



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:41 PM UTC

PDB ID : 2JF6 / pdb_00002jff6
Title : Structure of inactive mutant of Strictosidine Glucosidase in complex with strictosidine
Authors : Barleben, L.; Panjikar, S.; Ruppert, M.; Koepke, J.; Stockigt, J.
Deposited on : 2007-01-26
Resolution : 2.82 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

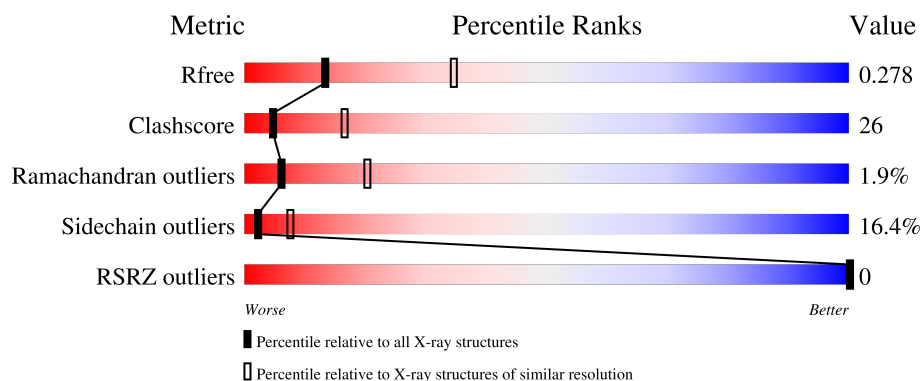
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

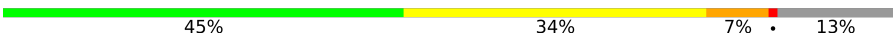
The reported resolution of this entry is 2.82 Å.

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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	532	
1	B	532	

2 Entry composition [i](#)

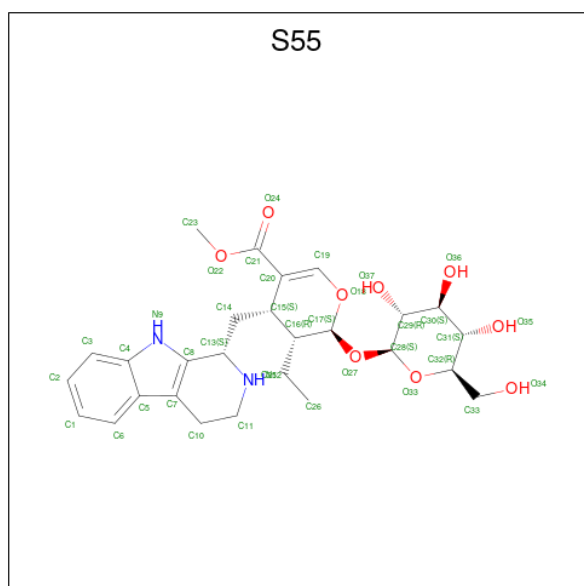
There are 3 unique types of molecules in this entry. The entry contains 7759 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STRICTOSIDINE-O-BETA-D-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3774	2430	628	701	15			
1	B	472	Total	C	N	O	S	0	0	0
			3833	2465	639	714	15			

- Molecule 2 is METHYL (2S,3R,4S)-3-ETHYL-2-(BETA-D-GLUCOPYRANOSYLOXY)-4-[(1S)-2,3,4,9-TETRAHYDRO-1H-BETA-CARBOLIN-1-YLMETHYL]-3,4-DIHYDRO-2H-PYRAN-5-CARBOXYLATE (CCD ID: S55) (formula: C₂₇H₃₆N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	27	2	9		
2	B	1	Total	C	N	O	0	0
			37	27	2	8		

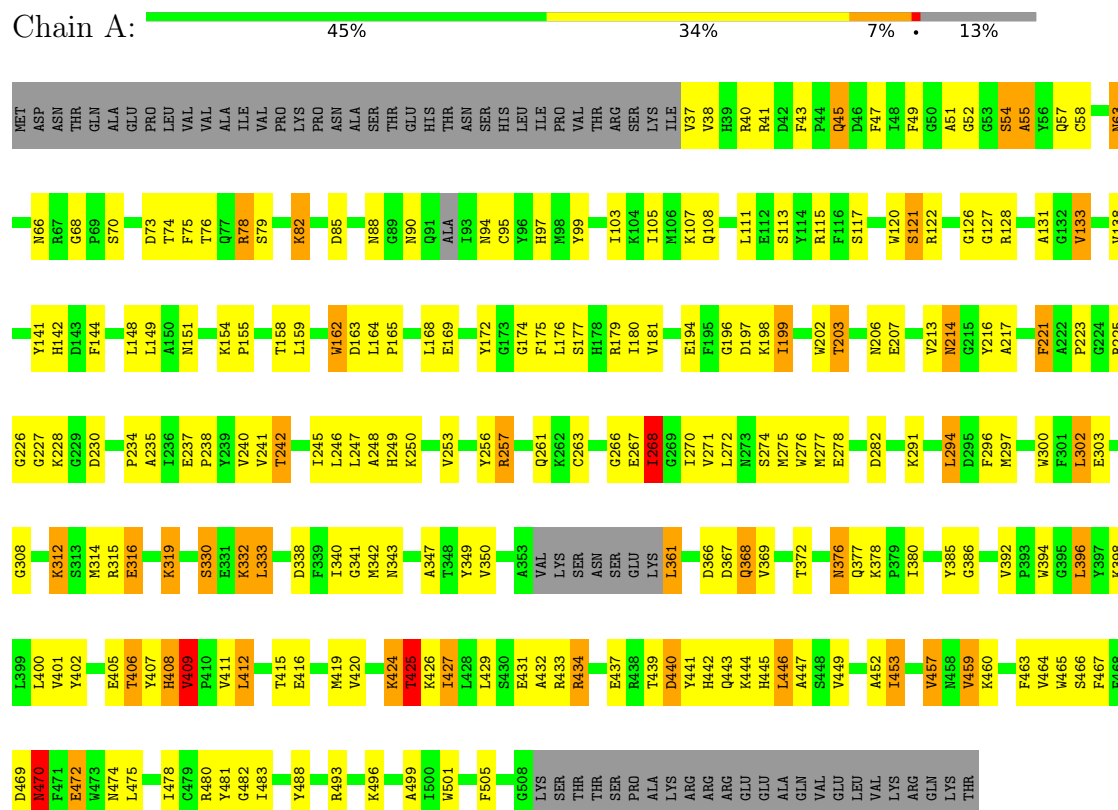
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total 42	O 42	0	0
3	B	35	Total 35	O 35	0	0

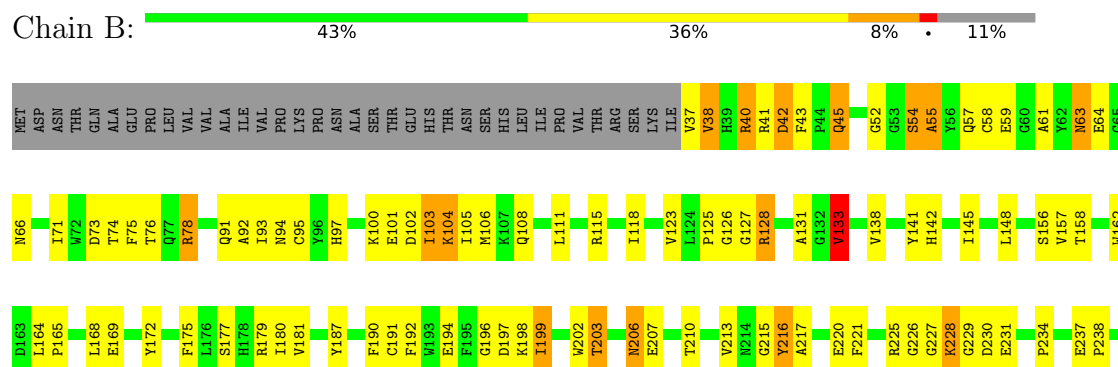
3 Residue-property plots

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

• Molecule 1: STRICTOSIDINE-O-BETA-D-GLUCOSIDASE



• Molecule 1: STRICTOSIDINE-O-BETA-D-GLUCOSIDASE



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.00Å 159.00Å 102.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.82 20.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.82) 99.5 (20.00-2.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.58 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.280 0.217 , 0.278	Depositor DCC
R_{free} test set	1621 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 6.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7759	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: S55

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	1/3885 (0.0%)	1.09	14/5260 (0.3%)
1	B	0.87	2/3946 (0.1%)	1.13	13/5344 (0.2%)
All	All	0.85	3/7831 (0.0%)	1.11	27/10604 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	VAL	CA-CB	6.73	1.62	1.54
1	B	133	VAL	CA-CB	5.95	1.61	1.54
1	A	133	VAL	CA-CB	5.60	1.60	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	VAL	N-CA-C	8.19	121.74	113.47
1	B	123	VAL	N-CA-C	-7.86	105.05	111.81
1	B	425	THR	N-CA-C	-6.46	100.96	110.52
1	A	246	LEU	N-CA-C	-6.41	104.38	111.36
1	A	268	ILE	CB-CA-C	-6.22	102.22	110.98
1	B	357	ASN	O-C-N	6.09	125.34	120.83
1	B	97	HIS	N-CA-C	-5.93	106.59	113.88
1	B	275	MET	N-CA-C	-5.84	101.87	110.52
1	B	157	VAL	N-CA-C	5.78	116.12	107.51
1	A	425	THR	N-CA-C	-5.72	102.05	110.52
1	A	470	ASN	N-CA-C	5.68	115.61	108.45
1	B	356	SER	N-CA-C	5.65	119.64	111.56
1	A	408	HIS	CA-C-N	-5.54	117.94	123.04
1	A	408	HIS	C-N-CA	-5.54	117.94	123.04
1	B	268	ILE	CB-CA-C	-5.49	103.50	111.68
1	A	409	VAL	CA-C-N	5.47	126.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	C-N-CA	5.47	126.67	119.84
1	A	366	ASP	N-CA-C	5.43	118.70	111.75
1	A	240	VAL	N-CA-C	-5.42	105.25	110.72
1	B	341	GLY	N-CA-C	-5.36	104.86	112.37
1	B	470	ASN	N-CA-C	5.28	115.25	108.34
1	A	52	GLY	N-CA-C	5.27	118.80	111.10
1	B	52	GLY	N-CA-C	5.23	118.92	111.12
1	A	172	TYR	N-CA-C	5.21	119.19	112.41
1	B	172	TYR	N-CA-C	5.20	119.16	112.41
1	A	221	PHE	N-CA-C	-5.15	101.47	109.24
1	A	275	MET	N-CA-C	-5.09	102.99	110.52

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	3774	0	3576	187	0
1	B	3833	0	3640	195	0
2	A	38	0	36	18	0
2	B	37	0	36	13	0
3	A	42	0	0	7	0
3	B	35	0	0	7	0
All	All	7759	0	7288	384	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 26.

All (384) 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)
2:B:1509:S55:H232	2:B:1509:S55:H19	1.25	1.16
2:A:1509:S55:H19	2:A:1509:S55:C23	1.80	1.10
1:B:242:THR:HG21	1:B:300:TRP:CZ2	1.92	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:TYR:HB3	1:B:268:ILE:HD11	1.38	1.01
1:B:367:ASP:O	1:B:369:VAL:N	1.91	1.00
2:A:1509:S55:H19	2:A:1509:S55:H232	1.39	0.98
1:A:367:ASP:O	1:A:369:VAL:N	2.00	0.94
1:B:63:ASN:HD22	1:B:63:ASN:H	1.18	0.91
2:B:1509:S55:H19	2:B:1509:S55:C23	2.01	0.90
1:A:434:ARG:HG2	1:A:434:ARG:HH11	1.37	0.89
1:A:66:ASN:HD21	1:B:66:ASN:H	1.17	0.89
1:B:199:ILE:HD11	1:B:202:TRP:CZ2	2.08	0.88
1:B:419:MET:HE1	1:B:437:GLU:HB3	1.56	0.86
1:A:199:ILE:HD11	1:A:202:TRP:CZ2	2.11	0.84
1:A:164:LEU:HD12	1:A:165:PRO:HD2	1.58	0.84
1:B:256:TYR:HB3	1:B:268:ILE:CD1	2.07	0.84
1:A:73:ASP:O	1:A:76:THR:HG22	1.79	0.83
1:A:196:GLY:HA2	1:A:199:ILE:CD1	2.09	0.82
2:A:1509:S55:H232	2:A:1509:S55:C19	2.12	0.79
1:B:106:MET:HG2	1:B:467:PHE:CE2	2.17	0.79
1:A:54:SER:CB	1:A:57:GLN:HE21	1.96	0.78
1:B:164:LEU:HD12	1:B:165:PRO:HD2	1.65	0.78
1:B:206:ASN:C	1:B:206:ASN:HD22	1.92	0.78
1:A:199:ILE:HD11	1:A:202:TRP:CE2	2.19	0.78
1:A:268:ILE:O	1:A:338:ASP:HB2	1.83	0.77
1:B:274:SER:HA	1:B:297:MET:HE2	1.64	0.77
1:B:40:ARG:HH21	1:B:43:PHE:HB2	1.49	0.76
1:A:402:TYR:O	1:A:406:THR:OG1	2.03	0.76
1:B:45:GLN:HA	1:B:45:GLN:HE21	1.50	0.76
1:A:425:THR:O	1:A:426:LYS:HB2	1.84	0.76
1:A:452:ALA:O	1:A:457:VAL:HG13	1.86	0.76
1:A:470:ASN:HD22	1:A:470:ASN:H	1.34	0.75
2:A:1509:S55:H19	2:A:1509:S55:H233	1.66	0.75
1:B:227:GLY:O	1:B:230:ASP:HB2	1.87	0.75
1:B:452:ALA:O	1:B:457:VAL:HG13	1.85	0.75
1:A:272:LEU:HD12	1:A:302:LEU:HD22	1.68	0.75
1:A:276:TRP:HE1	1:A:278:GLU:HG2	1.51	0.75
1:B:386:GLY:HA3	2:B:1509:S55:C1	2.17	0.74
1:A:434:ARG:HG2	1:A:434:ARG:NH1	1.96	0.74
1:A:261:GLN:NE2	1:A:266:GLY:O	2.20	0.74
1:A:434:ARG:HH11	1:A:434:ARG:CG	2.00	0.74
1:A:221:PHE:HZ	2:A:1509:S55:H261	1.53	0.73
1:A:442:HIS:CE1	1:A:464:VAL:HG22	2.23	0.73
1:A:460:LYS:HE2	3:A:2039:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:MET:HG3	1:B:294:LEU:HD22	1.70	0.73
1:A:470:ASN:HD22	1:A:470:ASN:N	1.85	0.73
1:B:73:ASP:O	1:B:76:THR:HG22	1.88	0.72
1:A:466:SER:O	1:A:482:GLY:HA2	1.89	0.72
1:A:278:GLU:HG3	1:A:394:TRP:HH2	1.54	0.72
1:B:93:ILE:O	1:B:493:ARG:NH2	2.23	0.72
1:A:68:GLY:O	1:A:121:SER:HB2	1.90	0.71
1:B:242:THR:HG21	1:B:300:TRP:CE2	2.24	0.71
1:A:66:ASN:ND2	1:B:66:ASN:H	1.87	0.71
1:A:386:GLY:HA3	2:A:1509:S55:C1	2.20	0.71
1:A:460:LYS:CE	3:A:2039:HOH:O	2.38	0.71
1:B:141:TYR:O	1:B:145:ILE:HG12	1.91	0.70
1:A:63:ASN:H	1:A:63:ASN:HD22	1.40	0.70
1:B:314:MET:O	1:B:318:VAL:HG23	1.91	0.70
1:B:343:ASN:CG	1:B:416:GLU:HB2	2.17	0.70
1:A:424:LYS:O	1:A:427:ILE:HD11	1.92	0.69
1:A:105:ILE:HA	1:A:108:GLN:NE2	2.08	0.69
1:A:221:PHE:CZ	2:A:1509:S55:H261	2.27	0.69
1:B:277:MET:CG	1:B:294:LEU:HD22	2.23	0.69
1:A:105:ILE:HA	1:A:108:GLN:HE21	1.57	0.68
1:B:412:LEU:HD23	1:B:457:VAL:HG23	1.76	0.68
2:B:1509:S55:H232	2:B:1509:S55:C19	2.12	0.68
1:A:277:MET:CG	1:A:294:LEU:HD22	2.24	0.67
1:A:94:ASN:HD21	1:A:97:HIS:HD2	1.42	0.67
1:B:466:SER:O	1:B:482:GLY:HA2	1.94	0.67
1:A:45:GLN:HA	1:A:45:GLN:HE21	1.59	0.66
1:A:54:SER:HB3	1:A:57:GLN:HE21	1.60	0.66
1:B:42:ASP:N	1:B:42:ASP:OD2	2.28	0.66
1:B:268:ILE:O	1:B:338:ASP:HB2	1.96	0.66
1:A:226:GLY:O	1:A:234:PRO:HG3	1.95	0.66
1:B:40:ARG:HH21	1:B:43:PHE:CB	2.08	0.65
1:A:221:PHE:HZ	2:A:1509:S55:C26	2.09	0.65
1:A:349:TYR:CE1	1:A:380:ILE:HB	2.32	0.65
1:B:386:GLY:HA3	2:B:1509:S55:H1	1.79	0.64
1:B:106:MET:HG2	1:B:467:PHE:HE2	1.59	0.64
1:A:221:PHE:CZ	2:A:1509:S55:C26	2.80	0.64
1:A:312:LYS:HZ2	1:A:315:ARG:HG3	1.63	0.64
1:A:277:MET:HG3	1:A:294:LEU:HD22	1.80	0.63
1:B:226:GLY:O	1:B:234:PRO:HG3	1.98	0.63
1:B:175:PHE:CE1	1:B:180:ILE:HG12	2.33	0.63
1:B:57:GLN:HG2	1:B:471:PHE:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLY:CA	2:B:1509:S55:H1	2.29	0.63
1:A:196:GLY:HA2	1:A:199:ILE:HD13	1.79	0.63
1:B:445:HIS:O	1:B:449:VAL:HG23	1.97	0.63
1:A:445:HIS:O	1:A:449:VAL:HG23	1.98	0.63
1:A:213:VAL:O	1:A:217:ALA:HB3	1.98	0.62
1:A:274:SER:HA	1:A:297:MET:SD	2.39	0.62
1:B:115:ARG:HG2	1:B:156:SER:HB3	1.81	0.62
1:B:181:VAL:HG21	1:B:247:LEU:HB3	1.80	0.61
1:A:177:SER:O	1:A:180:ILE:HG22	1.99	0.61
1:A:278:GLU:HG3	1:A:394:TRP:CH2	2.35	0.61
1:B:253:VAL:HA	1:B:268:ILE:HD12	1.81	0.61
1:A:347:ALA:O	1:A:380:ILE:HD13	2.00	0.61
1:A:88:ASN:OD1	1:A:90:ASN:HB2	1.99	0.61
1:B:261:GLN:NE2	1:B:338:ASP:OD1	2.34	0.61
1:A:158:THR:HG23	1:A:203:THR:HG22	1.82	0.61
1:B:220:GLU:O	1:B:221:PHE:HD1	1.83	0.61
1:A:214:ASN:HD22	1:A:214:ASN:N	1.99	0.60
1:B:474:ASN:ND2	1:B:475:LEU:HD13	2.15	0.60
1:A:303:GLU:OE2	1:A:407:TYR:HE1	1.84	0.60
1:B:63:ASN:HD22	1:B:63:ASN:N	1.91	0.60
1:A:386:GLY:HA3	2:A:1509:S55:H1	1.83	0.60
1:A:416:GLU:HG2	1:A:465:TRP:HB2	1.84	0.60
1:B:296:PHE:CE2	1:B:314:MET:HG2	2.38	0.59
1:B:271:VAL:HG12	1:B:341:GLY:HA3	1.85	0.59
1:A:79:SER:HB3	1:A:82:LYS:HG3	1.86	0.58
1:A:175:PHE:HB3	1:A:241:VAL:HG13	1.86	0.58
1:B:357:ASN:N	1:B:357:ASN:HD22	2.01	0.58
1:A:367:ASP:O	1:A:367:ASP:CG	2.46	0.58
1:B:105:ILE:HA	1:B:108:GLN:HE21	1.68	0.58
1:A:253:VAL:HG13	1:A:268:ILE:HD13	1.85	0.58
1:B:242:THR:CG2	1:B:300:TRP:CZ2	2.79	0.58
1:B:301:PHE:O	1:B:304:PRO:HD2	2.03	0.58
1:A:206:ASN:HA	1:A:271:VAL:HG22	1.86	0.57
1:B:388:TRP:HZ2	2:B:1509:S55:C23	2.17	0.57
1:A:163:ASP:OD1	3:A:2015:HOH:O	2.17	0.57
1:B:430:SER:O	1:B:434:ARG:NH1	2.37	0.57
1:A:419:MET:HE1	1:A:437:GLU:HB3	1.85	0.57
1:B:257:ARG:HH22	1:B:336:CYS:HA	1.69	0.57
1:B:315:ARG:HH22	1:B:324:LYS:HA	1.70	0.57
1:A:51:ALA:HB3	1:A:111:LEU:HD21	1.86	0.56
1:B:142:HIS:NE2	1:B:194:GLU:OE2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ILE:HA	1:B:457:VAL:O	2.04	0.56
1:A:420:VAL:HG23	1:A:481:TYR:CE1	2.40	0.56
1:B:296:PHE:CD1	1:B:367:ASP:HB3	2.40	0.56
1:B:471:PHE:HD1	1:B:477:TYR:CZ	2.23	0.56
1:A:57:GLN:O	1:A:470:ASN:HB2	2.05	0.56
1:B:337:TYR:OH	1:B:409:VAL:HB	2.06	0.56
1:A:54:SER:O	1:A:55:ALA:C	2.49	0.55
1:B:242:THR:HB	3:B:2016:HOH:O	2.06	0.55
1:A:386:GLY:CA	2:A:1509:S55:H1	2.35	0.55
1:B:177:SER:O	1:B:180:ILE:HG22	2.06	0.55
1:B:475:LEU:O	1:B:478:ILE:HG12	2.07	0.55
1:B:477:TYR:HB3	1:B:488:TYR:CD1	2.41	0.55
1:A:149:LEU:HD21	1:A:155:PRO:HD3	1.89	0.55
1:A:66:ASN:HD22	1:B:66:ASN:HA	1.71	0.55
1:A:168:LEU:O	1:A:169:GLU:C	2.50	0.55
1:A:396:LEU:HD22	1:A:400:LEU:CD1	2.37	0.55
1:A:276:TRP:NE1	1:A:278:GLU:HG2	2.21	0.54
1:B:312:LYS:NZ	1:B:315:ARG:HG3	2.22	0.54
1:B:425:THR:O	1:B:426:LYS:HB2	2.08	0.54
1:A:163:ASP:OD2	3:A:2014:HOH:O	2.18	0.54
1:B:338:ASP:O	1:B:411:VAL:CG2	2.55	0.54
1:A:196:GLY:C	1:A:198:LYS:H	2.16	0.54
1:B:221:PHE:HE2	2:B:1509:S55:C26	2.21	0.54
1:B:301:PHE:HZ	3:B:2016:HOH:O	1.90	0.53
1:B:277:MET:HB2	1:B:294:LEU:CD2	2.39	0.53
1:B:210:THR:HG21	2:B:1509:S55:H263	1.90	0.53
1:A:199:ILE:HD11	1:A:202:TRP:NE1	2.23	0.53
1:A:99:TYR:O	1:A:103:ILE:HG12	2.09	0.53
1:B:216:TYR:N	1:B:216:TYR:CD2	2.75	0.53
1:A:312:LYS:NZ	1:A:315:ARG:HG3	2.23	0.52
1:A:469:ASP:OD1	1:A:480:ARG:HD3	2.09	0.52
1:A:58:CYS:HB3	1:A:95:CYS:SG	2.50	0.52
1:B:54:SER:O	1:B:55:ALA:C	2.52	0.52
1:A:95:CYS:HB3	3:A:2008:HOH:O	2.09	0.52
1:B:231:GLU:HB2	3:B:2019:HOH:O	2.08	0.52
1:B:256:TYR:O	1:B:257:ARG:C	2.53	0.52
1:B:78:ARG:HB3	3:B:2003:HOH:O	2.10	0.52
1:B:162:TRP:CD1	1:B:162:TRP:N	2.73	0.52
1:B:336:CYS:O	1:B:336:CYS:SG	2.67	0.52
1:A:368:GLN:NE2	3:A:2028:HOH:O	2.43	0.52
1:A:470:ASN:N	1:A:470:ASN:ND2	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ASP:O	1:B:367:ASP:CG	2.53	0.52
1:B:55:ALA:HA	1:B:59:GLU:HG3	1.92	0.52
1:A:396:LEU:HD22	1:A:400:LEU:HD12	1.92	0.51
1:B:78:ARG:CB	3:B:2003:HOH:O	2.59	0.51
1:B:272:LEU:HB3	3:B:2022:HOH:O	2.10	0.51
1:B:465:TRP:CE2	1:B:466:SER:HB3	2.45	0.51
1:A:85:ASP:OD1	1:A:85:ASP:N	2.38	0.51
1:B:292:ARG:HH22	1:B:352:ASN:HB2	1.75	0.51
1:B:221:PHE:CE2	2:B:1509:S55:C26	2.92	0.51
1:B:474:ASN:HD21	1:B:475:LEU:HD13	1.74	0.51
1:A:149:LEU:CD2	1:A:155:PRO:HD3	2.41	0.51
2:A:1509:S55:C23	2:A:1509:S55:C19	2.57	0.51
1:A:235:ALA:HB2	1:A:361:LEU:O	2.11	0.51
1:A:343:ASN:CG	1:A:416:GLU:HB2	2.35	0.51
1:A:113:SER:HB2	1:A:154:LYS:HB2	1.92	0.51
1:A:126:GLY:HA3	1:A:131:ALA:CB	2.41	0.51
1:B:465:TRP:NE1	2:B:1509:S55:O35	2.44	0.51
1:A:66:ASN:HD21	1:B:66:ASN:N	1.97	0.51
1:A:256:TYR:O	1:A:257:ARG:C	2.54	0.51
1:B:126:GLY:HA3	1:B:131:ALA:CB	2.41	0.51
1:B:206:ASN:C	1:B:206:ASN:ND2	2.59	0.51
1:B:376:ASN:C	1:B:378:LYS:H	2.19	0.51
1:A:453:ILE:HA	1:A:457:VAL:O	2.11	0.51
1:B:402:TYR:O	1:B:406:THR:OG1	2.29	0.51
1:A:94:ASN:HD21	1:A:97:HIS:CD2	2.27	0.50
1:A:444:LYS:O	1:A:447:ALA:HB3	2.11	0.50
1:B:353:ALA:HB2	1:B:370:THR:OG1	2.11	0.50
1:B:419:MET:HE1	1:B:437:GLU:CB	2.35	0.50
1:B:92:ALA:HA	1:B:477:TYR:OH	2.12	0.50
1:A:214:ASN:HB2	1:A:221:PHE:CD2	2.47	0.50
1:A:396:LEU:HD13	1:A:449:VAL:HG22	1.92	0.50
1:B:396:LEU:HD22	1:B:400:LEU:CD1	2.42	0.50
1:B:306:THR:O	1:B:334:LYS:HG2	2.12	0.50
1:A:296:PHE:CG	1:A:367:ASP:HB3	2.47	0.49
1:B:217:ALA:HB2	1:B:238:PRO:HG3	1.94	0.49
1:B:249:HIS:CE1	1:B:270:ILE:HB	2.47	0.49
1:B:300:TRP:CD1	1:B:314:MET:HE1	2.47	0.49
1:B:168:LEU:O	1:B:169:GLU:C	2.55	0.49
1:B:296:PHE:CD1	1:B:367:ASP:CB	2.96	0.49
1:A:107:LYS:HD3	1:A:151:ASN:HD22	1.78	0.49
1:B:225:ARG:NH1	1:B:237:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLU:OE1	1:A:472:GLU:HA	2.11	0.49
1:B:385:TYR:CD2	1:B:422:GLU:HB2	2.48	0.49
1:A:207:GLU:OE1	1:A:343:ASN:ND2	2.32	0.49
1:A:238:PRO:O	1:A:242:THR:HG23	2.12	0.49
1:A:316:GLU:O	1:A:319:LYS:HD2	2.13	0.49
1:B:102:ASP:O	1:B:106:MET:HG3	2.12	0.49
1:A:70:SER:N	1:A:73:ASP:OD1	2.37	0.49
1:A:433:ARG:NH2	1:A:434:ARG:HH12	2.10	0.49
1:B:133:VAL:HG21	1:B:190:PHE:CZ	2.47	0.49
1:A:296:PHE:CE1	1:A:314:MET:HG2	2.48	0.49
1:A:465:TRP:CE2	1:A:466:SER:HB3	2.48	0.49
1:B:216:TYR:N	1:B:216:TYR:HD2	2.11	0.49
1:B:388:TRP:CZ2	2:B:1509:S55:C23	2.96	0.49
2:B:1509:S55:C23	2:B:1509:S55:C19	2.76	0.49
1:A:47:PHE:HE1	1:A:453:ILE:HD11	1.78	0.49
1:A:54:SER:HB2	1:A:57:GLN:HE21	1.74	0.49
1:A:250:LYS:HD3	1:A:333:LEU:HG	1.95	0.49
1:B:158:THR:HA	1:B:203:THR:HB	1.94	0.48
1:B:486:VAL:HG22	1:B:493:ARG:HG2	1.95	0.48
1:B:253:VAL:HA	1:B:268:ILE:CD1	2.42	0.48
1:B:337:TYR:CE1	1:B:340:ILE:HG12	2.49	0.48
1:A:164:LEU:HD12	1:A:165:PRO:CD	2.38	0.48
1:B:276:TRP:HB3	1:B:347:ALA:HB2	1.96	0.48
1:A:242:THR:HA	1:A:245:ILE:HD12	1.96	0.47
1:B:228:LYS:HD3	1:B:229:GLY:N	2.28	0.47
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.68	0.47
1:A:257:ARG:NH1	1:A:338:ASP:OD2	2.44	0.47
1:A:300:TRP:CD1	1:A:314:MET:HE1	2.48	0.47
1:A:122:ARG:HD2	1:A:141:TYR:HE2	1.78	0.47
1:A:176:LEU:HD21	1:A:237:GLU:OE1	2.13	0.47
1:B:164:LEU:HD12	1:B:165:PRO:CD	2.40	0.47
1:B:196:GLY:C	1:B:198:LYS:H	2.21	0.47
1:B:312:LYS:HZ2	1:B:315:ARG:HG3	1.79	0.47
1:A:308:GLY:O	1:A:330:SER:OG	2.31	0.47
1:B:243:HIS:CE1	1:B:325:PHE:CE2	3.03	0.47
1:A:340:ILE:HG12	1:A:409:VAL:HG21	1.95	0.47
1:B:299:GLY:O	1:B:300:TRP:C	2.58	0.47
1:A:223:PRO:HG2	1:A:225:ARG:HG3	1.95	0.47
1:A:429:LEU:HD23	1:A:429:LEU:O	2.15	0.47
1:B:276:TRP:HE1	1:B:278:GLU:HG2	1.79	0.47
1:B:382:HIS:O	1:B:390:HIS:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:PHE:CE1	1:A:505:PHE:HE1	2.32	0.47
1:A:440:ASP:OD1	1:A:444:LYS:NZ	2.48	0.47
1:A:302:LEU:HD13	1:A:302:LEU:HA	1.80	0.46
1:A:297:MET:HE1	2:A:1509:S55:H231	1.97	0.46
1:B:103:ILE:HG23	1:B:148:LEU:HD23	1.96	0.46
1:B:465:TRP:HA	1:B:466:SER:HA	1.69	0.46
1:A:300:TRP:CG	1:A:314:MET:HE1	2.50	0.46
1:B:175:PHE:CD1	1:B:180:ILE:HG21	2.51	0.46
1:A:441:TYR:CE2	1:A:445:HIS:CE1	3.02	0.46
1:A:78:ARG:HD2	1:B:128:ARG:CZ	2.46	0.46
1:B:471:PHE:CE1	1:B:476:GLY:HA2	2.51	0.46
1:B:207:GLU:HG2	1:B:273:ASN:OD1	2.16	0.46
1:B:351:THR:HG23	1:B:352:ASN:O	2.15	0.46
1:A:271:VAL:HG12	1:A:341:GLY:HA3	1.98	0.46
1:A:429:LEU:O	1:A:433:ARG:HG2	2.15	0.46
1:B:278:GLU:O	1:B:349:TYR:HA	2.16	0.45
1:B:342:MET:HE3	1:B:399:LEU:HD21	1.97	0.45
1:A:66:ASN:ND2	1:B:66:ASN:N	2.59	0.45
1:B:206:ASN:HD22	1:B:207:GLU:HB2	1.80	0.45
1:B:238:PRO:O	1:B:242:THR:HG22	2.16	0.45
1:A:41:ARG:C	1:A:43:PHE:H	2.25	0.45
1:B:303:GLU:HB3	1:B:304:PRO:HD3	1.99	0.45
1:A:115:ARG:HG3	1:A:463:PHE:CE2	2.52	0.45
1:B:216:TYR:CD1	1:B:241:VAL:HG21	2.51	0.45
1:A:294:LEU:HG	1:A:402:TYR:CE1	2.51	0.45
1:A:439:THR:HG23	1:A:501:TRP:CG	2.52	0.45
1:B:45:GLN:HA	1:B:45:GLN:NE2	2.25	0.45
1:B:237:GLU:O	1:B:238:PRO:C	2.60	0.45
1:A:175:PHE:CB	1:A:241:VAL:HG13	2.47	0.45
1:A:250:LYS:HD2	1:A:332:LYS:HB2	1.98	0.45
1:A:466:SER:O	1:A:467:PHE:C	2.60	0.45
1:A:207:GLU:OE1	2:A:1509:S55:O37	2.17	0.45
1:B:440:ASP:HA	1:B:443:GLN:HG3	1.97	0.45
1:A:75:PHE:O	1:A:79:SER:HB2	2.17	0.45
1:B:41:ARG:C	1:B:43:PHE:H	2.25	0.44
1:A:66:ASN:ND2	1:B:66:ASN:HA	2.32	0.44
1:A:126:GLY:HA3	1:A:131:ALA:HB1	2.00	0.44
1:A:225:ARG:NH1	1:A:237:GLU:CD	2.75	0.44
1:A:439:THR:O	1:A:440:ASP:C	2.61	0.44
1:A:465:TRP:CE2	2:A:1509:S55:O35	2.70	0.44
1:A:181:VAL:HG13	1:A:248:ALA:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HA	1:A:271:VAL:CG2	2.46	0.44
1:A:216:TYR:HB3	1:A:237:GLU:HB2	1.98	0.44
1:B:61:ALA:HB1	1:B:64:GLU:HB2	2.00	0.44
1:A:340:ILE:HG22	1:A:341:GLY:O	2.17	0.44
1:A:412:LEU:O	1:A:459:VAL:HA	2.18	0.44
1:B:71:ILE:HD13	1:B:164:LEU:HD23	1.99	0.44
1:B:301:PHE:C	1:B:304:PRO:HD2	2.41	0.44
1:B:276:TRP:NE1	1:B:278:GLU:HG2	2.32	0.44
1:B:338:ASP:O	1:B:411:VAL:HG23	2.18	0.44
1:B:338:ASP:O	1:B:411:VAL:HG21	2.17	0.44
1:A:297:MET:HE1	2:A:1509:S55:C23	2.48	0.44
1:B:187:TYR:CE2	1:B:191:CYS:SG	3.11	0.44
1:A:49:PHE:HE1	1:A:446:LEU:HD21	1.83	0.44
1:A:120:TRP:HB2	3:A:2013:HOH:O	2.18	0.43
1:A:127:GLY:HA3	1:A:168:LEU:HG	1.99	0.43
1:B:215:GLY:C	1:B:216:TYR:CD2	2.95	0.43
1:B:357:ASN:N	1:B:357:ASN:ND2	2.66	0.43
1:A:47:PHE:CE1	1:A:453:ILE:HD11	2.52	0.43
1:A:291:LYS:HD2	1:A:291:LYS:HA	1.65	0.43
1:B:74:THR:O	1:B:75:PHE:C	2.60	0.43
1:A:55:ALA:N	1:A:117:SER:OG	2.47	0.43
1:B:175:PHE:CD1	1:B:180:ILE:HG12	2.53	0.43
1:B:312:LYS:HD3	1:B:315:ARG:HB2	2.01	0.43
1:A:149:LEU:HD21	1:A:155:PRO:CD	2.48	0.43
1:B:357:ASN:HB2	1:B:358:SER:H	1.40	0.43
1:A:199:ILE:CD1	1:A:202:TRP:CZ2	2.94	0.43
1:A:225:ARG:NH1	1:A:237:GLU:OE1	2.51	0.43
1:B:399:LEU:O	1:B:402:TYR:HB3	2.18	0.43
1:B:248:ALA:O	1:B:249:HIS:C	2.61	0.43
1:A:469:ASP:HB3	1:A:488:TYR:OH	2.19	0.43
1:B:91:GLN:O	1:B:92:ALA:C	2.60	0.43
1:A:303:GLU:OE2	1:A:407:TYR:CE1	2.69	0.42
1:B:373:PHE:O	1:B:379:PRO:HA	2.19	0.42
1:A:174:GLY:O	1:A:180:ILE:HB	2.19	0.42
1:A:196:GLY:C	1:A:198:LYS:N	2.77	0.42
1:B:469:ASP:OD2	1:B:496:LYS:NZ	2.51	0.42
1:A:482:GLY:O	1:A:496:LYS:HD2	2.19	0.42
1:A:162:TRP:N	1:A:162:TRP:CD1	2.86	0.42
1:A:425:THR:O	1:A:426:LYS:CB	2.58	0.42
1:B:420:VAL:HG22	1:B:421:GLU:N	2.34	0.42
1:B:241:VAL:O	1:B:245:ILE:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:PHE:CD2	1:B:413:TYR:HD1	2.37	0.42
1:B:357:ASN:C	1:B:359:GLU:H	2.28	0.42
1:A:103:ILE:HD11	1:A:144:PHE:CE2	2.55	0.42
1:B:63:ASN:N	1:B:63:ASN:ND2	2.62	0.42
1:B:106:MET:HA	1:B:467:PHE:CZ	2.54	0.42
1:B:191:CYS:O	1:B:192:PHE:C	2.61	0.42
1:B:435:ASP:OD2	1:B:438:ARG:HD2	2.19	0.42
1:B:57:GLN:O	1:B:470:ASN:HB2	2.20	0.42
1:A:465:TRP:CZ2	2:A:1509:S55:O35	2.69	0.42
1:A:465:TRP:NE1	2:A:1509:S55:O35	2.53	0.42
1:A:385:TYR:OH	1:A:478:ILE:HD13	2.20	0.41
1:B:127:GLY:HA3	1:B:168:LEU:HG	2.02	0.41
1:A:74:THR:O	1:A:75:PHE:C	2.62	0.41
1:B:125:PRO:HB3	3:B:2002:HOH:O	2.20	0.41
1:B:126:GLY:HA3	1:B:131:ALA:HB1	2.03	0.41
1:B:277:MET:HB2	1:B:294:LEU:HD22	2.03	0.41
1:B:441:TYR:CD1	1:B:441:TYR:C	2.98	0.41
1:B:443:GLN:O	1:B:444:LYS:C	2.63	0.41
1:A:237:GLU:O	1:A:238:PRO:C	2.62	0.41
1:B:199:ILE:HD11	1:B:202:TRP:CH2	2.55	0.41
1:B:402:TYR:CD1	1:B:402:TYR:C	2.99	0.41
1:A:294:LEU:HD13	1:A:294:LEU:HA	1.71	0.41
1:A:376:ASN:C	1:A:378:LYS:H	2.28	0.41
1:A:103:ILE:HG23	1:A:148:LEU:HD23	2.03	0.41
1:A:441:TYR:CZ	1:A:445:HIS:CE1	3.08	0.41
1:A:465:TRP:HA	1:A:466:SER:HA	1.72	0.41
1:B:58:CYS:HB3	1:B:95:CYS:SG	2.61	0.41
1:B:296:PHE:CD2	1:B:314:MET:HG2	2.56	0.41
1:B:303:GLU:O	1:B:304:PRO:C	2.60	0.41
1:B:303:GLU:OE2	1:B:303:GLU:HA	2.21	0.41
1:B:413:TYR:CE2	1:B:460:LYS:HB2	2.55	0.41
1:B:439:THR:O	1:B:440:ASP:C	2.63	0.41
1:A:108:GLN:HE21	1:A:108:GLN:HB2	1.59	0.41
1:A:483:ILE:O	1:A:499:ALA:HB2	2.20	0.41
1:B:505:PHE:CD1	1:B:505:PHE:C	2.98	0.41
1:A:216:TYR:HD1	1:A:237:GLU:OE1	2.04	0.41
1:A:277:MET:HG2	1:A:294:LEU:HD22	2.02	0.41
1:B:196:GLY:C	1:B:198:LYS:N	2.79	0.41
1:B:350:VAL:HG22	1:B:369:VAL:HG11	2.03	0.41
1:B:101:GLU:O	1:B:104:LYS:CB	2.69	0.41
1:A:407:TYR:O	1:A:408:HIS:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:VAL:O	1:B:217:ALA:HB3	2.21	0.40
1:B:407:TYR:O	1:B:408:HIS:C	2.63	0.40
1:B:436:ALA:O	1:B:437:GLU:C	2.63	0.40
1:B:442:HIS:CE1	1:B:464:VAL:HG22	2.56	0.40
1:A:227:GLY:O	1:A:230:ASP:HB2	2.21	0.40
1:A:249:HIS:CE1	1:A:270:ILE:HB	2.56	0.40
1:B:278:GLU:HA	1:B:279:PRO:HD2	1.92	0.40
1:A:142:HIS:NE2	1:A:194:GLU:OE2	2.42	0.40
1:B:118:ILE:HA	1:B:141:TYR:CE1	2.57	0.40
1:B:199:ILE:O	1:B:199:ILE:HG12	2.21	0.40
1:B:207:GLU:HG2	1:B:273:ASN:CG	2.46	0.40
1:B:453:ILE:HD11	1:B:459:VAL:HB	2.02	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	458/532 (86%)	408 (89%)	42 (9%)	8 (2%)	7	23
1	B	470/532 (88%)	411 (87%)	49 (10%)	10 (2%)	5	18
All	All	928/1064 (87%)	819 (88%)	91 (10%)	18 (2%)	6	20

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	368	GLN
1	B	38	VAL
1	B	355	LYS
1	B	368	GLN
1	A	38	VAL

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Mol	Chain	Res	Type
1	B	358	SER
1	A	377	GLN
1	A	432	ALA
1	B	55	ALA
1	B	197	ASP
1	B	443	GLN
1	A	443	GLN
1	B	440	ASP
1	A	197	ASP
1	A	440	ASP
1	B	377	GLN
1	B	408	HIS

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	394/456 (86%)	333 (84%)	61 (16%)	2	9
1	B	401/456 (88%)	332 (83%)	69 (17%)	2	6
All	All	795/912 (87%)	665 (84%)	130 (16%)	2	7

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	40	ARG
1	A	45	GLN
1	A	54	SER
1	A	63	ASN
1	A	78	ARG
1	A	82	LYS
1	A	121	SER
1	A	128	ARG
1	A	133	VAL
1	A	138	VAL

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Mol	Chain	Res	Type
1	A	162	TRP
1	A	179	ARG
1	A	199	ILE
1	A	203	THR
1	A	214	ASN
1	A	228	LYS
1	A	242	THR
1	A	247	LEU
1	A	257	ARG
1	A	263	CYS
1	A	267	GLU
1	A	268	ILE
1	A	282	ASP
1	A	294	LEU
1	A	302	LEU
1	A	312	LYS
1	A	316	GLU
1	A	319	LYS
1	A	330	SER
1	A	332	LYS
1	A	333	LEU
1	A	342	MET
1	A	350	VAL
1	A	361	LEU
1	A	372	THR
1	A	376	ASN
1	A	392	VAL
1	A	396	LEU
1	A	398	LYS
1	A	401	VAL
1	A	405	GLU
1	A	406	THR
1	A	409	VAL
1	A	411	VAL
1	A	412	LEU
1	A	415	THR
1	A	424	LYS
1	A	425	THR
1	A	427	ILE
1	A	431	GLU
1	A	434	ARG
1	A	446	LEU

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Mol	Chain	Res	Type
1	A	453	ILE
1	A	457	VAL
1	A	459	VAL
1	A	470	ASN
1	A	472	GLU
1	A	474	ASN
1	A	475	LEU
1	A	493	ARG
1	B	37	VAL
1	B	38	VAL
1	B	40	ARG
1	B	42	ASP
1	B	45	GLN
1	B	54	SER
1	B	63	ASN
1	B	78	ARG
1	B	94	ASN
1	B	100	LYS
1	B	103	ILE
1	B	104	LYS
1	B	111	LEU
1	B	128	ARG
1	B	133	VAL
1	B	138	VAL
1	B	179	ARG
1	B	199	ILE
1	B	203	THR
1	B	206	ASN
1	B	216	TYR
1	B	228	LYS
1	B	242	THR
1	B	247	LEU
1	B	257	ARG
1	B	263	CYS
1	B	268	ILE
1	B	271	VAL
1	B	287	ILE
1	B	294	LEU
1	B	302	LEU
1	B	307	THR
1	B	312	LYS
1	B	319	LYS

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Mol	Chain	Res	Type
1	B	326	SER
1	B	334	LYS
1	B	350	VAL
1	B	351	THR
1	B	352	ASN
1	B	354	VAL
1	B	357	ASN
1	B	358	SER
1	B	359	GLU
1	B	364	GLU
1	B	368	GLN
1	B	371	LYS
1	B	372	THR
1	B	374	GLU
1	B	378	LYS
1	B	391	VAL
1	B	396	LEU
1	B	406	THR
1	B	408	HIS
1	B	409	VAL
1	B	411	VAL
1	B	412	LEU
1	B	415	THR
1	B	424	LYS
1	B	427	ILE
1	B	429	LEU
1	B	437	GLU
1	B	443	GLN
1	B	455	ASP
1	B	457	VAL
1	B	470	ASN
1	B	472	GLU
1	B	474	ASN
1	B	475	LEU
1	B	489	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	57	GLN
1	A	63	ASN

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Mol	Chain	Res	Type
1	A	66	ASN
1	A	77	GLN
1	A	94	ASN
1	A	97	HIS
1	A	108	GLN
1	A	151	ASN
1	A	166	GLN
1	A	206	ASN
1	A	214	ASN
1	A	261	GLN
1	A	273	ASN
1	A	284	GLN
1	A	352	ASN
1	A	368	GLN
1	A	389	GLN
1	A	470	ASN
1	A	474	ASN
1	A	504	ASN
1	B	45	GLN
1	B	57	GLN
1	B	63	ASN
1	B	66	ASN
1	B	77	GLN
1	B	94	ASN
1	B	108	GLN
1	B	178	HIS
1	B	206	ASN
1	B	214	ASN
1	B	264	GLN
1	B	352	ASN
1	B	357	ASN
1	B	389	GLN
1	B	470	ASN
1	B	474	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	S55	A	1509	-	41,42,42	1.58	4 (9%)	48,61,61	2.07	19 (39%)
2	S55	B	1509	-	39,41,42	1.44	5 (12%)	43,59,61	1.66	9 (20%)

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	S55	A	1509	-	-	5/18/65/65	0/5/5/5
2	S55	B	1509	-	-	8/15/62/65	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1509	S55	O18-C19	5.50	1.45	1.35
2	A	1509	S55	O18-C19	5.50	1.45	1.35
2	A	1509	S55	O22-C21	5.47	1.45	1.33
2	A	1509	S55	C8-N9	-3.67	1.34	1.38
2	B	1509	S55	C8-N9	-3.54	1.34	1.38
2	B	1509	S55	C5-C7	-3.33	1.38	1.44
2	A	1509	S55	C5-C7	-3.05	1.38	1.44
2	B	1509	S55	C5-C4	-2.55	1.38	1.41
2	B	1509	S55	C4-N9	-2.25	1.34	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1509	S55	O22-C21-C20	5.04	119.12	112.65
2	A	1509	S55	C14-C13-C8	-4.47	104.32	112.63
2	A	1509	S55	C26-C25-C16	-4.03	105.70	114.15
2	B	1509	S55	C26-C25-C16	-3.72	106.35	114.15
2	B	1509	S55	C17-O18-C19	3.71	123.88	116.41
2	A	1509	S55	O22-C21-O24	-3.66	116.51	123.50
2	B	1509	S55	O33-C32-C31	-3.59	103.22	109.70
2	A	1509	S55	O27-C28-O33	-3.37	101.81	110.69
2	B	1509	S55	C28-C29-C30	3.26	116.86	110.01
2	A	1509	S55	O33-C28-C29	3.19	116.93	110.37
2	B	1509	S55	C14-C13-C8	-3.14	106.79	112.63
2	A	1509	S55	C23-O22-C21	3.07	121.54	115.85
2	A	1509	S55	O18-C19-C20	-2.87	121.08	125.60
2	A	1509	S55	O35-C31-C30	-2.81	103.75	110.38
2	A	1509	S55	C17-O18-C19	2.60	121.65	116.41
2	A	1509	S55	O37-C29-C30	-2.55	104.37	110.38
2	A	1509	S55	C5-C7-C8	-2.52	105.19	106.90
2	B	1509	S55	C10-C7-C8	2.50	125.03	122.07
2	A	1509	S55	C10-C11-N12	2.43	115.25	109.98
2	A	1509	S55	C28-C29-C30	2.43	115.11	110.01
2	A	1509	S55	C10-C7-C8	2.42	124.94	122.07
2	A	1509	S55	C6-C5-C4	2.41	121.33	118.84
2	A	1509	S55	O33-C32-C31	-2.36	105.45	109.70
2	B	1509	S55	C3-C4-C5	-2.33	119.94	122.19
2	B	1509	S55	C5-C7-C8	-2.29	105.34	106.90
2	A	1509	S55	O36-C30-C29	-2.27	105.02	110.38
2	A	1509	S55	O33-C32-C33	-2.11	101.21	106.44
2	B	1509	S55	C28-O33-C32	-2.04	109.73	113.72

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1509	S55	C20-C21-O22-C23
2	A	1509	S55	O33-C28-O27-C17
2	B	1509	S55	C15-C20-C21-O22
2	B	1509	S55	O33-C28-O27-C17
2	A	1509	S55	O24-C21-O22-C23
2	B	1509	S55	O33-C32-C33-O34
2	A	1509	S55	O33-C32-C33-O34
2	A	1509	S55	C31-C32-C33-O34
2	B	1509	S55	C31-C32-C33-O34
2	B	1509	S55	C20-C21-O22-C23

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Mol	Chain	Res	Type	Atoms
2	B	1509	S55	C16-C17-O27-C28
2	B	1509	S55	C19-C20-C21-O22
2	B	1509	S55	O18-C17-O27-C28

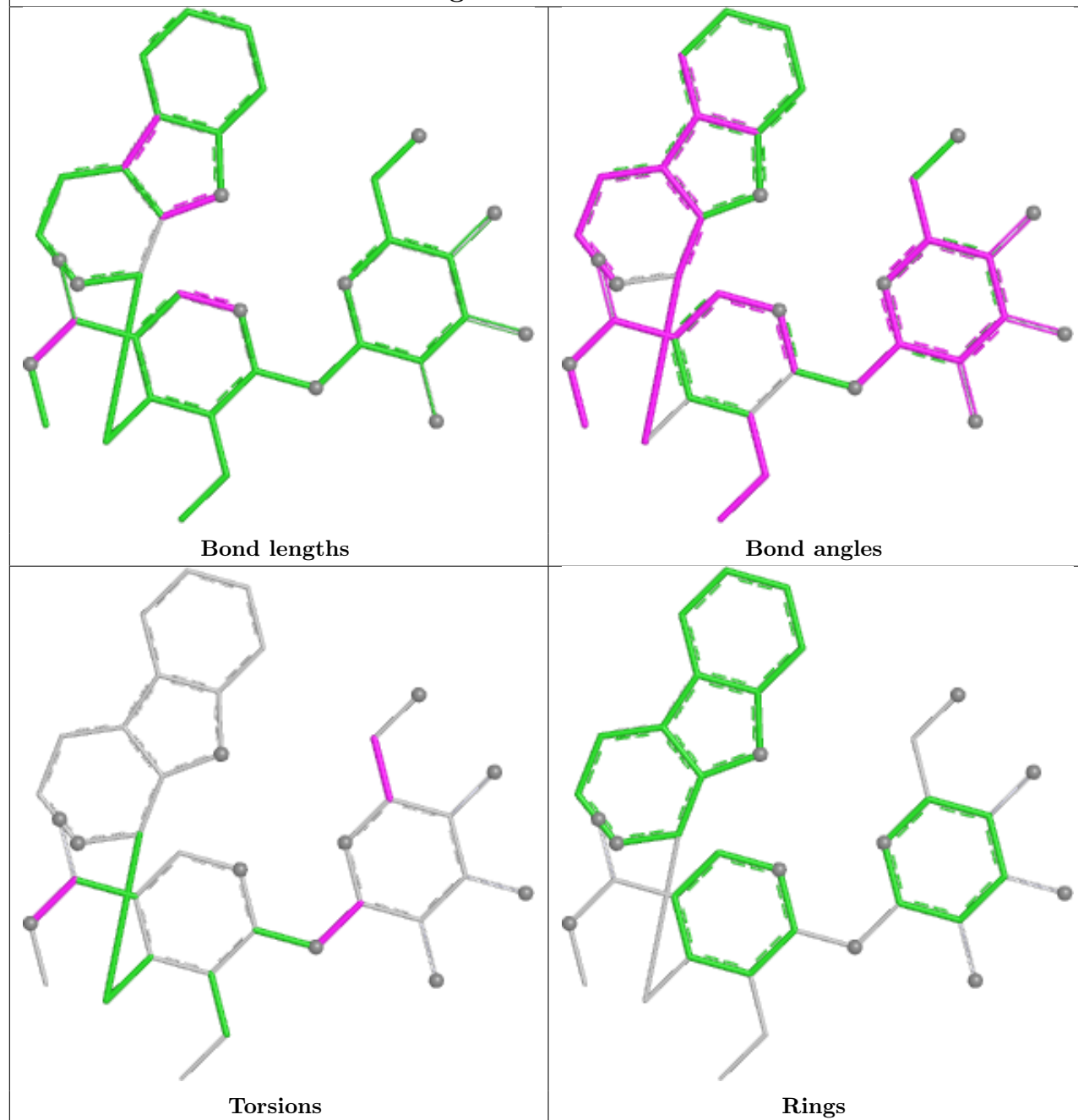
There are no ring outliers.

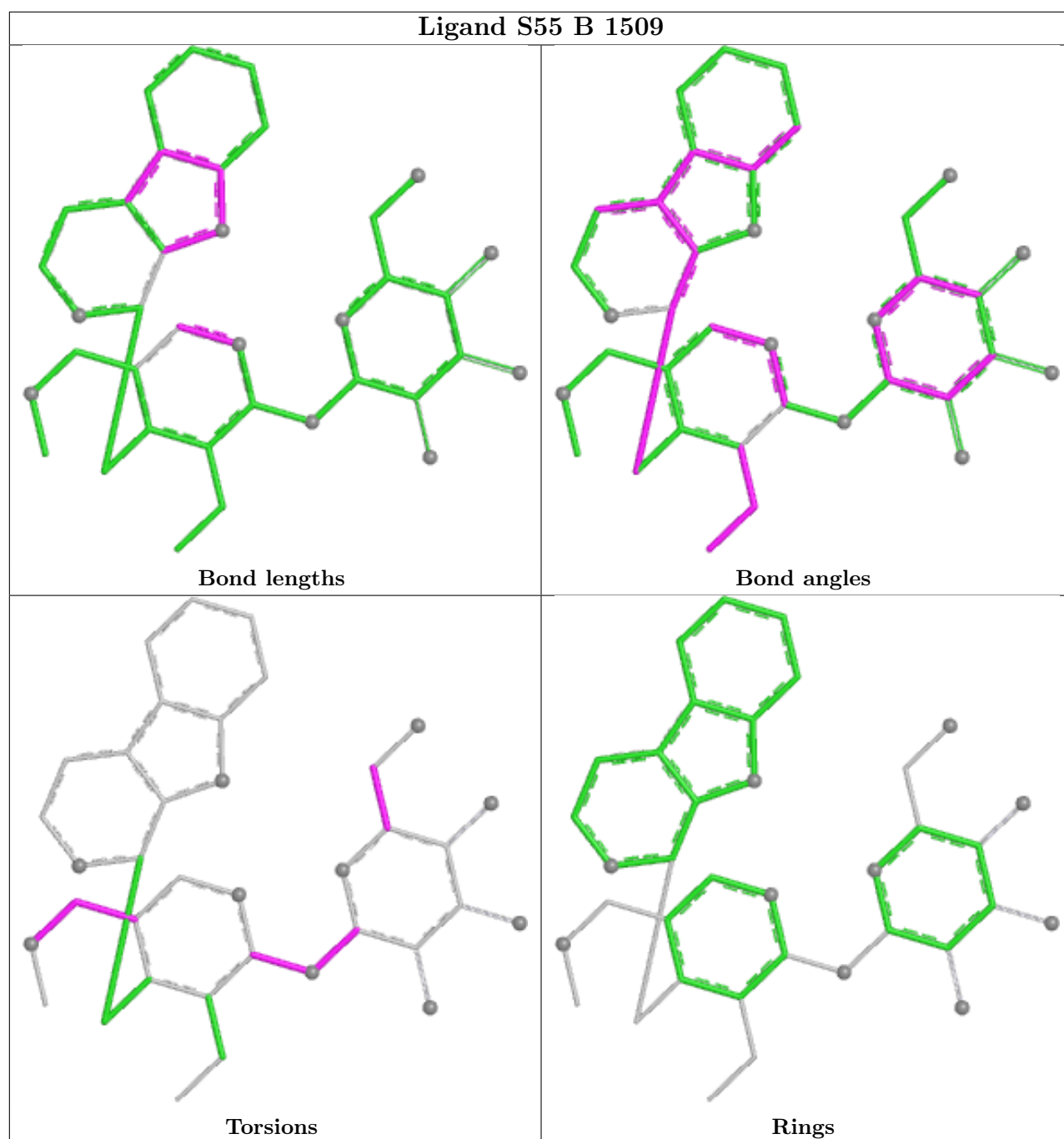
2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1509	S55	18	0
2	B	1509	S55	13	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 S55 A 1509





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	464/532 (87%)	-0.43	0 100 100	3, 8, 13, 17	0
1	B	472/532 (88%)	-0.48	0 100 100	3, 9, 16, 34	0
All	All	936/1064 (87%)	-0.45	0 100 100	3, 9, 14, 34	0

There are no RSRZ outliers to report.

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](#)

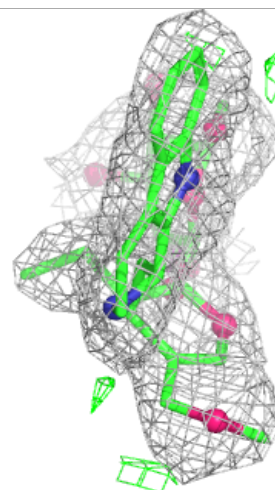
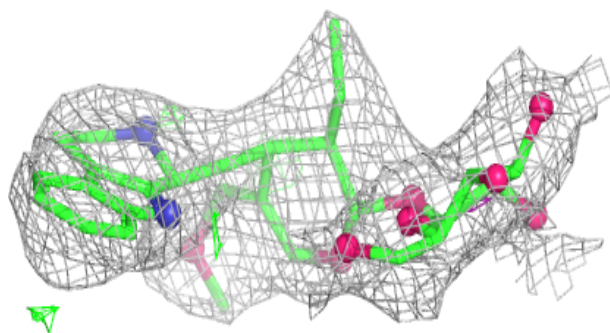
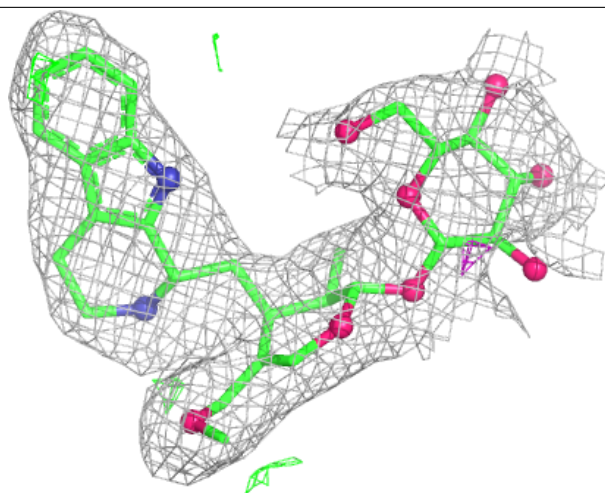
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

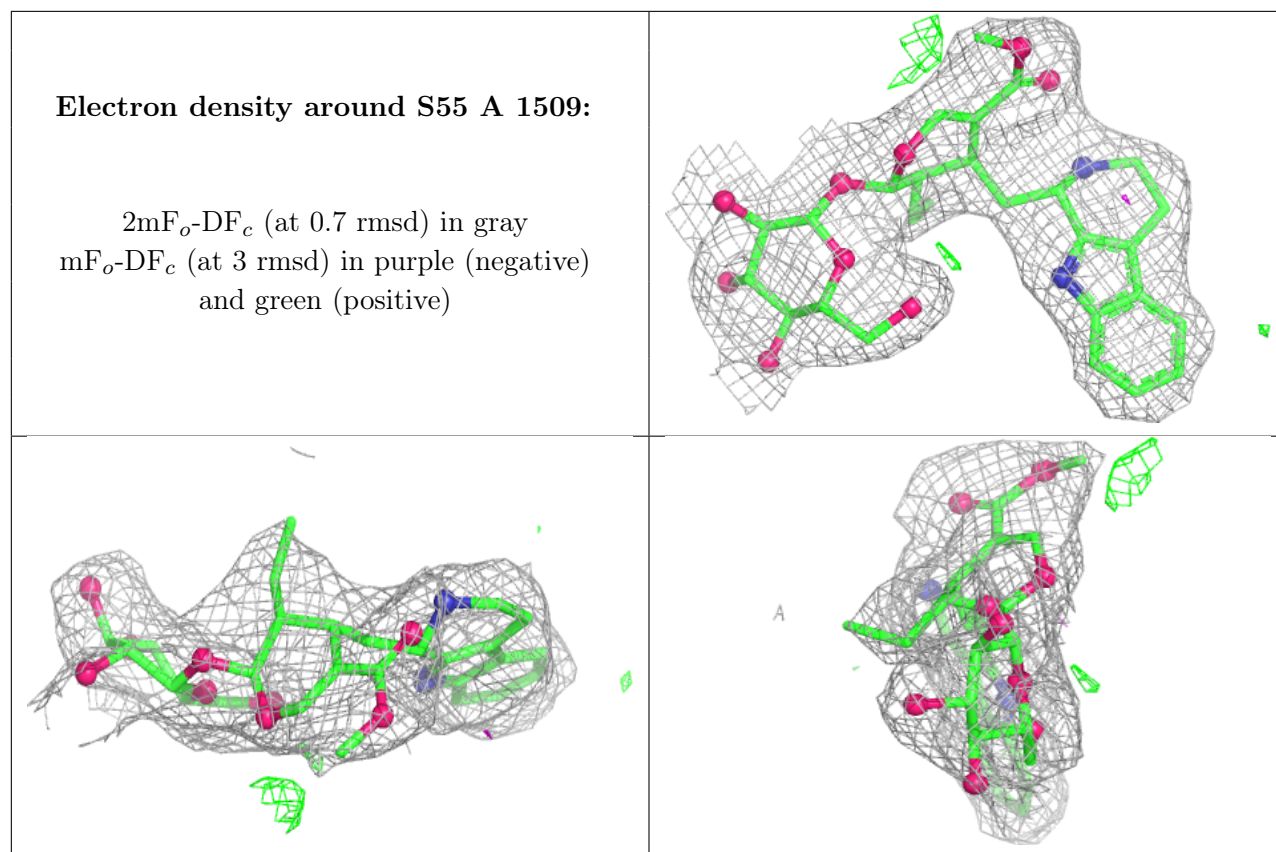
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	S55	B	1509	37/38	0.93	0.08	10,17,25,30	0
2	S55	A	1509	38/38	0.94	0.08	2,18,23,28	0

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 S55 B 1509:

$2mF_o-DF_c$ (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.