



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 06:45 PM EDT

PDB ID : 3DRR  
Title : HIV reverse transcriptase Y181C mutant in complex with inhibitor R8e  
Authors : Yan, Y.  
Deposited on : 2008-07-11  
Resolution : 2.89 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

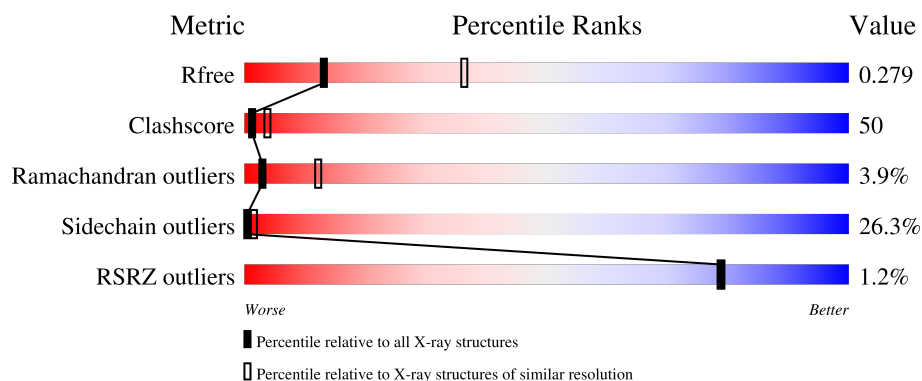
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

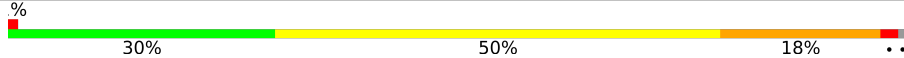
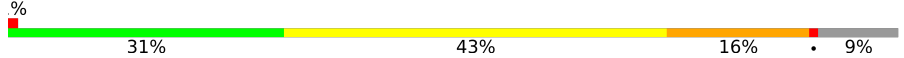
The reported resolution of this entry is 2.89 Å.

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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 30% 50% 18% 2% 1%
2	B	443	 31% 43% 16% 8% 2%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8249 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4536	2928	760	839	9			

There are 4 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
A	181	CYS	TYR	engineered mutation	UNP P04585

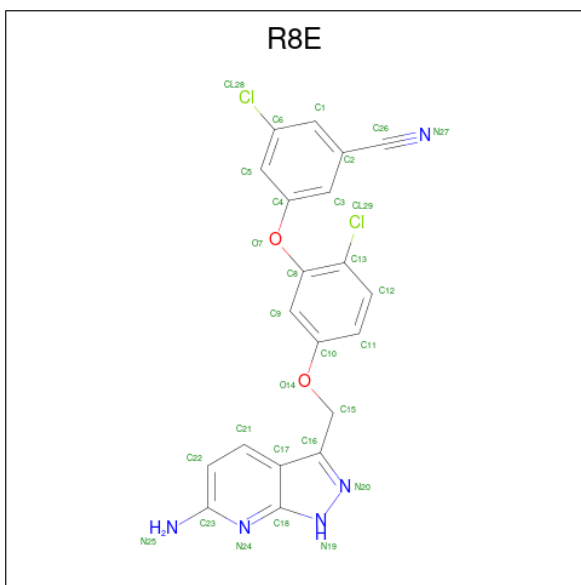
- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3338	2170	554	607	7			

There are 4 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
B	181	CYS	TYR	engineered mutation	UNP P04585

- Molecule 3 is 3-{5-[(6-amino-1H-pyrazolo[3,4-b]pyridin-3-yl)methoxy]-2-chlorophenoxy}-5-chlorobenzonitrile (three-letter code: R8E) (formula: C<sub>20</sub>H<sub>13</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			29	20	2	5	2		

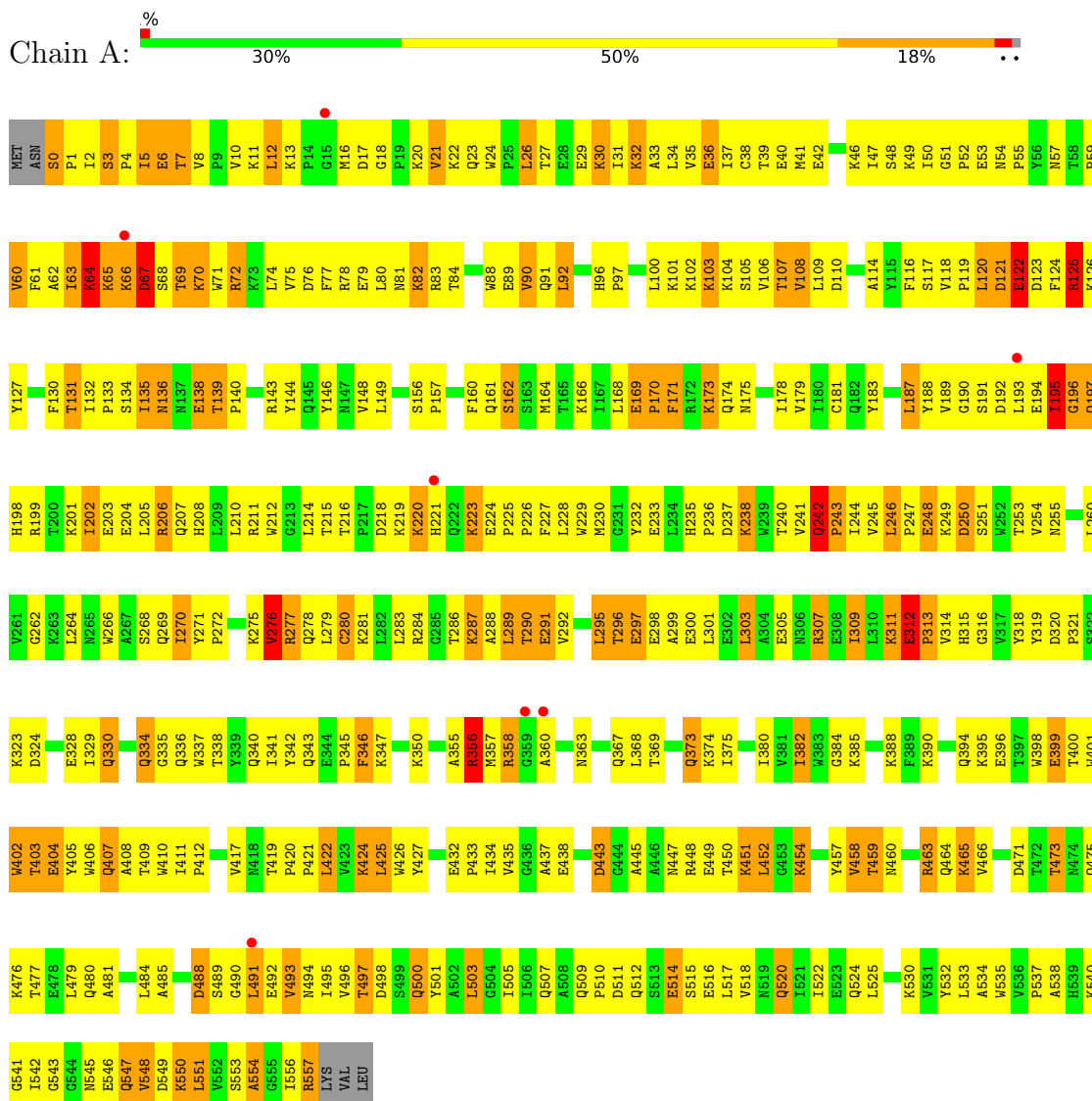
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	195	Total O 195 195	0	0
4	B	151	Total O 151 151	0	0

### 3 Residue-property plots

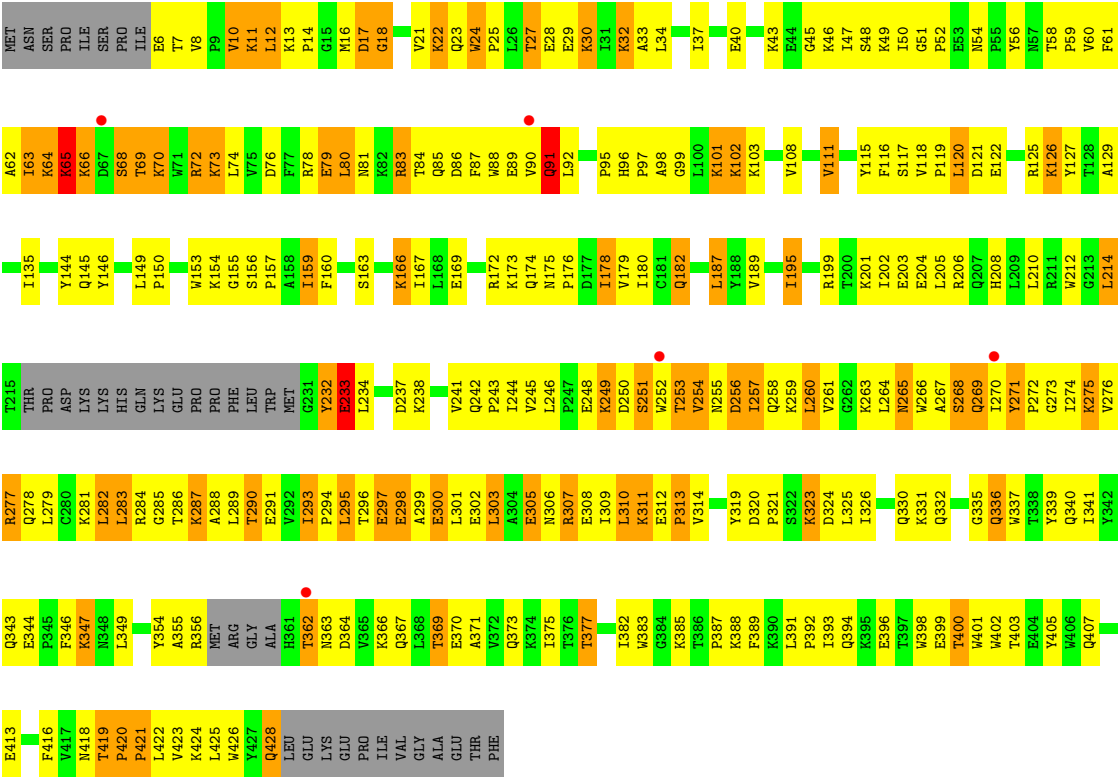
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Reverse transcriptase/ribonuclease H



#### • Molecule 2: p51 RT





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.93Å 154.68Å 154.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.89 47.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.89) 99.6 (47.14-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.91 (at 2.91Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, $R_{free}$	0.183 , 0.269 0.192 , 0.279	Depositor DCC
$R_{free}$ test set	1617 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 81.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R8E

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	0.64	0/4652	0.88	4/6320 (0.1%)
2	B	0.63	0/3431	0.84	4/4661 (0.1%)
All	All	0.64	0/8083	0.86	8/10981 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	C-N-CD	-13.44	91.04	120.60
2	B	420	PRO	C-N-CD	-11.79	94.67	120.60
2	B	51	GLY	C-N-CD	-6.55	106.19	120.60
1	A	216	THR	C-N-CD	6.06	141.12	128.40
1	A	242	GLN	C-N-CD	-6.05	107.30	120.60
2	B	419	THR	C-N-CD	-5.82	107.80	120.60
2	B	233	GLU	N-CA-C	5.54	125.95	111.00
1	A	149	LEU	C-N-CD	5.25	139.43	128.40

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	4536	0	4591	499	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3338	0	3365	325	0
3	A	29	0	13	5	0
4	A	195	0	0	15	0
4	B	151	0	0	8	0
All	All	8249	0	7969	796	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 50.

All (796) 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:65:LYS:HE3	1:A:70:LYS:HG2	1.19	1.16
1:A:255:ASN:HB2	1:A:289:LEU:HD22	1.16	1.14
1:A:63:ILE:HD11	1:A:74:LEU:HD21	1.19	1.13
2:B:260:LEU:HD22	2:B:264:LEU:HD12	1.30	1.13
1:A:473:THR:HG23	1:A:476:LYS:HD2	1.20	1.11
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.24	1.10
1:A:63:ILE:HD12	1:A:72:ARG:HG3	1.22	1.10
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.34	1.07
1:A:195:ILE:HG23	1:A:199:ARG:HD2	1.36	1.07
1:A:296:THR:HG22	1:A:299:ALA:H	1.11	1.06
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.40	1.04
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.56	1.03
2:B:362:THR:HG22	2:B:366:LYS:HG2	1.42	1.00
1:A:64:LYS:HZ1	1:A:69:THR:HG22	1.20	1.00
1:A:175:ASN:ND2	1:A:201:LYS:HZ2	1.59	0.99
1:A:500:GLN:HG3	2:B:422:LEU:HD11	1.46	0.97
2:B:422:LEU:HA	2:B:425:LEU:HD21	1.46	0.96
2:B:175:ASN:HB3	2:B:178:ILE:HG13	1.45	0.96
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.04	0.95
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.50	0.94
2:B:258:GLN:HG3	2:B:283:LEU:HD21	1.52	0.90
2:B:298:GLU:HA	2:B:301:LEU:CD1	2.02	0.90
1:A:63:ILE:HG12	1:A:74:LEU:HD11	1.52	0.90
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.35	0.90
1:A:65:LYS:HE3	1:A:70:LYS:CG	2.02	0.89
1:A:104:LYS:CB	1:A:192:ASP:HA	2.03	0.89
2:B:279:LEU:HA	2:B:282:LEU:HD11	1.53	0.89
1:A:287:LYS:HA	1:A:287:LYS:HE2	1.54	0.88
2:B:24:TRP:CE3	2:B:25:PRO:HD2	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.03	0.87
2:B:362:THR:CG2	2:B:366:LYS:HG2	2.04	0.87
2:B:298:GLU:HA	2:B:301:LEU:HG	1.56	0.87
1:A:296:THR:CG2	1:A:299:ALA:H	1.86	0.87
1:A:500:GLN:HG3	2:B:422:LEU:CD1	2.04	0.87
1:A:473:THR:CG2	1:A:476:LYS:HD2	2.03	0.87
2:B:65:LYS:HE3	2:B:68:SER:CB	2.05	0.87
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.39	0.85
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.11	0.85
1:A:131:THR:HG23	1:A:143:ARG:HD2	1.56	0.85
1:A:466:VAL:CG2	1:A:551:LEU:HD23	2.07	0.84
1:A:63:ILE:HD12	1:A:72:ARG:CG	2.07	0.84
1:A:296:THR:HG22	1:A:299:ALA:N	1.92	0.84
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.07	0.83
2:B:65:LYS:HE3	2:B:68:SER:HB3	1.58	0.83
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.07	0.83
1:A:63:ILE:CD1	1:A:74:LEU:HD21	2.07	0.82
1:A:125:ARG:HG2	1:A:146:TYR:O	1.78	0.82
1:A:241:VAL:HG23	1:A:244:ILE:HD11	1.62	0.82
2:B:254:VAL:HG21	2:B:288:ALA:O	1.79	0.81
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.16	0.81
2:B:268:SER:O	2:B:269:GLN:HG3	1.80	0.81
2:B:298:GLU:HA	2:B:301:LEU:CG	2.12	0.80
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.64	0.80
1:A:7:THR:HG22	4:A:629:HOH:O	1.81	0.80
1:A:65:LYS:HD3	1:A:70:LYS:O	1.82	0.80
1:A:175:ASN:HD21	1:A:201:LYS:HZ2	0.82	0.79
1:A:3:SER:OG	1:A:5:ILE:HG23	1.82	0.79
1:A:223:LYS:H	1:A:223:LYS:HD2	1.46	0.79
1:A:223:LYS:H	1:A:223:LYS:CD	1.95	0.79
2:B:18:GLY:HA3	2:B:56:TYR:CE1	2.18	0.79
2:B:425:LEU:HD23	2:B:425:LEU:H	1.47	0.79
1:A:206:ARG:NH1	1:A:218:ASP:HA	1.98	0.78
2:B:253:THR:HG23	2:B:289:LEU:O	1.83	0.78
1:A:5:ILE:HG22	1:A:212:TRP:HE3	1.48	0.78
1:A:35:VAL:O	1:A:39:THR:HG23	1.82	0.78
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.47	0.78
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.18	0.77
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.66	0.77
2:B:274:ILE:HG23	2:B:306:ASN:ND2	1.99	0.77
2:B:284:ARG:H	2:B:287:LYS:HZ2	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LYS:O	2:B:370:GLU:HG3	1.84	0.77
2:B:241:VAL:CG2	2:B:243:PRO:HG3	2.15	0.76
1:A:195:ILE:CG2	1:A:199:ARG:HD2	2.12	0.76
1:A:271:TYR:CE1	1:A:314:VAL:HG23	2.20	0.76
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.67	0.76
1:A:516:GLU:O	1:A:520:GLN:HG2	1.86	0.76
1:A:181:CYS:HB2	1:A:188:TYR:HB2	1.66	0.76
1:A:204:GLU:HB2	4:A:660:HOH:O	1.84	0.76
1:A:65:LYS:HG2	1:A:68:SER:HB3	1.67	0.76
1:A:278:GLN:HG2	1:A:298:GLU:HB2	1.66	0.76
1:A:79:GLU:CG	1:A:83:ARG:HH21	1.98	0.76
1:A:91:GLN:HE21	1:A:92:LEU:N	1.84	0.76
1:A:515:SER:HB3	1:A:518:VAL:HG23	1.68	0.75
2:B:279:LEU:HA	2:B:282:LEU:CD1	2.15	0.75
1:A:287:LYS:HE2	1:A:287:LYS:CA	2.09	0.75
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.82	0.75
1:A:473:THR:HG23	1:A:476:LYS:CD	2.11	0.75
1:A:5:ILE:HG12	1:A:6:GLU:N	2.00	0.74
2:B:298:GLU:CD	2:B:298:GLU:H	1.89	0.74
1:A:511:ASP:OD2	1:A:512:GLN:HG3	1.87	0.74
2:B:260:LEU:HD22	2:B:264:LEU:CD1	2.15	0.74
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.17	0.74
2:B:8:VAL:HG11	2:B:159:ILE:HG12	1.68	0.74
1:A:2:ILE:HD11	1:A:46:LYS:NZ	2.02	0.74
2:B:373:GLN:HE22	2:B:407:GLN:H	1.33	0.74
2:B:344:GLU:HB3	2:B:347:LYS:HD3	1.67	0.74
2:B:418:ASN:O	2:B:420:PRO:HD3	1.87	0.74
1:A:76:ASP:OD2	1:A:78:ARG:HG3	1.88	0.74
1:A:219:LYS:HG3	1:A:220:LYS:H	1.53	0.73
1:A:424:LYS:HE2	1:A:426:TRP:CH2	2.23	0.73
1:A:64:LYS:NZ	1:A:69:THR:HG22	2.01	0.73
1:A:466:VAL:HG23	1:A:551:LEU:HD23	1.69	0.73
1:A:134:SER:OG	1:A:139:THR:HB	1.89	0.73
2:B:298:GLU:CA	2:B:301:LEU:HG	2.19	0.73
1:A:211:ARG:O	1:A:211:ARG:HD3	1.88	0.73
1:A:435:VAL:HG23	2:B:290:THR:HG21	1.71	0.73
2:B:303:LEU:O	2:B:307:ARG:HB2	1.89	0.72
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.70	0.72
1:A:458:VAL:HG13	1:A:548:VAL:HG13	1.71	0.72
2:B:335:GLY:HA3	2:B:356:ARG:HG2	1.70	0.72
1:A:201:LYS:HE2	1:A:204:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HB3	1:A:382:ILE:HD13	1.70	0.72
2:B:282:LEU:HB3	2:B:293:ILE:CD1	2.19	0.71
1:A:277:ARG:NH1	1:A:278:GLN:NE2	2.37	0.71
1:A:90:VAL:HG12	1:A:91:GLN:N	2.05	0.71
2:B:34:LEU:CD2	2:B:73:LYS:HB2	2.21	0.71
1:A:277:ARG:CD	1:A:334:GLN:HE21	2.03	0.71
2:B:270:ILE:HB	2:B:346:PHE:HB3	1.71	0.71
2:B:125:ARG:CB	2:B:145:GLN:HE21	2.03	0.71
1:A:450:THR:OG1	1:A:452:LEU:HB2	1.91	0.70
1:A:454:LYS:HB2	1:A:556:ILE:HG13	1.72	0.70
1:A:52:PRO:HD2	1:A:53:GLU:OE2	1.91	0.70
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.27	0.70
2:B:271:TYR:CD1	2:B:310:LEU:HD12	2.25	0.70
1:A:503:LEU:HD22	1:A:507:GLN:HG3	1.74	0.70
1:A:65:LYS:CE	1:A:70:LYS:HG2	2.10	0.70
1:A:324:ASP:OD2	1:A:388:LYS:HE2	1.90	0.70
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.27	0.70
2:B:270:ILE:HG13	2:B:346:PHE:O	1.92	0.70
1:A:373:GLN:OE1	2:B:400:THR:HG21	1.91	0.70
2:B:284:ARG:H	2:B:287:LYS:NZ	1.88	0.69
2:B:8:VAL:HG11	2:B:159:ILE:CG1	2.22	0.69
1:A:535:TRP:CZ3	1:A:537:PRO:HD3	2.27	0.69
2:B:282:LEU:HB3	2:B:293:ILE:HD11	1.75	0.69
2:B:306:ASN:O	2:B:310:LEU:HD22	1.92	0.69
1:A:13:LYS:O	1:A:16:MET:HB2	1.93	0.69
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.25	0.69
2:B:50:ILE:HG21	2:B:145:GLN:HB2	1.75	0.69
1:A:12:LEU:HD23	1:A:124:PHE:HE1	1.57	0.69
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.85	0.69
2:B:267:ALA:O	2:B:270:ILE:HG23	1.93	0.68
1:A:63:ILE:HG12	1:A:74:LEU:CD1	2.22	0.68
1:A:23:GLN:NE2	1:A:26:LEU:HD21	2.08	0.68
2:B:293:ILE:HG13	2:B:293:ILE:O	1.92	0.68
2:B:116:PHE:HB2	4:B:465:HOH:O	1.92	0.68
1:A:454:LYS:NZ	1:A:554:ALA:O	2.27	0.68
2:B:373:GLN:NE2	2:B:407:GLN:H	1.91	0.68
2:B:256:ASP:O	2:B:260:LEU:HB2	1.92	0.68
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.58	0.68
2:B:87:PHE:CZ	2:B:159:ILE:HD11	2.29	0.68
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.29	0.68
2:B:28:GLU:O	2:B:32:LYS:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:TRP:HE1	2:B:367:GLN:NE2	1.92	0.67
1:A:104:LYS:HB2	1:A:191:SER:O	1.95	0.67
2:B:8:VAL:CG1	2:B:159:ILE:HG12	2.24	0.67
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.28	0.67
1:A:203:GLU:OE2	1:A:206:ARG:NH1	2.27	0.67
1:A:32:LYS:NZ	1:A:36:GLU:OE2	2.26	0.67
1:A:244:ILE:HD12	1:A:244:ILE:N	2.09	0.67
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.30	0.67
2:B:422:LEU:HA	2:B:425:LEU:CD2	2.24	0.67
1:A:241:VAL:CG2	1:A:244:ILE:HD11	2.25	0.66
1:A:402:TRP:CE3	1:A:403:THR:HB	2.29	0.66
1:A:369:THR:HG22	1:A:411:ILE:HD11	1.77	0.66
2:B:308:GLU:O	2:B:311:LYS:HG2	1.95	0.66
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.31	0.66
1:A:89:GLU:CB	1:A:92:LEU:HD11	2.26	0.66
1:A:312:GLU:HB2	4:A:737:HOH:O	1.96	0.66
1:A:169:GLU:O	1:A:173:LYS:HE2	1.96	0.66
1:A:358:ARG:NH1	2:B:396:GLU:OE2	2.28	0.66
1:A:65:LYS:HE2	1:A:72:ARG:CZ	2.25	0.66
1:A:266:TRP:O	1:A:269:GLN:HG3	1.95	0.66
2:B:18:GLY:HA3	2:B:56:TYR:CD1	2.31	0.65
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.26	0.65
1:A:134:SER:HB3	1:A:139:THR:O	1.96	0.65
1:A:277:ARG:HD2	1:A:334:GLN:HE21	1.62	0.65
2:B:274:ILE:HG22	2:B:275:LYS:N	2.11	0.65
2:B:260:LEU:O	2:B:264:LEU:HB2	1.97	0.65
2:B:195:ILE:O	2:B:199:ARG:HG3	1.96	0.65
2:B:98:ALA:O	2:B:101:LYS:NZ	2.29	0.65
1:A:233:GLU:HG2	1:A:235:HIS:HE1	1.60	0.64
1:A:503:LEU:HD22	1:A:507:GLN:CG	2.27	0.64
1:A:278:GLN:CG	1:A:298:GLU:HB2	2.27	0.64
2:B:253:THR:O	2:B:257:ILE:HG12	1.98	0.64
1:A:249:LYS:HG2	1:A:251:SER:O	1.97	0.64
2:B:95:PRO:HG3	4:B:562:HOH:O	1.96	0.64
2:B:108:VAL:HB	2:B:232:TYR:HD2	1.62	0.64
2:B:306:ASN:O	2:B:309:ILE:HB	1.98	0.64
2:B:279:LEU:HD23	2:B:302:GLU:OE1	1.97	0.64
2:B:373:GLN:O	2:B:377:THR:HG23	1.98	0.64
2:B:30:LYS:HG2	2:B:62:ALA:HB3	1.80	0.64
1:A:5:ILE:HG12	1:A:6:GLU:O	1.98	0.63
1:A:106:VAL:HG22	1:A:227:PHE:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.79	0.63
2:B:159:ILE:HG22	2:B:160:PHE:N	2.12	0.63
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.27	0.63
1:A:175:ASN:CB	1:A:178:ILE:HD13	2.20	0.63
2:B:274:ILE:HG22	2:B:275:LYS:H	1.61	0.63
1:A:206:ARG:HH22	1:A:218:ASP:HB3	1.63	0.63
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.28	0.63
1:A:553:SER:HA	1:A:557:ARG:HD3	1.80	0.63
1:A:2:ILE:HG12	4:A:698:HOH:O	1.98	0.63
1:A:465:LYS:HG3	1:A:466:VAL:N	2.13	0.63
1:A:102:LYS:HZ3	1:A:237:ASP:CB	2.12	0.63
2:B:396:GLU:O	2:B:400:THR:HG22	1.99	0.62
1:A:17:ASP:O	1:A:83:ARG:HD3	1.98	0.62
2:B:92:LEU:HD23	4:B:492:HOH:O	1.98	0.62
1:A:171:PHE:O	1:A:175:ASN:HB2	1.98	0.62
1:A:277:ARG:HD2	1:A:334:GLN:NE2	2.13	0.62
1:A:131:THR:HG23	1:A:143:ARG:CD	2.29	0.62
1:A:102:LYS:NZ	1:A:237:ASP:HB3	2.14	0.62
2:B:214:LEU:N	2:B:214:LEU:HD23	2.15	0.62
1:A:249:LYS:HG3	1:A:250:ASP:H	1.65	0.61
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.30	0.61
1:A:498:ASP:OD2	1:A:538:ALA:HB2	2.00	0.61
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.65	0.61
1:A:303:LEU:O	1:A:307:ARG:HG3	2.00	0.61
1:A:434:ILE:HG21	1:A:492:GLU:OE1	1.99	0.61
2:B:258:GLN:HG3	2:B:283:LEU:CD2	2.28	0.61
1:A:406:TRP:HZ3	2:B:392:PRO:CB	2.13	0.61
2:B:87:PHE:CZ	2:B:92:LEU:HD12	2.36	0.61
2:B:274:ILE:O	2:B:275:LYS:HD3	2.00	0.61
1:A:135:ILE:O	1:A:136:ASN:HB2	2.01	0.60
2:B:273:GLY:O	2:B:275:LYS:NZ	2.30	0.60
1:A:89:GLU:HB2	1:A:92:LEU:HD11	1.81	0.60
2:B:97:PRO:HG3	4:B:522:HOH:O	2.00	0.60
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.37	0.60
2:B:324:ASP:O	2:B:343:GLN:HG2	2.00	0.60
1:A:79:GLU:HG2	1:A:83:ARG:HH21	1.66	0.60
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.32	0.60
1:A:107:THR:HG23	1:A:198:HIS:CE1	2.37	0.60
2:B:64:LYS:NZ	2:B:69:THR:O	2.34	0.60
1:A:223:LYS:NZ	4:A:627:HOH:O	2.24	0.60
1:A:360:ALA:HA	1:A:514:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HA	1:A:511:ASP:OD2	2.02	0.60
2:B:261:VAL:O	2:B:265:ASN:HB3	2.01	0.60
1:A:65:LYS:HE2	1:A:72:ARG:NH1	2.17	0.60
1:A:277:ARG:NH1	1:A:278:GLN:HE21	1.97	0.60
2:B:241:VAL:HG23	2:B:243:PRO:HG3	1.83	0.60
2:B:295:LEU:HD12	2:B:299:ALA:HB3	1.82	0.59
2:B:87:PHE:CE1	2:B:92:LEU:HD12	2.37	0.59
1:A:170:PRO:O	1:A:173:LYS:N	2.27	0.59
1:A:219:LYS:HG3	1:A:220:LYS:N	2.17	0.59
1:A:253:THR:HA	1:A:291:GLU:O	2.02	0.59
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.38	0.59
1:A:244:ILE:HD12	1:A:244:ILE:H	1.66	0.59
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.37	0.59
2:B:175:ASN:N	2:B:176:PRO:HD3	2.18	0.59
1:A:437:ALA:HB3	1:A:494:ASN:HD21	1.68	0.59
1:A:66:LYS:O	1:A:67:ASP:HB2	2.02	0.59
1:A:515:SER:HB3	1:A:518:VAL:CG2	2.31	0.58
2:B:90:VAL:HG23	2:B:90:VAL:O	2.03	0.58
1:A:400:THR:O	1:A:404:GLU:HG3	2.03	0.58
2:B:320:ASP:OD2	2:B:323:LYS:HD2	2.02	0.58
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.38	0.58
1:A:70:LYS:NZ	1:A:72:ARG:HH21	2.01	0.58
1:A:70:LYS:NZ	1:A:72:ARG:NH2	2.51	0.58
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.30	0.58
1:A:238:LYS:HB2	1:A:315:HIS:HD2	1.68	0.58
1:A:108:VAL:HG13	1:A:223:LYS:HD3	1.86	0.58
1:A:384:GLY:O	2:B:27:THR:HB	2.03	0.58
2:B:76:ASP:OD2	2:B:78:ARG:HG3	2.03	0.58
2:B:420:PRO:HB2	2:B:423:VAL:HG23	1.83	0.58
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.38	0.58
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.03	0.58
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.68	0.58
1:A:287:LYS:HG2	1:A:291:GLU:OE1	2.02	0.58
2:B:241:VAL:HG21	2:B:243:PRO:HG3	1.86	0.58
1:A:195:ILE:HG23	1:A:199:ARG:CD	2.24	0.58
2:B:271:TYR:O	2:B:274:ILE:HG12	2.04	0.58
1:A:90:VAL:HG12	1:A:91:GLN:H	1.68	0.57
1:A:106:VAL:HA	1:A:189:VAL:O	2.04	0.57
1:A:420:PRO:HA	1:A:421:PRO:C	2.24	0.57
2:B:65:LYS:HE2	2:B:70:LYS:O	2.04	0.57
1:A:23:GLN:HG3	1:A:24:TRP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MET:HA	1:A:230:MET:HE2	1.86	0.57
1:A:465:LYS:HG3	1:A:466:VAL:H	1.69	0.57
1:A:29:GLU:HG2	4:A:669:HOH:O	2.04	0.57
1:A:21:VAL:HG22	1:A:59:PRO:CD	2.26	0.57
2:B:11:LYS:O	2:B:11:LYS:HG2	2.05	0.57
2:B:13:LYS:HB2	2:B:16:MET:HE3	1.86	0.57
1:A:405:TYR:CE2	1:A:407:GLN:HG2	2.39	0.57
1:A:105:SER:O	1:A:190:GLY:HA2	2.05	0.57
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.20	0.57
1:A:373:GLN:HE22	2:B:401:TRP:HE1	1.51	0.57
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.87	0.57
1:A:122:GLU:HB2	4:A:624:HOH:O	2.05	0.57
2:B:13:LYS:HB2	2:B:16:MET:CE	2.35	0.57
2:B:34:LEU:HD23	2:B:73:LYS:HB2	1.87	0.57
2:B:65:LYS:N	2:B:65:LYS:HD3	2.19	0.56
2:B:399:GLU:HG2	4:B:512:HOH:O	2.03	0.56
1:A:195:ILE:HD13	1:A:199:ARG:CD	2.35	0.56
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.87	0.56
1:A:346:PHE:N	1:A:346:PHE:CD1	2.70	0.56
1:A:434:ILE:H	1:A:434:ILE:HD12	1.70	0.56
1:A:445:ALA:O	1:A:477:THR:HG21	2.05	0.56
1:A:171:PHE:HA	1:A:174:GLN:HE21	1.71	0.56
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.22	0.56
1:A:296:THR:HG22	1:A:299:ALA:CB	2.36	0.56
1:A:369:THR:HG21	1:A:398:TRP:CH2	2.41	0.56
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.20	0.56
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.14	0.56
1:A:203:GLU:HA	1:A:206:ARG:HG3	1.88	0.56
2:B:122:GLU:HA	2:B:125:ARG:NE	2.21	0.56
1:A:277:ARG:HD3	1:A:334:GLN:HE21	1.69	0.56
1:A:406:TRP:CZ2	2:B:418:ASN:HA	2.40	0.56
2:B:167:ILE:HG12	2:B:212:TRP:CG	2.41	0.56
2:B:275:LYS:H	2:B:306:ASN:HD21	1.54	0.56
1:A:41:MET:HB2	1:A:47:ILE:HG12	1.88	0.56
1:A:70:LYS:HZ3	1:A:72:ARG:NH2	2.04	0.56
1:A:193:LEU:HD13	1:A:197:GLN:HB2	1.86	0.56
2:B:65:LYS:HD2	2:B:72:ARG:HB2	1.87	0.56
1:A:2:ILE:HD11	1:A:46:LYS:HZ2	1.67	0.56
1:A:104:LYS:CG	1:A:192:ASP:HA	2.35	0.56
1:A:399:GLU:O	1:A:402:TRP:HE3	1.89	0.56
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:O	1:A:103:LYS:NZ	2.29	0.56
1:A:107:THR:OG1	1:A:202:ILE:HD11	2.05	0.56
1:A:164:MET:O	1:A:168:LEU:HD12	2.06	0.56
1:A:547:GLN:HA	1:A:550:LYS:HE2	1.88	0.56
1:A:226:PRO:O	1:A:228:LEU:HD12	2.05	0.56
2:B:103:LYS:CE	2:B:179:VAL:HG23	2.36	0.56
2:B:275:LYS:HE3	2:B:305:GLU:OE1	2.06	0.56
1:A:305:GLU:O	1:A:309:ILE:HG13	2.05	0.56
1:A:465:LYS:O	1:A:466:VAL:HG23	2.06	0.55
1:A:490:GLY:O	1:A:492:GLU:N	2.40	0.55
2:B:12:LEU:HD23	2:B:17:ASP:HA	1.87	0.55
2:B:129:ALA:HA	2:B:144:TYR:O	2.06	0.55
2:B:332:GLN:HA	2:B:424:LYS:HE3	1.88	0.55
2:B:14:PRO:HA	4:B:541:HOH:O	2.05	0.55
1:A:245:VAL:O	1:A:247:PRO:HD3	2.07	0.55
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.07	0.55
1:A:238:LYS:HB2	1:A:315:HIS:CD2	2.41	0.55
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.36	0.55
2:B:274:ILE:C	2:B:275:LYS:HD3	2.26	0.55
1:A:311:LYS:O	1:A:312:GLU:HB3	2.04	0.55
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.35	0.55
1:A:540:LYS:O	1:A:542:ILE:N	2.40	0.55
2:B:72:ARG:HH11	2:B:72:ARG:CG	2.18	0.55
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.27	0.55
1:A:262:GLY:HA2	4:A:675:HOH:O	2.07	0.55
2:B:252:TRP:HB3	2:B:257:ILE:HD13	1.89	0.55
1:A:369:THR:HG21	1:A:398:TRP:CZ3	2.41	0.55
2:B:80:LEU:O	2:B:84:THR:HG23	2.07	0.55
1:A:106:VAL:HG22	1:A:227:PHE:HE2	1.68	0.55
1:A:194:GLU:CD	1:A:194:GLU:H	2.10	0.55
2:B:398:TRP:O	2:B:402:TRP:HD1	1.90	0.55
1:A:26:LEU:CD2	1:A:133:PRO:HG3	2.37	0.55
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.42	0.55
2:B:267:ALA:O	2:B:271:TYR:HB2	2.06	0.55
2:B:344:GLU:HB3	2:B:347:LYS:HZ2	1.72	0.55
1:A:173:LYS:HA	1:A:173:LYS:HZ2	1.72	0.54
2:B:8:VAL:HG23	4:B:498:HOH:O	2.07	0.54
1:A:319:TYR:OH	1:A:385:LYS:HE2	2.06	0.54
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.42	0.54
1:A:426:TRP:O	1:A:427:TYR:HB3	2.08	0.54
1:A:229:TRP:CD2	1:A:230:MET:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:O	1:A:10:VAL:HG23	2.08	0.54
1:A:460:ASN:HD22	2:B:288:ALA:N	2.05	0.54
2:B:298:GLU:HA	2:B:301:LEU:HD12	1.87	0.54
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.43	0.54
1:A:171:PHE:HA	1:A:174:GLN:NE2	2.22	0.54
2:B:369:THR:HG22	2:B:370:GLU:N	2.22	0.54
2:B:422:LEU:O	2:B:425:LEU:HD23	2.06	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.43	0.54
2:B:204:GLU:O	2:B:208:HIS:HD2	1.90	0.54
2:B:425:LEU:H	2:B:425:LEU:CD2	2.17	0.54
1:A:70:LYS:HZ1	1:A:72:ARG:HH21	1.55	0.53
1:A:183:TYR:HB3	1:A:188:TYR:HE1	1.72	0.53
1:A:290:THR:HB	4:A:633:HOH:O	2.08	0.53
1:A:91:GLN:HE21	1:A:92:LEU:H	1.54	0.53
1:A:433:PRO:CG	2:B:255:ASN:HD22	2.21	0.53
2:B:253:THR:HG22	2:B:255:ASN:N	2.24	0.53
2:B:428:GLN:NE2	2:B:428:GLN:HA	2.23	0.53
2:B:261:VAL:O	2:B:265:ASN:N	2.27	0.53
2:B:246:LEU:HD11	2:B:310:LEU:HD21	1.89	0.53
1:A:2:ILE:CD1	1:A:46:LYS:HZ2	2.22	0.53
1:A:515:SER:CB	1:A:518:VAL:HG23	2.36	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.43	0.53
1:A:193:LEU:HB3	1:A:197:GLN:HG2	1.89	0.53
1:A:120:LEU:HD12	1:A:121:ASP:N	2.24	0.53
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.53
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.91	0.53
1:A:411:ILE:HG23	1:A:412:PRO:HD2	1.91	0.53
1:A:454:LYS:HD3	1:A:556:ILE:HD11	1.91	0.53
1:A:447:ASN:OD1	1:A:449:GLU:HG2	2.09	0.53
2:B:12:LEU:HD12	2:B:84:THR:HG22	1.91	0.52
2:B:64:LYS:O	2:B:65:LYS:O	2.27	0.52
2:B:297:GLU:O	2:B:301:LEU:HG	2.09	0.52
1:A:51:GLY:O	1:A:143:ARG:NH1	2.42	0.52
2:B:11:LYS:HE2	2:B:11:LYS:N	2.23	0.52
2:B:371:ALA:O	2:B:375:ILE:HG13	2.09	0.52
1:A:104:LYS:HG3	1:A:192:ASP:O	2.09	0.52
1:A:171:PHE:N	1:A:174:GLN:NE2	2.57	0.52
1:A:410:TRP:CE3	2:B:363:ASN:CB	2.93	0.52
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.44	0.52
1:A:454:LYS:CD	1:A:556:ILE:HD11	2.39	0.52
1:A:48:SER:O	1:A:144:TYR:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD12	1:A:178:ILE:H	1.75	0.52
1:A:202:ILE:HG22	1:A:203:GLU:N	2.25	0.52
1:A:277:ARG:HH11	1:A:278:GLN:NE2	2.07	0.52
2:B:296:THR:O	2:B:300:GLU:OE1	2.27	0.52
2:B:373:GLN:HE22	2:B:407:GLN:N	2.06	0.52
1:A:406:TRP:HZ2	2:B:418:ASN:OD1	1.93	0.52
2:B:267:ALA:O	2:B:271:TYR:N	2.43	0.52
2:B:362:THR:HG23	2:B:366:LYS:CE	2.39	0.52
2:B:257:ILE:HA	2:B:260:LEU:HB2	1.90	0.52
1:A:270:ILE:O	1:A:272:PRO:HD3	2.09	0.52
1:A:417:VAL:O	1:A:417:VAL:HG13	2.10	0.52
1:A:464:GLN:HG2	1:A:465:LYS:N	2.24	0.52
2:B:34:LEU:HD21	2:B:73:LYS:HB2	1.90	0.52
2:B:326:ILE:O	2:B:341:ILE:HA	2.10	0.52
2:B:80:LEU:O	2:B:80:LEU:HD22	2.09	0.52
2:B:87:PHE:HE1	2:B:159:ILE:HD12	1.75	0.52
1:A:12:LEU:CD2	1:A:124:PHE:HE1	2.22	0.51
1:A:230:MET:CE	1:A:230:MET:CA	2.88	0.51
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.73	0.51
2:B:189:VAL:HB	2:B:202:ILE:HD11	1.91	0.51
1:A:102:LYS:HZ3	1:A:237:ASP:HB3	1.75	0.51
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.40	0.51
2:B:256:ASP:O	2:B:260:LEU:N	2.43	0.51
2:B:271:TYR:HD1	2:B:310:LEU:HD12	1.72	0.51
1:A:100:LEU:O	1:A:318:TYR:HB3	2.10	0.51
1:A:219:LYS:O	1:A:220:LYS:HG2	2.10	0.51
1:A:355:ALA:O	1:A:356:ARG:O	2.28	0.51
2:B:99:GLY:O	2:B:102:LYS:HB2	2.10	0.51
2:B:331:LYS:O	2:B:424:LYS:NZ	2.35	0.51
1:A:79:GLU:OE1	1:A:82:LYS:HE2	2.10	0.51
1:A:435:VAL:HG23	2:B:290:THR:CG2	2.40	0.51
1:A:542:ILE:O	1:A:545:ASN:HB3	2.11	0.51
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.09	0.51
2:B:257:ILE:O	2:B:261:VAL:HG13	2.10	0.51
1:A:497:THR:OG1	1:A:498:ASP:N	2.43	0.51
1:A:497:THR:O	1:A:535:TRP:HA	2.11	0.51
1:A:92:LEU:N	1:A:92:LEU:HD22	2.26	0.51
2:B:282:LEU:HB3	2:B:293:ILE:HD13	1.91	0.51
1:A:298:GLU:CA	1:A:301:LEU:HD12	2.38	0.51
1:A:400:THR:O	1:A:404:GLU:OE2	2.29	0.51
1:A:434:ILE:HD13	1:A:493:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:CG2	2:B:73:LYS:HD2	2.41	0.51
2:B:268:SER:HB3	2:B:274:ILE:HB	1.93	0.51
2:B:273:GLY:O	2:B:275:LYS:HD3	2.10	0.51
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.58	0.51
1:A:50:ILE:HG13	1:A:143:ARG:CB	2.40	0.51
1:A:363:ASN:O	1:A:367:GLN:HG3	2.10	0.51
1:A:12:LEU:CD2	1:A:124:PHE:CE1	2.94	0.50
1:A:295:LEU:HD23	1:A:295:LEU:N	2.26	0.50
1:A:296:THR:HG23	1:A:298:GLU:OE2	2.11	0.50
1:A:432:GLU:HB3	1:A:433:PRO:HD2	1.93	0.50
1:A:62:ALA:HA	1:A:72:ARG:O	2.11	0.50
1:A:70:LYS:HG3	1:A:71:TRP:N	2.26	0.50
2:B:166:LYS:HA	2:B:166:LYS:CE	2.40	0.50
1:A:2:ILE:HG22	1:A:2:ILE:O	2.11	0.50
1:A:91:GLN:NE2	1:A:92:LEU:H	2.08	0.50
1:A:135:ILE:O	1:A:138:GLU:OE2	2.29	0.50
1:A:406:TRP:CH2	1:A:407:GLN:HB2	2.46	0.50
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.92	0.50
1:A:63:ILE:CD1	1:A:72:ARG:HG3	2.17	0.50
1:A:104:LYS:HB2	1:A:192:ASP:CA	2.18	0.50
1:A:249:LYS:HG3	1:A:250:ASP:N	2.27	0.50
1:A:233:GLU:HB3	1:A:240:THR:HG22	1.93	0.50
1:A:406:TRP:HZ3	2:B:392:PRO:CA	2.23	0.50
2:B:362:THR:HG23	2:B:366:LYS:HE3	1.94	0.50
1:A:26:LEU:HD23	1:A:133:PRO:HG3	1.93	0.50
1:A:402:TRP:CE3	1:A:403:THR:CB	2.95	0.50
1:A:489:SER:CB	1:A:493:VAL:CG1	2.90	0.50
2:B:8:VAL:O	2:B:121:ASP:HB2	2.12	0.50
1:A:156:SER:N	1:A:157:PRO:CD	2.75	0.50
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.92	0.50
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.45	0.50
2:B:210:LEU:O	2:B:210:LEU:HG	2.12	0.50
1:A:65:LYS:HE2	1:A:72:ARG:HD2	1.94	0.49
1:A:475:GLN:NE2	1:A:501:TYR:CG	2.80	0.49
2:B:61:PHE:HE2	2:B:76:ASP:HB2	1.77	0.49
1:A:104:LYS:N	1:A:192:ASP:OD2	2.44	0.49
1:A:400:THR:O	1:A:403:THR:HG22	2.12	0.49
2:B:244:ILE:HD13	2:B:266:TRP:CH2	2.47	0.49
2:B:244:ILE:CG2	2:B:263:LYS:HE2	2.42	0.49
1:A:13:LYS:HE3	1:A:84:THR:O	2.11	0.49
1:A:104:LYS:HG3	1:A:192:ASP:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE2	1:A:298:GLU:N	2.29	0.49
2:B:12:LEU:HD22	2:B:127:TYR:CZ	2.46	0.49
2:B:87:PHE:CE1	2:B:159:ILE:HD12	2.48	0.49
1:A:79:GLU:HG3	1:A:83:ARG:NE	2.26	0.49
2:B:303:LEU:O	2:B:307:ARG:N	2.30	0.49
1:A:79:GLU:HG3	1:A:83:ARG:HH21	1.76	0.49
1:A:106:VAL:CG2	1:A:227:PHE:CE2	2.95	0.49
1:A:369:THR:CG2	1:A:398:TRP:CZ3	2.95	0.49
1:A:297:GLU:O	1:A:301:LEU:HG	2.13	0.49
1:A:20:LYS:HG2	1:A:55:PRO:O	2.13	0.49
1:A:91:GLN:NE2	1:A:92:LEU:N	2.58	0.49
1:A:230:MET:HE2	1:A:230:MET:CA	2.43	0.49
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.48	0.49
2:B:80:LEU:HD22	2:B:84:THR:HG23	1.94	0.49
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.95	0.49
1:A:475:GLN:NE2	1:A:501:TYR:CD1	2.81	0.49
2:B:87:PHE:O	2:B:91:GLN:HB3	2.13	0.49
2:B:115:TYR:HB3	2:B:149:LEU:CB	2.38	0.49
2:B:274:ILE:CG2	2:B:275:LYS:H	2.25	0.49
2:B:428:GLN:NE2	2:B:428:GLN:O	2.34	0.49
1:A:402:TRP:CZ3	1:A:403:THR:HB	2.47	0.49
1:A:406:TRP:CZ3	1:A:407:GLN:CB	2.95	0.49
2:B:241:VAL:C	2:B:243:PRO:HD3	2.34	0.49
1:A:12:LEU:HD23	1:A:124:PHE:CE1	2.43	0.48
1:A:296:THR:HG21	4:A:750:HOH:O	2.14	0.48
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.95	0.48
2:B:87:PHE:HZ	2:B:159:ILE:HD11	1.77	0.48
1:A:64:LYS:HE2	1:A:69:THR:C	2.32	0.48
2:B:87:PHE:CE1	2:B:159:ILE:CD1	2.96	0.48
2:B:257:ILE:HG12	2:B:257:ILE:H	1.39	0.48
2:B:275:LYS:N	2:B:306:ASN:HD21	2.10	0.48
1:A:532:TYR:HE2	1:A:534:ALA:HB2	1.76	0.48
1:A:540:LYS:O	1:A:542:ILE:HG13	2.13	0.48
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.96	0.48
1:A:402:TRP:CZ3	1:A:403:THR:CB	2.96	0.48
1:A:443:ASP:HB2	1:A:548:VAL:HB	1.96	0.48
1:A:500:GLN:HG3	2:B:422:LEU:CG	2.43	0.48
2:B:279:LEU:H	2:B:279:LEU:CD2	2.27	0.48
2:B:419:THR:HA	2:B:420:PRO:HD2	1.78	0.48
1:A:64:LYS:O	1:A:65:LYS:HD2	2.13	0.48
1:A:106:VAL:CG1	3:A:601:R8E:C18	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:TRP:CZ2	2:B:154:LYS:HE3	2.47	0.48
2:B:301:LEU:O	2:B:305:GLU:HB2	2.13	0.48
1:A:5:ILE:CG1	1:A:6:GLU:N	2.74	0.48
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.56	0.48
1:A:396:GLU:HB2	4:A:611:HOH:O	2.14	0.48
1:A:556:ILE:HD13	1:A:556:ILE:N	2.28	0.48
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.95	0.48
2:B:312:GLU:O	2:B:313:PRO:O	2.32	0.48
1:A:92:LEU:N	1:A:92:LEU:CD2	2.77	0.47
1:A:105:SER:HB3	1:A:198:HIS:CE1	2.49	0.47
1:A:454:LYS:HD3	1:A:556:ILE:CG1	2.44	0.47
1:A:547:GLN:OE1	2:B:285:GLY:HA2	2.14	0.47
1:A:547:GLN:N	1:A:547:GLN:HE21	2.12	0.47
2:B:65:LYS:CE	2:B:68:SER:HB3	2.38	0.47
2:B:66:LYS:HG2	2:B:407:GLN:HE22	1.79	0.47
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.96	0.47
2:B:120:LEU:O	2:B:125:ARG:NH2	2.47	0.47
1:A:27:THR:OG1	1:A:30:LYS:HD2	2.14	0.47
1:A:29:GLU:HG3	1:A:30:LYS:N	2.30	0.47
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.97	0.47
1:A:403:THR:CG2	1:A:404:GLU:N	2.77	0.47
1:A:404:GLU:HG3	1:A:404:GLU:H	1.55	0.47
1:A:406:TRP:CE2	1:A:407:GLN:HB3	2.50	0.47
1:A:492:GLU:HA	1:A:530:LYS:O	2.15	0.47
2:B:274:ILE:CG2	2:B:275:LYS:N	2.77	0.47
1:A:410:TRP:CE3	2:B:363:ASN:HB3	2.50	0.47
2:B:250:ASP:O	2:B:251:SER:HB3	2.15	0.47
2:B:283:LEU:HA	2:B:287:LYS:NZ	2.30	0.47
1:A:65:LYS:NZ	1:A:72:ARG:NH1	2.62	0.47
1:A:194:GLU:C	1:A:196:GLY:N	2.67	0.47
1:A:219:LYS:C	1:A:221:HIS:H	2.18	0.47
1:A:219:LYS:CG	1:A:220:LYS:N	2.78	0.47
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.30	0.47
1:A:518:VAL:O	1:A:522:ILE:HD12	2.15	0.47
2:B:87:PHE:CZ	2:B:159:ILE:CD1	2.96	0.47
1:A:12:LEU:HD13	1:A:83:ARG:HB3	1.97	0.47
1:A:101:LYS:O	3:A:601:R8E:H11	2.15	0.47
2:B:271:TYR:CD1	2:B:310:LEU:CD1	2.97	0.47
2:B:420:PRO:O	2:B:422:LEU:N	2.48	0.47
2:B:253:THR:HB	2:B:256:ASP:OD1	2.15	0.47
2:B:428:GLN:NE2	2:B:428:GLN:CA	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HH11	1:A:278:GLN:HE22	1.63	0.46
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.97	0.46
1:A:228:LEU:HD12	1:A:228:LEU:N	2.31	0.46
1:A:270:ILE:HD11	1:A:316:GLY:CA	2.45	0.46
2:B:125:ARG:HG2	2:B:146:TYR:O	2.16	0.46
1:A:3:SER:HB2	1:A:117:SER:O	2.15	0.46
1:A:337:TRP:N	1:A:337:TRP:CD1	2.83	0.46
1:A:402:TRP:CE3	1:A:403:THR:N	2.83	0.46
2:B:253:THR:HG22	2:B:255:ASN:H	1.80	0.46
2:B:268:SER:C	2:B:270:ILE:H	2.18	0.46
2:B:391:LEU:HA	2:B:392:PRO:HD2	1.79	0.46
1:A:489:SER:CB	1:A:493:VAL:HG11	2.46	0.46
1:A:291:GLU:HG3	1:A:292:VAL:N	2.30	0.46
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.30	0.46
2:B:241:VAL:HG23	2:B:243:PRO:CG	2.46	0.46
2:B:268:SER:O	2:B:270:ILE:HG22	2.15	0.46
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.97	0.46
2:B:13:LYS:CB	2:B:16:MET:HE3	2.46	0.46
1:A:266:TRP:CD2	1:A:269:GLN:NE2	2.84	0.46
1:A:406:TRP:CE3	1:A:406:TRP:C	2.89	0.46
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.97	0.46
2:B:281:LYS:O	2:B:284:ARG:HD3	2.16	0.46
1:A:108:VAL:HG22	1:A:223:LYS:HE3	1.98	0.46
1:A:275:LYS:HB3	1:A:336:GLN:HE22	1.79	0.46
2:B:279:LEU:CD2	2:B:279:LEU:N	2.79	0.46
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.52	0.45
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.98	0.45
1:A:173:LYS:CA	1:A:173:LYS:NZ	2.79	0.45
1:A:65:LYS:CE	1:A:72:ARG:NH1	2.79	0.45
2:B:246:LEU:CD1	2:B:310:LEU:HD23	2.45	0.45
1:A:202:ILE:CG2	1:A:203:GLU:N	2.79	0.45
1:A:335:GLY:O	1:A:355:ALA:HA	2.16	0.45
1:A:443:ASP:O	1:A:481:ALA:HB2	2.16	0.45
2:B:258:GLN:HE22	2:B:289:LEU:CD2	2.30	0.45
2:B:271:TYR:CE1	2:B:310:LEU:HD12	2.50	0.45
1:A:134:SER:OG	1:A:135:ILE:N	2.50	0.45
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.75	0.45
2:B:363:ASN:O	2:B:367:GLN:HG3	2.17	0.45
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.17	0.45
2:B:79:GLU:O	2:B:83:ARG:HG2	2.16	0.45
2:B:87:PHE:CZ	2:B:92:LEU:CD1	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:LEU:O	2:B:282:LEU:HD12	2.16	0.45
1:A:60:VAL:HG13	1:A:75:VAL:HG22	1.98	0.45
1:A:270:ILE:CD1	1:A:316:GLY:HA3	2.46	0.45
2:B:270:ILE:HD12	2:B:346:PHE:HA	1.98	0.45
1:A:61:PHE:CE2	1:A:63:ILE:HG23	2.52	0.45
1:A:65:LYS:HB3	1:A:68:SER:O	2.16	0.45
1:A:406:TRP:CD2	1:A:407:GLN:HB3	2.51	0.45
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.99	0.45
1:A:33:ALA:O	1:A:37:ILE:HG13	2.17	0.45
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.79	0.45
1:A:3:SER:HA	1:A:4:PRO:HD2	1.47	0.45
1:A:50:ILE:HG13	1:A:143:ARG:HB2	1.99	0.45
1:A:173:LYS:HA	1:A:173:LYS:NZ	2.32	0.45
1:A:206:ARG:NH2	1:A:218:ASP:HB3	2.30	0.45
2:B:244:ILE:HG23	2:B:263:LYS:HE2	1.99	0.45
1:A:107:THR:CG2	1:A:198:HIS:CE1	3.00	0.44
1:A:169:GLU:OE2	1:A:173:LYS:HE3	2.17	0.44
1:A:248:GLU:H	1:A:248:GLU:HG2	1.49	0.44
1:A:537:PRO:HB2	1:A:540:LYS:HG3	1.98	0.44
1:A:29:GLU:HG3	1:A:30:LYS:HG3	1.98	0.44
2:B:66:LYS:HG2	2:B:407:GLN:NE2	2.32	0.44
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.52	0.44
2:B:330:GLN:CD	2:B:340:GLN:HE22	2.19	0.44
1:A:400:THR:HG22	1:A:404:GLU:OE2	2.17	0.44
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.64	0.44
2:B:8:VAL:HG11	2:B:159:ILE:HG13	1.97	0.44
1:A:64:LYS:HZ1	1:A:69:THR:CG2	2.10	0.44
1:A:411:ILE:HG22	1:A:412:PRO:O	2.18	0.44
1:A:433:PRO:HG2	2:B:255:ASN:HD22	1.81	0.44
1:A:460:ASN:HD21	2:B:288:ALA:HB2	1.83	0.44
1:A:498:ASP:N	1:A:498:ASP:OD1	2.49	0.44
2:B:72:ARG:CG	2:B:72:ARG:NH1	2.79	0.44
2:B:81:ASN:ND2	2:B:154:LYS:HG3	2.32	0.44
2:B:319:TYR:O	2:B:321:PRO:HD3	2.18	0.44
1:A:1:PRO:O	1:A:2:ILE:HD13	2.17	0.44
1:A:30:LYS:HE2	1:A:61:PHE:HE1	1.82	0.44
2:B:270:ILE:HD12	2:B:346:PHE:CB	2.48	0.44
2:B:298:GLU:CD	2:B:298:GLU:N	2.65	0.44
1:A:106:VAL:CG2	1:A:227:PHE:HE2	2.31	0.44
1:A:420:PRO:HA	1:A:422:LEU:HD13	1.99	0.44
2:B:254:VAL:O	2:B:258:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.32	0.44
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.52	0.44
1:A:194:GLU:HA	4:A:775:HOH:O	2.18	0.44
2:B:80:LEU:HD13	2:B:153:TRP:CD1	2.53	0.43
2:B:249:LYS:HE2	2:B:249:LYS:HB3	1.31	0.43
1:A:522:ILE:HA	1:A:525:LEU:HD12	2.00	0.43
2:B:243:PRO:O	2:B:245:VAL:HG23	2.18	0.43
2:B:271:TYR:HB3	2:B:274:ILE:HD11	2.00	0.43
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.53	0.43
1:A:20:LYS:HE2	1:A:55:PRO:HB2	2.00	0.43
1:A:218:ASP:HB2	4:A:725:HOH:O	2.16	0.43
1:A:484:LEU:HA	1:A:484:LEU:HD23	1.70	0.43
2:B:43:LYS:C	2:B:45:GLY:H	2.22	0.43
2:B:244:ILE:HG23	2:B:263:LYS:CE	2.48	0.43
1:A:12:LEU:HD22	1:A:12:LEU:HA	1.69	0.43
1:A:47:ILE:HD12	1:A:144:TYR:CG	2.54	0.43
1:A:295:LEU:HB3	1:A:300:GLU:HG2	2.00	0.43
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.52	0.43
1:A:424:LYS:HE2	1:A:426:TRP:CE2	2.53	0.43
1:A:466:VAL:HG23	1:A:551:LEU:CD2	2.42	0.43
2:B:270:ILE:HD12	2:B:346:PHE:CD2	2.53	0.43
1:A:110:ASP:OD1	1:A:223:LYS:HE2	2.18	0.43
1:A:235:HIS:O	3:A:601:R8E:C22	2.66	0.43
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.25	0.43
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.72	0.43
2:B:252:TRP:HB3	2:B:257:ILE:CD1	2.48	0.43
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.85	0.43
1:A:208:HIS:O	1:A:212:TRP:HD1	2.02	0.43
2:B:63:ILE:HD13	2:B:74:LEU:HB2	2.01	0.43
2:B:86:ASP:HA	2:B:90:VAL:HG22	2.00	0.43
2:B:108:VAL:HB	2:B:232:TYR:CD2	2.48	0.43
2:B:287:LYS:H	2:B:287:LYS:HG2	1.68	0.43
1:A:402:TRP:CZ3	1:A:403:THR:OG1	2.69	0.43
2:B:416:PHE:CD2	2:B:416:PHE:N	2.86	0.43
1:A:8:VAL:O	1:A:121:ASP:HB2	2.19	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43
2:B:336:GLN:HE21	2:B:336:GLN:HB2	1.48	0.43
1:A:63:ILE:HD11	4:A:644:HOH:O	2.17	0.43
1:A:139:THR:HA	1:A:140:PRO:HD3	1.52	0.43
1:A:178:ILE:HD12	1:A:178:ILE:N	2.33	0.43
1:A:195:ILE:HD13	1:A:199:ARG:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:OE1	2:B:60:VAL:HG12	2.19	0.43
2:B:253:THR:CG2	2:B:255:ASN:H	2.32	0.43
1:A:65:LYS:HE2	1:A:72:ARG:CD	2.49	0.43
1:A:77:PHE:O	1:A:81:ASN:HB2	2.19	0.43
1:A:162:SER:CB	2:B:52:PRO:HG3	2.49	0.43
1:A:270:ILE:O	1:A:270:ILE:HG13	2.18	0.43
2:B:118:VAL:HG21	2:B:160:PHE:HD1	1.84	0.43
2:B:234:LEU:HD23	2:B:234:LEU:HA	1.75	0.43
2:B:305:GLU:O	2:B:309:ILE:HD12	2.18	0.43
1:A:236:PRO:HA	3:A:601:R8E:N24	2.34	0.42
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.54	0.42
1:A:447:ASN:O	1:A:451:LYS:N	2.46	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CZ	2.53	0.42
1:A:194:GLU:C	1:A:196:GLY:H	2.21	0.42
1:A:230:MET:HA	1:A:230:MET:CE	2.49	0.42
1:A:277:ARG:HE	1:A:336:GLN:CD	2.23	0.42
2:B:244:ILE:CD1	2:B:266:TRP:CH2	3.02	0.42
2:B:428:GLN:HE21	2:B:428:GLN:C	2.19	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD2	1.63	0.42
1:A:438:GLU:OE1	1:A:459:THR:OG1	2.26	0.42
2:B:199:ARG:NH1	2:B:233:GLU:OE1	2.53	0.42
2:B:330:GLN:NE2	2:B:340:GLN:HE22	2.18	0.42
2:B:339:TYR:O	2:B:340:GLN:HG3	2.19	0.42
1:A:80:LEU:HD11	1:A:124:PHE:CZ	2.55	0.42
1:A:225:PRO:HB3	3:A:601:R8E:N25	2.34	0.42
1:A:244:ILE:H	1:A:244:ILE:CD1	2.32	0.42
1:A:419:THR:HA	1:A:420:PRO:HD2	1.85	0.42
1:A:23:GLN:NE2	1:A:26:LEU:CD2	2.81	0.42
1:A:75:VAL:HG11	1:A:77:PHE:CZ	2.55	0.42
1:A:138:GLU:H	1:A:138:GLU:HG3	1.46	0.42
1:A:170:PRO:HB2	1:A:171:PHE:H	1.51	0.42
1:A:401:TRP:HB2	1:A:425:LEU:HD21	2.01	0.42
1:A:438:GLU:OE2	1:A:463:ARG:NH2	2.39	0.42
1:A:485:ALA:O	1:A:489:SER:HB3	2.19	0.42
1:A:102:LYS:NZ	1:A:237:ASP:CB	2.75	0.42
1:A:80:LEU:HD13	1:A:127:TYR:HB3	2.02	0.42
1:A:105:SER:HB2	1:A:198:HIS:ND1	2.34	0.42
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.33	0.42
1:A:501:TYR:CZ	1:A:505:ILE:CD1	3.02	0.42
2:B:58:THR:HG23	2:B:76:ASP:O	2.20	0.42
2:B:13:LYS:CB	2:B:16:MET:CE	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.50	0.42
1:A:65:LYS:HE2	1:A:72:ARG:NE	2.35	0.41
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.65	0.41
2:B:13:LYS:HE2	2:B:16:MET:HE3	2.01	0.41
2:B:260:LEU:CD2	2:B:264:LEU:HD12	2.23	0.41
1:A:173:LYS:N	1:A:173:LYS:HZ3	2.17	0.41
1:A:240:THR:HG23	1:A:241:VAL:O	2.19	0.41
1:A:424:LYS:HE2	1:A:426:TRP:CZ3	2.55	0.41
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.55	0.41
1:A:65:LYS:CG	1:A:68:SER:HB3	2.45	0.41
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.55	0.41
2:B:33:ALA:O	2:B:37:ILE:HD12	2.20	0.41
2:B:203:GLU:OE1	2:B:203:GLU:HA	2.19	0.41
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.55	0.41
2:B:294:PRO:HB3	4:B:451:HOH:O	2.19	0.41
1:A:21:VAL:O	1:A:57:ASN:HB3	2.20	0.41
2:B:195:ILE:HD12	2:B:195:ILE:HA	1.64	0.41
2:B:253:THR:O	2:B:257:ILE:CG1	2.66	0.41
2:B:253:THR:HG22	2:B:255:ASN:CB	2.50	0.41
1:A:105:SER:HB2	4:A:603:HOH:O	2.20	0.41
1:A:452:LEU:HD22	1:A:452:LEU:HA	1.84	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.41
2:B:81:ASN:CG	2:B:154:LYS:HG3	2.41	0.41
2:B:271:TYR:HD2	2:B:271:TYR:HA	1.63	0.41
2:B:335:GLY:O	2:B:355:ALA:HA	2.20	0.41
2:B:363:ASN:ND2	2:B:363:ASN:H	2.18	0.41
1:A:34:LEU:HB3	1:A:132:ILE:HD13	2.02	0.41
1:A:104:LYS:HG3	1:A:192:ASP:CA	2.50	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.73	0.41
1:A:242:GLN:HA	1:A:243:PRO:HD3	1.84	0.41
1:A:342:TYR:CD1	1:A:342:TYR:C	2.93	0.41
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.50	0.41
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.02	0.41
2:B:156:SER:HB2	2:B:157:PRO:HD3	2.02	0.41
2:B:362:THR:HG23	2:B:366:LYS:HG2	1.97	0.41
1:A:96:HIS:CB	1:A:382:ILE:HD13	2.45	0.41
1:A:109:LEU:HB2	1:A:187:LEU:HB2	2.03	0.41
1:A:169:GLU:CB	1:A:170:PRO:CD	2.94	0.41
1:A:194:GLU:CD	1:A:194:GLU:N	2.74	0.41
1:A:276:VAL:O	1:A:280:CYS:HB2	2.21	0.41
1:A:520:GLN:HG2	1:A:520:GLN:H	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLN:HB3	2:B:92:LEU:H	1.76	0.41
1:A:0:SER:HA	1:A:1:PRO:HD3	1.74	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.76	0.41
1:A:254:VAL:HG21	1:A:288:ALA:O	2.21	0.41
1:A:406:TRP:HE3	1:A:406:TRP:O	2.04	0.41
1:A:464:GLN:HG2	1:A:465:LYS:H	1.84	0.41
1:A:466:VAL:CG2	1:A:551:LEU:CD2	2.91	0.41
1:A:480:GLN:NE2	1:A:480:GLN:HA	2.35	0.41
2:B:13:LYS:HD2	2:B:85:GLN:HB3	2.03	0.41
2:B:396:GLU:O	2:B:400:THR:CG2	2.66	0.41
1:A:105:SER:CB	1:A:198:HIS:ND1	2.84	0.41
1:A:296:THR:HG23	1:A:297:GLU:N	2.36	0.41
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.91	0.40
1:A:406:TRP:CE3	1:A:407:GLN:CA	3.04	0.40
2:B:30:LYS:CG	2:B:62:ALA:HB3	2.50	0.40
1:A:109:LEU:O	1:A:187:LEU:HB2	2.20	0.40
1:A:206:ARG:HH22	1:A:218:ASP:CB	2.33	0.40
2:B:22:LYS:O	2:B:59:PRO:HG3	2.21	0.40
2:B:54:ASN:HD21	2:B:126:LYS:CB	2.35	0.40
1:A:26:LEU:HD22	1:A:133:PRO:HG3	2.03	0.40
1:A:287:LYS:HA	1:A:287:LYS:CE	2.39	0.40
2:B:167:ILE:HG12	2:B:212:TRP:CD1	2.57	0.40
2:B:421:PRO:O	2:B:425:LEU:HD22	2.21	0.40
1:A:27:THR:O	1:A:31:ILE:HG13	2.21	0.40
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.56	0.40
1:A:63:ILE:HG13	1:A:74:LEU:HG	2.02	0.40
1:A:324:ASP:O	1:A:343:GLN:HG2	2.22	0.40
2:B:354:TYR:OH	2:B:370:GLU:OE2	2.40	0.40
2:B:382:ILE:HG22	2:B:383:TRP:CG	2.56	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	556/563 (99%)	466 (84%)	62 (11%)	28 (5%)	2	7
2	B	398/443 (90%)	350 (88%)	39 (10%)	9 (2%)	6	23
All	All	954/1006 (95%)	816 (86%)	101 (11%)	37 (4%)	3	12

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	90	VAL
1	A	136	ASN
1	A	170	PRO
1	A	286	THR
1	A	356	ARG
1	A	491	LEU
2	B	65	LYS
2	B	313	PRO
2	B	421	PRO
1	A	64	LYS
1	A	171	PHE
1	A	195	ILE
1	A	196	GLY
1	A	243	PRO
1	A	541	GLY
1	A	543	GLY
2	B	18	GLY
1	A	18	GLY
1	A	67	ASP
1	A	121	ASP
1	A	122	GLU
1	A	313	PRO
2	B	91	GLN
2	B	237	ASP
2	B	272	PRO
2	B	277	ARG
1	A	125	ARG
1	A	139	THR
1	A	554	ALA
2	B	251	SER
1	A	312	GLU
1	A	346	PHE
1	A	345	PRO
1	A	276	VAL

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Mol	Chain	Res	Type
1	A	119	PRO
1	A	135	ILE

### 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	498/503 (99%)	368 (74%)	130 (26%)	0	1
2	B	368/403 (91%)	270 (73%)	98 (27%)	0	1
All	All	866/906 (96%)	638 (74%)	228 (26%)	0	1

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	11	LYS
1	A	12	LEU
1	A	21	VAL
1	A	22	LYS
1	A	26	LEU
1	A	30	LYS
1	A	32	LYS
1	A	36	GLU
1	A	40	GLU
1	A	60	VAL
1	A	63	ILE
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	67	ASP
1	A	69	THR
1	A	70	LYS

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Mol	Chain	Res	Type
1	A	72	ARG
1	A	82	LYS
1	A	92	LEU
1	A	103	LYS
1	A	107	THR
1	A	108	VAL
1	A	118	VAL
1	A	120	LEU
1	A	122	GLU
1	A	123	ASP
1	A	125	ARG
1	A	126	LYS
1	A	131	THR
1	A	138	GLU
1	A	161	GLN
1	A	162	SER
1	A	166	LYS
1	A	169	GLU
1	A	173	LYS
1	A	179	VAL
1	A	187	LEU
1	A	195	ILE
1	A	197	GLN
1	A	202	ILE
1	A	205	LEU
1	A	206	ARG
1	A	207	GLN
1	A	215	THR
1	A	220	LYS
1	A	223	LYS
1	A	224	GLU
1	A	238	LYS
1	A	242	GLN
1	A	246	LEU
1	A	248	GLU
1	A	250	ASP
1	A	260	LEU
1	A	268	SER
1	A	270	ILE
1	A	276	VAL
1	A	277	ARG
1	A	279	LEU

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Mol	Chain	Res	Type
1	A	280	CYS
1	A	281	LYS
1	A	284	ARG
1	A	287	LYS
1	A	289	LEU
1	A	290	THR
1	A	291	GLU
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	307	ARG
1	A	309	ILE
1	A	311	LYS
1	A	330	GLN
1	A	334	GLN
1	A	341	ILE
1	A	347	LYS
1	A	350	LYS
1	A	356	ARG
1	A	357	MET
1	A	358	ARG
1	A	368	LEU
1	A	373	GLN
1	A	374	LYS
1	A	380	ILE
1	A	382	ILE
1	A	394	GLN
1	A	395	LYS
1	A	399	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU
1	A	407	GLN
1	A	409	THR
1	A	422	LEU
1	A	424	LYS
1	A	425	LEU
1	A	443	ASP
1	A	448	ARG
1	A	451	LYS
1	A	452	LEU

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Mol	Chain	Res	Type
1	A	454	LYS
1	A	458	VAL
1	A	459	THR
1	A	463	ARG
1	A	465	LYS
1	A	471	ASP
1	A	473	THR
1	A	479	LEU
1	A	488	ASP
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	503	LEU
1	A	514	GLU
1	A	517	LEU
1	A	520	GLN
1	A	546	GLU
1	A	547	GLN
1	A	548	VAL
1	A	549	ASP
1	A	550	LYS
1	A	551	LEU
1	A	557	ARG
2	B	6	GLU
2	B	10	VAL
2	B	11	LYS
2	B	12	LEU
2	B	17	ASP
2	B	22	LYS
2	B	24	TRP
2	B	27	THR
2	B	29	GLU
2	B	30	LYS
2	B	32	LYS
2	B	40	GLU
2	B	46	LYS
2	B	48	SER
2	B	49	LYS
2	B	63	ILE
2	B	64	LYS

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Mol	Chain	Res	Type
2	B	65	LYS
2	B	66	LYS
2	B	68	SER
2	B	69	THR
2	B	70	LYS
2	B	72	ARG
2	B	73	LYS
2	B	79	GLU
2	B	80	LEU
2	B	83	ARG
2	B	89	GLU
2	B	91	GLN
2	B	101	LYS
2	B	102	LYS
2	B	111	VAL
2	B	117	SER
2	B	120	LEU
2	B	126	LYS
2	B	159	ILE
2	B	163	SER
2	B	166	LYS
2	B	169	GLU
2	B	173	LYS
2	B	174	GLN
2	B	178	ILE
2	B	182	GLN
2	B	187	LEU
2	B	195	ILE
2	B	205	LEU
2	B	206	ARG
2	B	214	LEU
2	B	232	TYR
2	B	233	GLU
2	B	238	LYS
2	B	242	GLN
2	B	248	GLU
2	B	249	LYS
2	B	253	THR
2	B	254	VAL
2	B	256	ASP
2	B	257	ILE
2	B	259	LYS

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Mol	Chain	Res	Type
2	B	260	LEU
2	B	265	ASN
2	B	268	SER
2	B	269	GLN
2	B	271	TYR
2	B	275	LYS
2	B	276	VAL
2	B	277	ARG
2	B	278	GLN
2	B	282	LEU
2	B	283	LEU
2	B	286	THR
2	B	287	LYS
2	B	290	THR
2	B	291	GLU
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	303	LEU
2	B	305	GLU
2	B	307	ARG
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	323	LYS
2	B	336	GLN
2	B	347	LYS
2	B	349	LEU
2	B	362	THR
2	B	369	THR
2	B	377	THR
2	B	388	LYS
2	B	394	GLN
2	B	400	THR
2	B	403	THR
2	B	413	GLU
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	147	ASN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	222	GLN
1	A	235	HIS
1	A	258	GLN
1	A	278	GLN
1	A	315	HIS
1	A	330	GLN
1	A	334	GLN
1	A	460	ASN
1	A	480	GLN
1	A	494	ASN
1	A	519	ASN
1	A	524	GLN
1	A	547	GLN
2	B	54	ASN
2	B	137	ASN
2	B	145	GLN
2	B	161	GLN
2	B	175	ASN
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	306	ASN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	361	HIS
2	B	367	GLN
2	B	373	GLN
2	B	407	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides 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	R8E	A	601	-	31,32,32	2.40	8 (25%)	36,45,45	3.13	15 (41%)

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	R8E	A	601	-	-	3/9/11/11	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8E	C2-C26	-10.11	1.22	1.44
3	A	601	R8E	C23-N25	3.58	1.45	1.35
3	A	601	R8E	C5-C4	-2.96	1.33	1.38
3	A	601	R8E	C18-N24	-2.54	1.31	1.36
3	A	601	R8E	C26-N27	-2.36	1.09	1.14
3	A	601	R8E	C16-N20	2.29	1.36	1.34
3	A	601	R8E	C17-C18	-2.13	1.37	1.43
3	A	601	R8E	C8-C13	-2.02	1.36	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	R8E	C2-C1-C6	-10.11	110.92	119.13
3	A	601	R8E	C5-C6-CL28	-6.63	110.86	119.15
3	A	601	R8E	C8-C13-CL29	-5.49	112.98	119.43
3	A	601	R8E	C1-C6-CL28	4.72	125.05	119.15
3	A	601	R8E	C3-C2-C26	-4.40	113.69	119.54
3	A	601	R8E	N25-C23-N24	-4.28	114.71	118.26
3	A	601	R8E	C8-O7-C4	4.07	128.15	118.00
3	A	601	R8E	C21-C22-C23	-4.01	116.35	119.48
3	A	601	R8E	C4-C5-C6	3.97	122.77	118.14
3	A	601	R8E	C1-C2-C3	3.20	124.81	119.71
3	A	601	R8E	C15-O14-C10	3.17	125.47	117.65
3	A	601	R8E	C22-C21-C17	-2.77	117.27	121.13
3	A	601	R8E	C12-C13-CL29	2.44	123.29	118.41
3	A	601	R8E	C12-C13-C8	2.09	123.73	120.78
3	A	601	R8E	C11-C12-C13	-2.06	117.03	120.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	R8E	C9-C10-O14-C15
3	A	601	R8E	C11-C10-O14-C15
3	A	601	R8E	C13-C8-O7-C4

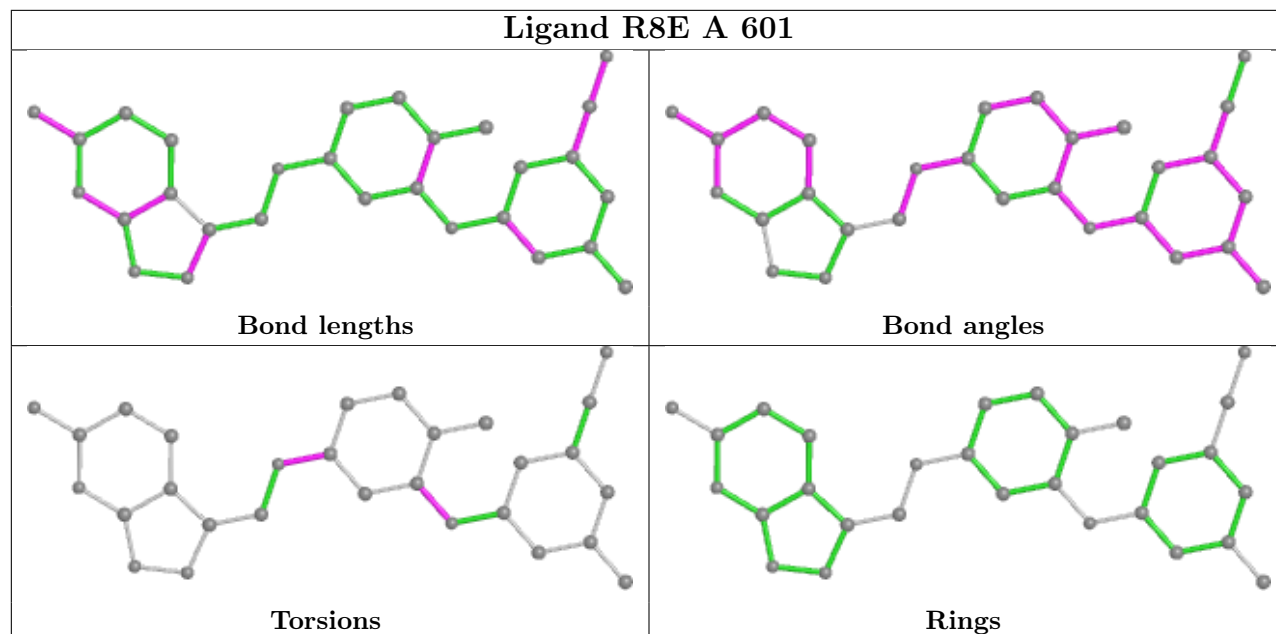
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	R8E	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	558/563 (99%)	-0.08	7 (1%) 77 77	21, 50, 83, 112	0
2	B	404/443 (91%)	-0.14	5 (1%) 79 79	24, 49, 100, 118	0
All	All	962/1006 (95%)	-0.10	12 (1%) 79 79	21, 50, 94, 118	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	3.0
2	B	90	VAL	3.0
2	B	67	ASP	2.7
2	B	270	ILE	2.7
1	A	66	LYS	2.5
1	A	491	LEU	2.3
2	B	362	THR	2.3
1	A	15	GLY	2.2
1	A	360	ALA	2.2
1	A	221	HIS	2.2
2	B	252	TRP	2.2
1	A	359	GLY	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 monosaccharides in this entry.

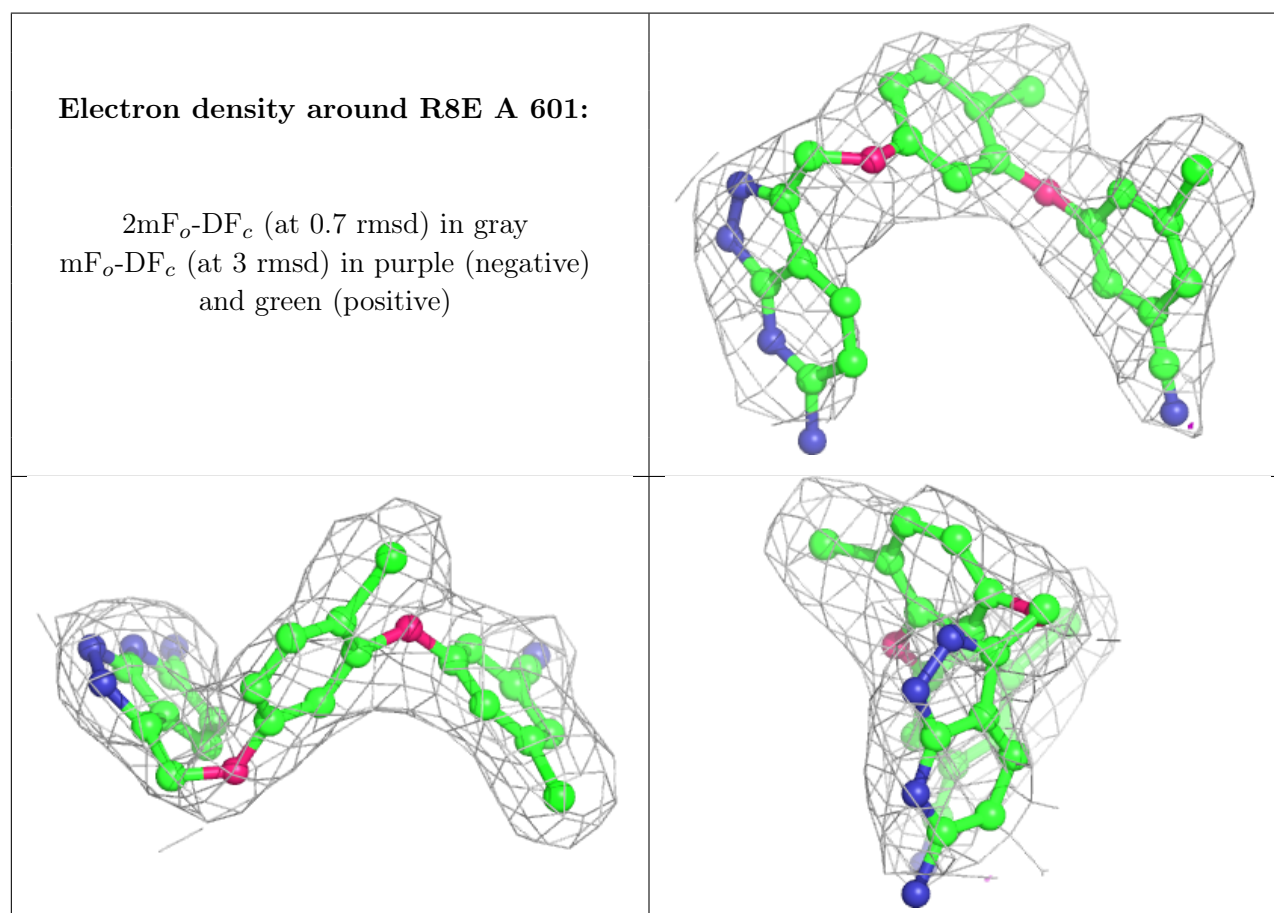


## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	R8E	A	601	29/29	0.96	0.23	42,52,75,78	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.