Chain	Res	Type
1	A	930	LYS
1	A	944	MET
1	A	948	SER
1	A	965	MET
1	A	966	THR
1	A	979	PHE
1	A	1020	GLN
1	A	1037	VAL
1	A	1039	ASN
1	A	1048	VAL
1	A	1052	LEU
1	A	1090	VAL
1	A	1111	ILE
1	A	1163	THR
1	A	1167	ASP
1	A	1168	LYS
1	A	1254	GLN
1	B	33	VAL
1	B	35	VAL
1	B	75	THR
1	B	129	VAL
1	B	133	CYS
1	B	211	THR
1	B	217	ILE
1	B	220	VAL
1	B	277	LEU
1	B	279	GLU
1	B	282	ARG
1	B	283	LEU
1	B	294	SER
1	B	305	SER
1	B	310	PHE
1	B	333	SER
1	B	335	LEU
1	B	377	SER
1	B	383	ASN
1	B	409	LEU
1	B	419	VAL
1	B	468	VAL
1	B	474	VAL
1	B	478	THR
1	B	483	ASN

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Mol	Chain	Res	Type
1	B	593	VAL
1	B	601	VAL
1	B	603	VAL
1	B	688	VAL
1	B	702	THR
1	B	720	LEU
1	B	725	SER
1	B	729	SER
1	B	748	SER
1	B	755	PHE
1	B	848	ILE
1	B	854	THR
1	B	908	ARG
1	B	930	LYS
1	B	944	MET
1	B	945	MET
1	B	948	SER
1	B	967	PHE
1	B	1019	THR
1	B	1022	LEU
1	B	1037	VAL
1	B	1048	VAL
1	B	1052	LEU
1	B	1058	LYS
1	B	1090	VAL
1	B	1111	ILE
1	B	1137	SER
1	B	1163	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	266	GLN
1	A	514	HIS
1	A	515	GLN
1	A	744	GLN
1	A	834	GLN
1	A	838	ASN
1	A	910	GLN
1	A	1151	HIS
1	A	1191	HIS

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Mol	Chain	Res	Type
1	A	1255	GLN
1	B	153	ASN
1	B	191	GLN
1	B	387	ASN
1	B	394	HIS
1	B	410	ASN
1	B	514	HIS
1	B	515	GLN
1	B	608	HIS
1	B	700	ASN
1	B	769	GLN
1	B	795	GLN
1	B	820	GLN
1	B	834	GLN
1	B	838	ASN
1	B	942	GLN
1	B	969	ASN
1	B	986	GLN
1	B	1025	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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$
2	2J8	B	6004	-	16,18,39	1.70	4 (25%)	20,24,57	3.31	4 (20%)
2	2J8	B	6003	-	33,39,39	1.98	10 (30%)	51,57,57	1.81	16 (31%)
2	2J8	A	6002	-	16,18,39	2.08	5 (31%)	20,24,57	3.60	6 (30%)
2	2J8	A	6001	-	33,39,39	1.77	10 (30%)	51,57,57	1.78	11 (21%)

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	2J8	B	6004	-	-	8/14/16/48	0/2/2/4
2	2J8	B	6003	-	-	25/42/48/48	0/4/4/4
2	2J8	A	6002	-	-	7/14/16/48	0/2/2/4
2	2J8	A	6001	-	-	29/42/48/48	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6002	2J8	SE1-C05	4.33	1.97	1.88
2	B	6003	2J8	SE3-C19	4.25	1.97	1.88
2	A	6001	2J8	SE1-C05	4.18	1.97	1.88
2	B	6003	2J8	SE2-C12	4.06	1.96	1.88
2	B	6003	2J8	SE1-C05	4.01	1.96	1.88
2	A	6002	2J8	SE3-C19	4.00	1.97	1.86
2	B	6004	2J8	SE3-C19	3.84	1.96	1.86
2	A	6001	2J8	C02-N03	3.36	1.41	1.34
2	A	6001	2J8	SE3-C19	3.26	1.95	1.88
2	B	6003	2J8	C01-C02	3.24	1.54	1.48
2	B	6003	2J8	C08-C09	3.21	1.54	1.48
2	A	6001	2J8	C09-N10	3.19	1.40	1.34
2	A	6001	2J8	SE2-C12	3.16	1.94	1.88
2	B	6003	2J8	C28-C04	3.14	1.63	1.54
2	B	6003	2J8	C02-N03	3.14	1.40	1.34
2	A	6002	2J8	C19-N22	3.00	1.31	1.28
2	B	6003	2J8	C09-N10	2.86	1.40	1.34
2	A	6002	2J8	C01-C02	2.86	1.54	1.48
2	A	6002	2J8	C02-N03	2.85	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	2J8	C31-C11	2.77	1.62	1.54
2	B	6003	2J8	C16-N17	2.62	1.39	1.34
2	B	6004	2J8	C19-N22	2.59	1.30	1.28
2	B	6004	2J8	C02-N03	2.46	1.39	1.34
2	B	6004	2J8	SE1-C05	2.28	1.93	1.88
2	A	6001	2J8	C28-C04	2.18	1.60	1.54
2	B	6003	2J8	C31-C11	2.13	1.60	1.54
2	A	6001	2J8	C08-C09	2.11	1.52	1.48
2	A	6001	2J8	C18-N17	-2.02	1.41	1.45
2	A	6001	2J8	C07-C08	2.01	1.38	1.35

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6002	2J8	C08-N24-C05	12.29	116.18	104.86
2	B	6004	2J8	C08-N24-C05	11.33	115.30	104.86
2	B	6004	2J8	C19-N22-C01	7.22	115.81	109.51
2	A	6002	2J8	C19-N22-C01	6.74	115.39	109.51
2	A	6001	2J8	C18-N17-C16	5.30	132.36	121.57
2	A	6002	2J8	C04-N03-C02	5.10	131.94	121.57
2	A	6001	2J8	C01-C02-N03	4.77	122.00	115.22
2	B	6003	2J8	C04-N03-C02	4.44	130.59	121.57
2	B	6004	2J8	C04-N03-C02	3.85	129.41	121.57
2	B	6003	2J8	C08-C09-N10	3.49	120.19	115.22
2	A	6001	2J8	C01-N22-C19	3.40	116.86	113.49
2	A	6001	2J8	C11-N10-C09	3.31	128.30	121.57
2	A	6001	2J8	C08-C09-N10	3.11	119.64	115.22
2	B	6003	2J8	C01-C02-N03	3.09	119.62	115.22
2	A	6002	2J8	C05-C04-N03	3.03	112.74	108.05
2	B	6003	2J8	C15-N23-C12	3.01	116.47	113.49
2	B	6003	2J8	C01-N22-C19	3.01	116.47	113.49
2	B	6003	2J8	C11-N10-C09	3.01	127.70	121.57
2	B	6003	2J8	C18-N17-C16	3.01	127.69	121.57
2	B	6003	2J8	C15-C16-N17	2.90	119.34	115.22
2	A	6001	2J8	C04-N03-C02	2.88	127.42	121.57
2	B	6003	2J8	C28-C04-C05	2.77	116.04	111.76
2	B	6003	2J8	C18-C19-N22	2.71	127.47	123.89
2	B	6003	2J8	C29-C28-C04	2.59	118.27	111.16
2	B	6004	2J8	C01-C02-N03	2.54	118.84	115.22
2	A	6001	2J8	C19-C18-N17	-2.54	104.12	108.05
2	A	6002	2J8	C30-C28-C04	2.50	118.02	111.16
2	B	6003	2J8	C33-C31-C11	2.43	117.82	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6003	2J8	C08-N24-C05	2.40	115.86	113.49
2	A	6001	2J8	C04-C05-N24	2.35	126.99	123.89
2	B	6003	2J8	C04-C05-N24	2.32	126.94	123.89
2	A	6001	2J8	C11-C12-N23	2.14	126.71	123.89
2	B	6003	2J8	C30-C28-C04	2.12	116.97	111.16
2	A	6002	2J8	C01-C02-N03	2.11	118.22	115.22
2	A	6001	2J8	C15-N23-C12	2.07	115.54	113.49
2	B	6003	2J8	C11-C12-N23	2.04	126.58	123.89
2	A	6001	2J8	C30-C28-C04	2.03	116.73	111.16

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6001	2J8	C21-C01-C02-N03
2	A	6001	2J8	C21-C01-C02-O25
2	A	6001	2J8	N22-C01-C02-N03
2	A	6001	2J8	N22-C01-C02-O25
2	A	6001	2J8	N03-C04-C05-N24
2	A	6001	2J8	N03-C04-C28-C30
2	A	6001	2J8	C05-C04-C28-C29
2	A	6001	2J8	C05-C04-C28-C30
2	A	6001	2J8	C07-C08-C09-N10
2	A	6001	2J8	C07-C08-C09-O26
2	A	6001	2J8	N24-C08-C09-N10
2	A	6001	2J8	N24-C08-C09-O26
2	A	6001	2J8	C31-C11-C12-N23
2	A	6001	2J8	C12-C11-C31-C32
2	A	6001	2J8	C12-C11-C31-C33
2	A	6001	2J8	C14-C15-C16-N17
2	A	6001	2J8	C14-C15-C16-O27
2	A	6001	2J8	N23-C15-C16-N17
2	A	6001	2J8	N23-C15-C16-O27
2	A	6001	2J8	C34-C18-C19-N22
2	A	6001	2J8	C19-C18-C34-C35
2	A	6001	2J8	C19-C18-C34-C36
2	A	6002	2J8	C21-C01-C02-N03
2	A	6002	2J8	C21-C01-C02-O25
2	A	6002	2J8	N22-C01-C02-N03
2	A	6002	2J8	N22-C01-C02-O25
2	A	6002	2J8	C28-C04-C05-N24
2	B	6003	2J8	C21-C01-C02-N03

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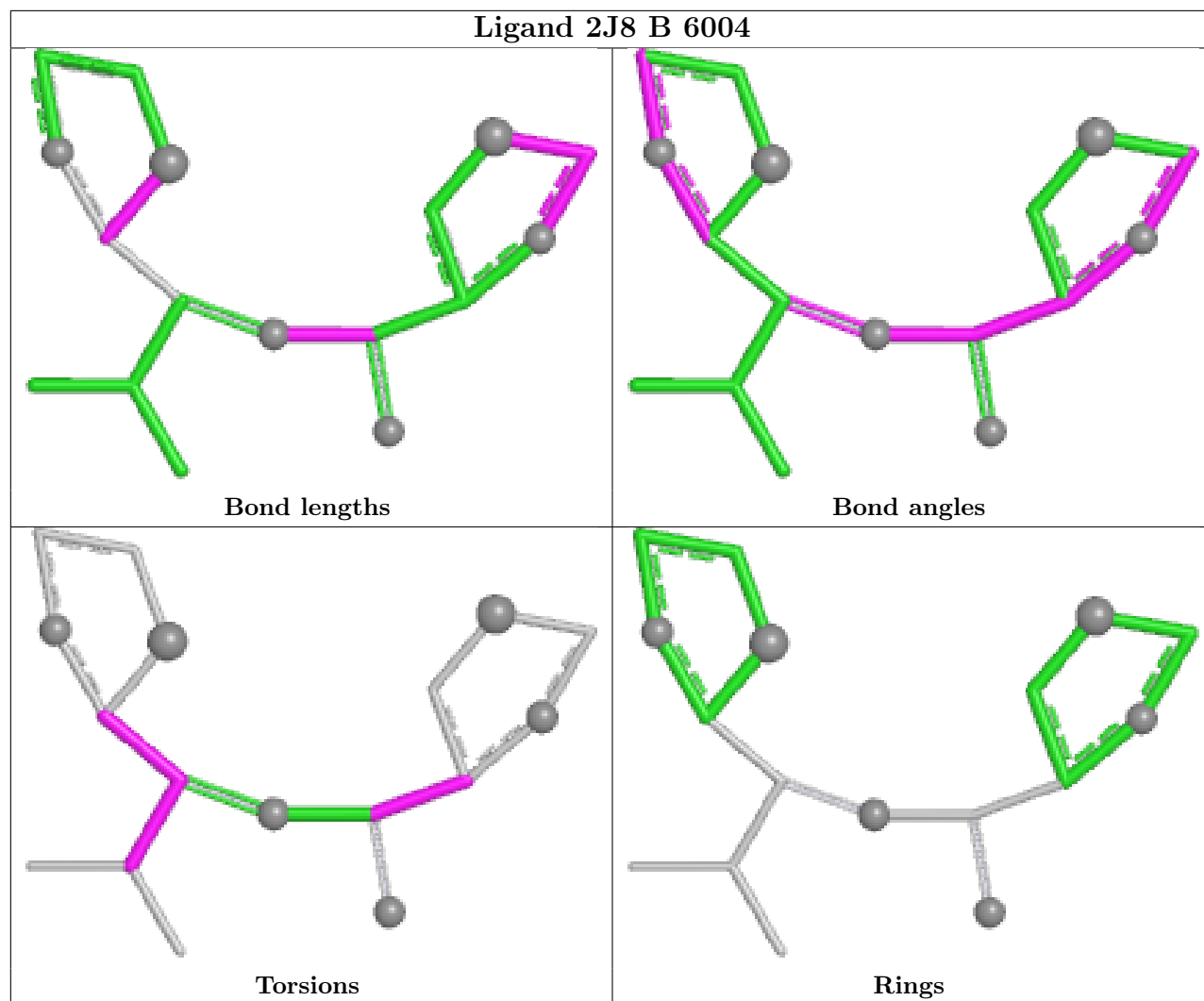
Mol	Chain	Res	Type	Atoms
2	B	6003	2J8	C21-C01-C02-O25
2	B	6003	2J8	N22-C01-C02-N03
2	B	6003	2J8	N22-C01-C02-O25
2	B	6003	2J8	C28-C04-C05-N24
2	B	6003	2J8	C07-C08-C09-N10
2	B	6003	2J8	C07-C08-C09-O26
2	B	6003	2J8	N24-C08-C09-N10
2	B	6003	2J8	N24-C08-C09-O26
2	B	6003	2J8	C31-C11-C12-N23
2	B	6003	2J8	C12-C11-C31-C33
2	B	6003	2J8	C14-C15-C16-N17
2	B	6003	2J8	C14-C15-C16-O27
2	B	6003	2J8	N23-C15-C16-N17
2	B	6003	2J8	N23-C15-C16-O27
2	B	6003	2J8	C34-C18-C19-N22
2	B	6003	2J8	N17-C18-C34-C36
2	B	6003	2J8	C19-C18-C34-C35
2	B	6003	2J8	C19-C18-C34-C36
2	B	6004	2J8	C21-C01-C02-N03
2	B	6004	2J8	C21-C01-C02-O25
2	B	6004	2J8	N22-C01-C02-N03
2	B	6004	2J8	N22-C01-C02-O25
2	B	6004	2J8	N03-C04-C05-N24
2	B	6004	2J8	C28-C04-C05-N24
2	A	6001	2J8	N17-C18-C34-C35
2	A	6001	2J8	N17-C18-C34-C36
2	B	6003	2J8	N17-C18-C34-C35
2	A	6001	2J8	N03-C04-C28-C29
2	A	6001	2J8	N10-C11-C31-C32
2	A	6001	2J8	N10-C11-C31-C33
2	B	6003	2J8	N10-C11-C31-C33
2	B	6003	2J8	N10-C11-C31-C32
2	B	6003	2J8	C12-C11-C31-C32
2	B	6003	2J8	C05-C04-C28-C30
2	B	6004	2J8	C05-C04-C28-C30
2	B	6003	2J8	N03-C04-C28-C30
2	A	6001	2J8	C05-C04-N03-C02
2	A	6001	2J8	C28-C04-C05-N24
2	B	6004	2J8	N03-C04-C28-C30
2	A	6002	2J8	C05-C04-N03-C02
2	A	6002	2J8	N03-C04-C28-C30

There are no ring outliers.

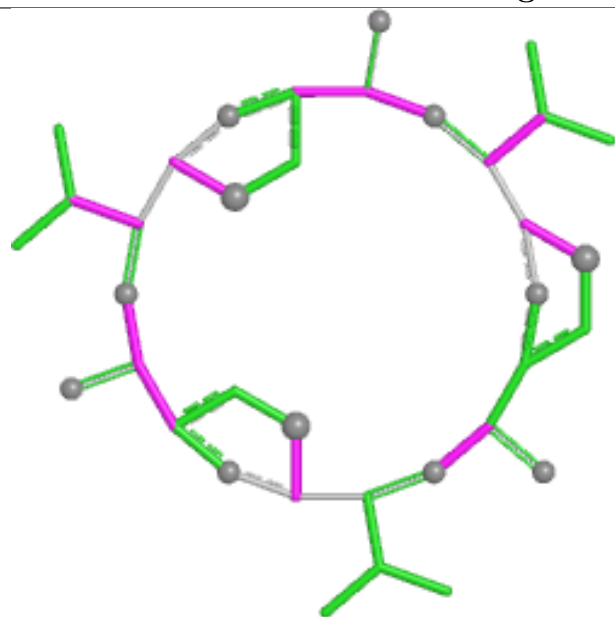
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6004	2J8	3	0
2	B	6003	2J8	3	0
2	A	6002	2J8	3	0
2	A	6001	2J8	3	0

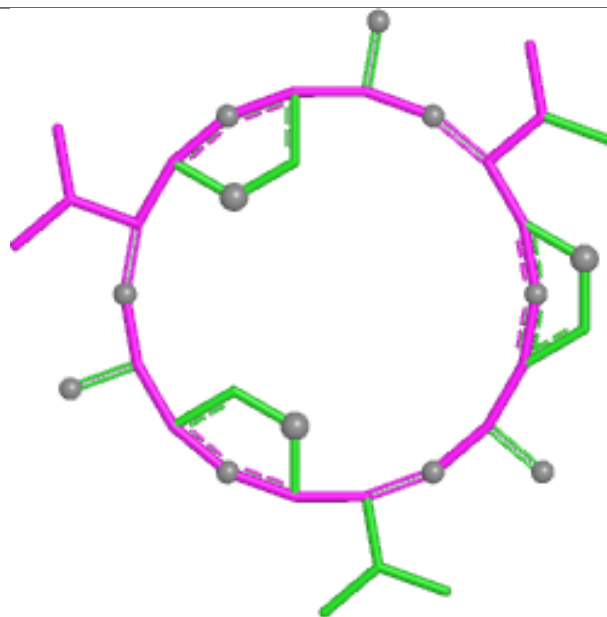
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



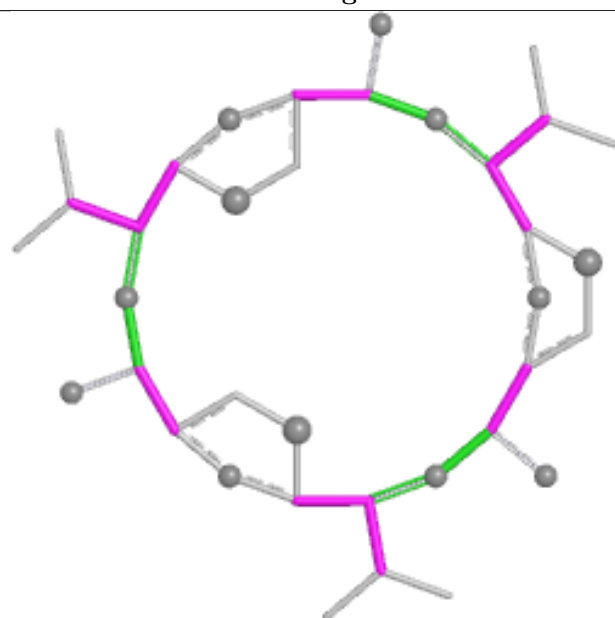
Ligand 2J8 B 6003



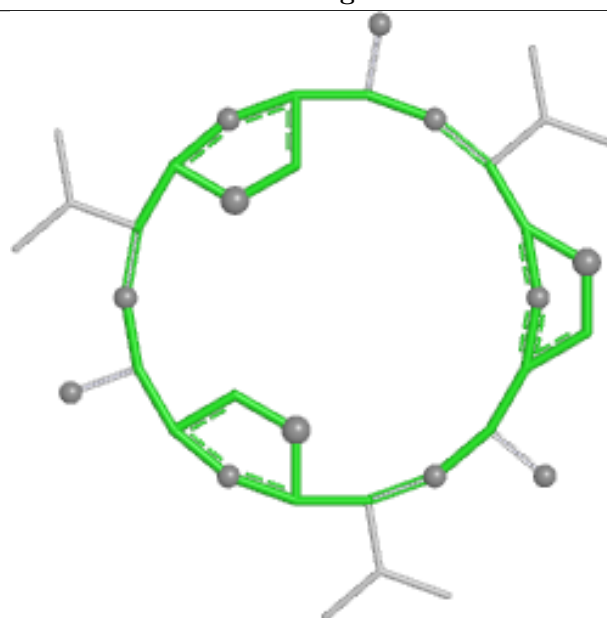
Bond lengths



Bond angles

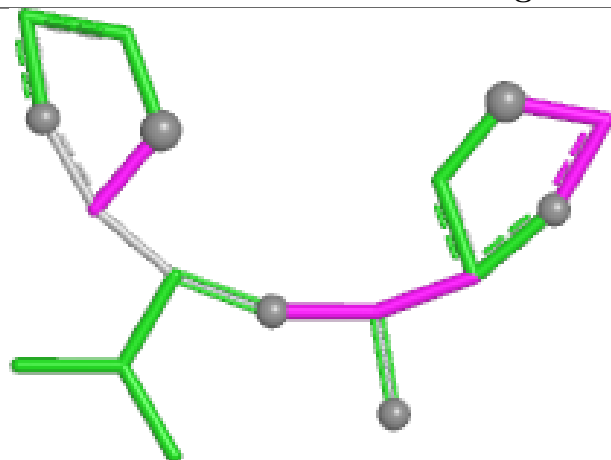


Torsions

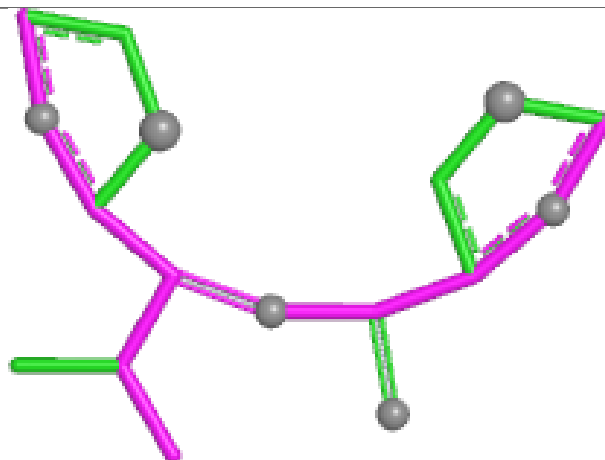


Rings

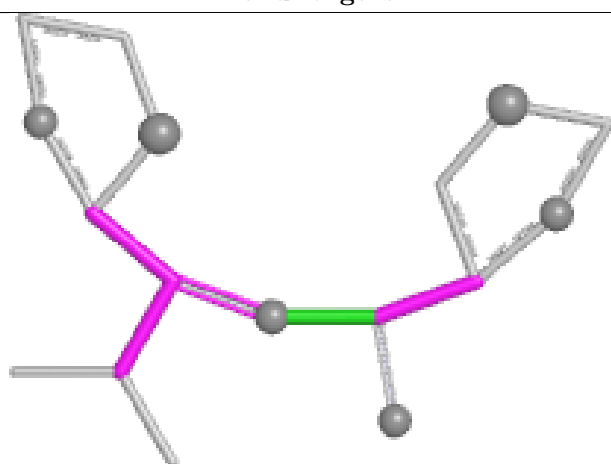
Ligand 2J8 A 6002



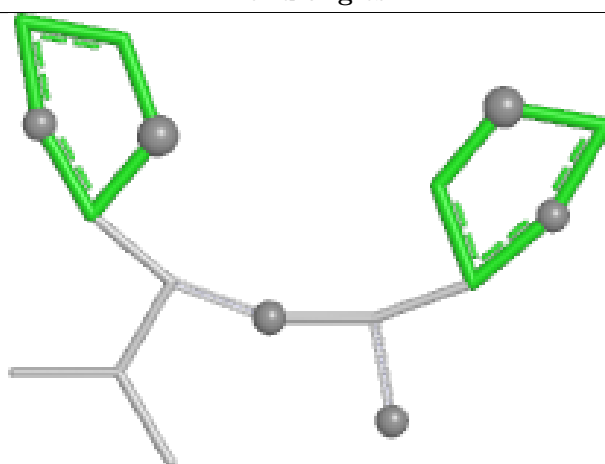
Bond lengths



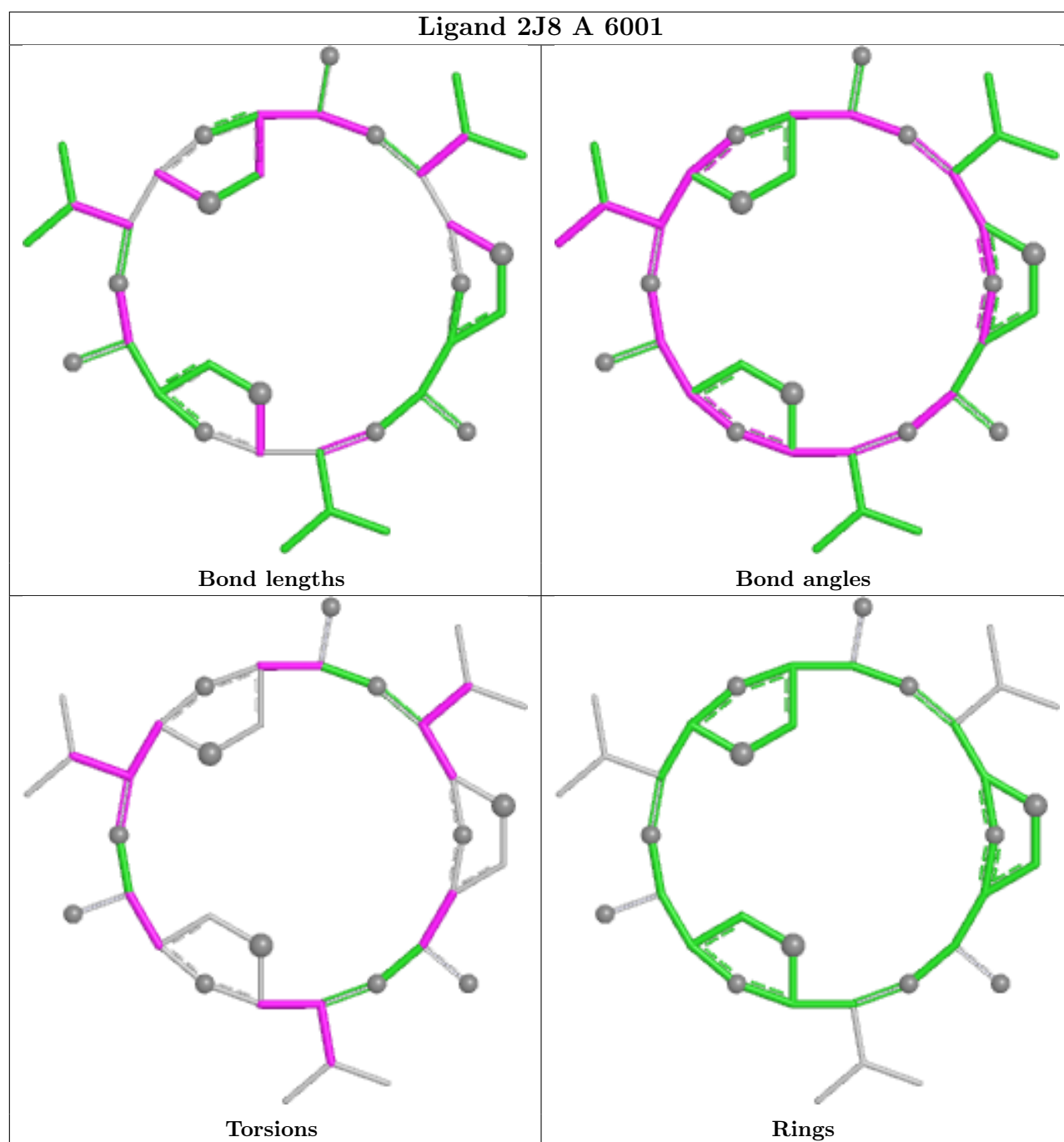
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1188/1282 (92%)	-0.36	4 (0%)	90 80	115, 186, 284, 381	0
1	B	1180/1282 (92%)	-0.36	4 (0%)	90 80	120, 197, 296, 512	0
All	All	2368/2564 (92%)	-0.36	8 (0%)	90 80	115, 191, 291, 512	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	VAL	3.9
1	B	990	PHE	3.7
1	B	1198	ALA	2.6
1	A	460	ARG	2.4
1	B	952	CYS	2.3
1	A	128	GLN	2.2
1	A	202	ILE	2.2
1	B	800	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

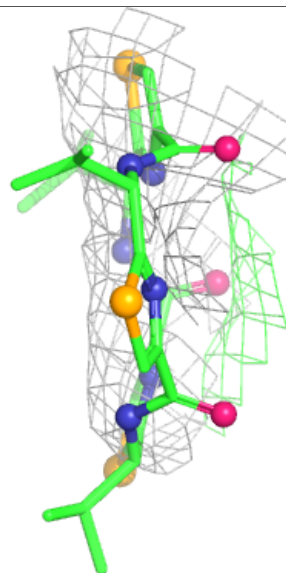
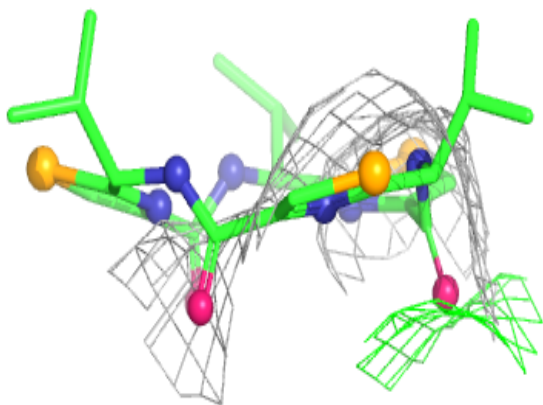
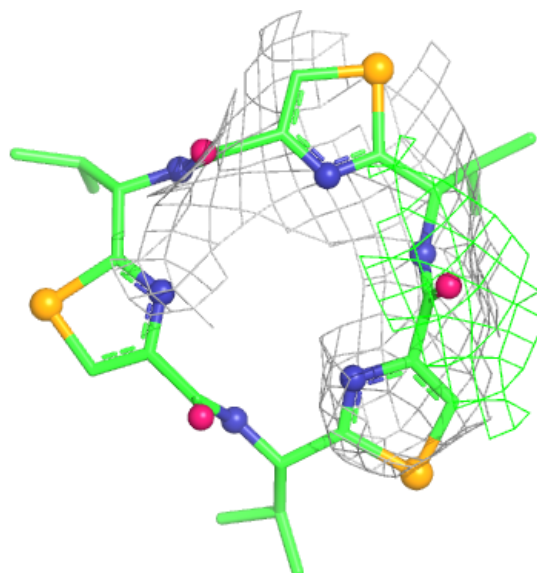
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	2J8	B	6003	36/36	0.71	0.14	191,311,336,550	0
2	2J8	B	6004	17/36	0.72	0.12	149,240,316,443	0
2	2J8	A	6002	17/36	0.81	0.12	234,240,512,514	0
2	2J8	A	6001	36/36	0.86	0.11	149,241,277,497	0

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

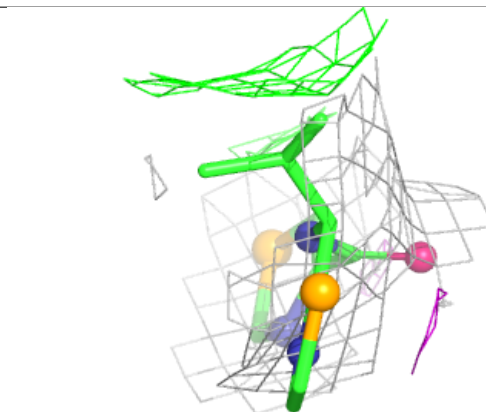
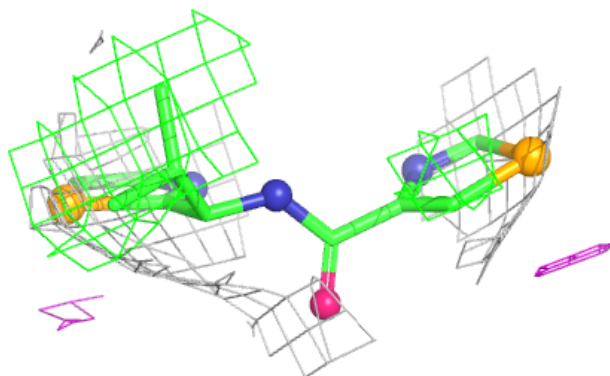
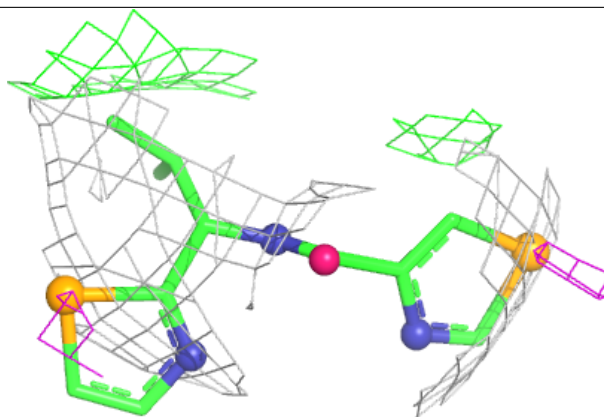
Electron density around 2J8 B 6003:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

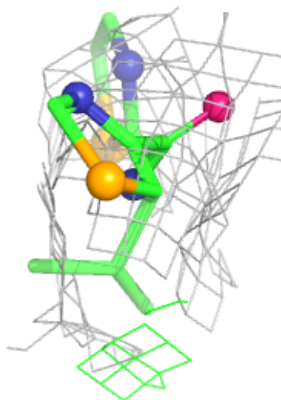
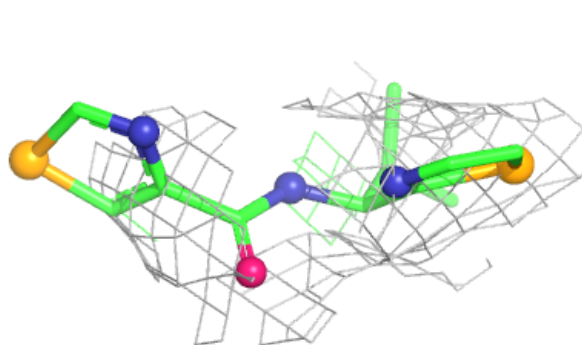
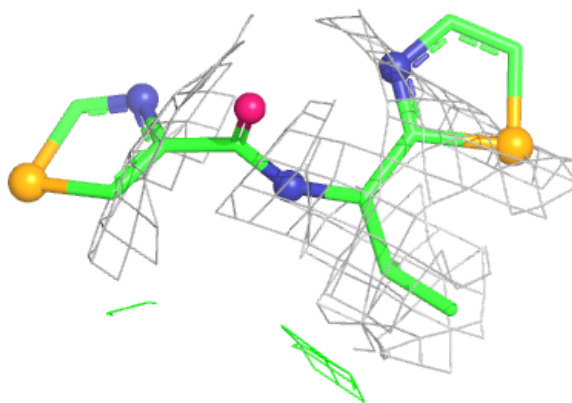


Electron density around 2J8 B 6004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

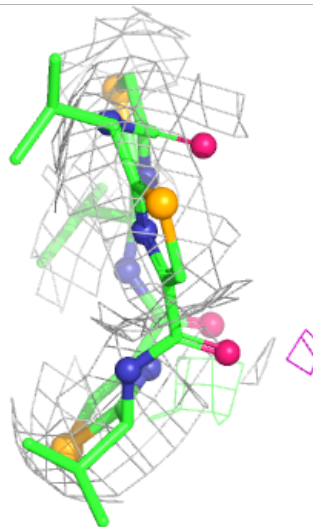
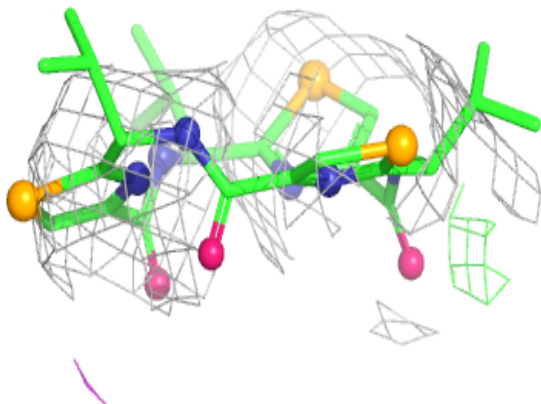
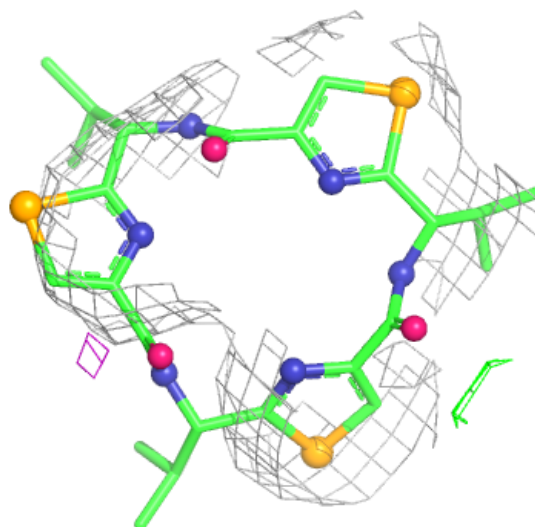
**Electron density around 2J8 A 6002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2J8 A 6001:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.