



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:38 PM GMT

PDB ID : 2RF2  
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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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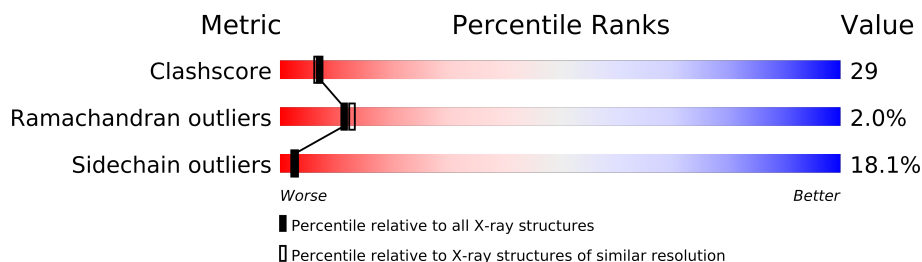
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	563	
2	B	443	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8593 atoms, of which 0 are hydrogen and 0 are deuterium.

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/ribonucleaseH (EC 2.7.7.49) (EC 2.7.7.7) (EC 3.1.26.4) (p66 RT).

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

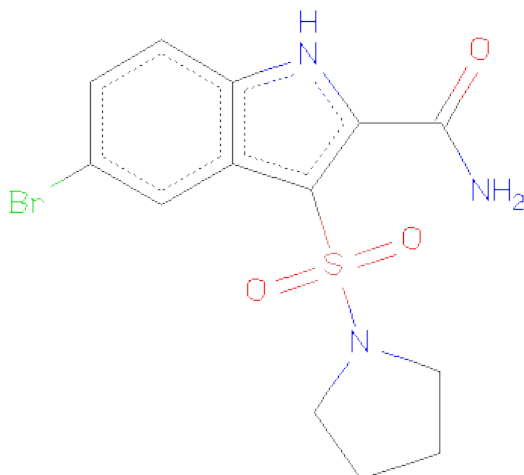
- Molecule 2 is a protein called Reverse transcriptase/ribonucleaseH (EC 2.7.7.49) (EC 2.7.7.7) (EC 3.1.26.4) (p66 RT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	0	0
			3352	2182	555	609	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 5-BROMO-3-(PYRROLIDIN-1-YLSULFONYL)-1H-INDOLE-2-CARBOXYAMIDE (three-letter code: MRX) (formula: C<sub>13</sub>H<sub>14</sub>BrN<sub>3</sub>O<sub>3</sub>S).

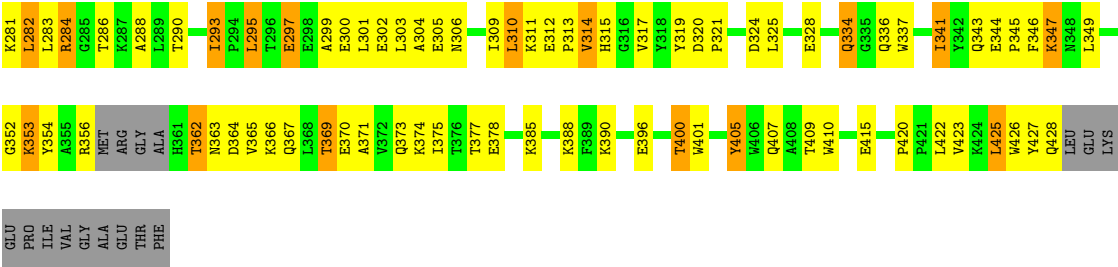


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	S	0	0
			21	1	13	3	3	1		

- 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		





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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.	Xtriage
Total number of atoms	8593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.62	0/4625	0.79	1/6282 (0.0%)
2	B	0.62	0/3446	0.82	4/4682 (0.1%)
All	All	0.62	0/8071	0.80	5/10964 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	LYS	C-N-CD	-16.25	84.85	120.60
2	B	271	TYR	C-N-CD	-7.60	103.88	120.60
2	B	120	LEU	CA-CB-CG	5.89	128.84	115.30
2	B	244	ILE	N-CA-C	-5.33	96.60	111.00
1	A	86	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4510	0	4558	258	0
2	B	3352	0	3380	204	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	452	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (452) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HD23	2:B:214:LEU:H	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: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
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.41	0.85
1:A:297:GLU:O	1:A:298:GLU:N	2.07	0.85
1:A:356:ARG:NE	1:A:358:ARG:HG3	1.92	0.84
1:A:195:ILE:H	1:A:195:ILE:HD12	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
2:B:274:ILE:HA	2:B:306:ASN:ND2	1.93	0.83
1:A:399:GLU:O	1:A:403:THR:HB	1.79	0.83
1:A:478:GLU:HG3	4:A:596:HOH:O	1.80	0.82
1:A:411:ILE:HG22	1:A:412:PRO:O	1.79	0.82
1:A:199:ARG:HH11	1:A:199:ARG:HG2	1.44	0.81
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.62	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:454:LYS:HZ3	1:A:556:ILE:HD11	1.50	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
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
2:B:214:LEU:N	2:B:214:LEU:HD23	2.03	0.73
2:B:125:ARG:HG2	2:B:146:TYR:O	1.88	0.73
1:A:219:LYS:O	1:A:220:LYS:HB3	1.89	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:H	2:B:303:LEU:HD23	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:399:GLU:HA	1:A:402:TRP:HE3	1.52	0.70
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.74	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:296:THR:HG21	4:A:597:HOH:O	1.93	0.68
1:A:223:LYS:CD	1:A:223:LYS:H	2.03	0.68
2:B:297:GLU:O	2:B:301:LEU:HG	1.92	0.68
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
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.19	0.68
1:A:367:GLN:NE2	1:A:512:GLN:OE1	2.27	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
2:B:295:LEU:HD23	2:B:299:ALA:HB3	1.77	0.66
1:A:540:LYS:CB	1:A:542:ILE:HD11	2.26	0.66
1:A:454:LYS:HZ3	1:A:556:ILE:CD1	2.09	0.66
1:A:223:LYS:N	1:A:223:LYS:HD2	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
2:B:282:LEU:HD12	2:B:293:ILE:CD1	2.26	0.65
1:A:139:THR:HG22	1:A:140:PRO:N	2.12	0.65
2:B:363:ASN:HA	4:B:580:HOH:O	1.97	0.65
2:B:345:PRO:O	2:B:346:PHE:HB2	1.96	0.65
2:B:16:MET:HA	2:B:16:MET:HE2	1.78	0.65
1:A:51:GLY:O	1:A:143:ARG:NH1	2.30	0.65
1:A:171:PHE:O	1:A:175:ASN:ND2	2.29	0.64
2:B:377:THR:HG22	2:B:410:TRP:HZ2	1.61	0.64
2:B:276:VAL:HG12	2:B:280:CYS:SG	2.36	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
2:B:253:THR:HG23	2:B:255:ASN:N	2.12	0.63
2:B:282:LEU:HD21	2:B:299:ALA:CB	2.29	0.63
2:B:40:GLU:O	2:B:44:GLU:HG3	1.98	0.63
2:B:273:GLY:O	2:B:275:LYS:HG2	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:103:LYS:HE3	2:B:179:VAL:HG13	1.81	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:NH1	1:A:463:ARG:HG2	1.99	0.62
2:B:195:ILE:O	2:B:199:ARG:HG3	1.98	0.62
2:B:16:MET:CE	2:B:16:MET:HA	2.28	0.62
2:B:253:THR:HG23	2:B:255:ASN:H	1.65	0.61
1:A:472:THR:HG22	1:A:476:LYS:CB	2.30	0.61
1:A:365:VAL:O	1:A:369:THR:HG23	2.01	0.61
2:B:295:LEU:HD22	2:B:300:GLU:HG2	1.82	0.61
1:A:362:THR:CG2	1:A:367:GLN:HE21	2.14	0.60
1:A:94:ILE:HD13	1:A:230:MET:HG3	1.82	0.60
2:B:362:THR:HG23	2:B:366:LYS:HZ2	1.66	0.60
1:A:106:VAL:HG11	3:A:561:MRX:BR	2.56	0.60
1:A:28:GLU:HG2	1:A:135:ILE:HG12	1.82	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
2:B:279:LEU:O	2:B:282:LEU:HB2	2.02	0.60
1:A:3:SER:CB	1:A:5:ILE:HG12	2.31	0.60
1:A:556:ILE:N	1:A:556:ILE:HD12	2.17	0.60
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.37	0.60
2:B:286:THR:O	2:B:286:THR:HG23	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: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:277:ARG:HD3	1:A:336:GLN:CD	2.24	0.58
1:A:432:GLU:OE1	1:A:433:PRO:HD2	2.03	0.58
1:A:24:TRP:N	1:A:24:TRP:CD1	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
2:B:252:TRP:CD1	2:B:295:LEU:HD12	2.39	0.58
1:A:399:GLU:HB2	1:A:402:TRP:CZ3	2.38	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:PRO:HD3	4:A:639:HOH:O	2.03	0.58
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.84	0.58
1:A:432:GLU:OE1	1:A:432:GLU:HA	2.04	0.57
1:A:324:ASP:O	1:A:343:GLN:HG2	2.03	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
1:A:500:GLN:HG2	2:B:422:LEU:HD12	1.87	0.57
1:A:199:ARG:NH1	1:A:199:ARG:HG2	2.17	0.57
2:B:317:VAL:HG13	2:B:347:LYS:HB3	1.87	0.57
1:A:556:ILE:O	1:A:556:ILE:HG22	2.05	0.57
1:A:441:TYR:O	1:A:548:VAL:HG21	2.05	0.56
1:A:303:LEU:HD13	1:A:307:ARG:NH1	2.20	0.56
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.34	0.56
2:B:282:LEU:CD2	2:B:299:ALA:HB2	2.34	0.56
2:B:266:TRP:CH2	2:B:427:TYR:CZ	2.92	0.56
2:B:86:ASP:O	2:B:90:VAL:HG22	2.04	0.56
1:A:211:ARG:O	1:A:211:ARG:NH1	2.28	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:422:LEU:O	2:B:425:LEU:HG	2.05	0.55
2:B:278:GLN:NE2	2:B:281:LYS:NZ	2.54	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
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
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:466:VAL:HG21	1:A:551:LEU:CD1	2.37	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:138:GLU:O	1:A:139:THR:HB	2.08	0.54
1:A:555:GLY:C	1:A:556:ILE:HD12	2.27	0.54
1:A:3:SER:HB3	1:A:5:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:240:THR:O	2:B:241:VAL:O	2.26	0.54
1:A:311:LYS:O	1:A:312:GLU:HB3	2.08	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
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
2:B:362:THR:HG22	2:B:367:GLN:HG3	1.89	0.53
1:A:502:ALA:O	1:A:506:ILE:HD12	2.08	0.53
1:A:278:GLN:OE1	1:A:281:LYS:NZ	2.31	0.53
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.43	0.53
1:A:64:LYS:HE2	1:A:69:THR:CG2	2.14	0.53
1:A:69:THR:HG22	1:A:69:THR:O	2.08	0.53
1:A:180:ILE:HG22	1:A:189:VAL:HG13	1.91	0.53
2:B:334:GLN:HG3	2:B:334:GLN:O	2.09	0.53
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.09	0.53
2:B:300:GLU:HA	2:B:303:LEU:HD21	1.90	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
1:A:296:THR:HG22	1:A:299:ALA:HB3	1.90	0.53
2:B:254:VAL:HG21	2:B:288:ALA:O	2.09	0.53
2:B:409:THR:HG21	4:B:451:HOH:O	2.09	0.52
2:B:157:PRO:HG3	2:B:184:MET:HA	1.91	0.52
1:A:296:THR:HG22	1:A:299:ALA:HB2	1.90	0.52
1:A:134:SER:HB2	1:A:140:PRO:O	2.10	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:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.52
1:A:41:MET:HE2	1:A:47:ILE:HG23	1.91	0.52
1:A:40:GLU:O	1:A:44:GLU:HG3	2.08	0.52
1:A:356:ARG:HH21	1:A:358:ARG:HD2	1.74	0.52
1:A:298:GLU:OE2	1:A:298:GLU:N	2.42	0.52
1:A:312:GLU:HB2	4:A:922:HOH:O	2.08	0.52
2:B:301:LEU:O	2:B:304:ALA:HB3	2.10	0.52
2:B:241:VAL:HB	2:B:243:PRO:HD3	1.91	0.52
2:B:278:GLN:HE22	2:B:281:LYS:HZ2	1.56	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
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:278:GLN:HA	2:B:281:LYS:HD3	1.92	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
1:A:31:ILE:HD13	1:A:133:PRO:O	2.10	0.51
2:B:297:GLU:OE1	2:B:300:GLU:OE2	2.29	0.51
2:B:261:VAL:HB	2:B:276:VAL:HG13	1.92	0.51
1:A:466:VAL:CG2	1:A:551:LEU:HD11	2.40	0.51
2:B:24:TRP:CZ3	2:B:59:PRO:CG	2.94	0.51
1:A:500:GLN:HG2	2:B:422:LEU:CD1	2.41	0.51
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.33	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
2:B:86:ASP:OD2	2:B:90:VAL:HG21	2.11	0.50
1:A:395:LYS:HD3	4:A:853:HOH:O	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:548:VAL:O	1:A:552:VAL:HB	2.11	0.50
1:A:466:VAL:CG2	1:A:551:LEU:HG	2.42	0.50
2:B:242:GLN:HG2	2:B:352:GLY:CA	2.42	0.50
2:B:266:TRP:O	2:B:268:SER:O	2.29	0.50
1:A:297:GLU:C	1:A:298:GLU:N	2.65	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
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:236:PRO:HA	2:B:239:TRP:CD2	2.46	0.49
2:B:233:GLU:HB2	4:B:510:HOH:O	2.12	0.49
2:B:108:VAL:HB	2:B:232:TYR:HB3	1.94	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:HG13	2:B:111:VAL:O	2.12	0.49
2:B:278:GLN:NE2	2:B:281:LYS:HZ3	2.09	0.49
1:A:148:VAL:O	1:A:150:PRO:HD3	2.13	0.49
2:B:303:LEU:HD23	2:B:303:LEU:N	2.25	0.49
2:B:101:LYS:O	2:B:236:PRO:HB2	2.13	0.49
1:A:137:ASN:OD1	1:A:137:ASN:O	2.30	0.49
1:A:139:THR:CG2	1:A:140:PRO:CD	2.90	0.49
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.28	0.48
1:A:139:THR:CG2	1:A:140:PRO:N	2.76	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:LYS:CD	1:A:219:LYS:H	2.21	0.48
1:A:276:VAL:HG13	1:A:280:CYS:SG	2.53	0.48
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.91	0.48
1:A:118:VAL:HG22	1:A:149:LEU:HG	1.93	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
2:B:44:GLU:OE2	2:B:46:LYS:HE2	2.14	0.48
1:A:424:LYS:NZ	1:A:426:TRP:CZ2	2.81	0.48
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.96	0.48
1:A:297:GLU:C	1:A:300:GLU:HB2	2.34	0.48
1:A:24:TRP:HE1	1:A:59:PRO:HB3	1.79	0.48
1:A:219:LYS:HD2	1:A:219:LYS:N	2.29	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:41:MET:HE2	1:A:47:ILE:CG2	2.44	0.47
2:B:295:LEU:HD23	2:B:299:ALA:CB	2.42	0.47
1:A:116:PHE:HZ	4:A:611:HOH:O	1.97	0.47
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.47
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.96	0.47
1:A:410:TRP:CE3	2:B:363:ASN:HB3	2.49	0.47
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.44	0.47
1:A:206:ARG:HG2	1:A:216:THR:OG1	2.14	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
2:B:266:TRP:CD1	2:B:426:TRP:CE3	3.02	0.47
1:A:451:LYS:N	1:A:451:LYS:HD3	2.29	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
1:A:402:TRP:CD1	1:A:402:TRP:C	2.87	0.47
2:B:396:GLU:O	2:B:400:THR:CG2	2.63	0.47
2:B:396:GLU:O	2:B:400:THR:HG23	2.15	0.47
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.77	0.47
1:A:101:LYS:N	1:A:101:LYS:HD3	2.29	0.47
1:A:5:ILE:HG21	1:A:167:ILE:HD11	1.97	0.47
1:A:108:VAL:HG21	1:A:223:LYS:HD3	1.96	0.46
1:A:72:ARG:HD3	4:A:899:HOH:O	2.15	0.46
2:B:261:VAL:O	2:B:265:ASN:HB3	2.15	0.46
2:B:64:LYS:HG3	2:B:68:SER:O	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:354:TYR:OH	2:B:370:GLU:OE2	2.31	0.46
1:A:449:GLU:H	1:A:449:GLU:HG2	1.52	0.46
1:A:219:LYS:N	1:A:219:LYS:CD	2.79	0.46
1:A:211:ARG:C	1:A:211:ARG:HD3	2.36	0.46
2:B:24:TRP:CZ3	2:B:59:PRO:HG2	2.51	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.14	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:463:ARG:CG	1:A:463:ARG:HH11	2.03	0.46
2:B:13:LYS:CE	2:B:86:ASP:N	2.79	0.46
1:A:466:VAL:CG2	1:A:551:LEU:CG	2.93	0.46
2:B:337:TRP:HE1	2:B:367:GLN:NE2	2.09	0.46
2:B:103:LYS:O	2:B:236:PRO:HD2	2.16	0.46
2:B:275:LYS:H	2:B:306:ASN:HD21	1.64	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
1:A:279:LEU:HD22	1:A:302:GLU:OE1	2.15	0.46
2:B:271:TYR:HA	2:B:272:PRO:HD2	1.75	0.46
1:A:136:ASN:C	1:A:138:GLU:H	2.19	0.45
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
2:B:90:VAL:CG2	2:B:91:GLN:N	2.80	0.45
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.98	0.45
2:B:244:ILE:CD1	2:B:266:TRP:CZ3	3.00	0.45
1:A:219:LYS:O	1:A:220:LYS:CB	2.63	0.45
2:B:100:LEU:HD13	2:B:179:VAL:HG22	1.99	0.45
1:A:543:GLY:O	1:A:545:ASN:N	2.50	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:275:LYS:HE3	1:A:305:GLU:OE2	2.17	0.45
2:B:205:LEU:HD22	2:B:209:LEU:HD22	1.99	0.45
2:B:305:GLU:HG2	2:B:305:GLU:O	2.17	0.45
1:A:125:ARG:HG2	1:A:146:TYR:O	2.16	0.45
1:A:1:PRO:HD2	4:A:608:HOH:O	2.16	0.45
1:A:174:GLN:H	1:A:174:GLN:HG2	1.60	0.45
2:B:242:GLN:HG2	2:B:352:GLY:C	2.38	0.45
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.99	0.45
1:A:199:ARG:NH1	1:A:199:ARG:CG	2.77	0.45
2:B:353:LYS:O	2:B:374:LYS:NZ	2.50	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:371:ALA:O	2:B:375:ILE:HD12	2.17	0.45
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.99	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
2:B:271:TYR:CD1	2:B:310:LEU:CD1	3.00	0.44
1:A:107:THR:CG2	1:A:198:HIS:CE1	2.90	0.44
1:A:100:LEU:HD22	3:A:561:MRX:H151	1.99	0.44
1:A:60:VAL:HG13	1:A:130:PHE:HB2	1.99	0.44
2:B:194:GLU:OE1	2:B:197:GLN:HG3	2.18	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
2:B:299:ALA:O	2:B:302:GLU:N	2.40	0.44
2:B:214:LEU:N	2:B:214:LEU:CD2	2.76	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
1:A:60:VAL:HG11	1:A:130:PHE:HD2	1.83	0.44
1:A:136:ASN:O	1:A:138:GLU:N	2.50	0.43
1:A:51:GLY:N	1:A:53:GLU:OE1	2.46	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
2:B:125:ARG:HD3	2:B:147:ASN:HD22	1.82	0.43
1:A:2:ILE:HD11	1:A:46:LYS:HD3	2.00	0.43
2:B:24:TRP:HZ3	2:B:59:PRO:HG2	1.84	0.43
1:A:173:LYS:HD2	1:A:173:LYS:HA	1.49	0.43
2:B:13:LYS:HE3	2:B:85:GLN:CA	2.49	0.43
1:A:542:ILE:H	1:A:542:ILE:HG12	1.37	0.43
1:A:287:LYS:HB2	1:A:291:GLU:CD	2.38	0.43
1:A:206:ARG:NH1	1:A:218:ASP:HB3	2.34	0.43
2:B:264:LEU:HD22	2:B:274:ILE:HG23	2.01	0.43
2:B:169:GLU:HG3	4:B:709:HOH:O	2.18	0.43
1:A:457:TYR:C	1:A:457:TYR:CD1	2.92	0.43
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.87	0.43
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.49	0.43
1:A:346:PHE:CD1	1:A:346:PHE:N	2.82	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:180:ILE:HD13	1:A:180:ILE:HG23	1.79	0.42
1:A:542:ILE:HG13	4:A:578:HOH:O	2.19	0.42
1:A:236:PRO:HA	3:A:561:MRX:H5	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:SER:OG	1:A:139:THR:HB	2.20	0.42
2:B:72:ARG:HH22	2:B:409:THR:HG21	1.81	0.42
2:B:24:TRP:CE3	2:B:61:PHE:HZ	2.37	0.42
2:B:250:ASP:O	2:B:251:SER:HB3	2.19	0.42
2:B:237:ASP:OD2	2:B:238:LYS:HD3	2.19	0.42
2:B:354:TYR:CD2	2:B:374:LYS:HD2	2.54	0.42
1:A:540:LYS:CB	1:A:542:ILE:CD1	2.97	0.42
2:B:388:LYS:HG2	4:B:535:HOH:O	2.18	0.42
2:B:324:ASP:O	2:B:343:GLN:HG2	2.19	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
2:B:293:ILE:HG13	2:B:293:ILE:O	2.20	0.42
1:A:395:LYS:HG3	1:A:414:TRP:CH2	2.55	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: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:439:THR:O	1:A:459:THR:HA	2.21	0.41
1:A:59:PRO:HB2	1:A:61:PHE:CZ	2.55	0.41
2:B:317:VAL:CG1	2:B:347:LYS:HB3	2.49	0.41
2:B:312:GLU:CB	2:B:313:PRO:CD	2.97	0.41
1:A:399:GLU:HB2	1:A:402:TRP:HZ3	1.83	0.41
1:A:47:ILE:HD12	1:A:144:TYR:CG	2.56	0.41
1:A:493:VAL:CG2	1:A:528:LYS:HE3	2.51	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:254:VAL:O	1:A:258:GLN:HG3	2.21	0.41
2:B:244:ILE:HD11	2:B:266:TRP:CZ3	2.55	0.41
2:B:24:TRP:HZ3	2:B:59:PRO:CG	2.34	0.41
1:A:434:ILE:HG21	1:A:492:GLU:OE2	2.20	0.41
2:B:346:PHE:HD2	2:B:346:PHE:HA	1.73	0.41
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:253:THR:CG2	2:B:255:ASN:HB3	2.52	0.40
2:B:88:TRP:CZ3	2:B:89:GLU:HB2	2.57	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

### 5.3.1 Protein backbone ⓘ

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%)	11	13
2	B	399/443 (90%)	372 (93%)	19 (5%)	8 (2%)	11	13
All	All	947/1006 (94%)	882 (93%)	46 (5%)	19 (2%)	11	13

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
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 ⓘ

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%)	402 (81%)	92 (19%)	2	2
2	B	369/403 (92%)	305 (83%)	64 (17%)	3	3
All	All	863/906 (95%)	707 (82%)	156 (18%)	2	3

All (156) 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	68	SER
1	A	70	LYS
1	A	72	ARG
1	A	74	LEU
1	A	82	LYS
1	A	92	LEU
1	A	94	ILE
1	A	101	LYS
1	A	103	LYS
1	A	104	LYS
1	A	107	THR
1	A	118	VAL
1	A	126	LYS
1	A	134	SER
1	A	142	ILE
1	A	162	SER
1	A	173	LYS
1	A	174	GLN
1	A	175	ASN

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Mol	Chain	Res	Type
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	211	ARG
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	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	291	GLU
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	312	GLU
1	A	334	GLN
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	431	LYS
1	A	449	GLU
1	A	451	LYS
1	A	454	LYS
1	A	459	THR
1	A	461	ARG

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Mol	Chain	Res	Type
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	514	GLU
1	A	516	GLU
1	A	523	GLU
1	A	529	GLU
1	A	540	LYS
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	91	GLN
2	B	111	VAL
2	B	120	LEU
2	B	162	SER
2	B	173	LYS

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Mol	Chain	Res	Type
2	B	179	VAL
2	B	199	ARG
2	B	205	LEU
2	B	209	LEU
2	B	211	ARG
2	B	212	TRP
2	B	214	LEU
2	B	237	ASP
2	B	238	LYS
2	B	240	THR
2	B	241	VAL
2	B	249	LYS
2	B	253	THR
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	282	LEU
2	B	284	ARG
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	334	GLN
2	B	336	GLN
2	B	341	ILE
2	B	347	LYS
2	B	349	LEU
2	B	353	LYS
2	B	356	ARG
2	B	362	THR
2	B	369	THR
2	B	400	THR
2	B	405	TYR
2	B	425	LEU

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Mol	Chain	Res	Type
2	B	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	137	ASN
1	A	147	ASN
1	A	151	GLN
1	A	198	HIS
1	A	258	GLN
1	A	330	GLN
1	A	500	GLN
1	A	507	GLN
1	A	509	GLN
1	A	519	ASN
1	A	547	GLN
2	B	96	HIS
2	B	147	ASN
2	B	175	ASN
2	B	182	GLN
2	B	278	GLN
2	B	306	ASN
2	B	336	GLN
2	B	367	GLN
2	B	373	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	-	23,23,23	3.22	7 (30%)	32,35,35	3.27	14 (43%)

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	-	-	0/6/23/23	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	MRX	S10-N11	9.17	1.77	1.63
3	A	561	MRX	C7-C2	8.43	1.50	1.41
3	A	561	MRX	C18-N20	4.62	1.43	1.33
3	A	561	MRX	O16-S10	3.84	1.48	1.43
3	A	561	MRX	C8-C18	-3.66	1.42	1.51
3	A	561	MRX	C1-C6	2.91	1.41	1.36
3	A	561	MRX	BR-C6	2.33	1.95	1.90

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	MRX	O17-S10-O16	7.57	132.88	119.38
3	A	561	MRX	C8-C18-N20	6.90	127.86	115.82
3	A	561	MRX	O17-S10-N11	-6.40	100.19	106.71
3	A	561	MRX	C5-C6-C1	-5.34	117.06	121.94
3	A	561	MRX	O19-C18-N20	-5.04	115.31	122.59
3	A	561	MRX	C12-N11-C15	-4.83	101.00	109.83
3	A	561	MRX	O16-S10-N11	-4.73	101.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	561	MRX	C8-N9-C3	4.07	114.50	108.18
3	A	561	MRX	BR-C6-C1	3.76	124.40	119.82
3	A	561	MRX	C14-C15-N11	3.53	109.24	103.64
3	A	561	MRX	O17-S10-C7	-3.35	103.04	108.94
3	A	561	MRX	C13-C12-N11	-2.83	99.15	103.64
3	A	561	MRX	C4-C5-C6	2.52	121.72	119.13
3	A	561	MRX	C7-S10-N11	2.46	108.98	103.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.