



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:56 AM UTC

PDB ID : 2RF2 / pdb_00002rf2
Title : HIV reverse transcriptase in complex with inhibitor 7e (NNRTI)
Authors : Yan, Y.; Prasad, S.
Deposited on : 2007-09-27
Resolution : 2.40 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

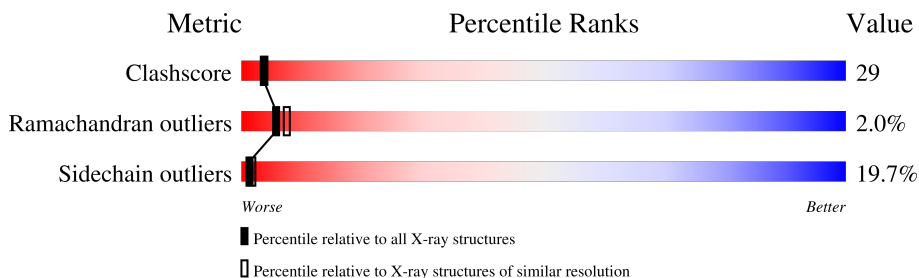
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	563	 53% 33% 10% . .
2	B	443	 46% 31% 13% . 9%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8593 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/ribonuclease H (EC 2.7.7.49) (EC 2.7.7.7) (EC 3.1.26.4) (p66 RT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4510	2915	754	833	8	0	0	0

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

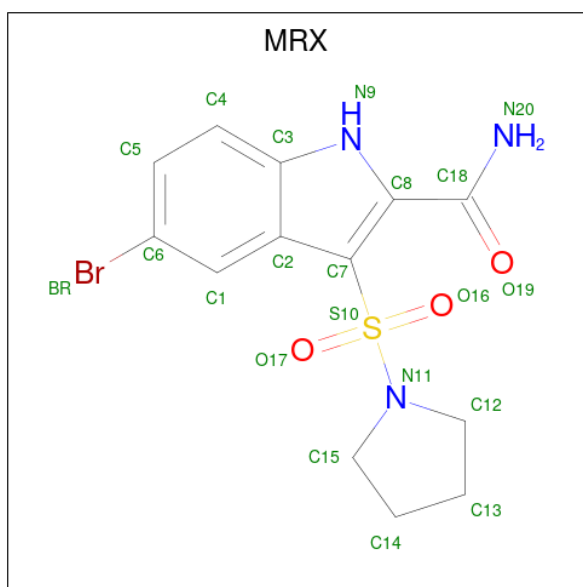
- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H (EC 2.7.7.49) (EC 2.7.7.7) (EC 3.1.26.4) (p66 RT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	405	3352	2182	555	609	6	0	0	0

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 5-bromo-3-(pyrrolidin-1-ylsulfonyl)-1H-indole-2-carboxamide (CCD ID: MRX) (formula: C₁₃H₁₄BrN₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	N	O			S
3	A	1	21	1	13	3	3	1	0	0

- Molecule 4 is water.

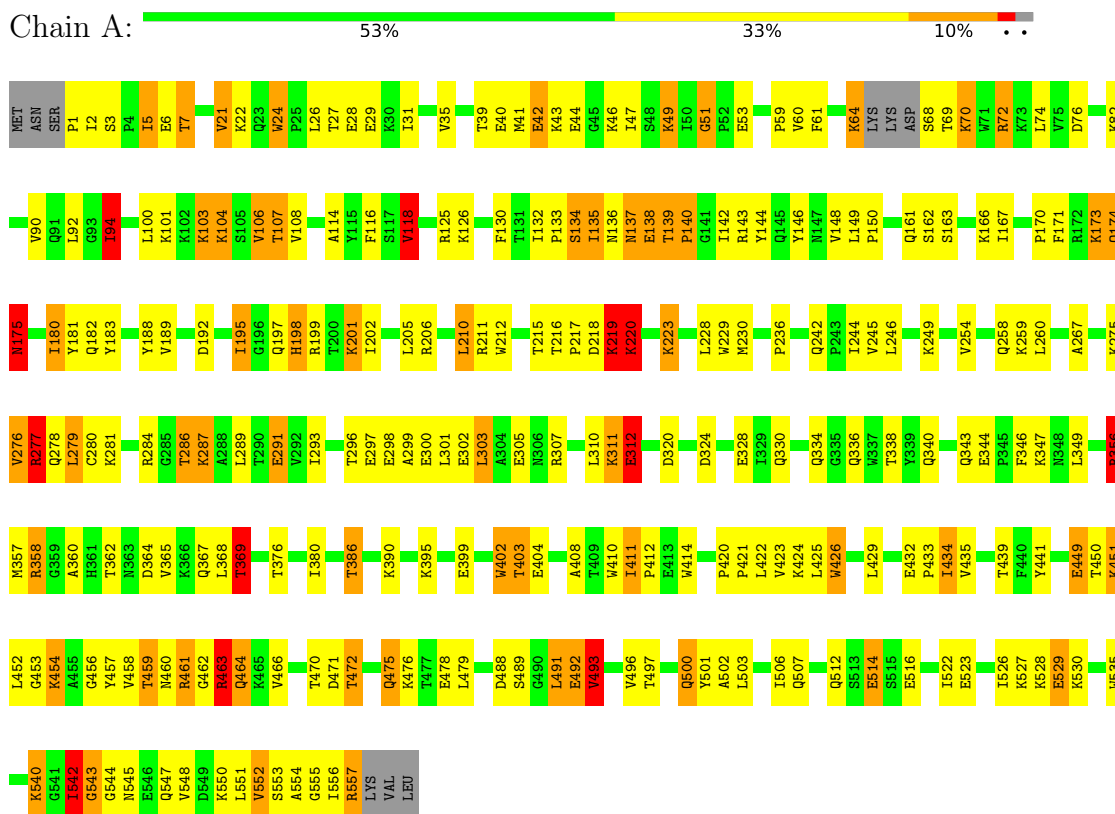
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	413	Total	O	0	0
			413	413		
4	B	297	Total	O	0	0
			297	297		

3 Residue-property plots

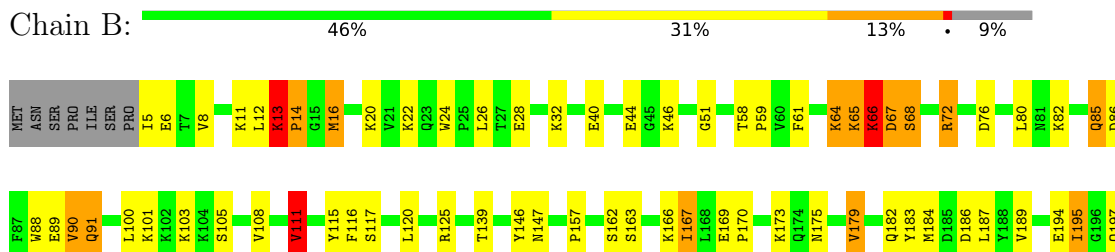
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Reverse transcriptase/ribonuclease H (EC 2.7.7.49) (EC 2.7.7.7) (EC 3.1.26.4) (p66 RT)



- Molecule 2: Reverse transcriptase/ribonuclease H (EC 2.7.7.49) (EC 2.7.7.7) (EC 3.1.26.4) (p66 RT)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.29Å 155.81Å 155.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.77 – 2.40	Depositor
% Data completeness (in resolution range)	99.2 (15.77-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.185 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8593	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.80	2/4625 (0.0%)	1.20	34/6282 (0.5%)
2	B	0.79	0/3446	1.23	40/4682 (0.9%)
All	All	0.80	2/8071 (0.0%)	1.21	74/10964 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	VAL	CA-CB	5.71	1.58	1.54
1	A	369	THR	CA-CB	5.40	1.62	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ILE	CA-C-N	-12.16	107.99	120.03
1	A	132	ILE	C-N-CA	-12.16	107.99	120.03
2	B	139	THR	CA-C-N	-10.43	109.08	120.14
2	B	139	THR	C-N-CA	-10.43	109.08	120.14
2	B	13	LYS	CA-C-N	10.05	132.40	119.84
2	B	13	LYS	C-N-CA	10.05	132.40	119.84
2	B	13	LYS	C-N-CD	-9.79	84.85	125.00
1	A	94	ILE	CA-C-N	-9.64	109.85	119.78
1	A	94	ILE	C-N-CA	-9.64	109.85	119.78
1	A	411	ILE	CA-C-N	-9.07	108.50	119.84
1	A	411	ILE	C-N-CA	-9.07	108.50	119.84
2	B	195	ILE	N-CA-C	8.96	120.83	110.62
1	A	118	VAL	CB-CA-C	8.85	118.71	110.13
2	B	175	ASN	CA-C-N	8.52	130.49	119.84
2	B	175	ASN	C-N-CA	8.52	130.49	119.84
2	B	249	LYS	N-CA-C	8.48	120.98	108.60
2	B	244	ILE	N-CA-C	-8.27	96.60	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	GLY	CA-C-N	7.69	127.40	119.56
2	B	51	GLY	C-N-CA	7.69	127.40	119.56
1	A	242	GLN	CA-C-N	7.43	129.13	119.84
1	A	242	GLN	C-N-CA	7.43	129.13	119.84
2	B	401	TRP	N-CA-C	7.41	122.45	113.41
1	A	118	VAL	CA-C-N	7.40	127.32	119.85
1	A	118	VAL	C-N-CA	7.40	127.32	119.85
2	B	246	LEU	CA-C-N	-7.37	112.33	120.14
2	B	246	LEU	C-N-CA	-7.37	112.33	120.14
1	A	277	ARG	N-CA-C	7.33	119.26	111.28
1	A	470	THR	N-CA-C	7.19	122.72	113.88
1	A	489	SER	N-CA-C	7.19	122.32	112.90
2	B	402	TRP	N-CA-C	7.03	119.83	111.33
1	A	493	VAL	CB-CA-C	-6.87	102.25	111.80
1	A	386	THR	CA-C-N	-6.85	113.45	120.85
1	A	386	THR	C-N-CA	-6.85	113.45	120.85
2	B	271	TYR	CA-C-N	6.83	127.85	120.13
2	B	271	TYR	C-N-CA	6.83	127.85	120.13
2	B	233	GLU	N-CA-C	6.75	119.84	108.02
2	B	320	ASP	CA-C-N	6.73	126.42	119.56
2	B	320	ASP	C-N-CA	6.73	126.42	119.56
2	B	344	GLU	CA-C-N	-6.71	112.85	119.76
2	B	344	GLU	C-N-CA	-6.71	112.85	119.76
2	B	235	HIS	CA-C-N	6.59	125.82	118.97
2	B	235	HIS	C-N-CA	6.59	125.82	118.97
1	A	462	GLY	N-CA-C	6.48	122.67	114.25
2	B	270	ILE	N-CA-C	-6.39	106.73	111.90
1	A	175	ASN	CA-C-N	6.16	127.54	119.84
1	A	175	ASN	C-N-CA	6.16	127.54	119.84
2	B	254	VAL	N-CA-C	-5.93	104.72	110.42
1	A	470	THR	CA-C-N	-5.91	114.36	122.87
1	A	470	THR	C-N-CA	-5.91	114.36	122.87
2	B	241	VAL	N-CA-C	5.77	121.34	109.34
1	A	198	HIS	N-CA-C	-5.73	104.40	111.40
2	B	115	TYR	N-CA-C	5.62	118.34	111.82
2	B	268	SER	N-CA-C	-5.62	103.49	110.41
1	A	138	GLU	N-CA-C	-5.57	101.61	109.96
2	B	189	VAL	CA-C-N	-5.52	117.44	122.80
2	B	189	VAL	C-N-CA	-5.52	117.44	122.80
2	B	310	LEU	N-CA-C	5.50	118.03	111.71
1	A	456	GLY	N-CA-C	5.50	119.56	110.55
1	A	51	GLY	CA-C-N	5.46	127.50	120.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLY	C-N-CA	5.46	127.50	120.89
1	A	219	LYS	N-CA-C	-5.40	103.22	110.24
2	B	85	GLN	N-CA-C	5.37	118.94	112.38
2	B	111	VAL	N-CA-CB	-5.34	105.00	111.94
2	B	382	ILE	N-CA-C	5.31	115.52	110.53
2	B	186	ASP	N-CA-C	5.28	118.19	109.85
1	A	349	LEU	N-CA-C	-5.27	105.20	111.69
1	A	461	ARG	CB-CA-C	5.25	119.47	111.02
1	A	426	TRP	N-CA-C	5.18	119.66	113.23
2	B	271	TYR	C-N-CD	-5.15	103.88	125.00
1	A	463	ARG	N-CA-C	5.08	116.66	110.41
1	A	320	ASP	CA-C-N	-5.04	114.62	119.87
1	A	320	ASP	C-N-CA	-5.04	114.62	119.87
2	B	167	ILE	N-CA-C	5.01	115.73	110.62
2	B	287	LYS	N-CA-C	5.01	117.94	110.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	4510	0	4558	264	0
2	B	3352	0	3380	205	0
3	A	21	0	14	3	0
4	A	413	0	0	18	0
4	B	297	0	0	12	0
All	All	8593	0	7952	459	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 29.

All (459) 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:64:LYS:HE2	1:A:69:THR:HG23	1.21	1.17
2:B:253:THR:HG22	2:B:256:ASP:H	1.07	1.10
2:B:422:LEU:HA	2:B:425:LEU:HD21	1.35	1.08
1:A:463:ARG:HG2	1:A:463:ARG:HH11	1.19	1.06
2:B:246:LEU:HD11	2:B:310:LEU:HD23	1.39	1.03
2:B:344:GLU:HB3	2:B:347:LYS:HD3	1.44	0.97
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.06	0.97
1:A:475:GLN:HG2	1:A:501:TYR:CE2	2.04	0.93
1:A:296:THR:HG23	1:A:299:ALA:H	1.33	0.92
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.04	0.92
1:A:107:THR:HG22	1:A:198:HIS:CE1	2.04	0.92
2:B:214:LEU:H	2:B:214:LEU:HD23	1.33	0.92
1:A:107:THR:HG22	1:A:198:HIS:HE1	1.33	0.91
1:A:356:ARG:HE	1:A:358:ARG:HG3	1.35	0.90
2:B:422:LEU:HA	2:B:425:LEU:CD2	2.02	0.89
1:A:24:TRP:H	1:A:24:TRP:CD1	1.88	0.89
1:A:223:LYS:H	1:A:223:LYS:HD2	1.36	0.88
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.03	0.87
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.55	0.87
2:B:253:THR:HG22	2:B:256:ASP:N	1.89	0.87
2:B:268:SER:O	2:B:269:GLN:HB2	1.75	0.86
1:A:297:GLU:O	1:A:298:GLU:N	2.07	0.85
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.41	0.85
1:A:356:ARG:NE	1:A:358:ARG:HG3	1.92	0.84
1:A:195:ILE:HD12	1:A:195:ILE:H	1.41	0.84
1:A:454:LYS:CD	1:A:556:ILE:HD13	2.08	0.84
1:A:24:TRP:H	1:A:24:TRP:HD1	1.24	0.84
1:A:399:GLU:O	1:A:403:THR:HB	1.79	0.83
2:B:274:ILE:HA	2:B:306:ASN:ND2	1.93	0.83
1:A:411:ILE:HG22	1:A:412:PRO:O	1.79	0.82
1:A:478:GLU:HG3	4:A:596:HOH:O	1.80	0.82
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.44	0.81
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.62	0.81
2:B:163:SER:HA	2:B:166:LYS:HE2	1.60	0.81
2:B:215:THR:HA	4:B:496:HOH:O	1.80	0.80
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.15	0.80
1:A:458:VAL:HG22	1:A:548:VAL:CG2	2.12	0.80
1:A:35:VAL:O	1:A:39:THR:HG23	1.82	0.79
1:A:64:LYS:CE	1:A:69:THR:HG23	2.08	0.79
1:A:296:THR:CG2	1:A:299:ALA:H	1.94	0.79
1:A:161:GLN:HG3	4:A:960:HOH:O	1.82	0.78
2:B:373:GLN:O	2:B:377:THR:HG23	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HD3	1:A:336:GLN:NE2	1.99	0.77
1:A:475:GLN:HG2	1:A:501:TYR:CD2	2.19	0.77
2:B:373:GLN:HE22	2:B:407:GLN:H	1.30	0.77
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.66	0.77
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.66	0.76
1:A:42:GLU:OE1	1:A:49:LYS:HE3	1.85	0.76
1:A:70:LYS:HE3	1:A:72:ARG:HG3	1.67	0.75
1:A:244:ILE:HD13	1:A:267:ALA:HB2	1.68	0.75
2:B:13:LYS:HE3	2:B:85:GLN:N	2.01	0.75
1:A:454:LYS:HZ3	1:A:556:ILE:HD11	1.52	0.74
2:B:253:THR:O	2:B:257:ILE:HG12	1.88	0.74
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.70	0.74
1:A:360:ALA:HA	1:A:514:GLU:OE1	1.87	0.74
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.85	0.74
1:A:219:LYS:O	1:A:220:LYS:HB3	1.89	0.73
2:B:125:ARG:HG2	2:B:146:TYR:O	1.88	0.73
2:B:214:LEU:HD23	2:B:214:LEU:N	2.03	0.73
2:B:14:PRO:HB3	4:B:571:HOH:O	1.88	0.73
1:A:108:VAL:CG2	1:A:223:LYS:HD3	2.19	0.72
1:A:61:PHE:HE2	1:A:76:ASP:HB2	1.54	0.72
2:B:373:GLN:NE2	2:B:407:GLN:H	1.87	0.72
1:A:458:VAL:HG22	1:A:548:VAL:HG23	1.72	0.71
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.35	0.71
2:B:366:LYS:O	2:B:370:GLU:HG3	1.90	0.71
2:B:303:LEU:HD23	2:B:303:LEU:H	1.56	0.71
2:B:312:GLU:OE2	2:B:313:PRO:HD3	1.91	0.71
2:B:300:GLU:O	2:B:304:ALA:HB2	1.91	0.71
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.74	0.70
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.52	0.70
1:A:29:GLU:HG2	4:A:689:HOH:O	1.92	0.70
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.74	0.70
2:B:282:LEU:HD21	2:B:299:ALA:HB2	1.72	0.69
1:A:3:SER:OG	1:A:5:ILE:HG12	1.91	0.69
2:B:105:SER:HB2	4:B:465:HOH:O	1.91	0.69
1:A:69:THR:HG21	4:A:869:HOH:O	1.92	0.69
2:B:266:TRP:HH2	2:B:427:TYR:CZ	2.11	0.69
2:B:254:VAL:O	2:B:258:GLN:HG3	1.93	0.69
2:B:253:THR:CG2	2:B:256:ASP:H	1.96	0.69
1:A:223:LYS:H	1:A:223:LYS:CD	2.03	0.68
1:A:296:THR:HG21	4:A:597:HOH:O	1.93	0.68
2:B:297:GLU:O	2:B:301:LEU:HG	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HD12	1:A:195:ILE:N	2.07	0.68
2:B:103:LYS:HE3	2:B:179:VAL:CG1	2.24	0.68
1:A:540:LYS:HB2	1:A:542:ILE:HD11	1.73	0.68
1:A:454:LYS:HD2	1:A:556:ILE:HD13	1.76	0.68
2:B:72:ARG:NH2	2:B:409:THR:HG21	2.09	0.68
1:A:367:GLN:NE2	1:A:512:GLN:OE1	2.27	0.68
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.19	0.68
1:A:454:LYS:HE2	1:A:554:ALA:O	1.92	0.68
1:A:556:ILE:O	1:A:557:ARG:HB3	1.92	0.68
1:A:297:GLU:HB3	1:A:298:GLU:N	2.09	0.67
1:A:540:LYS:CB	1:A:542:ILE:HD11	2.26	0.66
2:B:295:LEU:HD23	2:B:299:ALA:HB3	1.77	0.66
1:A:223:LYS:HD2	1:A:223:LYS:N	2.09	0.66
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.30	0.66
1:A:195:ILE:H	1:A:195:ILE:CD1	2.03	0.66
1:A:296:THR:HG22	1:A:299:ALA:CB	2.24	0.66
1:A:27:THR:O	1:A:31:ILE:HG13	1.97	0.65
1:A:195:ILE:O	1:A:199:ARG:HG3	1.96	0.65
1:A:139:THR:HG22	1:A:140:PRO:N	2.12	0.65
2:B:282:LEU:HD12	2:B:293:ILE:CD1	2.26	0.65
2:B:363:ASN:HA	4:B:580:HOH:O	1.97	0.65
1:A:454:LYS:HZ3	1:A:556:ILE:CD1	2.10	0.65
1:A:51:GLY:O	1:A:143:ARG:NH1	2.30	0.65
2:B:345:PRO:O	2:B:346:PHE:HB2	1.96	0.65
1:A:171:PHE:O	1:A:175:ASN:ND2	2.29	0.64
2:B:276:VAL:HG12	2:B:280:CYS:SG	2.36	0.64
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.61	0.64
2:B:278:GLN:HE22	2:B:281:LYS:NZ	1.96	0.64
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.27	0.64
1:A:277:ARG:HD3	1:A:336:GLN:CD	2.24	0.63
2:B:16:MET:HE2	2:B:16:MET:HA	1.80	0.63
2:B:253:THR:HG23	2:B:255:ASN:N	2.12	0.63
2:B:40:GLU:O	2:B:44:GLU:HG3	1.98	0.63
2:B:282:LEU:HD21	2:B:299:ALA:CB	2.29	0.63
2:B:103:LYS:HE3	2:B:179:VAL:HG13	1.81	0.63
2:B:273:GLY:O	2:B:275:LYS:HG2	1.99	0.63
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.29	0.63
2:B:85:GLN:O	2:B:89:GLU:HB3	1.99	0.62
1:A:108:VAL:HG23	1:A:223:LYS:HD3	1.79	0.62
1:A:463:ARG:HG2	1:A:463:ARG:NH1	1.99	0.62
2:B:16:MET:HA	2:B:16:MET:CE	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ILE:O	2:B:199:ARG:HG3	1.98	0.62
1:A:365:VAL:O	1:A:369:THR:HG23	2.01	0.61
1:A:472:THR:HG22	1:A:476:LYS:CB	2.30	0.61
2:B:253:THR:HG23	2:B:255:ASN:H	1.65	0.61
2:B:295:LEU:HD22	2:B:300:GLU:HG2	1.82	0.61
1:A:94:ILE:HD13	1:A:230:MET:HG3	1.82	0.60
1:A:362:THR:CG2	1:A:367:GLN:HE21	2.14	0.60
1:A:28:GLU:HG2	1:A:135:ILE:HG12	1.82	0.60
1:A:106:VAL:HG11	3:A:561:MRX:BR	2.56	0.60
1:A:182:GLN:HB3	4:A:618:HOH:O	2.00	0.60
2:B:210:LEU:O	2:B:210:LEU:HG	2.01	0.60
1:A:3:SER:CB	1:A:5:ILE:HG12	2.31	0.60
2:B:279:LEU:O	2:B:282:LEU:HB2	2.02	0.60
1:A:556:ILE:HD12	1:A:556:ILE:N	2.17	0.60
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.37	0.60
2:B:286:THR:HG23	2:B:286:THR:O	2.02	0.60
2:B:312:GLU:HB3	2:B:313:PRO:CD	2.31	0.60
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.84	0.60
1:A:211:ARG:HB2	4:A:832:HOH:O	2.01	0.59
1:A:555:GLY:C	1:A:556:ILE:HD12	2.27	0.59
1:A:454:LYS:CE	1:A:556:ILE:HD13	2.32	0.59
1:A:170:PRO:O	1:A:174:GLN:HG2	2.03	0.59
2:B:28:GLU:CG	2:B:32:LYS:HE2	2.33	0.59
1:A:454:LYS:CG	1:A:556:ILE:HD13	2.33	0.59
2:B:163:SER:O	2:B:167:ILE:HG13	2.03	0.59
2:B:353:LYS:HE2	4:B:730:HOH:O	2.03	0.59
1:A:500:GLN:CG	2:B:422:LEU:HD12	2.33	0.59
1:A:432:GLU:OE1	1:A:433:PRO:HD2	2.03	0.58
1:A:24:TRP:CD1	1:A:24:TRP:N	2.65	0.58
2:B:242:GLN:H	2:B:243:PRO:CD	2.16	0.58
2:B:246:LEU:CD1	2:B:310:LEU:HD23	2.26	0.58
1:A:399:GLU:HB2	1:A:402:TRP:CZ3	2.38	0.58
2:B:252:TRP:CD1	2:B:295:LEU:HD12	2.39	0.58
1:A:1:PRO:HD3	4:A:639:HOH:O	2.03	0.58
2:B:28:GLU:HG3	2:B:32:LYS:HE2	1.84	0.58
2:B:66:LYS:HE2	2:B:67:ASP:HB2	1.85	0.58
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.84	0.58
1:A:324:ASP:O	1:A:343:GLN:HG2	2.03	0.57
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.04	0.57
2:B:303:LEU:HA	2:B:306:ASN:HB2	1.85	0.57
2:B:13:LYS:O	2:B:16:MET:HB2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.17	0.57
1:A:500:GLN:HG2	2:B:422:LEU:HD12	1.87	0.57
1:A:556:ILE:O	1:A:556:ILE:HG22	2.05	0.57
2:B:317:VAL:HG13	2:B:347:LYS:HB3	1.87	0.57
1:A:303:LEU:HD13	1:A:307:ARG:NH1	2.20	0.56
1:A:441:TYR:O	1:A:548:VAL:HG21	2.05	0.56
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.34	0.56
1:A:211:ARG:O	1:A:211:ARG:NH1	2.28	0.56
2:B:86:ASP:O	2:B:90:VAL:HG22	2.04	0.56
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.92	0.56
2:B:282:LEU:CD2	2:B:299:ALA:HB2	2.34	0.56
1:A:460:ASN:HA	2:B:286:THR:HG23	1.88	0.56
1:A:61:PHE:CE2	1:A:76:ASP:HB2	2.37	0.56
1:A:216:THR:HB	1:A:217:PRO:HD2	1.86	0.56
2:B:278:GLN:NE2	2:B:281:LYS:NZ	2.54	0.55
2:B:422:LEU:O	2:B:425:LEU:HG	2.05	0.55
2:B:266:TRP:CG	2:B:426:TRP:CE3	2.95	0.55
2:B:13:LYS:CE	2:B:86:ASP:H	2.19	0.55
2:B:212:TRP:HH2	4:B:576:HOH:O	1.90	0.55
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.55
1:A:557:ARG:O	1:A:557:ARG:HG2	2.05	0.55
2:B:271:TYR:CD1	2:B:310:LEU:HD12	2.41	0.55
1:A:211:ARG:O	1:A:211:ARG:HD3	2.06	0.55
1:A:472:THR:HG22	1:A:476:LYS:HB2	1.87	0.55
2:B:328:GLU:HG3	2:B:390:LYS:HD3	1.88	0.55
1:A:297:GLU:C	1:A:298:GLU:N	2.65	0.55
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.88	0.55
1:A:24:TRP:CE2	1:A:61:PHE:HE1	2.24	0.54
1:A:399:GLU:HB3	4:A:662:HOH:O	2.07	0.54
1:A:466:VAL:HG21	1:A:551:LEU:CD1	2.37	0.54
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.42	0.54
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.89	0.54
1:A:138:GLU:O	1:A:139:THR:HB	2.08	0.54
2:B:297:GLU:HA	2:B:300:GLU:HG3	1.89	0.54
2:B:377:THR:HG22	2:B:410:TRP:CZ2	2.42	0.54
1:A:3:SER:HB3	1:A:5:ILE:HG12	1.89	0.54
1:A:311:LYS:O	1:A:312:GLU:HB3	2.08	0.54
2:B:240:THR:O	2:B:241:VAL:O	2.26	0.54
2:B:314:VAL:O	2:B:315:HIS:HB3	2.08	0.54
1:A:5:ILE:HD11	1:A:118:VAL:HB	1.89	0.54
1:A:286:THR:HG23	1:A:287:LYS:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLY:HA2	1:A:556:ILE:HG21	1.90	0.54
1:A:108:VAL:HG23	1:A:223:LYS:CD	2.37	0.53
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.43	0.53
1:A:278:GLN:OE1	1:A:281:LYS:NZ	2.31	0.53
1:A:502:ALA:O	1:A:506:ILE:HD12	2.08	0.53
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.89	0.53
1:A:64:LYS:HE2	1:A:69:THR:CG2	2.14	0.53
1:A:180:ILE:HG22	1:A:189:VAL:HG13	1.91	0.53
1:A:69:THR:O	1:A:69:THR:HG22	2.08	0.53
2:B:334:GLN:O	2:B:334:GLN:HG3	2.09	0.53
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.09	0.53
1:A:542:ILE:O	1:A:543:GLY:O	2.27	0.53
2:B:241:VAL:O	2:B:242:GLN:HB2	2.08	0.53
2:B:300:GLU:HA	2:B:303:LEU:HD21	1.90	0.53
1:A:296:THR:HG22	1:A:299:ALA:HB3	1.90	0.53
2:B:278:GLN:HE22	2:B:281:LYS:HZ2	1.55	0.53
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.53
2:B:254:VAL:HG21	2:B:288:ALA:O	2.09	0.53
2:B:157:PRO:HG3	2:B:184:MET:HA	1.91	0.52
2:B:409:THR:HG21	4:B:451:HOH:O	2.09	0.52
1:A:134:SER:HB2	1:A:140:PRO:O	2.10	0.52
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.90	0.52
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.52
2:B:244:ILE:CD1	2:B:266:TRP:HZ3	2.23	0.52
2:B:268:SER:HB3	2:B:274:ILE:HB	1.92	0.52
1:A:297:GLU:C	1:A:300:GLU:HB2	2.34	0.52
1:A:40:GLU:O	1:A:44:GLU:HG3	2.08	0.52
1:A:298:GLU:N	1:A:298:GLU:OE2	2.42	0.52
1:A:312:GLU:HB2	4:A:922:HOH:O	2.08	0.52
1:A:356:ARG:HH21	1:A:358:ARG:HD2	1.74	0.52
2:B:241:VAL:HB	2:B:243:PRO:HD3	1.91	0.52
2:B:301:LEU:O	2:B:304:ALA:HB3	2.10	0.52
1:A:402:TRP:CD1	1:A:402:TRP:C	2.87	0.52
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.45	0.51
1:A:7:THR:HG22	4:A:888:HOH:O	2.10	0.51
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.45	0.51
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.75	0.51
2:B:266:TRP:CD1	2:B:426:TRP:CZ3	2.99	0.51
1:A:103:LYS:HE3	4:A:591:HOH:O	2.10	0.51
2:B:242:GLN:HG2	2:B:352:GLY:HA2	1.92	0.51
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HA	2:B:281:LYS:HD3	1.92	0.51
1:A:31:ILE:HD13	1:A:133:PRO:O	2.10	0.51
1:A:466:VAL:CG2	1:A:551:LEU:HD11	2.40	0.51
2:B:261:VAL:HB	2:B:276:VAL:HG13	1.92	0.51
2:B:297:GLU:OE1	2:B:300:GLU:OE2	2.29	0.51
1:A:211:ARG:HD3	1:A:211:ARG:C	2.36	0.51
2:B:24:TRP:CZ3	2:B:59:PRO:CG	2.94	0.51
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.33	0.51
1:A:500:GLN:HG2	2:B:422:LEU:CD1	2.41	0.51
1:A:491:LEU:HB2	1:A:529:GLU:HB2	1.93	0.51
1:A:108:VAL:HG11	1:A:188:TYR:CE2	2.45	0.50
1:A:395:LYS:HD3	4:A:853:HOH:O	2.11	0.50
2:B:86:ASP:OD2	2:B:90:VAL:HG21	2.11	0.50
1:A:108:VAL:CG1	1:A:188:TYR:CE2	2.94	0.50
2:B:281:LYS:O	2:B:284:ARG:HD2	2.10	0.50
1:A:475:GLN:HG2	1:A:501:TYR:CZ	2.46	0.50
1:A:41:MET:HE2	1:A:47:ILE:HG23	1.92	0.50
1:A:136:ASN:C	1:A:138:GLU:H	2.19	0.50
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.42	0.50
1:A:548:VAL:O	1:A:552:VAL:HB	2.11	0.50
2:B:242:GLN:HG2	2:B:352:GLY:CA	2.42	0.50
1:A:472:THR:HG22	1:A:476:LYS:HB3	1.93	0.50
2:B:242:GLN:H	2:B:243:PRO:HD3	1.76	0.50
2:B:266:TRP:O	2:B:268:SER:O	2.29	0.50
1:A:362:THR:HG23	1:A:367:GLN:HE21	1.76	0.50
1:A:180:ILE:HA	1:A:188:TYR:O	2.12	0.50
2:B:5:ILE:HG22	2:B:6:GLU:N	2.27	0.50
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.94	0.49
2:B:233:GLU:HB2	4:B:510:HOH:O	2.12	0.49
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.46	0.49
1:A:466:VAL:HG21	1:A:551:LEU:HD11	1.93	0.49
1:A:94:ILE:HD12	1:A:229:TRP:CH2	2.47	0.49
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.27	0.49
2:B:111:VAL:O	2:B:111:VAL:HG13	2.12	0.49
1:A:148:VAL:O	1:A:150:PRO:HD3	2.13	0.49
1:A:137:ASN:OD1	1:A:137:ASN:O	2.30	0.49
2:B:101:LYS:O	2:B:236:PRO:HB2	2.13	0.49
2:B:303:LEU:HD23	2:B:303:LEU:N	2.25	0.49
1:A:139:THR:CG2	1:A:140:PRO:CD	2.90	0.49
2:B:242:GLN:HG2	2:B:352:GLY:C	2.38	0.49
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:CG2	1:A:140:PRO:N	2.76	0.48
1:A:219:LYS:H	1:A:219:LYS:CD	2.21	0.48
1:A:276:VAL:HG13	1:A:280:CYS:SG	2.53	0.48
1:A:118:VAL:HG22	1:A:149:LEU:HG	1.93	0.48
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.91	0.48
1:A:522:ILE:O	1:A:526:ILE:HG13	2.13	0.48
1:A:107:THR:HG21	1:A:202:ILE:CG1	2.39	0.48
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.49	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CZ2	2.81	0.48
2:B:44:GLU:OE2	2:B:46:LYS:HE2	2.14	0.48
1:A:24:TRP:HE1	1:A:59:PRO:HB3	1.79	0.48
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.96	0.48
1:A:219:LYS:HD2	1:A:219:LYS:N	2.29	0.48
2:B:278:GLN:NE2	2:B:281:LYS:HZ3	2.11	0.48
1:A:287:LYS:HB2	1:A:291:GLU:CD	2.38	0.48
1:A:21:VAL:CG2	1:A:59:PRO:HG3	2.44	0.48
2:B:242:GLN:N	2:B:243:PRO:CD	2.77	0.48
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.95	0.48
1:A:457:TYR:CD1	1:A:457:TYR:C	2.92	0.47
1:A:116:PHE:HZ	4:A:611:HOH:O	1.97	0.47
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.96	0.47
2:B:295:LEU:HD23	2:B:299:ALA:CB	2.42	0.47
1:A:206:ARG:HG2	1:A:216:THR:OG1	2.14	0.47
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.44	0.47
1:A:410:TRP:CE3	2:B:363:ASN:HB3	2.49	0.47
1:A:424:LYS:NZ	1:A:426:TRP:CE2	2.83	0.47
1:A:492:GLU:HA	1:A:530:LYS:O	2.14	0.47
1:A:451:LYS:HD3	1:A:451:LYS:N	2.29	0.47
2:B:266:TRP:CD1	2:B:426:TRP:CE3	3.02	0.47
1:A:103:LYS:O	1:A:236:PRO:HB2	2.15	0.47
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.94	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.15	0.47
2:B:268:SER:HA	2:B:271:TYR:O	2.15	0.47
2:B:396:GLU:O	2:B:400:THR:CG2	2.63	0.47
1:A:101:LYS:N	1:A:101:LYS:HD3	2.29	0.47
1:A:210:LEU:HD23	1:A:210:LEU:HA	1.77	0.47
2:B:396:GLU:O	2:B:400:THR:HG23	2.15	0.47
1:A:5:ILE:HG21	1:A:167:ILE:HD11	1.97	0.47
1:A:72:ARG:HD3	4:A:899:HOH:O	2.15	0.46
1:A:108:VAL:HG21	1:A:223:LYS:HD3	1.96	0.46
2:B:64:LYS:HG3	2:B:68:SER:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:O	2:B:265:ASN:HB3	2.15	0.46
1:A:449:GLU:H	1:A:449:GLU:HG2	1.52	0.46
2:B:354:TYR:OH	2:B:370:GLU:OE2	2.31	0.46
1:A:219:LYS:CD	1:A:219:LYS:N	2.79	0.46
2:B:24:TRP:CZ3	2:B:59:PRO:HG2	2.51	0.46
1:A:330:GLN:HE21	1:A:338:THR:HG23	1.81	0.46
2:B:263:LYS:HB2	4:B:736:HOH:O	2.16	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.14	0.46
1:A:463:ARG:HH11	1:A:463:ARG:CG	2.03	0.46
1:A:466:VAL:CG2	1:A:551:LEU:CG	2.93	0.46
2:B:13:LYS:CE	2:B:86:ASP:N	2.79	0.46
2:B:103:LYS:O	2:B:236:PRO:HD2	2.16	0.46
2:B:337:TRP:HE1	2:B:367:GLN:NE2	2.09	0.46
1:A:279:LEU:HD22	1:A:302:GLU:OE1	2.15	0.46
1:A:362:THR:HG21	1:A:367:GLN:HE21	1.81	0.46
2:B:24:TRP:CZ3	2:B:59:PRO:CB	2.99	0.46
2:B:275:LYS:H	2:B:306:ASN:HD21	1.64	0.46
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.75	0.46
1:A:138:GLU:O	1:A:139:THR:CB	2.64	0.45
2:B:72:ARG:NH2	2:B:409:THR:CG2	2.78	0.45
2:B:388:LYS:HE3	2:B:415:GLU:HG3	1.98	0.45
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.98	0.45
1:A:219:LYS:O	1:A:220:LYS:CB	2.63	0.45
1:A:543:GLY:O	1:A:545:ASN:N	2.50	0.45
2:B:100:LEU:HD13	2:B:179:VAL:HG22	1.99	0.45
2:B:244:ILE:CD1	2:B:266:TRP:CZ3	3.00	0.45
1:A:275:LYS:HE3	1:A:305:GLU:OE2	2.17	0.45
1:A:297:GLU:CA	1:A:298:GLU:N	2.80	0.45
2:B:281:LYS:O	2:B:284:ARG:HG3	2.17	0.45
1:A:125:ARG:HG2	1:A:146:TYR:O	2.16	0.45
2:B:205:LEU:HD22	2:B:209:LEU:HD22	1.99	0.45
2:B:305:GLU:O	2:B:305:GLU:HG2	2.17	0.45
1:A:1:PRO:HD2	4:A:608:HOH:O	2.16	0.45
1:A:174:GLN:HG2	1:A:174:GLN:H	1.60	0.45
2:B:116:PHE:C	2:B:116:PHE:CD2	2.95	0.45
1:A:199:ARG:NH1	1:A:199:ARG:CG	2.77	0.45
1:A:365:VAL:O	1:A:369:THR:CG2	2.65	0.45
1:A:376:THR:HG23	1:A:386:THR:HG22	1.99	0.45
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.99	0.45
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.99	0.45
2:B:353:LYS:O	2:B:374:LYS:NZ	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ALA:O	2:B:375:ILE:HD12	2.17	0.45
1:A:5:ILE:HD13	1:A:163:SER:HB3	1.98	0.44
2:B:270:ILE:HG12	2:B:271:TYR:N	2.32	0.44
2:B:354:TYR:HD2	2:B:374:LYS:HD2	1.82	0.44
1:A:454:LYS:NZ	1:A:556:ILE:CD1	2.80	0.44
1:A:60:VAL:HG13	1:A:130:PHE:HB2	1.99	0.44
1:A:100:LEU:HD22	3:A:561:MRX:H151	1.99	0.44
1:A:107:THR:CG2	1:A:198:HIS:CE1	2.90	0.44
2:B:194:GLU:OE1	2:B:197:GLN:HG3	2.18	0.44
2:B:271:TYR:CD1	2:B:310:LEU:CD1	3.00	0.44
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.99	0.44
1:A:297:GLU:CB	1:A:298:GLU:N	2.80	0.44
1:A:21:VAL:HG22	1:A:59:PRO:CD	2.38	0.44
1:A:466:VAL:HG21	1:A:551:LEU:CG	2.48	0.44
2:B:214:LEU:N	2:B:214:LEU:CD2	2.76	0.44
2:B:299:ALA:O	2:B:302:GLU:N	2.40	0.44
1:A:60:VAL:HG11	1:A:130:PHE:HD2	1.83	0.44
1:A:51:GLY:N	1:A:53:GLU:OE1	2.46	0.43
1:A:136:ASN:O	1:A:138:GLU:N	2.50	0.43
1:A:457:TYR:O	1:A:464:GLN:HA	2.18	0.43
1:A:107:THR:CG2	1:A:202:ILE:HD11	2.48	0.43
1:A:174:GLN:HB2	4:A:849:HOH:O	2.18	0.43
1:A:2:ILE:HD11	1:A:46:LYS:HD3	2.00	0.43
2:B:90:VAL:CG2	2:B:91:GLN:N	2.80	0.43
2:B:125:ARG:HD3	2:B:147:ASN:HD22	1.82	0.43
1:A:173:LYS:HD2	1:A:173:LYS:HA	1.49	0.43
2:B:24:TRP:HZ3	2:B:59:PRO:HG2	1.84	0.43
1:A:357:MET:HE3	1:A:360:ALA:O	2.18	0.43
1:A:542:ILE:H	1:A:542:ILE:HG12	1.37	0.43
2:B:13:LYS:HE3	2:B:85:GLN:CA	2.49	0.43
1:A:206:ARG:NH1	1:A:218:ASP:HB3	2.34	0.43
2:B:169:GLU:HG3	4:B:709:HOH:O	2.18	0.43
2:B:264:LEU:HD22	2:B:274:ILE:HG23	2.01	0.43
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.87	0.43
1:A:346:PHE:N	1:A:346:PHE:CD1	2.82	0.43
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.49	0.43
2:B:244:ILE:HD13	2:B:266:TRP:HZ3	1.83	0.42
1:A:356:ARG:NH2	1:A:358:ARG:HH11	2.17	0.42
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.23	0.42
1:A:180:ILE:HG23	1:A:180:ILE:HD13	1.79	0.42
1:A:236:PRO:HA	3:A:561:MRX:H5	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG13	4:A:578:HOH:O	2.19	0.42
2:B:312:GLU:CD	2:B:313:PRO:HD3	2.44	0.42
1:A:134:SER:OG	1:A:139:THR:HB	2.20	0.42
2:B:24:TRP:CE3	2:B:61:PHE:HZ	2.37	0.42
2:B:72:ARG:HH22	2:B:409:THR:HG21	1.81	0.42
2:B:250:ASP:O	2:B:251:SER:HB3	2.19	0.42
1:A:298:GLU:N	1:A:298:GLU:CD	2.78	0.42
2:B:237:ASP:OD2	2:B:238:LYS:HD3	2.19	0.42
1:A:540:LYS:CB	1:A:542:ILE:CD1	2.97	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.19	0.42
2:B:354:TYR:CD2	2:B:374:LYS:HD2	2.54	0.42
2:B:388:LYS:HG2	4:B:535:HOH:O	2.18	0.42
1:A:497:THR:O	1:A:535:TRP:HA	2.20	0.42
1:A:311:LYS:O	1:A:312:GLU:CB	2.67	0.42
2:B:182:GLN:NE2	4:B:605:HOH:O	2.24	0.42
1:A:395:LYS:HG3	1:A:414:TRP:CH2	2.55	0.42
2:B:293:ILE:O	2:B:293:ILE:HG13	2.20	0.42
1:A:500:GLN:CG	2:B:422:LEU:CD1	2.97	0.41
2:B:274:ILE:CD1	2:B:309:ILE:HG21	2.50	0.41
2:B:90:VAL:HG23	2:B:91:GLN:N	2.35	0.41
2:B:239:TRP:CZ2	2:B:378:GLU:HG2	2.55	0.41
1:A:41:MET:HE2	1:A:47:ILE:CG2	2.50	0.41
1:A:439:THR:O	1:A:459:THR:HA	2.21	0.41
1:A:500:GLN:HE21	1:A:500:GLN:HB3	1.67	0.41
1:A:553:SER:OG	1:A:557:ARG:NH1	2.54	0.41
2:B:13:LYS:HE2	2:B:86:ASP:N	2.35	0.41
1:A:59:PRO:HB2	1:A:61:PHE:CZ	2.55	0.41
2:B:312:GLU:CB	2:B:313:PRO:CD	2.97	0.41
2:B:317:VAL:CG1	2:B:347:LYS:HB3	2.49	0.41
1:A:47:ILE:HD12	1:A:144:TYR:CG	2.56	0.41
1:A:399:GLU:HB2	1:A:402:TRP:HZ3	1.83	0.41
1:A:493:VAL:CG2	1:A:528:LYS:HE3	2.51	0.41
1:A:254:VAL:O	1:A:258:GLN:HG3	2.21	0.41
1:A:403:THR:HG22	1:A:404:GLU:N	2.36	0.41
1:A:433:PRO:HB2	2:B:290:THR:HG23	2.03	0.41
1:A:3:SER:OG	1:A:212:TRP:O	2.35	0.41
1:A:277:ARG:CD	1:A:336:GLN:CD	2.93	0.41
1:A:434:ILE:HG21	1:A:492:GLU:OE2	2.20	0.41
2:B:24:TRP:HZ3	2:B:59:PRO:CG	2.34	0.41
2:B:244:ILE:HD11	2:B:266:TRP:CZ3	2.55	0.41
2:B:346:PHE:HD2	2:B:346:PHE:HA	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.46	0.40
1:A:454:LYS:CG	1:A:556:ILE:CD1	2.98	0.40
2:B:65:LYS:HG2	2:B:407:GLN:O	2.20	0.40
2:B:282:LEU:HD12	2:B:293:ILE:HD12	2.02	0.40
2:B:88:TRP:CZ3	2:B:89:GLU:HB2	2.57	0.40
2:B:253:THR:CG2	2:B:255:ASN:HB3	2.52	0.40
2:B:345:PRO:O	2:B:347:LYS:HD2	2.22	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	548/563 (97%)	510 (93%)	27 (5%)	11 (2%)	6 7
2	B	399/443 (90%)	372 (93%)	19 (5%)	8 (2%)	6 7
All	All	947/1006 (94%)	882 (93%)	46 (5%)	19 (2%)	6 7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	THR
1	A	356	ARG
1	A	543	GLY
2	B	14	PRO
2	B	241	VAL
2	B	242	GLN
2	B	243	PRO
1	A	114	ALA
1	A	140	PRO
1	A	492	GLU
1	A	542	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	544	GLY
2	B	66	LYS
1	A	137	ASN
1	A	312	GLU
2	B	13	LYS
2	B	269	GLN
2	B	251	SER
1	A	220	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/503 (98%)	390 (79%)	104 (21%)	1	1
2	B	369/403 (92%)	303 (82%)	66 (18%)	2	2
All	All	863/906 (95%)	693 (80%)	170 (20%)	1	2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	22	LYS
1	A	24	TRP
1	A	26	LEU
1	A	42	GLU
1	A	43	LYS
1	A	49	LYS
1	A	64	LYS
1	A	68	SER
1	A	70	LYS
1	A	72	ARG
1	A	74	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	82	LYS
1	A	90	VAL
1	A	92	LEU
1	A	94	ILE
1	A	103	LYS
1	A	104	LYS
1	A	106	VAL
1	A	107	THR
1	A	118	VAL
1	A	126	LYS
1	A	134	SER
1	A	135	ILE
1	A	142	ILE
1	A	162	SER
1	A	166	LYS
1	A	173	LYS
1	A	174	GLN
1	A	175	ASN
1	A	180	ILE
1	A	195	ILE
1	A	197	GLN
1	A	201	LYS
1	A	205	LEU
1	A	210	LEU
1	A	215	THR
1	A	219	LYS
1	A	220	LYS
1	A	223	LYS
1	A	228	LEU
1	A	245	VAL
1	A	249	LYS
1	A	259	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	287	LYS
1	A	289	LEU
1	A	291	GLU
1	A	293	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	312	GLU
1	A	334	GLN
1	A	344	GLU
1	A	347	LYS
1	A	356	ARG
1	A	358	ARG
1	A	368	LEU
1	A	369	THR
1	A	402	TRP
1	A	403	THR
1	A	422	LEU
1	A	425	LEU
1	A	429	LEU
1	A	434	ILE
1	A	435	VAL
1	A	449	GLU
1	A	451	LYS
1	A	452	LEU
1	A	454	LYS
1	A	459	THR
1	A	461	ARG
1	A	463	ARG
1	A	464	GLN
1	A	471	ASP
1	A	472	THR
1	A	475	GLN
1	A	479	LEU
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	503	LEU
1	A	507	GLN
1	A	514	GLU
1	A	516	GLU
1	A	523	GLU
1	A	527	LYS
1	A	529	GLU
1	A	540	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	542	ILE
1	A	547	GLN
1	A	550	LYS
1	A	552	VAL
1	A	557	ARG
2	B	8	VAL
2	B	11	LYS
2	B	12	LEU
2	B	13	LYS
2	B	16	MET
2	B	20	LYS
2	B	22	LYS
2	B	26	LEU
2	B	64	LYS
2	B	65	LYS
2	B	66	LYS
2	B	67	ASP
2	B	68	SER
2	B	72	ARG
2	B	80	LEU
2	B	82	LYS
2	B	90	VAL
2	B	91	GLN
2	B	111	VAL
2	B	117	SER
2	B	120	LEU
2	B	162	SER
2	B	173	LYS
2	B	179	VAL
2	B	187	LEU
2	B	199	ARG
2	B	205	LEU
2	B	209	LEU
2	B	211	ARG
2	B	214	LEU
2	B	215	THR
2	B	237	ASP
2	B	238	LYS
2	B	240	THR
2	B	241	VAL
2	B	249	LYS
2	B	253	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	259	LYS
2	B	260	LEU
2	B	261	VAL
2	B	265	ASN
2	B	270	ILE
2	B	275	LYS
2	B	277	ARG
2	B	278	GLN
2	B	279	LEU
2	B	281	LYS
2	B	282	LEU
2	B	284	ARG
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	309	ILE
2	B	310	LEU
2	B	314	VAL
2	B	317	VAL
2	B	336	GLN
2	B	341	ILE
2	B	347	LYS
2	B	349	LEU
2	B	356	ARG
2	B	362	THR
2	B	369	THR
2	B	400	THR
2	B	425	LEU
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	137	ASN
1	A	147	ASN
1	A	151	GLN
1	A	161	GLN
1	A	197	GLN
1	A	198	HIS
1	A	235	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	ASN
1	A	330	GLN
1	A	394	GLN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
2	B	96	HIS
2	B	147	ASN
2	B	175	ASN
2	B	265	ASN
2	B	278	GLN
2	B	306	ASN
2	B	336	GLN
2	B	373	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	MRX	A	561	-	21,23,23	2.28	8 (38%)	29,35,35	3.07	14 (48%)

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	MRX	A	561	-	-	0/14/23/23	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	MRX	O16-S10	5.17	1.48	1.43
3	A	561	MRX	C2-C7	4.39	1.50	1.45
3	A	561	MRX	C18-N20	3.45	1.43	1.33
3	A	561	MRX	C8-C18	-3.31	1.42	1.47
3	A	561	MRX	BR-C6	2.76	1.95	1.90
3	A	561	MRX	C8-C7	2.67	1.43	1.39
3	A	561	MRX	C1-C2	2.57	1.43	1.39
3	A	561	MRX	C5-C6	2.28	1.42	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	MRX	O17-S10-O16	9.19	132.88	119.69
3	A	561	MRX	C12-N11-C15	-7.39	101.00	111.22
3	A	561	MRX	C3-N9-C8	5.01	114.50	109.00
3	A	561	MRX	O17-S10-N11	-4.06	100.19	107.26
3	A	561	MRX	BR-C6-C1	3.65	124.40	119.23
3	A	561	MRX	O19-C18-N20	-3.38	115.31	122.89
3	A	561	MRX	C14-C15-N11	3.20	109.24	103.52
3	A	561	MRX	C5-C6-C1	-3.11	117.06	121.53
3	A	561	MRX	O16-S10-N11	-3.08	101.89	107.26
3	A	561	MRX	C13-C12-N11	-2.45	99.15	103.52
3	A	561	MRX	O17-S10-C7	-2.26	103.04	107.67
3	A	561	MRX	C1-C2-C3	-2.18	117.27	119.39
3	A	561	MRX	C4-C5-C6	2.12	121.72	119.18
3	A	561	MRX	C2-C1-C6	2.10	122.61	118.99

There are no chirality outliers.

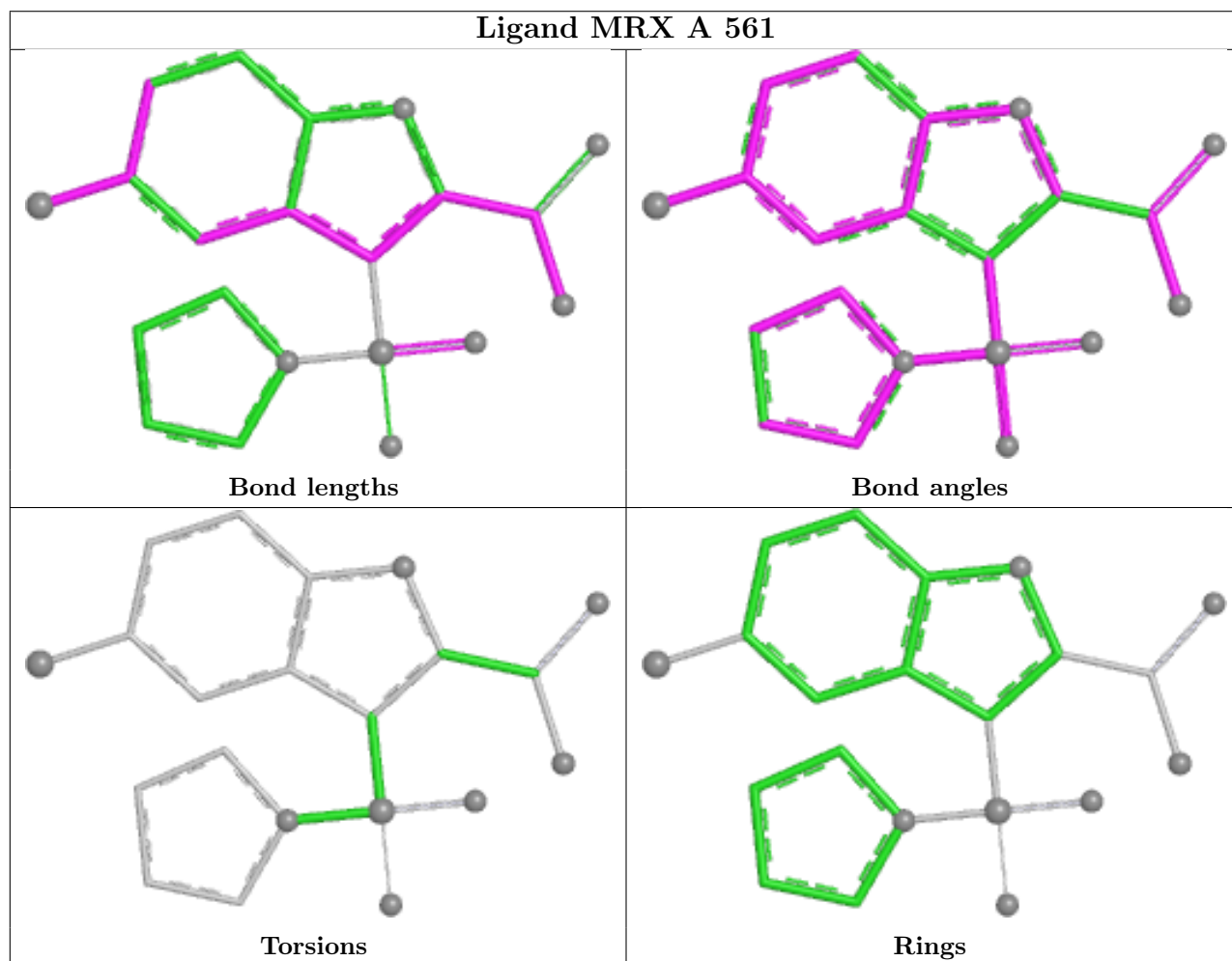
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	MRX	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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	297:GLU	C	298:GLU	N	2.65

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.