



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:53 AM UTC

PDB ID : 3C6T / pdb_00003c6t
Title : Crystal Structure of HIV Reverse Transcriptase in complex with inhibitor 14
Authors : Yan, Y.; Prasad, S.
Deposited on : 2008-02-05
Resolution : 2.70 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

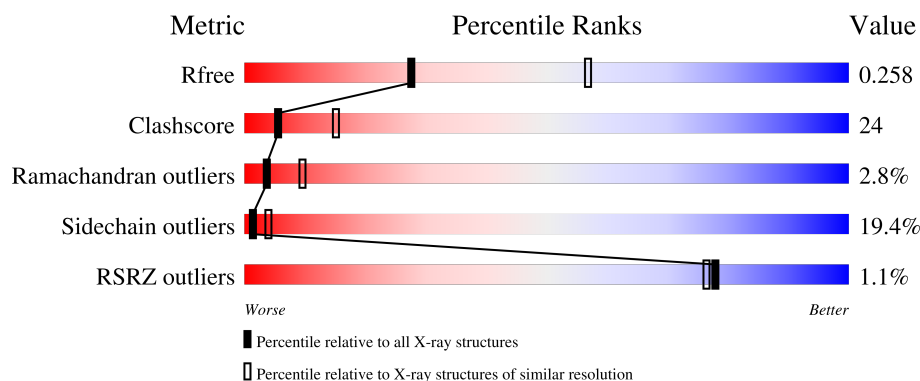
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	563	50%38%10%..
2	B	443	2% 42%37%11%•9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	M14	A	561	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8293 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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4550	2938	762	842	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P04585
A	-1	ASN	-	expression tag	UNP P04585
A	0	SER	-	expression tag	UNP P04585

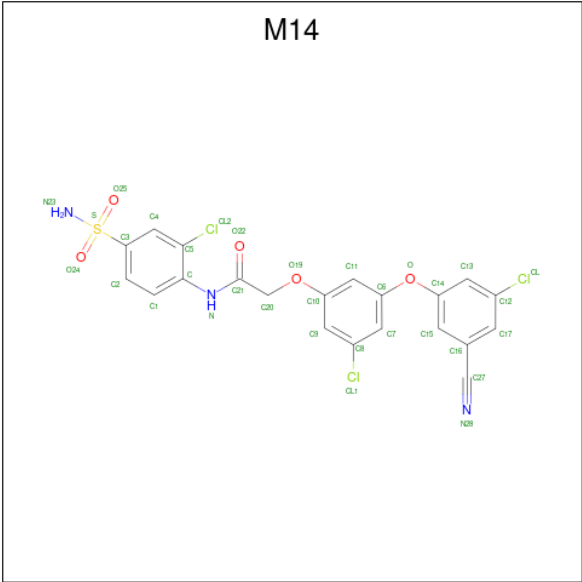
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3344	2176	554	608	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P04585
B	-1	ASN	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585

- Molecule 3 is 2-[3-chloro-5-(3-chloro-5-cyanophenoxy)phenoxy]-N-(2-chloro-4-sulfamoylphenyl)acetamide (CCD ID: M14) (formula: C₂₁H₁₄Cl₃N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	33	21	3	3	5	0	0

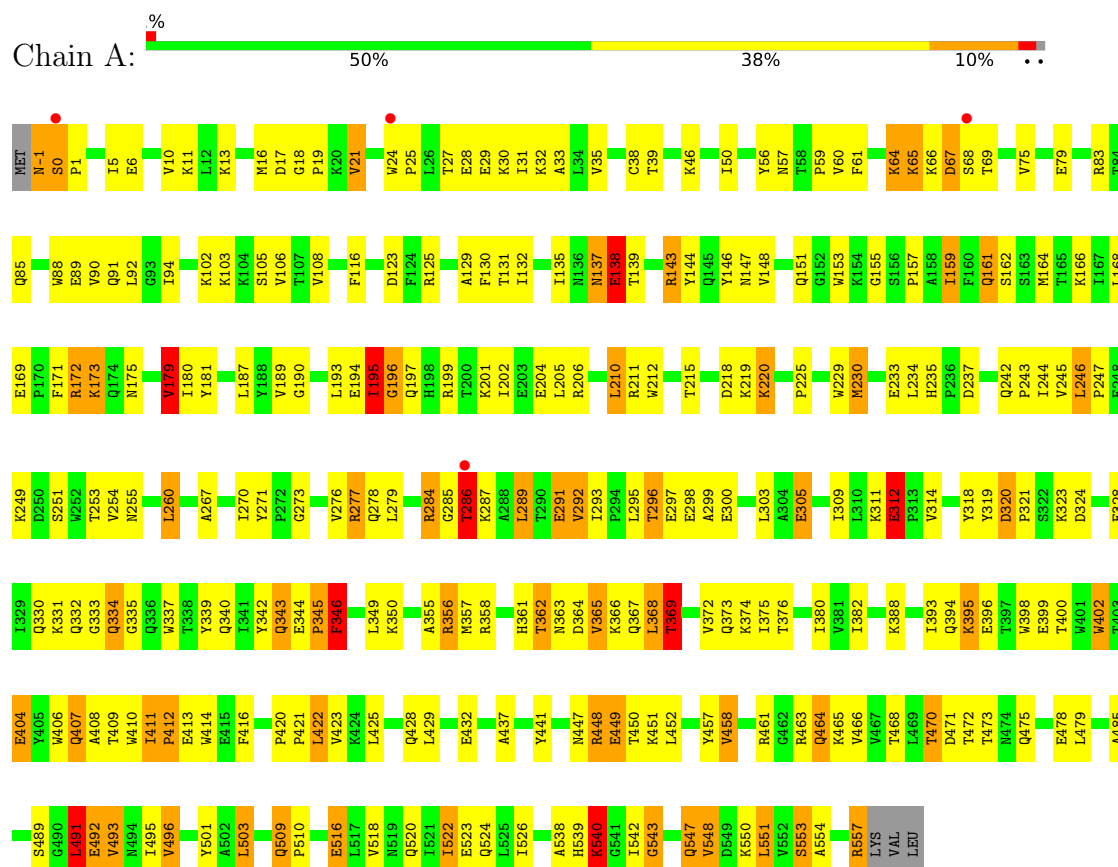
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	209	Total	O	0	0
			209	209		
4	B	157	Total	O	0	0
			157	157		

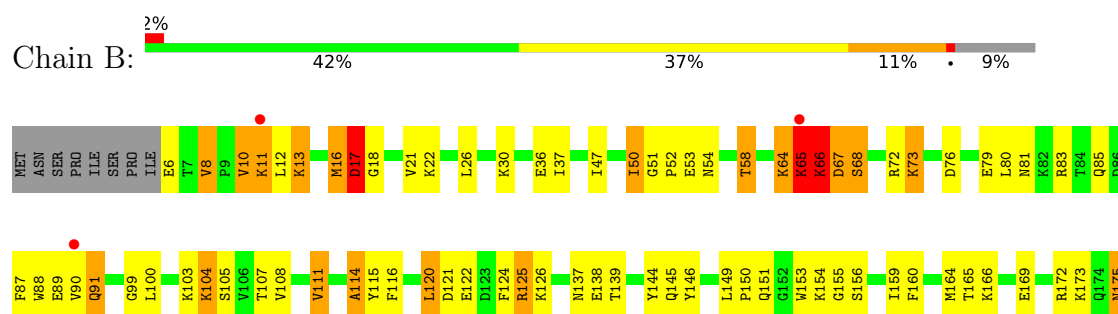
3 Residue-property plots

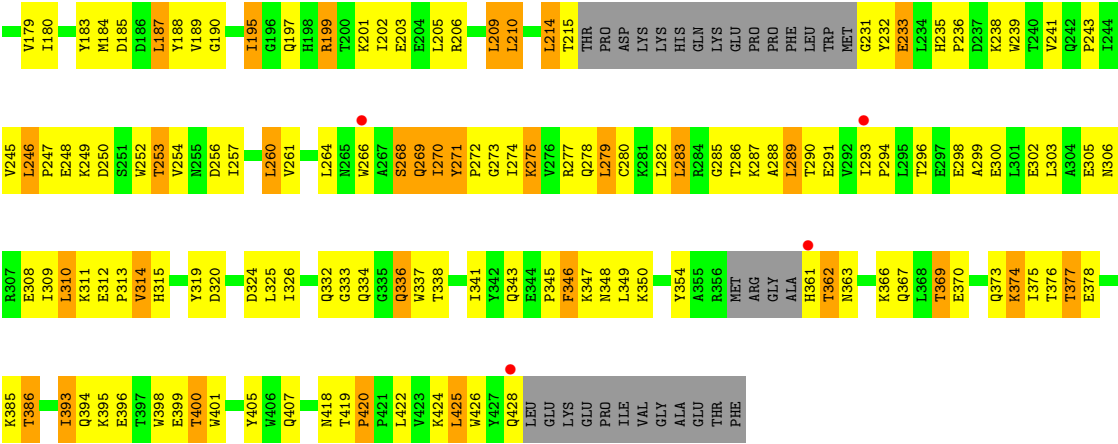
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: Reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.29Å 154.51Å 155.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 2.70 47.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.3 (47.22-2.70) 93.4 (47.22-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.281 (Not available) , 0.258	Depositor DCC
R_{free} test set	1857 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8293	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: M14

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	1.10	7/4667 (0.1%)	1.26	35/6341 (0.6%)
2	B	1.06	2/3438 (0.1%)	1.24	22/4671 (0.5%)
All	All	1.08	9/8105 (0.1%)	1.25	57/11012 (0.5%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	VAL	CA-CB	6.83	1.62	1.54
1	A	496	VAL	CA-CB	6.12	1.62	1.54
1	A	509	GLN	C-O	-5.93	1.21	1.23
1	A	369	THR	CA-CB	5.49	1.62	1.53
2	B	114	ALA	CA-CB	-5.39	1.44	1.53
2	B	50	ILE	CA-C	-5.17	1.47	1.52
1	A	365	VAL	C-O	-5.13	1.18	1.24
1	A	21	VAL	CA-CB	5.09	1.61	1.54
1	A	179	VAL	CA-CB	5.03	1.60	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	0	SER	CA-C-N	12.14	135.01	119.84
1	A	0	SER	C-N-CA	12.14	135.01	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	420	PRO	CA-C-N	9.05	129.63	119.32
2	B	420	PRO	C-N-CA	9.05	129.63	119.32
1	A	540	LYS	N-CA-C	-8.94	92.00	107.20
2	B	233	GLU	N-CA-C	8.59	123.72	107.75
1	A	382	ILE	N-CA-C	8.37	118.29	110.42
1	A	172	ARG	N-CA-C	-8.25	102.24	111.07
1	A	493	VAL	CB-CA-C	-8.12	97.88	110.95
1	A	320	ASP	CA-C-N	7.52	127.69	119.87
1	A	320	ASP	C-N-CA	7.52	127.69	119.87
1	A	246	LEU	CA-C-N	7.30	128.97	119.84
1	A	246	LEU	C-N-CA	7.30	128.97	119.84
1	A	344	GLU	CA-C-N	7.21	128.86	119.84
1	A	344	GLU	C-N-CA	7.21	128.86	119.84
1	A	414	TRP	N-CA-C	6.86	120.15	109.52
2	B	156	SER	CA-C-N	-6.40	113.10	119.56
2	B	156	SER	C-N-CA	-6.40	113.10	119.56
1	A	346	PHE	CB-CA-C	6.31	119.15	110.06
2	B	386	THR	CA-C-N	6.30	126.82	120.14
2	B	386	THR	C-N-CA	6.30	126.82	120.14
1	A	286	THR	N-CA-C	6.19	123.98	110.80
1	A	491	LEU	N-CA-C	6.13	123.86	110.80
2	B	398	TRP	N-CA-C	-6.02	104.62	111.07
1	A	432	GLU	CA-C-N	6.00	126.01	119.89
1	A	432	GLU	C-N-CA	6.00	126.01	119.89
1	A	470	THR	CA-C-N	-5.93	115.08	123.03
1	A	470	THR	C-N-CA	-5.93	115.08	123.03
2	B	268	SER	N-CA-C	-5.88	102.20	110.50
2	B	348	ASN	N-CA-C	5.88	118.23	109.59
2	B	13	LYS	CA-C-N	5.68	125.69	119.89
2	B	13	LYS	C-N-CA	5.68	125.69	119.89
2	B	51	GLY	CA-C-N	5.62	125.73	119.32
2	B	51	GLY	C-N-CA	5.62	125.73	119.32
1	A	411	ILE	CA-C-N	5.62	126.86	119.84
1	A	411	ILE	C-N-CA	5.62	126.86	119.84
1	A	423	VAL	CB-CA-C	5.54	117.78	110.91
2	B	271	TYR	CA-C-N	5.37	126.55	119.84
2	B	271	TYR	C-N-CA	5.37	126.55	119.84
1	A	343	GLN	N-CA-C	-5.33	105.90	112.72
1	A	0	SER	N-CA-C	5.29	121.50	109.81
2	B	362	THR	N-CA-C	5.27	118.28	107.37
1	A	18	GLY	CA-C-N	-5.23	114.57	119.85
1	A	18	GLY	C-N-CA	-5.23	114.57	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LEU	N-CA-C	5.21	116.65	111.07
2	B	54	ASN	CA-C-N	5.21	126.24	120.45
2	B	54	ASN	C-N-CA	5.21	126.24	120.45
1	A	461	ARG	N-CA-C	-5.21	104.37	111.56
1	A	495	ILE	CA-C-N	-5.13	115.86	122.99
1	A	495	ILE	C-N-CA	-5.13	115.86	122.99
1	A	492	GLU	N-CA-C	5.08	117.24	107.44
2	B	17	ASP	N-CA-C	5.07	114.84	108.45
2	B	144	TYR	CB-CA-C	-5.07	101.19	110.62
1	A	161	GLN	N-CA-C	-5.07	105.84	111.36
2	B	195	ILE	N-CA-C	5.07	115.79	110.62
1	A	503	LEU	N-CA-C	-5.05	105.67	111.07
1	A	473	THR	N-CA-C	-5.02	101.66	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4550	0	4601	232	0
2	B	3344	0	3369	157	0
3	A	33	0	14	10	0
4	A	209	0	0	22	0
4	B	157	0	0	10	0
All	All	8293	0	7984	376	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 24.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HD21	1:A:201:LYS:CE	1.54	1.20
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.16	1.08
1:A:175:ASN:HD21	1:A:201:LYS:HE3	1.17	1.07
1:A:175:ASN:ND2	1:A:201:LYS:HE2	1.68	1.07
1:A:237:ASP:HB3	4:A:756:HOH:O	1.59	0.99
1:A:35:VAL:O	1:A:39:THR:HG23	1.61	0.99
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.30	0.96
1:A:277:ARG:CD	1:A:334:GLN:NE2	2.27	0.96
2:B:333:GLY:O	2:B:336:GLN:NE2	2.01	0.93
2:B:253:THR:HG22	2:B:256:ASP:H	1.36	0.91
1:A:125:ARG:HG2	1:A:146:TYR:O	1.73	0.89
1:A:197:GLN:HB2	4:A:662:HOH:O	1.76	0.86
2:B:270:ILE:HG22	2:B:346:PHE:HB3	1.57	0.86
1:A:296:THR:HG22	1:A:299:ALA:H	1.40	0.86
2:B:396:GLU:O	2:B:400:THR:HG22	1.74	0.86
2:B:250:ASP:HA	4:B:583:HOH:O	1.77	0.85
1:A:516:GLU:O	1:A:520:GLN:HG3	1.75	0.85
2:B:345:PRO:O	2:B:346:PHE:HB2	1.78	0.84
2:B:350:LYS:HE2	2:B:378:GLU:OE1	1.78	0.84
1:A:466:VAL:CG2	1:A:551:LEU:HD23	2.09	0.83
1:A:273:GLY:HA2	1:A:332:GLN:NE2	1.93	0.83
1:A:296:THR:HG23	1:A:298:GLU:OE2	1.79	0.82
1:A:277:ARG:HD3	1:A:334:GLN:NE2	1.94	0.82
1:A:437:ALA:HB1	1:A:492:GLU:O	1.79	0.82
1:A:66:LYS:O	1:A:67:ASP:HB2	1.80	0.80
1:A:277:ARG:HD3	1:A:334:GLN:HE21	1.48	0.78
2:B:273:GLY:O	2:B:275:LYS:HG2	1.83	0.78
1:A:175:ASN:ND2	1:A:201:LYS:HE3	1.91	0.78
1:A:173:LYS:HE3	1:A:173:LYS:HA	1.64	0.77
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.66	0.77
1:A:175:ASN:HD22	1:A:201:LYS:HE2	1.48	0.77
1:A:16:MET:HE2	1:A:83:ARG:HA	1.66	0.77
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.18	0.77
2:B:214:LEU:H	2:B:214:LEU:HD23	1.48	0.76
1:A:173:LYS:HA	1:A:173:LYS:CE	2.16	0.76
1:A:522:ILE:O	1:A:526:ILE:HG13	1.86	0.75
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.35	0.75
1:A:24:TRP:HB3	4:A:572:HOH:O	1.84	0.75
1:A:123:ASP:OD1	1:A:123:ASP:N	2.20	0.74
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.69	0.74
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.23	0.74
2:B:319:TYR:OH	2:B:385:LYS:HD2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLN:OE1	2:B:400:THR:HG21	1.88	0.73
2:B:66:LYS:HB2	4:B:624:HOH:O	1.86	0.73
2:B:363:ASN:O	2:B:367:GLN:HG3	1.89	0.73
1:A:211:ARG:O	1:A:211:ARG:HD3	1.89	0.72
1:A:172:ARG:HH21	1:A:180:ILE:HB	1.52	0.72
1:A:478:GLU:HG2	4:A:576:HOH:O	1.89	0.72
1:A:162:SER:CB	2:B:52:PRO:HG3	2.20	0.71
2:B:85:GLN:O	2:B:89:GLU:HB3	1.90	0.71
1:A:91:GLN:HG2	4:A:640:HOH:O	1.91	0.71
1:A:311:LYS:O	1:A:312:GLU:OE1	2.09	0.71
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.55	0.70
1:A:277:ARG:HG3	1:A:334:GLN:HE22	1.55	0.70
2:B:260:LEU:HD22	2:B:264:LEU:HD12	1.75	0.69
1:A:195:ILE:HG12	1:A:199:ARG:HE	1.58	0.69
2:B:195:ILE:O	2:B:199:ARG:HG2	1.93	0.69
1:A:376:THR:O	1:A:380:ILE:HD12	1.94	0.68
1:A:365:VAL:O	1:A:369:THR:CG2	2.42	0.68
1:A:400:THR:O	1:A:404:GLU:HG3	1.94	0.67
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.76	0.67
1:A:255:ASN:HB2	1:A:289:LEU:HD22	1.77	0.66
2:B:268:SER:O	2:B:269:GLN:HB2	1.94	0.66
1:A:365:VAL:O	1:A:369:THR:HG22	1.96	0.66
2:B:305:GLU:O	2:B:309:ILE:HG13	1.95	0.66
1:A:277:ARG:CG	1:A:334:GLN:HE22	2.09	0.65
1:A:66:LYS:O	1:A:67:ASP:CB	2.45	0.65
2:B:314:VAL:O	2:B:315:HIS:HB3	1.97	0.65
2:B:373:GLN:O	2:B:377:THR:HG23	1.96	0.65
1:A:331:LYS:HE3	1:A:364:ASP:OD1	1.96	0.65
1:A:448:ARG:HH11	1:A:448:ARG:CG	2.08	0.65
2:B:13:LYS:HB2	2:B:16:MET:HE3	1.80	0.64
2:B:283:LEU:HA	2:B:287:LYS:HZ1	1.62	0.64
1:A:277:ARG:HD2	1:A:334:GLN:NE2	2.11	0.64
1:A:16:MET:CE	1:A:83:ARG:HA	2.27	0.64
2:B:396:GLU:O	2:B:400:THR:CG2	2.45	0.64
1:A:273:GLY:HA2	1:A:332:GLN:HE21	1.63	0.63
2:B:11:LYS:HE2	2:B:11:LYS:N	2.14	0.63
1:A:16:MET:HE3	1:A:83:ARG:HG2	1.80	0.63
1:A:172:ARG:NH2	1:A:180:ILE:HB	2.13	0.63
1:A:173:LYS:HE3	1:A:173:LYS:CA	2.29	0.63
2:B:64:LYS:O	2:B:65:LYS:HB2	1.98	0.63
2:B:210:LEU:HD12	2:B:210:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:O	1:A:31:ILE:HG13	1.98	0.62
2:B:260:LEU:HD22	2:B:264:LEU:CD1	2.29	0.62
1:A:428:GLN:HG2	4:A:704:HOH:O	1.97	0.62
1:A:194:GLU:CD	1:A:194:GLU:H	2.08	0.62
1:A:277:ARG:CG	1:A:334:GLN:NE2	2.62	0.62
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.81	0.61
1:A:210:LEU:C	1:A:212:TRP:H	2.07	0.61
1:A:466:VAL:CG2	1:A:551:LEU:CD2	2.79	0.61
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.34	0.61
2:B:185:ASP:HB2	4:B:498:HOH:O	2.01	0.61
1:A:543:GLY:O	1:A:547:GLN:NE2	2.34	0.60
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.34	0.60
1:A:64:LYS:HE2	1:A:69:THR:HA	1.83	0.60
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.67	0.60
1:A:394:GLN:HG3	4:A:635:HOH:O	2.02	0.60
2:B:306:ASN:O	2:B:310:LEU:HB2	2.01	0.60
2:B:314:VAL:O	2:B:315:HIS:CB	2.49	0.60
2:B:270:ILE:O	2:B:272:PRO:HD3	2.01	0.59
2:B:422:LEU:HD23	2:B:425:LEU:HD21	1.83	0.59
1:A:162:SER:HB3	2:B:52:PRO:HG3	1.84	0.59
2:B:111:VAL:O	2:B:111:VAL:CG1	2.49	0.59
1:A:543:GLY:HA2	2:B:285:GLY:O	2.03	0.59
2:B:246:LEU:HD21	2:B:310:LEU:HD21	1.84	0.59
1:A:210:LEU:C	1:A:212:TRP:N	2.55	0.59
1:A:287:LYS:HB2	1:A:291:GLU:HG2	1.85	0.59
1:A:318:TYR:CZ	3:A:561:M14:H20A	2.38	0.59
1:A:277:ARG:HG3	1:A:334:GLN:NE2	2.17	0.59
1:A:409:THR:HG22	1:A:410:TRP:N	2.17	0.58
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.85	0.58
1:A:289:LEU:HD12	4:A:800:HOH:O	2.03	0.58
1:A:475:GLN:HG2	1:A:501:TYR:CD2	2.38	0.58
2:B:175:ASN:ND2	2:B:201:LYS:HD2	2.18	0.58
1:A:449:GLU:HG3	4:A:705:HOH:O	2.02	0.58
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.85	0.58
1:A:466:VAL:HG23	1:A:551:LEU:CD2	2.34	0.58
1:A:246:LEU:HD22	1:A:260:LEU:CD2	2.34	0.58
1:A:318:TYR:CD1	3:A:561:M14:H20A	2.39	0.58
1:A:457:TYR:CD1	1:A:457:TYR:C	2.82	0.58
1:A:318:TYR:CE2	3:A:561:M14:H20A	2.39	0.57
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.87	0.57
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:O	1:A:522:ILE:HD12	2.05	0.57
2:B:336:GLN:C	2:B:337:TRP:CD1	2.83	0.57
1:A:284:ARG:HH11	1:A:285:GLY:HA3	1.69	0.57
2:B:302:GLU:O	2:B:303:LEU:C	2.46	0.57
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.87	0.57
1:A:357:MET:HB3	4:A:786:HOH:O	2.05	0.56
2:B:308:GLU:O	2:B:311:LYS:HG2	2.05	0.56
1:A:318:TYR:CE1	3:A:561:M14:H20A	2.41	0.56
1:A:318:TYR:CD2	3:A:561:M14:H20A	2.40	0.56
1:A:466:VAL:HG23	1:A:551:LEU:HD23	1.86	0.56
1:A:284:ARG:O	1:A:284:ARG:NH1	2.39	0.56
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.88	0.56
1:A:396:GLU:HB2	4:A:580:HOH:O	2.06	0.56
1:A:543:GLY:CA	2:B:285:GLY:O	2.54	0.56
1:A:64:LYS:O	1:A:65:LYS:HB2	2.04	0.56
1:A:179:VAL:CG2	3:A:561:M14:CL1	2.91	0.56
1:A:171:PHE:CD1	1:A:171:PHE:C	2.84	0.55
2:B:124:PHE:O	2:B:125:ARG:C	2.46	0.55
2:B:246:LEU:HD21	2:B:310:LEU:CD2	2.36	0.55
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.36	0.55
1:A:56:TYR:O	1:A:143:ARG:NH2	2.34	0.55
2:B:21:VAL:CG2	2:B:79:GLU:HG3	2.37	0.55
1:A:91:GLN:C	1:A:92:LEU:HD22	2.31	0.55
1:A:157:PRO:HD2	4:A:568:HOH:O	2.06	0.55
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.42	0.54
1:A:194:GLU:O	1:A:195:ILE:C	2.50	0.54
1:A:210:LEU:O	1:A:212:TRP:N	2.39	0.54
1:A:318:TYR:CG	3:A:561:M14:H20A	2.43	0.54
1:A:320:ASP:O	1:A:343:GLN:NE2	2.40	0.54
1:A:106:VAL:HA	1:A:189:VAL:O	2.08	0.54
2:B:165:THR:C	2:B:166:LYS:HE2	2.32	0.54
2:B:232:TYR:HE1	4:B:570:HOH:O	1.90	0.54
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.88	0.54
2:B:247:PRO:HB2	2:B:249:LYS:HE3	1.89	0.54
1:A:312:GLU:O	1:A:312:GLU:CD	2.51	0.54
2:B:12:LEU:CD2	2:B:17:ASP:HA	2.38	0.54
2:B:293:ILE:HB	2:B:294:PRO:HD2	1.90	0.53
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.90	0.53
2:B:215:THR:HA	4:B:486:HOH:O	2.07	0.53
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.90	0.53
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:HG3	1:A:448:ARG:NH1	2.10	0.53
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.90	0.53
1:A:346:PHE:N	1:A:346:PHE:CD1	2.75	0.53
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.43	0.53
2:B:338:THR:HB	4:B:449:HOH:O	2.09	0.53
1:A:164:MET:HE3	1:A:187:LEU:HD21	1.90	0.52
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.74	0.52
2:B:13:LYS:HD2	2:B:85:GLN:N	2.24	0.52
1:A:300:GLU:HG3	4:A:801:HOH:O	2.09	0.52
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.44	0.52
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.43	0.52
1:A:210:LEU:O	1:A:211:ARG:C	2.53	0.52
1:A:450:THR:HB	1:A:452:LEU:HG	1.90	0.52
2:B:107:THR:HA	2:B:232:TYR:O	2.08	0.52
2:B:325:LEU:HD12	2:B:385:LYS:CG	2.40	0.52
1:A:409:THR:CG2	1:A:410:TRP:N	2.73	0.52
1:A:17:ASP:O	1:A:83:ARG:HD3	2.09	0.51
1:A:464:GLN:HG2	1:A:465:LYS:N	2.25	0.51
1:A:10:VAL:HG12	1:A:11:LYS:N	2.26	0.51
1:A:284:ARG:NH1	1:A:285:GLY:HA3	2.25	0.51
1:A:485:ALA:O	1:A:489:SER:HB3	2.09	0.51
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.39	0.51
2:B:254:VAL:CG1	2:B:289:LEU:HA	2.41	0.51
2:B:361:HIS:O	2:B:361:HIS:CG	2.64	0.51
2:B:324:ASP:O	2:B:343:GLN:HG2	2.11	0.51
1:A:5:ILE:HG22	1:A:212:TRP:CZ3	2.45	0.51
1:A:466:VAL:HG22	1:A:551:LEU:HD23	1.91	0.51
2:B:166:LYS:HE2	2:B:166:LYS:N	2.25	0.51
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.93	0.50
2:B:138:GLU:HG2	2:B:139:THR:HG23	1.93	0.50
1:A:225:PRO:HG3	3:A:561:M14:O25	2.11	0.50
2:B:122:GLU:O	2:B:125:ARG:HG3	2.12	0.50
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.47	0.50
1:A:333:GLY:O	1:A:335:GLY:N	2.45	0.50
1:A:366:LYS:NZ	4:A:685:HOH:O	2.43	0.49
2:B:422:LEU:CD2	2:B:425:LEU:HD21	2.42	0.49
2:B:199:ARG:HD3	2:B:233:GLU:OE1	2.12	0.49
2:B:206:ARG:HH21	2:B:231:GLY:N	2.10	0.49
2:B:282:LEU:HB3	2:B:293:ILE:HD11	1.93	0.49
2:B:312:GLU:OE2	2:B:313:PRO:HD2	2.12	0.49
1:A:25:PRO:HD2	4:A:572:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.43	0.49
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.94	0.49
1:A:447:ASN:OD1	1:A:447:ASN:C	2.55	0.49
1:A:229:TRP:CD2	1:A:230:MET:HB2	2.48	0.49
2:B:17:ASP:CG	2:B:18:GLY:N	2.70	0.49
1:A:273:GLY:HA2	1:A:332:GLN:HE22	1.74	0.48
1:A:30:LYS:HE3	1:A:61:PHE:CE1	2.48	0.48
1:A:253:THR:HA	1:A:291:GLU:O	2.12	0.48
1:A:116:PHE:O	1:A:148:VAL:HG11	2.12	0.48
2:B:64:LYS:HA	2:B:64:LYS:HD3	1.52	0.48
1:A:5:ILE:HG12	1:A:6:GLU:O	2.13	0.48
2:B:268:SER:O	2:B:269:GLN:CB	2.61	0.48
2:B:362:THR:HG22	2:B:367:GLN:HG2	1.95	0.48
1:A:441:TYR:O	1:A:548:VAL:HG21	2.14	0.48
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.49	0.48
2:B:175:ASN:HD21	2:B:201:LYS:HD2	1.79	0.48
1:A:365:VAL:O	1:A:369:THR:HG23	2.14	0.48
1:A:406:TRP:HH2	2:B:418:ASN:OD1	1.97	0.48
1:A:538:ALA:O	1:A:540:LYS:HD2	2.14	0.48
2:B:180:ILE:HA	2:B:188:TYR:O	2.14	0.48
2:B:366:LYS:HD2	2:B:405:TYR:CD1	2.49	0.48
2:B:114:ALA:CB	2:B:214:LEU:HD22	2.44	0.47
1:A:195:ILE:CG2	1:A:196:GLY:N	2.77	0.47
1:A:324:ASP:O	1:A:343:GLN:HG2	2.14	0.47
2:B:105:SER:O	2:B:190:GLY:HA2	2.14	0.47
2:B:373:GLN:NE2	2:B:407:GLN:H	2.12	0.47
1:A:254:VAL:HG11	1:A:286:THR:HG21	1.96	0.47
1:A:164:MET:HE1	1:A:187:LEU:HD11	1.97	0.47
1:A:171:PHE:CD1	1:A:171:PHE:O	2.68	0.47
1:A:94:ILE:O	1:A:94:ILE:HG13	2.14	0.47
1:A:102:LYS:HE3	1:A:237:ASP:HA	1.97	0.47
1:A:298:GLU:H	1:A:298:GLU:CD	2.21	0.47
2:B:362:THR:HG22	2:B:367:GLN:CG	2.45	0.47
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.55	0.47
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.30	0.47
1:A:155:GLY:O	1:A:159:ILE:HG13	2.15	0.47
2:B:279:LEU:O	2:B:282:LEU:HB2	2.14	0.47
1:A:-1:ASN:N	4:A:763:HOH:O	2.31	0.46
1:A:286:THR:HG23	1:A:287:LYS:O	2.16	0.46
1:A:367:GLN:O	1:A:368:LEU:C	2.58	0.46
1:A:396:GLU:HA	1:A:399:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:CE	1:A:187:LEU:HD11	2.46	0.46
1:A:179:VAL:HG22	3:A:561:M14:CL1	2.53	0.46
1:A:179:VAL:HG21	3:A:561:M14:CL1	2.53	0.46
2:B:165:THR:HG22	2:B:166:LYS:CE	2.46	0.46
2:B:278:GLN:O	2:B:282:LEU:HD23	2.15	0.46
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.75	0.46
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.97	0.46
2:B:111:VAL:O	2:B:111:VAL:HG13	2.15	0.46
1:A:29:GLU:HG2	4:A:648:HOH:O	2.15	0.46
2:B:17:ASP:CG	2:B:18:GLY:H	2.24	0.46
2:B:169:GLU:OE2	2:B:169:GLU:HA	2.16	0.46
2:B:376:THR:HG23	2:B:386:THR:HB	1.98	0.46
1:A:168:LEU:O	1:A:169:GLU:C	2.57	0.45
1:A:328:GLU:OE1	1:A:342:TYR:OH	2.28	0.45
1:A:402:TRP:CD1	1:A:402:TRP:C	2.94	0.45
1:A:449:GLU:HB2	4:A:705:HOH:O	2.16	0.45
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.99	0.45
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.52	0.45
1:A:398:TRP:CH2	1:A:411:ILE:CD1	2.99	0.45
2:B:124:PHE:O	2:B:126:LYS:N	2.49	0.45
2:B:197:GLN:HB3	4:B:457:HOH:O	2.17	0.45
2:B:282:LEU:HD21	2:B:299:ALA:HB2	1.97	0.45
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.74	0.45
1:A:251:SER:HB3	1:A:292:VAL:HG11	1.99	0.45
1:A:287:LYS:HD2	1:A:287:LYS:N	2.31	0.45
1:A:388:LYS:HD2	1:A:413:GLU:OE1	2.17	0.45
2:B:418:ASN:O	2:B:419:THR:C	2.58	0.45
1:A:28:GLU:HG3	4:A:585:HOH:O	2.17	0.45
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.52	0.45
1:A:296:THR:HG23	1:A:298:GLU:CD	2.39	0.45
1:A:362:THR:OG1	1:A:363:ASN:N	2.50	0.45
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.87	0.44
2:B:172:ARG:HD2	4:B:496:HOH:O	2.17	0.44
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.98	0.44
2:B:354:TYR:OH	2:B:370:GLU:OE2	2.34	0.44
2:B:373:GLN:HE22	2:B:407:GLN:H	1.65	0.44
1:A:50:ILE:HG22	4:A:609:HOH:O	2.18	0.44
2:B:99:GLY:O	2:B:100:LEU:C	2.61	0.44
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.53	0.44
1:A:355:ALA:O	1:A:356:ARG:C	2.61	0.44
2:B:67:ASP:O	2:B:68:SER:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:C	2:B:285:GLY:O	2.61	0.44
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.53	0.43
2:B:298:GLU:H	2:B:298:GLU:CD	2.25	0.43
1:A:19:PRO:HB3	1:A:79:GLU:HB3	2.00	0.43
1:A:458:VAL:HG13	1:A:548:VAL:HG22	2.01	0.43
1:A:245:VAL:HG13	1:A:245:VAL:O	2.17	0.43
2:B:337:TRP:CD1	2:B:337:TRP:N	2.86	0.43
2:B:341:ILE:HD11	2:B:375:ILE:CG2	2.45	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.43
2:B:232:TYR:CE1	4:B:570:HOH:O	2.56	0.43
1:A:509:GLN:N	1:A:510:PRO:CD	2.81	0.43
2:B:137:ASN:O	2:B:138:GLU:C	2.60	0.43
2:B:320:ASP:OD1	2:B:320:ASP:C	2.61	0.43
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.52	0.43
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.79	0.43
1:A:297:GLU:OE1	1:A:297:GLU:HA	2.19	0.43
2:B:210:LEU:HD12	2:B:210:LEU:C	2.44	0.43
2:B:374:LYS:O	2:B:374:LYS:HG2	2.19	0.43
1:A:64:LYS:CE	1:A:69:THR:HA	2.49	0.43
2:B:79:GLU:OE2	2:B:83:ARG:NE	2.44	0.43
1:A:273:GLY:C	1:A:332:GLN:HE22	2.27	0.42
2:B:166:LYS:HE2	2:B:166:LYS:HA	2.01	0.42
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.71	0.42
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.69	0.42
1:A:464:GLN:HG2	1:A:465:LYS:H	1.84	0.42
1:A:172:ARG:O	1:A:173:LYS:C	2.61	0.42
2:B:88:TRP:CZ2	2:B:154:LYS:HD3	2.54	0.42
1:A:164:MET:O	1:A:164:MET:HG3	2.17	0.42
1:A:172:ARG:NH2	1:A:180:ILE:O	2.53	0.42
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.55	0.42
1:A:105:SER:O	1:A:190:GLY:HA2	2.19	0.42
1:A:420:PRO:HA	1:A:421:PRO:C	2.44	0.42
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.55	0.42
1:A:32:LYS:O	1:A:33:ALA:C	2.61	0.42
2:B:104:LYS:HE3	2:B:104:LYS:HB2	1.73	0.42
2:B:428:GLN:NE2	2:B:428:GLN:HA	2.35	0.42
1:A:91:GLN:HG3	1:A:92:LEU:N	2.34	0.42
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.55	0.42
1:A:173:LYS:HE3	1:A:173:LYS:N	2.34	0.42
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.85	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ALA:HB2	2:B:214:LEU:HD22	2.01	0.42
1:A:251:SER:HB3	1:A:292:VAL:CG1	2.50	0.41
1:A:173:LYS:CE	1:A:173:LYS:CA	2.92	0.41
2:B:36:GLU:O	2:B:37:ILE:C	2.62	0.41
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.55	0.41
1:A:0:SER:OG	1:A:46:LYS:NZ	2.53	0.41
1:A:64:LYS:O	1:A:65:LYS:CB	2.67	0.41
2:B:243:PRO:O	2:B:245:VAL:HG23	2.20	0.41
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.50	0.41
2:B:199:ARG:CD	2:B:233:GLU:OE1	2.69	0.41
1:A:65:LYS:NZ	1:A:68:SER:HB3	2.35	0.41
1:A:137:ASN:O	1:A:138:GLU:C	2.63	0.41
1:A:334:GLN:HE21	1:A:334:GLN:HB3	1.62	0.41
2:B:10:VAL:HG13	2:B:87:PHE:CD2	2.56	0.41
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.56	0.41
1:A:194:GLU:CD	1:A:194:GLU:N	2.77	0.41
1:A:270:ILE:O	1:A:270:ILE:HG13	2.20	0.41
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.89	0.41
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.35	0.41
2:B:419:THR:HA	2:B:420:PRO:HD2	1.94	0.41
1:A:557:ARG:HB3	4:A:703:HOH:O	2.19	0.41
2:B:81:ASN:HB3	2:B:154:LYS:HD2	2.02	0.41
2:B:362:THR:CG2	2:B:367:GLN:HG2	2.50	0.41
1:A:395:LYS:HZ2	1:A:416:PHE:H	1.67	0.41
1:A:542:ILE:O	1:A:543:GLY:C	2.63	0.41
2:B:13:LYS:HD2	2:B:85:GLN:H	1.85	0.41
2:B:179:VAL:O	2:B:189:VAL:HA	2.21	0.41
2:B:169:GLU:C	2:B:169:GLU:CD	2.88	0.41
1:A:242:GLN:O	1:A:243:PRO:C	2.64	0.40
2:B:65:LYS:HD3	4:B:534:HOH:O	2.20	0.40
2:B:165:THR:HG22	2:B:166:LYS:HE2	2.03	0.40
2:B:332:GLN:HA	2:B:424:LYS:HE3	2.03	0.40
1:A:64:LYS:HE3	1:A:69:THR:HG22	2.03	0.40
1:A:406:TRP:CZ3	1:A:407:GLN:CB	3.04	0.40
2:B:166:LYS:HE2	2:B:166:LYS:CA	2.50	0.40
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.85	0.40
1:A:465:LYS:NZ	4:A:702:HOH:O	2.53	0.40
1:A:553:SER:OG	1:A:557:ARG:HD3	2.21	0.40
2:B:268:SER:HB3	2:B:274:ILE:HB	2.02	0.40
1:A:89:GLU:HB3	1:A:92:LEU:HD21	2.03	0.40
1:A:181:TYR:CD1	2:B:138:GLU:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:THR:O	2:B:291:GLU:C	2.63	0.40
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.87	0.40
1:A:129:ALA:HA	1:A:144:TYR:O	2.22	0.40
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.12	0.40
2:B:120:LEU:O	2:B:121:ASP:C	2.64	0.40
2:B:235:HIS:HA	2:B:236:PRO:HD3	1.82	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	557/563 (99%)	492 (88%)	48 (9%)	17 (3%)	3	8
2	B	398/443 (90%)	353 (89%)	35 (9%)	10 (2%)	4	11
All	All	955/1006 (95%)	845 (88%)	83 (9%)	27 (3%)	4	9

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	67	ASP
1	A	90	VAL
1	A	286	THR
1	A	412	PRO
2	B	288	ALA
1	A	64	LYS
1	A	138	GLU
1	A	195	ILE
1	A	196	GLY
1	A	356	ARG
1	A	491	LEU

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Mol	Chain	Res	Type
1	A	543	GLY
2	B	269	GLN
1	A	65	LYS
1	A	220	LYS
1	A	554	ALA
2	B	68	SER
2	B	91	GLN
2	B	125	ARG
1	A	312	GLU
2	B	65	LYS
2	B	66	LYS
2	B	67	ASP
2	B	346	PHE
1	A	345	PRO
2	B	241	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	384/503 (76%)	301 (78%)	83 (22%)	1	3
2	B	368/403 (91%)	305 (83%)	63 (17%)	2	6
All	All	752/906 (83%)	606 (81%)	146 (19%)	1	4

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
1	A	137	ASN
1	A	138	GLU
1	A	139	THR
1	A	143	ARG
1	A	151	GLN
1	A	159	ILE
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	166	LYS
1	A	173	LYS
1	A	179	VAL
1	A	193	LEU
1	A	195	ILE
1	A	202	ILE
1	A	204	GLU
1	A	205	LEU
1	A	210	LEU
1	A	215	THR
1	A	219	LYS
1	A	220	LYS
1	A	230	MET
1	A	234	LEU
1	A	249	LYS
1	A	260	LEU
1	A	276	VAL
1	A	277	ARG
1	A	279	LEU
1	A	284	ARG
1	A	286	THR
1	A	289	LEU
1	A	291	GLU
1	A	292	VAL
1	A	293	ILE
1	A	295	LEU
1	A	296	THR
1	A	303	LEU
1	A	305	GLU
1	A	312	GLU
1	A	323	LYS
1	A	334	GLN
1	A	345	PRO
1	A	346	PHE
1	A	350	LYS
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	374	LYS
1	A	393	ILE

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Mol	Chain	Res	Type
1	A	395	LYS
1	A	402	TRP
1	A	404	GLU
1	A	407	GLN
1	A	422	LEU
1	A	425	LEU
1	A	429	LEU
1	A	448	ARG
1	A	449	GLU
1	A	451	LYS
1	A	458	VAL
1	A	463	ARG
1	A	464	GLN
1	A	468	THR
1	A	470	THR
1	A	471	ASP
1	A	472	THR
1	A	479	LEU
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	516	GLU
1	A	522	ILE
1	A	523	GLU
1	A	539	HIS
1	A	540	LYS
1	A	547	GLN
1	A	548	VAL
1	A	550	LYS
1	A	551	LEU
1	A	553	SER
1	A	557	ARG
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	11	LYS
2	B	16	MET
2	B	17	ASP
2	B	22	LYS
2	B	26	LEU
2	B	30	LYS

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Mol	Chain	Res	Type
2	B	47	ILE
2	B	58	THR
2	B	64	LYS
2	B	65	LYS
2	B	66	LYS
2	B	72	ARG
2	B	73	LYS
2	B	80	LEU
2	B	90	VAL
2	B	91	GLN
2	B	104	LYS
2	B	111	VAL
2	B	120	LEU
2	B	173	LYS
2	B	175	ASN
2	B	187	LEU
2	B	199	ARG
2	B	202	ILE
2	B	203	GLU
2	B	205	LEU
2	B	209	LEU
2	B	210	LEU
2	B	214	LEU
2	B	238	LYS
2	B	246	LEU
2	B	248	GLU
2	B	253	THR
2	B	257	ILE
2	B	260	LEU
2	B	261	VAL
2	B	270	ILE
2	B	275	LYS
2	B	277	ARG
2	B	279	LEU
2	B	280	CYS
2	B	283	LEU
2	B	286	THR
2	B	289	LEU
2	B	296	THR
2	B	300	GLU
2	B	310	LEU
2	B	314	VAL

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Mol	Chain	Res	Type
2	B	326	ILE
2	B	334	GLN
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	369	THR
2	B	374	LYS
2	B	377	THR
2	B	393	ILE
2	B	394	GLN
2	B	400	THR
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	175	ASN
1	A	258	GLN
1	A	330	GLN
1	A	332	GLN
1	A	334	GLN
1	A	336	GLN
1	A	394	GLN
1	A	428	GLN
1	A	480	GLN
1	A	487	GLN
1	A	509	GLN
1	A	512	GLN
1	A	519	ASN
1	A	524	GLN
2	B	96	HIS
2	B	137	ASN
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	336	GLN

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Mol	Chain	Res	Type
2	B	367	GLN
2	B	373	GLN
2	B	394	GLN
2	B	407	GLN
2	B	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	M14	A	561	-	35,35,35	1.42	3 (8%)	50,50,50	2.30	15 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M14	A	561	-	-	5/21/21/21	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	M14	S-N23	5.52	1.71	1.60
3	A	561	M14	C16-C27	-3.37	1.37	1.44
3	A	561	M14	C9-C8	2.61	1.42	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	M14	O24-S-C3	-7.53	98.84	107.35
3	A	561	M14	C5-C-N	-4.71	111.99	119.25
3	A	561	M14	C16-C27-N28	-4.23	167.42	177.87
3	A	561	M14	C7-C8-CL1	-4.22	113.88	119.17
3	A	561	M14	C9-C8-CL1	3.37	123.39	119.17
3	A	561	M14	C17-C16-C27	-3.19	115.25	119.55
3	A	561	M14	O25-S-N23	3.16	111.91	107.35
3	A	561	M14	C3-S-N23	-3.12	104.06	108.40
3	A	561	M14	C1-C-N	3.03	128.84	121.82
3	A	561	M14	C11-C10-C9	-2.80	116.73	120.98
3	A	561	M14	C20-C21-N	-2.68	110.27	115.62
3	A	561	M14	C20-O19-C10	2.60	122.28	117.63
3	A	561	M14	O24-S-N23	2.55	111.03	107.35
3	A	561	M14	C17-C16-C15	2.51	123.58	119.70
3	A	561	M14	O19-C10-C9	2.49	131.72	119.74

There are no chirality outliers.

All (5) torsion outliers are listed below:

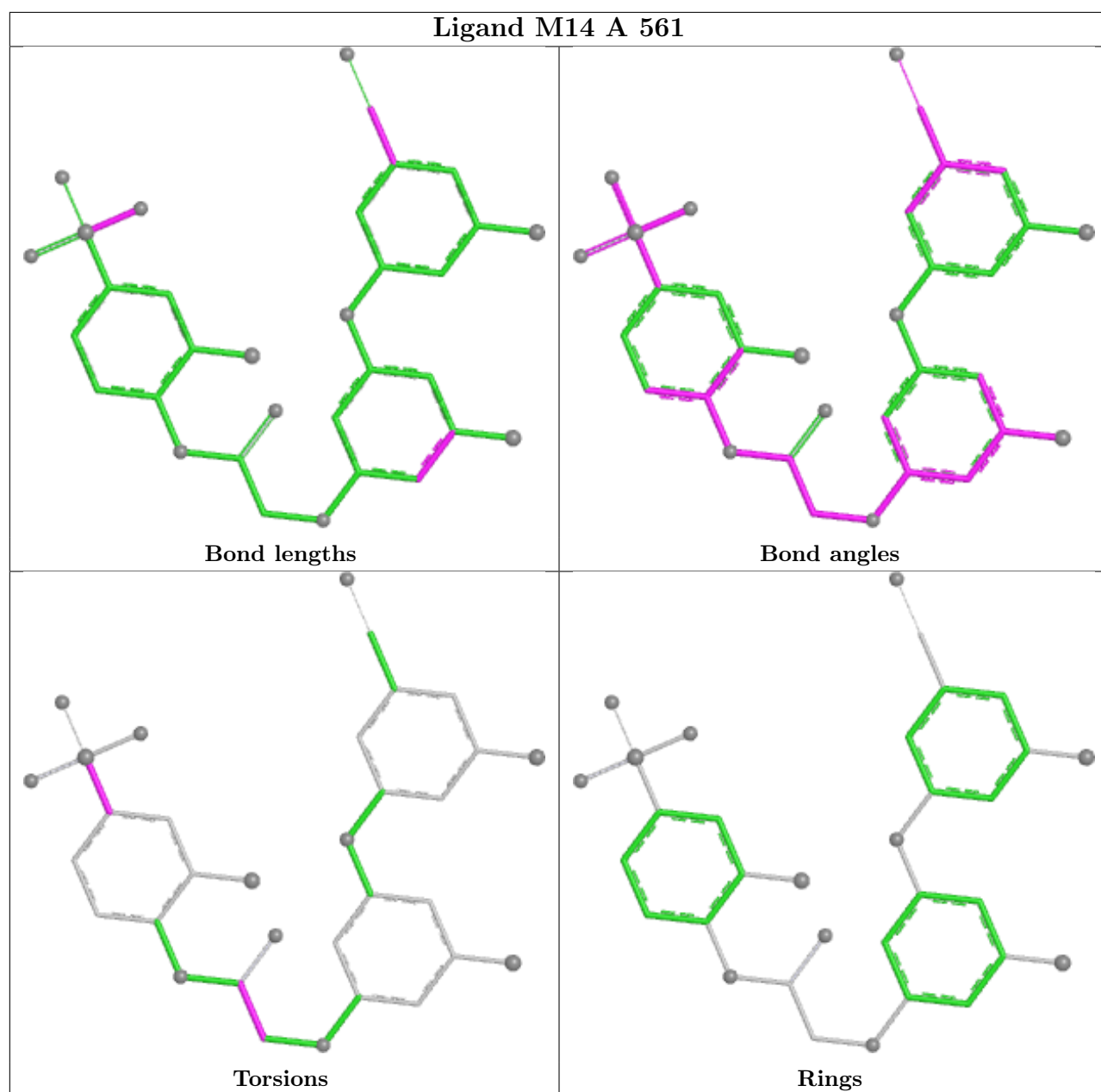
Mol	Chain	Res	Type	Atoms
3	A	561	M14	O19-C20-C21-O22
3	A	561	M14	C2-C3-S-O24
3	A	561	M14	C4-C3-S-O24
3	A	561	M14	C4-C3-S-N23
3	A	561	M14	C2-C3-S-N23

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	M14	10	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.



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	559/563 (99%)	-0.17	4 (0%) 84 83	24, 46, 68, 91	0
2	B	404/443 (91%)	-0.11	7 (1%) 69 67	24, 44, 82, 96	0
All	All	963/1006 (95%)	-0.14	11 (1%) 78 76	24, 46, 78, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	266	TRP	2.9
1	A	0	SER	2.4
2	B	11	LYS	2.3
2	B	361	HIS	2.3
1	A	286	THR	2.3
2	B	428	GLN	2.2
2	B	293	ILE	2.2
1	A	68	SER	2.2
2	B	90	VAL	2.1
1	A	24	TRP	2.1
2	B	65	LYS	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](#)

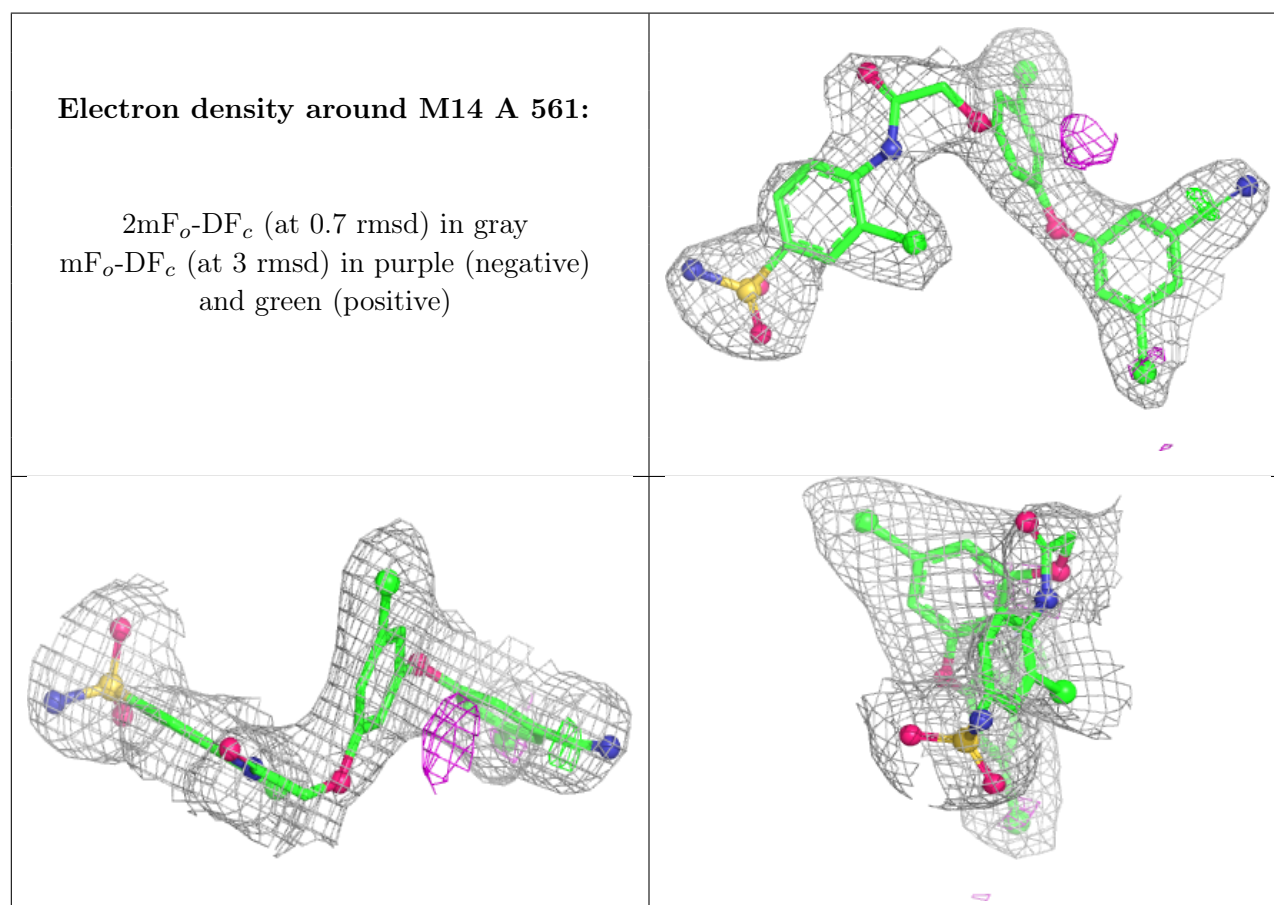
There are no oligosaccharides in this entry.

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
3	M14	A	561	33/33	0.94	0.09	38,48,54,58	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.