



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:39 am BST

PDB ID : 3DRP
Title : HIV reverse transcriptase in complex with inhibitor R8e
Authors : Yan, Y.; Prasad, S.
Deposited on : 2008-07-11
Resolution : 2.60 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 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 : 2.11
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) : 2.11

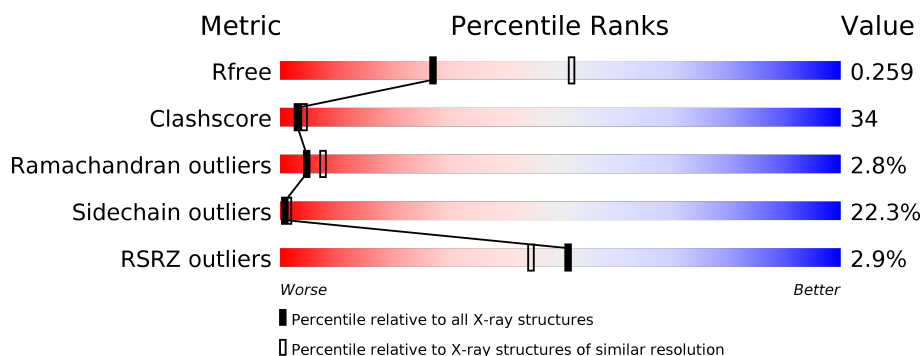
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 ≥ 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	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>38%</div> <div>14%</div> <div>••</div> </div> </div>
2	B	443	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>32%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8340 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
			4542	2934	760	840	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

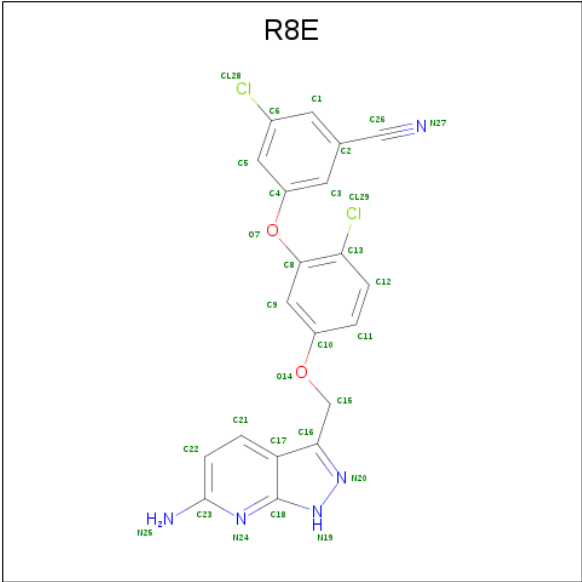
- Molecule 2 is a protein called p51 RT.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is 3-{5-[(6-amino-1H-pyrazolo[3,4-b]pyridin-3-yl)methoxy]-2-chlorophenoxy}-5-chlorobenzonitrile (three-letter code: R8E) (formula: C₂₀H₁₃Cl₂N₅O₂).



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

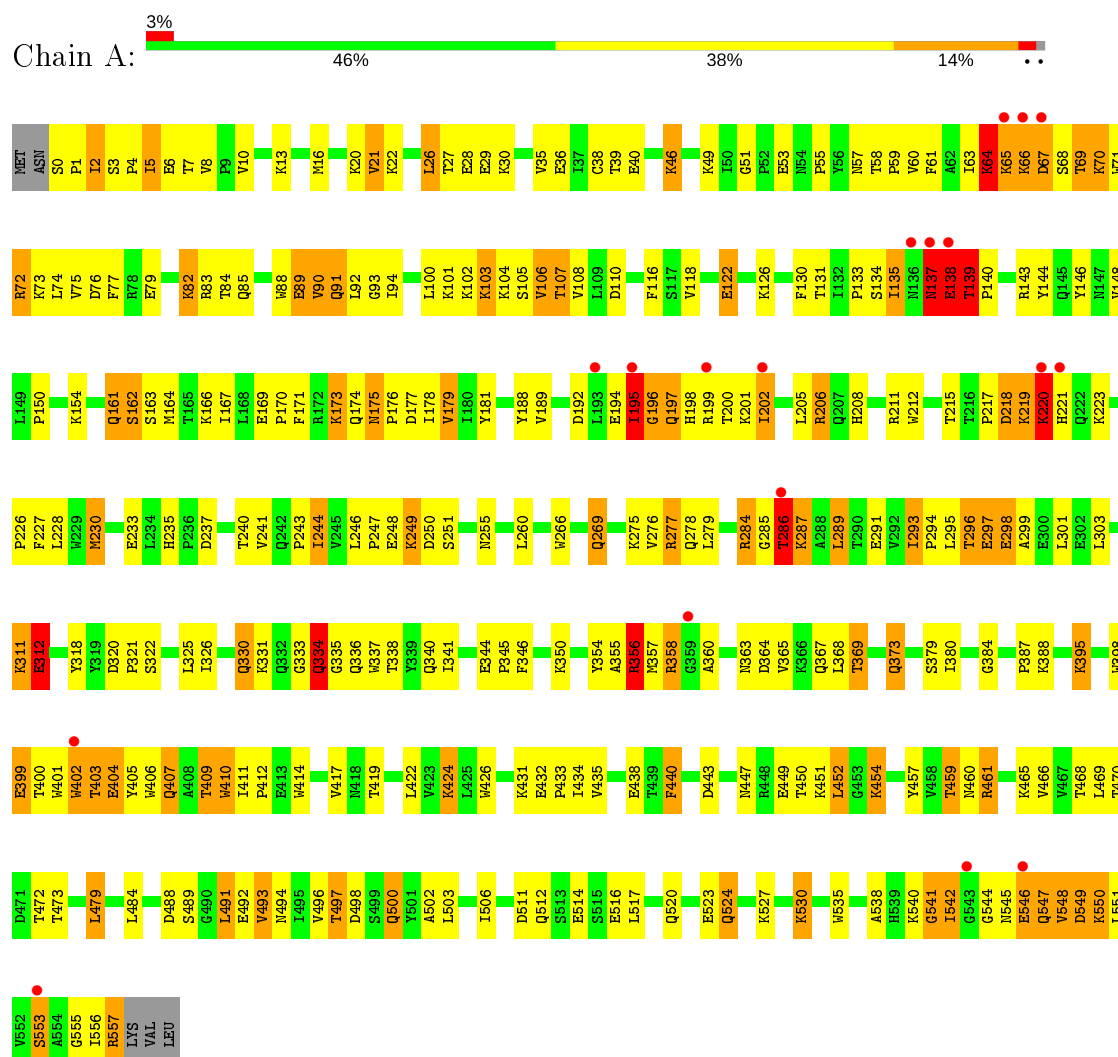
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		
4	B	193	Total	O	0	0
			193	193		

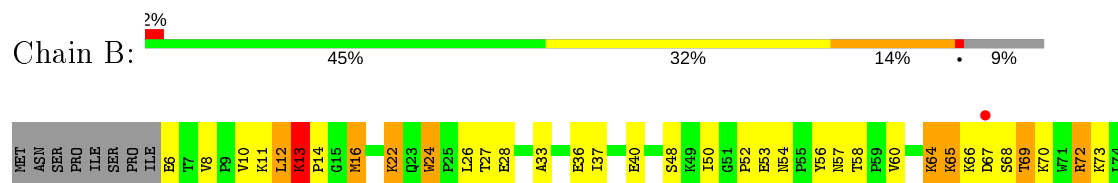
3 Residue-property plots

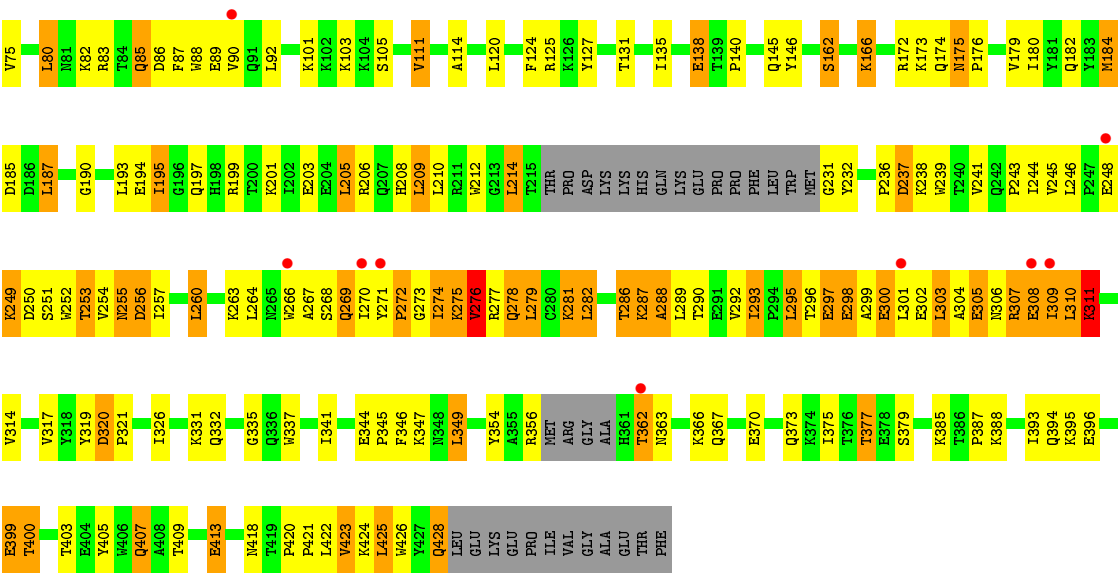
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, α , β , γ	118.86Å 155.03Å 155.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 2.60 47.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (94.49-2.60) 99.8 (47.16-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.85 (at 2.61Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.187 , 0.251 0.194 , 0.259	Depositor DCC
R_{free} test set	2245 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8340	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.66	0/4659	0.83	2/6330 (0.0%)
2	B	0.66	0/3438	0.81	3/4671 (0.1%)
All	All	0.66	0/8097	0.82	5/11001 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASN	C-N-CD	-9.03	100.73	120.60
2	B	13	LYS	C-N-CD	-7.11	104.95	120.60
1	A	312	GLU	C-N-CD	-6.80	105.65	120.60
2	B	205	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	320	ASP	C-N-CD	-5.13	109.32	120.60

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	4542	0	4595	349	0
2	B	3344	0	3369	220	0
3	A	29	0	13	2	0
4	A	232	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	193	0	0	7	0
All	All	8340	0	7977	541	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 34.

All (541) 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:296:THR:HG22	1:A:299:ALA:H	1.09	1.18
1:A:255:ASN:HB2	1:A:289:LEU:HD22	1.20	1.14
2:B:13:LYS:HE3	2:B:85:GLN:HB3	1.35	1.05
1:A:2:ILE:HD11	1:A:46:LYS:HZ1	1.20	1.04
2:B:209:LEU:HG	2:B:214:LEU:HD12	1.38	1.01
1:A:175:ASN:HD21	1:A:201:LYS:NZ	1.59	1.00
1:A:195:ILE:HD13	1:A:199:ARG:HE	1.26	1.00
1:A:406:TRP:CH2	2:B:418:ASN:HA	1.98	0.98
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	1.99	0.97
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.45	0.97
1:A:143:ARG:HH11	1:A:143:ARG:HG3	1.30	0.95
1:A:2:ILE:HD11	1:A:46:LYS:NZ	1.81	0.93
1:A:277:ARG:HH11	1:A:278:GLN:HE21	1.14	0.93
1:A:175:ASN:HD21	1:A:201:LYS:HZ1	1.06	0.92
2:B:362:THR:HG22	2:B:366:LYS:HG2	1.52	0.91
1:A:195:ILE:HD13	1:A:199:ARG:NE	1.85	0.90
1:A:63:ILE:HG12	1:A:74:LEU:HD11	1.55	0.89
2:B:268:SER:O	2:B:269:GLN:HG3	1.71	0.89
2:B:89:GLU:HG2	2:B:90:VAL:HG13	1.55	0.88
1:A:277:ARG:NH1	1:A:278:GLN:HE21	1.72	0.88
2:B:241:VAL:HG23	2:B:243:PRO:HD3	1.56	0.88
1:A:181:TYR:HB2	1:A:188:TYR:HB2	1.57	0.87
2:B:298:GLU:HA	2:B:301:LEU:HG	1.58	0.85
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.22	0.85
1:A:173:LYS:NZ	1:A:173:LYS:HA	1.91	0.85
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.11	0.84
1:A:28:GLU:HG2	1:A:135:ILE:HD12	1.59	0.84
1:A:296:THR:HG22	1:A:299:ALA:N	1.92	0.84
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.25	0.83
1:A:108:VAL:CG2	1:A:223:LYS:HD2	2.09	0.83
1:A:63:ILE:CD1	1:A:74:LEU:HD21	2.09	0.82
1:A:63:ILE:HD11	1:A:74:LEU:HD21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:O	1:A:312:GLU:HB3	1.79	0.81
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.62	0.81
1:A:64:LYS:O	1:A:65:LYS:HD2	1.80	0.81
1:A:3:SER:OG	1:A:5:ILE:HG23	1.81	0.80
2:B:422:LEU:HA	2:B:425:LEU:HD21	1.64	0.80
1:A:63:ILE:HG12	1:A:74:LEU:CD1	2.10	0.80
1:A:277:ARG:NH1	1:A:278:GLN:HG2	1.97	0.80
2:B:13:LYS:HE3	2:B:85:GLN:CB	2.12	0.80
1:A:454:LYS:HD2	1:A:556:ILE:HD11	1.62	0.80
2:B:13:LYS:CE	2:B:85:GLN:HB3	2.12	0.80
1:A:296:THR:CG2	1:A:299:ALA:H	1.92	0.80
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.46	0.79
1:A:255:ASN:CB	1:A:289:LEU:HD22	2.07	0.78
2:B:366:LYS:O	2:B:370:GLU:HG3	1.83	0.78
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.18	0.78
1:A:466:VAL:CG2	1:A:551:LEU:HD23	2.13	0.78
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.62	0.78
2:B:87:PHE:CZ	2:B:92:LEU:HD12	2.18	0.78
1:A:545:ASN:O	1:A:549:ASP:HB2	1.84	0.77
2:B:298:GLU:H	2:B:298:GLU:CD	1.86	0.77
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.66	0.77
1:A:70:LYS:HE2	1:A:71:TRP:O	1.84	0.77
1:A:35:VAL:O	1:A:39:THR:HG23	1.85	0.76
1:A:175:ASN:ND2	1:A:201:LYS:HZ1	1.82	0.76
1:A:91:GLN:NE2	1:A:92:LEU:H	1.83	0.76
1:A:237:ASP:HB3	4:A:800:HOH:O	1.85	0.76
2:B:195:ILE:O	2:B:199:ARG:HG3	1.85	0.75
1:A:70:LYS:HG3	1:A:71:TRP:N	1.99	0.75
1:A:63:ILE:CG1	1:A:74:LEU:HD11	2.17	0.75
2:B:279:LEU:O	2:B:282:LEU:HG	1.86	0.75
1:A:181:TYR:CE1	2:B:138:GLU:HG3	2.22	0.74
2:B:253:THR:HG23	2:B:289:LEU:O	1.87	0.74
1:A:107:THR:HG23	1:A:198:HIS:HE1	1.52	0.74
1:A:400:THR:O	1:A:404:GLU:HG3	1.87	0.74
1:A:424:LYS:HE2	1:A:426:TRP:CH2	2.22	0.74
1:A:255:ASN:HB2	1:A:289:LEU:CD2	2.12	0.74
2:B:271:TYR:CD1	2:B:310:LEU:HD12	2.22	0.74
1:A:233:GLU:HG2	1:A:235:HIS:CE1	2.23	0.74
2:B:87:PHE:CE2	2:B:92:LEU:HD12	2.23	0.73
1:A:540:LYS:O	1:A:542:ILE:N	2.21	0.73
2:B:422:LEU:HB3	2:B:426:TRP:CZ2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG22	1:A:223:LYS:HD2	1.69	0.73
2:B:13:LYS:CB	2:B:16:MET:HE3	2.18	0.73
1:A:360:ALA:HA	1:A:514:GLU:OE1	1.89	0.73
1:A:500:GLN:HG3	2:B:422:LEU:HD11	1.71	0.72
2:B:379:SER:OG	2:B:387:PRO:HD3	1.90	0.72
1:A:194:GLU:HG3	4:A:765:HOH:O	1.89	0.72
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.04	0.72
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.25	0.72
1:A:5:ILE:HG21	1:A:167:ILE:HD11	1.71	0.72
1:A:29:GLU:HG2	4:A:611:HOH:O	1.90	0.71
1:A:82:LYS:HD3	4:A:697:HOH:O	1.89	0.71
2:B:305:GLU:O	2:B:309:ILE:HB	1.89	0.71
2:B:270:ILE:HG13	2:B:346:PHE:O	1.90	0.71
1:A:211:ARG:O	1:A:211:ARG:HD3	1.90	0.71
2:B:36:GLU:HG2	4:B:576:HOH:O	1.91	0.71
2:B:206:ARG:HH21	2:B:231:GLY:N	1.88	0.70
1:A:298:GLU:OE2	1:A:298:GLU:N	2.22	0.70
1:A:244:ILE:HD12	1:A:244:ILE:N	2.07	0.70
2:B:303:LEU:O	2:B:307:ARG:HB2	1.92	0.70
1:A:63:ILE:CG2	1:A:74:LEU:HD11	2.22	0.69
1:A:206:ARG:HH12	1:A:218:ASP:HB2	1.56	0.69
1:A:63:ILE:CD1	1:A:72:ARG:HG3	2.21	0.69
2:B:279:LEU:HD13	2:B:282:LEU:HD11	1.75	0.69
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.01	0.69
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.28	0.69
1:A:395:LYS:HE2	1:A:414:TRP:CE2	2.28	0.69
1:A:354:TYR:CE1	1:A:356:ARG:HB2	2.28	0.69
2:B:420:PRO:HG2	2:B:423:VAL:HG21	1.75	0.69
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.22	0.68
2:B:241:VAL:CG2	2:B:243:PRO:HD3	2.23	0.68
2:B:362:THR:HG22	2:B:366:LYS:CG	2.23	0.68
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.27	0.68
1:A:173:LYS:HZ2	1:A:173:LYS:HA	1.58	0.68
2:B:52:PRO:HD2	2:B:53:GLU:OE1	1.94	0.68
1:A:106:VAL:CG2	1:A:227:PHE:HE2	2.06	0.67
1:A:411:ILE:HG23	1:A:412:PRO:HD2	1.76	0.67
1:A:65:LYS:CE	1:A:72:ARG:HH11	2.07	0.67
2:B:301:LEU:O	2:B:305:GLU:HB2	1.94	0.67
1:A:502:ALA:O	1:A:506:ILE:HD12	1.94	0.67
1:A:249:LYS:HG2	1:A:251:SER:O	1.95	0.67
2:B:13:LYS:HD2	2:B:86:ASP:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.77	0.67
1:A:202:ILE:O	1:A:206:ARG:HG3	1.95	0.66
1:A:169:GLU:N	1:A:170:PRO:HD2	2.11	0.65
2:B:72:ARG:NH2	2:B:409:THR:HG21	2.11	0.65
1:A:102:LYS:O	1:A:103:LYS:NZ	2.26	0.65
1:A:181:TYR:HE1	2:B:138:GLU:HG3	1.61	0.65
1:A:91:GLN:HG3	1:A:93:GLY:O	1.95	0.65
1:A:241:VAL:HG23	1:A:244:ILE:HD11	1.78	0.65
1:A:438:GLU:HG3	1:A:461:ARG:HB2	1.76	0.65
2:B:270:ILE:O	2:B:272:PRO:HD3	1.97	0.65
1:A:333:GLY:O	1:A:335:GLY:N	2.30	0.65
2:B:64:LYS:NZ	2:B:69:THR:O	2.29	0.65
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.12	0.65
1:A:326:ILE:CD1	1:A:388:LYS:HE3	2.26	0.65
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.62	0.65
1:A:65:LYS:HE3	1:A:72:ARG:HD2	1.78	0.65
2:B:256:ASP:O	2:B:260:LEU:HB2	1.97	0.64
1:A:176:PRO:HD2	1:A:177:ASP:H	1.62	0.64
1:A:177:ASP:HB2	4:A:826:HOH:O	1.97	0.64
1:A:500:GLN:HG3	2:B:422:LEU:CD1	2.27	0.64
1:A:194:GLU:H	1:A:194:GLU:CD	2.00	0.64
2:B:267:ALA:O	2:B:270:ILE:HG23	1.97	0.64
2:B:335:GLY:HA3	2:B:356:ARG:HG2	1.79	0.64
1:A:107:THR:HG23	1:A:198:HIS:CE1	2.33	0.64
1:A:175:ASN:HB3	1:A:178:ILE:HD13	1.79	0.64
1:A:395:LYS:HE2	1:A:414:TRP:CZ2	2.32	0.64
1:A:424:LYS:HE3	1:A:426:TRP:CD2	2.33	0.64
1:A:524:GLN:CA	1:A:524:GLN:HE21	2.09	0.64
1:A:63:ILE:HG13	1:A:72:ARG:HG3	1.79	0.64
1:A:13:LYS:O	1:A:16:MET:HB2	1.97	0.64
1:A:555:GLY:O	1:A:556:ILE:HD13	1.97	0.63
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.79	0.63
1:A:230:MET:HA	1:A:230:MET:HE2	1.80	0.63
2:B:66:LYS:HG2	2:B:407:GLN:HE21	1.63	0.63
1:A:520:GLN:O	1:A:523:GLU:HG2	1.98	0.63
2:B:422:LEU:O	2:B:425:LEU:HG	1.99	0.63
1:A:64:LYS:HD3	1:A:70:LYS:O	1.98	0.63
2:B:278:GLN:HB3	2:B:299:ALA:HA	1.80	0.63
1:A:107:THR:CG2	1:A:202:ILE:HD13	2.29	0.63
2:B:282:LEU:HD13	2:B:295:LEU:CD1	2.29	0.62
1:A:266:TRP:O	1:A:269:GLN:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:HG22	1:A:412:PRO:O	2.00	0.62
1:A:162:SER:CB	2:B:52:PRO:HG3	2.29	0.62
1:A:500:GLN:OE1	2:B:422:LEU:HG	2.00	0.62
1:A:65:LYS:HG2	1:A:68:SER:HB3	1.82	0.62
1:A:497:THR:O	1:A:535:TRP:HA	2.00	0.62
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.24	0.62
1:A:297:GLU:O	1:A:301:LEU:HG	1.99	0.62
1:A:101:LYS:HD3	1:A:321:PRO:HG3	1.82	0.61
2:B:210:LEU:O	2:B:210:LEU:HD12	2.00	0.61
2:B:111:VAL:HG21	2:B:187:LEU:HD22	1.80	0.61
1:A:450:THR:OG1	1:A:452:LEU:HB2	2.00	0.61
2:B:6:GLU:HA	4:B:544:HOH:O	2.00	0.61
1:A:399:GLU:O	1:A:403:THR:HB	2.00	0.61
1:A:195:ILE:HG23	1:A:199:ARG:CD	2.29	0.61
1:A:175:ASN:HD21	1:A:201:LYS:CE	2.13	0.60
1:A:65:LYS:CE	1:A:72:ARG:HD2	2.30	0.60
1:A:355:ALA:O	1:A:356:ARG:O	2.18	0.60
1:A:331:LYS:HE3	1:A:364:ASP:OD1	2.01	0.60
1:A:21:VAL:CG2	1:A:59:PRO:HG3	2.31	0.60
2:B:396:GLU:O	2:B:400:THR:HG22	2.01	0.60
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.32	0.60
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.84	0.59
1:A:5:ILE:HG22	1:A:212:TRP:CE3	2.37	0.59
1:A:547:GLN:O	1:A:550:LYS:HD2	2.03	0.59
2:B:253:THR:O	2:B:257:ILE:HG13	2.03	0.59
2:B:373:GLN:HE22	2:B:407:GLN:H	1.48	0.59
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.32	0.58
2:B:301:LEU:N	2:B:301:LEU:HD23	2.18	0.58
1:A:1:PRO:C	1:A:2:ILE:HD13	2.22	0.58
1:A:447:ASN:OD1	1:A:449:GLU:HB2	2.03	0.58
1:A:103:LYS:HE3	1:A:192:ASP:OD1	2.03	0.58
1:A:176:PRO:CD	1:A:177:ASP:H	2.16	0.58
1:A:173:LYS:HZ3	1:A:173:LYS:HA	1.65	0.58
1:A:244:ILE:H	1:A:244:ILE:HD12	1.65	0.58
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.19	0.58
2:B:268:SER:C	2:B:270:ILE:H	2.07	0.58
1:A:107:THR:CG2	1:A:198:HIS:HE1	2.16	0.58
1:A:411:ILE:CG2	1:A:412:PRO:HD2	2.33	0.58
2:B:13:LYS:HB3	2:B:16:MET:HE3	1.86	0.58
1:A:40:GLU:HA	1:A:40:GLU:OE1	2.02	0.57
2:B:362:THR:CG2	2:B:366:LYS:HG2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:HA	1:A:174:GLN:NE2	2.19	0.57
1:A:26:LEU:HD22	1:A:133:PRO:HG3	1.86	0.57
2:B:13:LYS:HB2	2:B:16:MET:HE3	1.86	0.57
1:A:195:ILE:HG23	1:A:199:ARG:HD2	1.85	0.57
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.50	0.57
1:A:523:GLU:HG2	1:A:524:GLN:N	2.20	0.57
2:B:278:GLN:HB2	2:B:302:GLU:OE2	2.05	0.57
1:A:298:GLU:H	1:A:298:GLU:CD	2.07	0.57
2:B:276:VAL:HA	2:B:302:GLU:OE1	2.05	0.57
1:A:63:ILE:HG12	1:A:74:LEU:CG	2.35	0.57
2:B:297:GLU:O	2:B:300:GLU:HB2	2.04	0.57
1:A:171:PHE:O	1:A:175:ASN:HB2	2.04	0.57
1:A:66:LYS:O	1:A:67:ASP:HB2	2.05	0.57
2:B:253:THR:HG22	2:B:255:ASN:N	2.20	0.57
2:B:268:SER:O	2:B:270:ILE:N	2.33	0.56
2:B:282:LEU:O	2:B:287:LYS:NZ	2.37	0.56
1:A:63:ILE:CG1	1:A:72:ARG:HG3	2.35	0.56
2:B:111:VAL:HG22	2:B:214:LEU:HD13	1.87	0.56
2:B:260:LEU:O	2:B:264:LEU:HB2	2.05	0.56
2:B:373:GLN:O	2:B:377:THR:HG23	2.04	0.56
2:B:296:THR:HB	2:B:298:GLU:OE2	2.06	0.56
1:A:102:LYS:HZ3	1:A:237:ASP:HB3	1.70	0.56
1:A:3:SER:HB3	1:A:5:ILE:HD13	1.86	0.56
2:B:162:SER:O	2:B:166:LYS:HG2	2.07	0.55
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.88	0.55
1:A:65:LYS:CG	1:A:68:SER:HB3	2.36	0.55
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.40	0.55
2:B:172:ARG:HH21	2:B:180:ILE:HB	1.70	0.55
2:B:273:GLY:O	2:B:275:LYS:HD3	2.07	0.55
2:B:317:VAL:HG12	2:B:349:LEU:CD1	2.36	0.55
1:A:373:GLN:OE1	2:B:400:THR:HG21	2.06	0.55
1:A:206:ARG:HH12	1:A:218:ASP:CB	2.19	0.55
1:A:108:VAL:HG21	1:A:223:LYS:HD2	1.87	0.55
2:B:393:ILE:HG12	2:B:394:GLN:H	1.72	0.55
1:A:3:SER:HB3	1:A:5:ILE:CD1	2.36	0.54
1:A:498:ASP:OD2	1:A:538:ALA:HB2	2.07	0.54
2:B:194:GLU:HB3	2:B:197:GLN:HG3	1.89	0.54
2:B:246:LEU:HD11	2:B:310:LEU:CD2	2.36	0.54
1:A:65:LYS:HE3	1:A:72:ARG:HH11	1.72	0.54
2:B:421:PRO:O	2:B:425:LEU:HD23	2.07	0.54
1:A:277:ARG:HD2	1:A:334:GLN:HE21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:HB2	4:B:601:HOH:O	2.07	0.54
1:A:296:THR:HG23	1:A:298:GLU:H	1.73	0.54
2:B:254:VAL:HG21	2:B:288:ALA:O	2.06	0.54
1:A:500:GLN:CG	2:B:422:LEU:HG	2.38	0.54
1:A:406:TRP:CZ3	2:B:418:ASN:HA	2.39	0.54
1:A:2:ILE:N	1:A:2:ILE:HD13	2.23	0.54
2:B:209:LEU:CG	2:B:214:LEU:HD12	2.26	0.54
2:B:101:LYS:HG2	4:B:535:HOH:O	2.07	0.54
2:B:267:ALA:O	2:B:271:TYR:HB2	2.07	0.54
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.23	0.54
1:A:356:ARG:CZ	1:A:358:ARG:HD2	2.38	0.53
1:A:297:GLU:HG2	4:A:668:HOH:O	2.08	0.53
1:A:194:GLU:O	1:A:196:GLY:N	2.41	0.53
1:A:27:THR:OG1	1:A:30:LYS:HG3	2.08	0.53
1:A:356:ARG:NE	1:A:358:ARG:HG3	2.24	0.53
1:A:466:VAL:HG23	1:A:551:LEU:HD23	1.90	0.53
2:B:268:SER:HA	2:B:274:ILE:HG13	1.91	0.53
2:B:306:ASN:O	2:B:310:LEU:N	2.33	0.53
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.24	0.52
1:A:540:LYS:HB2	1:A:542:ILE:HD12	1.92	0.52
1:A:296:THR:HG23	1:A:298:GLU:OE2	2.09	0.52
1:A:134:SER:OG	1:A:138:GLU:O	2.27	0.52
1:A:277:ARG:NH1	1:A:278:GLN:NE2	2.52	0.52
1:A:326:ILE:HD12	1:A:388:LYS:HE3	1.91	0.52
1:A:365:VAL:O	1:A:369:THR:HG23	2.09	0.52
1:A:277:ARG:HE	1:A:336:GLN:CD	2.13	0.52
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.25	0.52
2:B:422:LEU:HD13	2:B:426:TRP:CH2	2.45	0.52
1:A:405:TYR:CE2	1:A:407:GLN:HG2	2.44	0.52
2:B:373:GLN:NE2	2:B:407:GLN:H	2.08	0.52
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.92	0.52
1:A:8:VAL:O	1:A:10:VAL:HG23	2.10	0.52
1:A:85:GLN:O	1:A:154:LYS:HE2	2.10	0.52
2:B:396:GLU:O	2:B:400:THR:CG2	2.58	0.52
1:A:331:LYS:HB2	1:A:337:TRP:CZ3	2.45	0.51
2:B:10:VAL:HB	2:B:124:PHE:CD1	2.45	0.51
1:A:197:GLN:O	1:A:201:LYS:HB2	2.11	0.51
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.74	0.51
1:A:325:LEU:C	1:A:326:ILE:HD13	2.31	0.51
2:B:422:LEU:HD13	2:B:426:TRP:CZ2	2.45	0.51
1:A:58:THR:HG23	1:A:76:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:TYR:CE1	2:B:310:LEU:HD12	2.45	0.51
1:A:137:ASN:O	1:A:138:GLU:O	2.27	0.51
1:A:230:MET:CE	1:A:230:MET:CA	2.89	0.51
2:B:253:THR:HB	2:B:256:ASP:OD1	2.10	0.51
1:A:363:ASN:HA	1:A:511:ASP:OD2	2.11	0.51
1:A:500:GLN:HG2	2:B:421:PRO:HG2	1.93	0.51
1:A:312:GLU:O	1:A:312:GLU:OE2	2.30	0.50
2:B:208:HIS:O	2:B:212:TRP:HE3	1.93	0.50
2:B:292:VAL:HG12	2:B:293:ILE:N	2.26	0.50
1:A:277:ARG:HH12	1:A:278:GLN:HG2	1.74	0.50
1:A:195:ILE:CG2	1:A:199:ARG:HD2	2.42	0.50
1:A:28:GLU:HG2	1:A:135:ILE:HG23	1.94	0.50
1:A:175:ASN:HD22	1:A:178:ILE:CD1	2.25	0.50
2:B:250:ASP:OD2	2:B:250:ASP:N	2.42	0.50
2:B:266:TRP:O	2:B:270:ILE:HG22	2.12	0.50
1:A:409:THR:HG21	4:A:793:HOH:O	2.11	0.50
1:A:479:LEU:HD13	1:A:502:ALA:HB2	1.94	0.50
2:B:33:ALA:O	2:B:37:ILE:HD12	2.12	0.50
1:A:541:GLY:HA2	1:A:546:GLU:HG2	1.93	0.50
2:B:304:ALA:O	2:B:308:GLU:HB3	2.12	0.50
1:A:170:PRO:O	1:A:174:GLN:OE1	2.30	0.49
1:A:122:GLU:HB2	4:A:622:HOH:O	2.13	0.49
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.47	0.49
1:A:523:GLU:CG	1:A:524:GLN:N	2.75	0.49
2:B:362:THR:HG23	2:B:366:LYS:HZ2	1.78	0.49
1:A:424:LYS:HE2	1:A:426:TRP:CZ3	2.47	0.49
1:A:557:ARG:HH11	1:A:557:ARG:CG	2.25	0.49
2:B:252:TRP:CD1	2:B:252:TRP:N	2.79	0.49
1:A:167:ILE:HD13	1:A:212:TRP:HB3	1.94	0.49
1:A:284:ARG:C	1:A:286:THR:H	2.14	0.49
2:B:244:ILE:HG23	2:B:263:LYS:HE2	1.95	0.49
2:B:341:ILE:HD11	2:B:375:ILE:HG23	1.94	0.49
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.93	0.49
1:A:218:ASP:OD1	1:A:221:HIS:ND1	2.44	0.49
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.47	0.49
2:B:344:GLU:HB2	2:B:347:LYS:CD	2.29	0.49
1:A:135:ILE:O	1:A:138:GLU:OE2	2.30	0.49
1:A:68:SER:OG	1:A:69:THR:N	2.46	0.49
2:B:13:LYS:HE3	2:B:85:GLN:CA	2.42	0.49
2:B:306:ASN:O	2:B:309:ILE:HG22	2.13	0.49
1:A:354:TYR:CZ	1:A:356:ARG:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:O	1:A:148:VAL:HG11	2.13	0.48
1:A:135:ILE:HD11	4:A:722:HOH:O	2.12	0.48
1:A:198:HIS:CE1	1:A:202:ILE:CD1	2.97	0.48
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.13	0.48
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.94	0.48
2:B:395:LYS:HG3	2:B:399:GLU:OE1	2.13	0.48
2:B:268:SER:O	2:B:270:ILE:HG22	2.14	0.48
1:A:460:ASN:HB2	2:B:286:THR:O	2.13	0.48
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.95	0.48
2:B:56:TYR:O	2:B:57:ASN:HB2	2.13	0.48
2:B:66:LYS:HA	2:B:407:GLN:NE2	2.28	0.48
2:B:271:TYR:HB3	2:B:274:ILE:HD11	1.95	0.48
1:A:0:SER:O	1:A:2:ILE:HD13	2.14	0.48
1:A:511:ASP:OD2	1:A:512:GLN:HG2	2.14	0.48
2:B:273:GLY:O	2:B:275:LYS:NZ	2.29	0.48
1:A:417:VAL:HG13	1:A:419:THR:HG23	1.96	0.47
1:A:89:GLU:O	1:A:90:VAL:O	2.32	0.47
2:B:166:LYS:HE3	4:B:531:HOH:O	2.13	0.47
2:B:105:SER:HB2	4:B:455:HOH:O	2.14	0.47
1:A:233:GLU:OE2	1:A:235:HIS:HE1	1.96	0.47
1:A:492:GLU:HA	1:A:530:LYS:O	2.14	0.47
1:A:432:GLU:OE1	1:A:433:PRO:HD2	2.15	0.47
2:B:125:ARG:HG2	2:B:146:TYR:O	2.15	0.47
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.49	0.47
1:A:21:VAL:HG22	1:A:59:PRO:HD3	1.97	0.47
1:A:63:ILE:HG23	1:A:74:LEU:HD11	1.95	0.47
1:A:100:LEU:O	1:A:318:TYR:HB3	2.13	0.47
1:A:542:ILE:O	1:A:546:GLU:HG3	2.13	0.47
1:A:424:LYS:HE2	1:A:426:TRP:CZ2	2.50	0.47
1:A:459:THR:O	2:B:286:THR:OG1	2.30	0.47
1:A:3:SER:HA	1:A:4:PRO:HD2	1.68	0.47
1:A:179:VAL:O	1:A:189:VAL:HA	2.15	0.47
1:A:63:ILE:HD12	1:A:72:ARG:HG3	1.96	0.46
1:A:296:THR:HG23	1:A:298:GLU:CD	2.36	0.46
1:A:101:LYS:HD3	1:A:321:PRO:CG	2.44	0.46
2:B:22:LYS:HB2	2:B:22:LYS:HE3	1.48	0.46
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.51	0.46
2:B:278:GLN:HA	2:B:281:LYS:HD2	1.98	0.46
2:B:337:TRP:HE1	2:B:367:GLN:NE2	2.13	0.46
2:B:388:LYS:HD3	2:B:413:GLU:HB3	1.97	0.46
2:B:65:LYS:HD3	2:B:72:ARG:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.51	0.46
1:A:465:LYS:HG3	1:A:466:VAL:N	2.31	0.46
1:A:194:GLU:N	1:A:194:GLU:CD	2.67	0.46
1:A:440:PHE:HZ	1:A:488:ASP:O	1.98	0.46
1:A:406:TRP:CH2	2:B:418:ASN:CA	2.86	0.46
1:A:457:TYR:C	1:A:457:TYR:CD1	2.89	0.46
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.30	0.46
1:A:198:HIS:CE1	1:A:202:ILE:HD12	2.51	0.46
2:B:65:LYS:HE2	2:B:65:LYS:HB2	1.52	0.46
1:A:356:ARG:NH2	1:A:358:ARG:CD	2.78	0.45
1:A:63:ILE:HG23	1:A:74:LEU:CD1	2.46	0.45
2:B:249:LYS:CG	2:B:250:ASP:N	2.79	0.45
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.80	0.45
2:B:175:ASN:N	2:B:176:PRO:HD3	2.31	0.45
1:A:208:HIS:O	1:A:212:TRP:HD1	1.99	0.45
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.51	0.45
1:A:181:TYR:HD2	3:A:601:R8E:CL29	2.37	0.45
2:B:244:ILE:HG23	2:B:263:LYS:CE	2.46	0.45
2:B:276:VAL:HG13	2:B:276:VAL:O	2.16	0.45
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.64	0.45
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.47	0.45
2:B:208:HIS:O	2:B:212:TRP:CE3	2.69	0.45
2:B:308:GLU:HA	2:B:311:LYS:HD3	1.98	0.45
2:B:6:GLU:N	4:B:572:HOH:O	2.49	0.45
2:B:6:GLU:O	2:B:6:GLU:HG2	2.16	0.45
1:A:164:MET:HG3	1:A:164:MET:O	2.17	0.45
1:A:379:SER:OG	1:A:387:PRO:HG3	2.17	0.45
1:A:410:TRP:CE3	2:B:363:ASN:CB	3.00	0.45
2:B:268:SER:C	2:B:269:GLN:HG3	2.36	0.45
2:B:278:GLN:NE2	2:B:278:GLN:HA	2.30	0.45
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.52	0.45
1:A:405:TYR:O	2:B:331:LYS:HE2	2.17	0.45
4:A:726:HOH:O	2:B:140:PRO:HD3	2.17	0.45
2:B:274:ILE:HG23	2:B:306:ASN:ND2	2.32	0.45
2:B:354:TYR:OH	2:B:370:GLU:OE2	2.34	0.45
1:A:188:TYR:HB3	3:A:601:R8E:C4	2.47	0.45
2:B:422:LEU:CD1	2:B:426:TRP:CH2	3.00	0.45
1:A:546:GLU:HG3	1:A:546:GLU:H	1.36	0.45
1:A:63:ILE:HG12	1:A:74:LEU:HG	1.99	0.45
2:B:292:VAL:O	2:B:293:ILE:HG22	2.17	0.45
2:B:298:GLU:N	2:B:298:GLU:CD	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:O	1:A:220:LYS:HG2	2.18	0.44
1:A:230:MET:HE2	1:A:230:MET:CA	2.44	0.44
1:A:346:PHE:CD1	1:A:346:PHE:N	2.83	0.44
1:A:403:THR:CG2	1:A:404:GLU:N	2.80	0.44
1:A:426:TRP:N	1:A:426:TRP:CD1	2.84	0.44
1:A:440:PHE:N	1:A:440:PHE:CD1	2.85	0.44
2:B:297:GLU:O	2:B:301:LEU:HD23	2.17	0.44
2:B:428:GLN:O	2:B:428:GLN:NE2	2.32	0.44
2:B:282:LEU:CD1	2:B:295:LEU:HD11	2.47	0.44
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.69	0.44
1:A:175:ASN:HD22	1:A:178:ILE:HD11	1.83	0.44
1:A:424:LYS:CE	1:A:426:TRP:CZ3	3.00	0.44
2:B:253:THR:CG2	2:B:254:VAL:N	2.79	0.44
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.95	0.44
1:A:110:ASP:O	1:A:217:PRO:HD3	2.17	0.44
1:A:20:LYS:HG2	1:A:55:PRO:O	2.17	0.44
1:A:549:ASP:O	1:A:553:SER:HB2	2.16	0.44
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.48	0.44
2:B:422:LEU:CB	2:B:426:TRP:CH2	2.98	0.44
1:A:326:ILE:N	1:A:326:ILE:HD13	2.33	0.44
1:A:555:GLY:C	1:A:556:ILE:HD13	2.38	0.44
1:A:228:LEU:N	1:A:228:LEU:HD12	2.32	0.44
1:A:230:MET:HB2	1:A:230:MET:HE3	1.82	0.44
1:A:337:TRP:NE1	1:A:367:GLN:OE1	2.43	0.44
1:A:175:ASN:ND2	1:A:178:ILE:CD1	2.80	0.44
1:A:60:VAL:CG1	1:A:75:VAL:HG22	2.42	0.44
1:A:13:LYS:HE3	1:A:84:THR:O	2.18	0.44
1:A:293:ILE:HA	1:A:294:PRO:HD3	1.86	0.44
1:A:369:THR:HG21	1:A:398:TRP:CZ3	2.53	0.44
1:A:61:PHE:HB2	4:A:623:HOH:O	2.18	0.44
1:A:240:THR:HG23	1:A:241:VAL:O	2.18	0.43
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.18	0.43
1:A:161:GLN:NE2	4:A:693:HOH:O	2.50	0.43
1:A:320:ASP:OD1	1:A:322:SER:OG	2.35	0.43
1:A:409:THR:OG1	1:A:410:TRP:N	2.51	0.43
1:A:443:ASP:HB2	1:A:548:VAL:HB	2.00	0.43
2:B:12:LEU:HD22	2:B:127:TYR:CZ	2.53	0.43
2:B:184:MET:HB3	2:B:185:ASP:H	1.62	0.43
1:A:219:LYS:O	1:A:220:LYS:CB	2.65	0.43
1:A:457:TYR:O	1:A:457:TYR:CD1	2.71	0.43
1:A:472:THR:HB	1:A:473:THR:H	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:CB	1:A:548:VAL:HB	2.48	0.43
2:B:257:ILE:HG23	2:B:279:LEU:HD12	2.00	0.43
1:A:468:THR:C	1:A:469:LEU:HG	2.38	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.87	0.43
1:A:434:ILE:HG21	1:A:492:GLU:OE1	2.19	0.43
2:B:249:LYS:HB3	2:B:249:LYS:HE2	1.44	0.43
2:B:326:ILE:O	2:B:341:ILE:HA	2.18	0.43
1:A:3:SER:OG	1:A:212:TRP:O	2.25	0.43
1:A:424:LYS:CE	1:A:426:TRP:CE3	3.01	0.43
1:A:82:LYS:HG3	1:A:82:LYS:O	2.17	0.43
2:B:260:LEU:HD23	2:B:260:LEU:HA	1.70	0.43
2:B:266:TRP:O	2:B:268:SER:O	2.36	0.43
1:A:433:PRO:HB2	2:B:290:THR:CG2	2.49	0.43
1:A:63:ILE:HD13	1:A:74:LEU:HD21	1.94	0.43
1:A:404:GLU:HG3	1:A:404:GLU:H	1.63	0.43
1:A:380:ILE:HD13	2:B:27:THR:HG22	2.00	0.43
2:B:345:PRO:O	2:B:346:PHE:HB2	2.19	0.43
1:A:365:VAL:O	1:A:369:THR:CG2	2.67	0.42
1:A:479:LEU:CD1	1:A:502:ALA:HB2	2.48	0.42
1:A:557:ARG:NH1	1:A:557:ARG:CG	2.81	0.42
2:B:271:TYR:CB	2:B:274:ILE:HD11	2.48	0.42
2:B:80:LEU:O	2:B:80:LEU:HD22	2.19	0.42
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.52	0.42
1:A:64:LYS:HB3	1:A:65:LYS:H	1.55	0.42
1:A:433:PRO:HB2	2:B:290:THR:HG23	2.02	0.42
2:B:65:LYS:HB3	2:B:66:LYS:H	1.64	0.42
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.54	0.42
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.78	0.42
1:A:206:ARG:NH1	1:A:218:ASP:CB	2.82	0.42
1:A:466:VAL:HG22	1:A:551:LEU:HD23	1.99	0.42
2:B:253:THR:CG2	2:B:255:ASN:H	2.32	0.42
1:A:285:GLY:O	1:A:286:THR:O	2.37	0.42
1:A:424:LYS:CE	1:A:426:TRP:CD2	3.02	0.42
2:B:332:GLN:HA	2:B:424:LYS:HE3	2.02	0.42
1:A:230:MET:HA	1:A:230:MET:CE	2.48	0.42
1:A:91:GLN:NE2	1:A:92:LEU:N	2.62	0.42
2:B:332:GLN:HB3	2:B:428:GLN:OE1	2.20	0.42
2:B:103:LYS:HG3	2:B:190:GLY:C	2.40	0.42
2:B:72:ARG:HH22	2:B:409:THR:HG21	1.81	0.42
1:A:553:SER:OG	1:A:557:ARG:NH1	2.52	0.42
2:B:253:THR:HG22	2:B:255:ASN:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLY:O	2:B:27:THR:HB	2.19	0.42
1:A:88:TRP:HB2	2:B:54:ASN:O	2.20	0.42
1:A:424:LYS:CE	1:A:426:TRP:CE2	2.99	0.42
1:A:434:ILE:HD13	1:A:530:LYS:HB2	2.02	0.42
2:B:395:LYS:O	2:B:399:GLU:HB2	2.19	0.42
1:A:547:GLN:HA	1:A:550:LYS:CG	2.49	0.42
2:B:236:PRO:O	2:B:238:LYS:N	2.53	0.42
2:B:13:LYS:HB3	2:B:16:MET:CE	2.49	0.42
2:B:105:SER:O	2:B:190:GLY:HA2	2.19	0.42
2:B:57:ASN:OD1	2:B:131:THR:OG1	2.30	0.42
1:A:424:LYS:CE	1:A:426:TRP:CH2	3.00	0.41
2:B:319:TYR:O	2:B:321:PRO:HD3	2.20	0.41
2:B:82:LYS:HE3	2:B:413:GLU:OE2	2.20	0.41
1:A:388:LYS:HE3	1:A:388:LYS:HB2	1.82	0.41
1:A:65:LYS:HE2	1:A:72:ARG:HD2	2.00	0.41
2:B:174:GLN:C	2:B:176:PRO:HD3	2.40	0.41
1:A:523:GLU:HG2	1:A:524:GLN:H	1.81	0.41
1:A:424:LYS:CE	1:A:426:TRP:CZ2	3.04	0.41
1:A:460:ASN:HD22	2:B:288:ALA:H	1.67	0.41
2:B:244:ILE:CG2	2:B:263:LYS:HE2	2.51	0.41
2:B:296:THR:OG1	2:B:298:GLU:OE1	2.31	0.41
1:A:163:SER:O	1:A:167:ILE:HG13	2.20	0.41
1:A:284:ARG:NH1	1:A:285:GLY:HA3	2.36	0.41
1:A:410:TRP:O	1:A:410:TRP:CG	2.72	0.41
1:A:489:SER:CB	1:A:493:VAL:CG1	2.99	0.41
1:A:104:LYS:HG3	1:A:192:ASP:OD2	2.20	0.41
1:A:550:LYS:HG3	1:A:550:LYS:H	1.56	0.41
1:A:3:SER:OG	1:A:5:ILE:HD12	2.20	0.41
1:A:65:LYS:HZ1	1:A:72:ARG:NH1	2.18	0.41
2:B:88:TRP:CZ3	2:B:89:GLU:HB2	2.56	0.41
2:B:275:LYS:HE2	2:B:305:GLU:OE1	2.20	0.41
2:B:422:LEU:HB3	2:B:426:TRP:CE2	2.55	0.41
2:B:90:VAL:O	2:B:90:VAL:HG23	2.20	0.41
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.51	0.41
1:A:326:ILE:CD1	1:A:388:LYS:CE	2.98	0.41
2:B:87:PHE:CZ	2:B:92:LEU:CD1	2.99	0.41
1:A:206:ARG:NH1	1:A:218:ASP:CA	2.78	0.41
1:A:516:GLU:HA	1:A:516:GLU:OE1	2.20	0.41
2:B:253:THR:HG23	2:B:254:VAL:N	2.36	0.41
1:A:102:LYS:NZ	1:A:237:ASP:HB3	2.36	0.40
1:A:249:LYS:HE2	1:A:249:LYS:HB2	1.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG23	1:A:287:LYS:O	2.20	0.40
1:A:21:VAL:HG22	1:A:59:PRO:HG3	2.01	0.40
2:B:236:PRO:C	2:B:238:LYS:H	2.24	0.40
2:B:271:TYR:CD1	2:B:310:LEU:CD1	3.00	0.40
1:A:460:ASN:HD21	2:B:288:ALA:HB2	1.86	0.40
1:A:237:ASP:N	1:A:237:ASP:OD2	2.54	0.40
2:B:193:LEU:HB3	2:B:197:GLN:HB2	2.03	0.40
1:A:139:THR:HA	1:A:140:PRO:HD2	1.86	0.40
2:B:85:GLN:O	2:B:89:GLU:HB3	2.21	0.40
1:A:3:SER:CB	1:A:5:ILE:CD1	2.99	0.40
1:A:541:GLY:CA	1:A:546:GLU:HG2	2.51	0.40
2:B:13:LYS:HB3	2:B:14:PRO:HD2	2.03	0.40
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.51	0.40
2:B:245:VAL:O	2:B:245:VAL:HG12	2.20	0.40
2:B:274:ILE:C	2:B:275:LYS:HD3	2.42	0.40
1:A:233:GLU:HG2	1:A:235:HIS:HE1	1.81	0.40
1:A:451:LYS:O	1:A:470:THR:O	2.40	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	556/563 (99%)	486 (87%)	51 (9%)	19 (3%)	3	5
2	B	398/443 (90%)	369 (93%)	21 (5%)	8 (2%)	7	14
All	All	954/1006 (95%)	855 (90%)	72 (8%)	27 (3%)	5	7

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	195	ILE
1	A	286	THR
1	A	334	GLN
1	A	356	ARG
1	A	541	GLY
1	A	196	GLY
1	A	64	LYS
1	A	137	ASN
1	A	139	THR
1	A	220	LYS
1	A	312	GLU
1	A	410	TRP
1	A	491	LEU
2	B	237	ASP
2	B	288	ALA
2	B	423	VAL
1	A	135	ILE
1	A	250	ASP
2	B	269	GLN
2	B	311	LYS
2	B	85	GLN
1	A	345	PRO
2	B	272	PRO
2	B	276	VAL
1	A	243	PRO

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%)	384 (77%)	114 (23%)	1	1
2	B	368/403 (91%)	289 (78%)	79 (22%)	1	1
All	All	866/906 (96%)	673 (78%)	193 (22%)	1	1

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	21	VAL
1	A	22	LYS
1	A	26	LEU
1	A	36	GLU
1	A	46	LYS
1	A	49	LYS
1	A	64	LYS
1	A	65	LYS
1	A	66	LYS
1	A	67	ASP
1	A	69	THR
1	A	70	LYS
1	A	72	ARG
1	A	82	LYS
1	A	89	GLU
1	A	91	GLN
1	A	94	ILE
1	A	103	LYS
1	A	105	SER
1	A	106	VAL
1	A	107	THR
1	A	118	VAL
1	A	122	GLU
1	A	126	LYS
1	A	137	ASN
1	A	138	GLU
1	A	139	THR
1	A	161	GLN
1	A	162	SER
1	A	166	LYS
1	A	173	LYS
1	A	179	VAL
1	A	195	ILE
1	A	197	GLN
1	A	200	THR
1	A	202	ILE
1	A	205	LEU
1	A	206	ARG
1	A	215	THR

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Mol	Chain	Res	Type
1	A	218	ASP
1	A	219	LYS
1	A	220	LYS
1	A	230	MET
1	A	244	ILE
1	A	248	GLU
1	A	249	LYS
1	A	260	LEU
1	A	269	GLN
1	A	275	LYS
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
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	298	GLU
1	A	303	LEU
1	A	311	LYS
1	A	312	GLU
1	A	330	GLN
1	A	334	GLN
1	A	341	ILE
1	A	344	GLU
1	A	350	LYS
1	A	356	ARG
1	A	357	MET
1	A	358	ARG
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	395	LYS
1	A	399	GLU
1	A	402	TRP
1	A	403	THR
1	A	404	GLU

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	409	THR
1	A	422	LEU
1	A	424	LYS
1	A	431	LYS
1	A	435	VAL
1	A	440	PHE
1	A	452	LEU
1	A	454	LYS
1	A	459	THR
1	A	461	ARG
1	A	479	LEU
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	524	GLN
1	A	527	LYS
1	A	530	LYS
1	A	542	ILE
1	A	546	GLU
1	A	547	GLN
1	A	548	VAL
1	A	549	ASP
1	A	550	LYS
1	A	553	SER
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	22	LYS
2	B	24	TRP
2	B	26	LEU
2	B	40	GLU
2	B	48	SER
2	B	58	THR
2	B	64	LYS
2	B	65	LYS

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	68	SER
2	B	69	THR
2	B	70	LYS
2	B	72	ARG
2	B	73	LYS
2	B	80	LEU
2	B	83	ARG
2	B	111	VAL
2	B	120	LEU
2	B	138	GLU
2	B	162	SER
2	B	166	LYS
2	B	173	LYS
2	B	175	ASN
2	B	182	GLN
2	B	184	MET
2	B	187	LEU
2	B	195	ILE
2	B	203	GLU
2	B	205	LEU
2	B	209	LEU
2	B	214	LEU
2	B	232	TYR
2	B	237	ASP
2	B	248	GLU
2	B	249	LYS
2	B	251	SER
2	B	253	THR
2	B	255	ASN
2	B	256	ASP
2	B	260	LEU
2	B	274	ILE
2	B	275	LYS
2	B	276	VAL
2	B	277	ARG
2	B	278	GLN
2	B	279	LEU
2	B	281	LYS
2	B	282	LEU
2	B	286	THR
2	B	287	LYS

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Mol	Chain	Res	Type
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	308	GLU
2	B	309	ILE
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	349	LEU
2	B	362	THR
2	B	377	THR
2	B	399	GLU
2	B	400	THR
2	B	403	THR
2	B	405	TYR
2	B	407	GLN
2	B	413	GLU
2	B	425	LEU
2	B	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) 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	175	ASN
1	A	198	HIS
1	A	222	GLN
1	A	235	HIS
1	A	242	GLN
1	A	258	GLN
1	A	278	GLN
1	A	315	HIS
1	A	330	GLN
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	428	GLN
1	A	460	ASN
1	A	480	GLN
1	A	507	GLN
1	A	509	GLN
1	A	512	GLN
1	A	519	ASN
1	A	520	GLN
1	A	524	GLN
1	A	547	GLN
2	B	96	HIS
2	B	137	ASN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	367	GLN
2	B	373	GLN
2	B	394	GLN
2	B	407	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 carbohydrates 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	2.31	9 (29%)	36,45,45	2.23	12 (33%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8E	C2-C26	-7.02	1.29	1.44
3	A	601	R8E	C8-C13	-4.71	1.31	1.39
3	A	601	R8E	C23-N25	4.49	1.48	1.35
3	A	601	R8E	C5-C6	2.85	1.43	1.38
3	A	601	R8E	C11-C10	-2.49	1.33	1.38
3	A	601	R8E	C18-N19	-2.39	1.30	1.34
3	A	601	R8E	C9-C10	-2.36	1.34	1.38
3	A	601	R8E	C21-C22	2.36	1.41	1.36
3	A	601	R8E	C6-CL28	2.05	1.79	1.74

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	R8E	C8-C13-CL29	-6.04	112.33	119.43
3	A	601	R8E	C11-C12-C13	-4.64	113.29	120.00
3	A	601	R8E	C1-C6-CL28	-4.49	113.54	119.15
3	A	601	R8E	C12-C11-C10	4.07	124.71	119.73
3	A	601	R8E	C15-O14-C10	3.34	125.89	117.65
3	A	601	R8E	O7-C8-C13	-3.32	111.73	119.58
3	A	601	R8E	C5-C6-CL28	3.05	122.96	119.15
3	A	601	R8E	C12-C13-CL29	2.85	124.12	118.41
3	A	601	R8E	N25-C23-N24	-2.42	116.25	118.26
3	A	601	R8E	C21-C22-C23	-2.33	117.66	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	R8E	C8-C9-C10	-2.16	115.25	119.05
3	A	601	R8E	C9-C8-C13	2.12	122.19	119.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

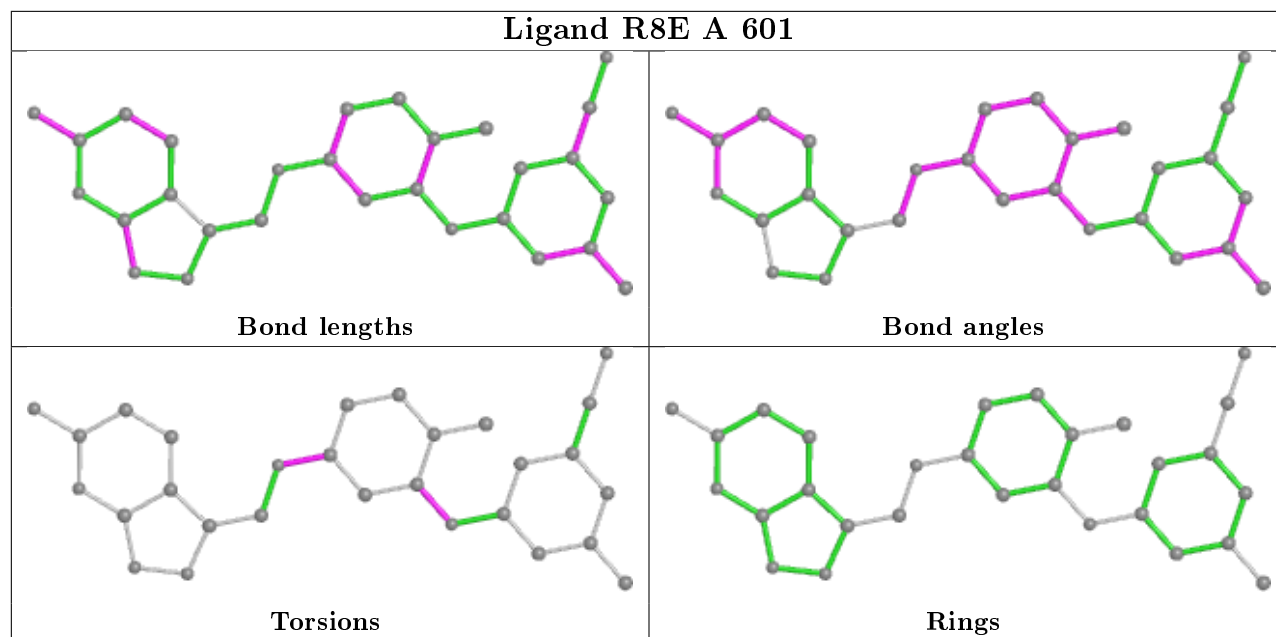
Mol	Chain	Res	Type	Atoms
3	A	601	R8E	C9-C10-O14-C15
3	A	601	R8E	C11-C10-O14-C15
3	A	601	R8E	C13-C8-O7-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	R8E	2	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	558/563 (99%)	-0.09	18 (3%) 47 40	28, 55, 93, 125	0
2	B	404/443 (91%)	-0.15	10 (2%) 57 51	27, 50, 108, 126	0
All	All	962/1006 (95%)	-0.11	28 (2%) 51 45	27, 54, 102, 126	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	3.9
1	A	66	LYS	3.7
1	A	67	ASP	3.7
2	B	362	THR	3.5
1	A	402	TRP	3.2
1	A	286	THR	3.2
1	A	220	LYS	3.0
2	B	67	ASP	3.0
1	A	65	LYS	2.8
1	A	553	SER	2.8
1	A	221	HIS	2.8
1	A	543	GLY	2.7
2	B	270	ILE	2.7
1	A	136	ASN	2.5
2	B	266	TRP	2.3
2	B	271	TYR	2.3
2	B	309	ILE	2.3
1	A	359	GLY	2.3
2	B	248	GLU	2.2
1	A	199	ARG	2.2
1	A	195	ILE	2.2
1	A	202	ILE	2.1
1	A	546	GLU	2.1
2	B	308	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	138	GLU	2.1
2	B	90	VAL	2.1
1	A	137	ASN	2.0
2	B	301	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

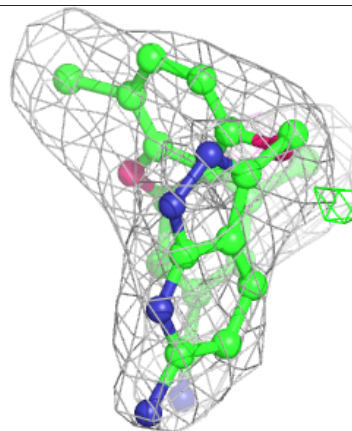
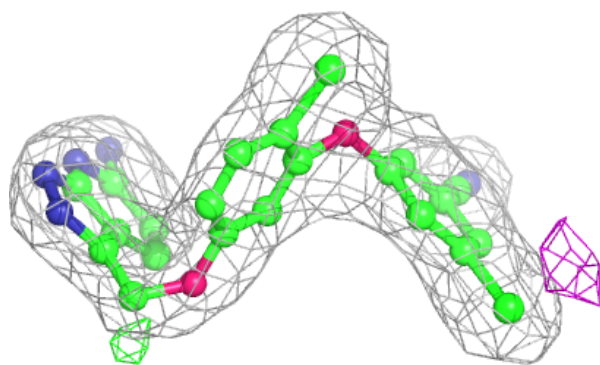
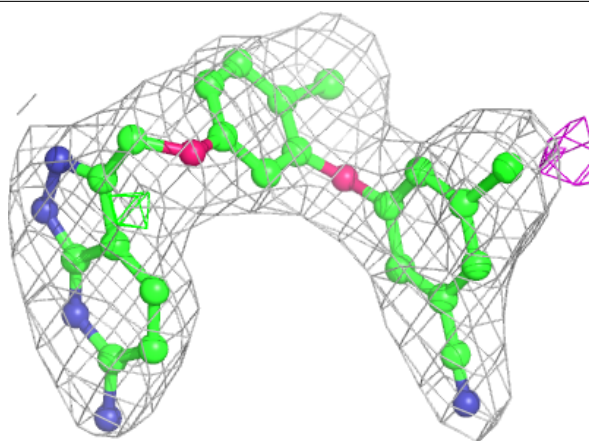
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	R8E	A	601	29/29	0.98	0.14	43,50,59,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around R8E A 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.