



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:04 PM UTC

PDB ID : 3DRP / pdb_00003drp
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

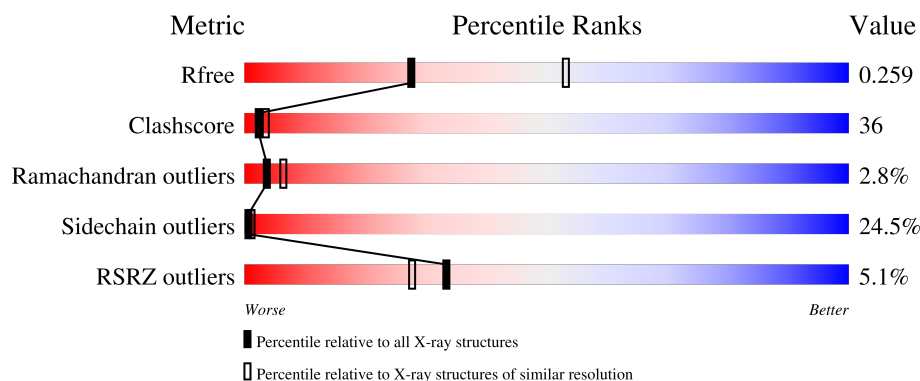
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	563	4% 41% 38% 16% ••
2	B	443	6% 41% 33% 15% • 9%

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

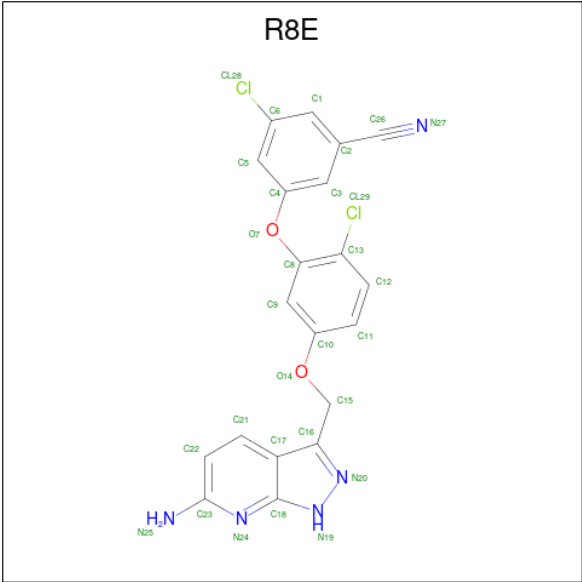
- Molecule 2 is a protein called p51 RT.

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 (CCD ID: R8E) (formula: C₂₀H₁₃Cl₂N₅O₂).



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

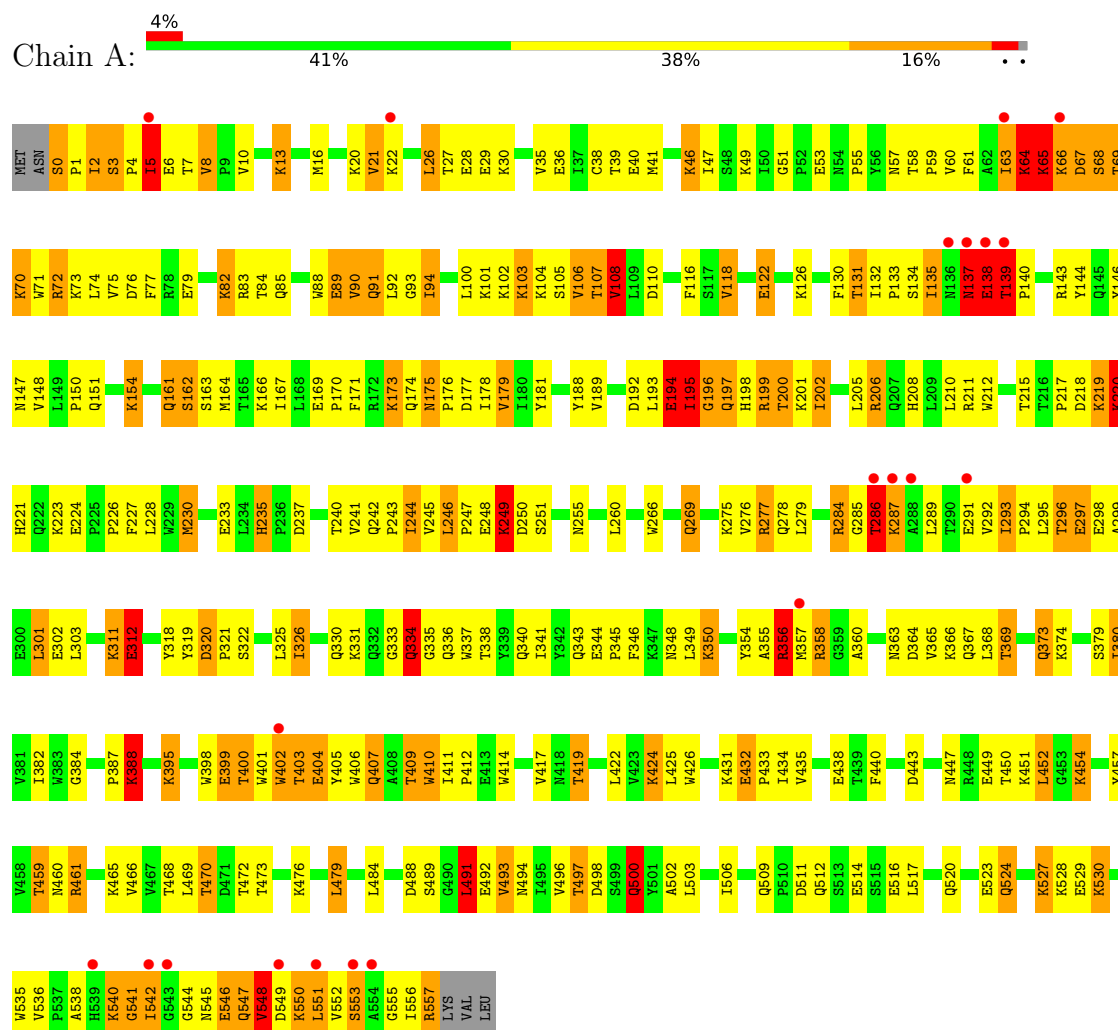
- Molecule 4 is water.

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

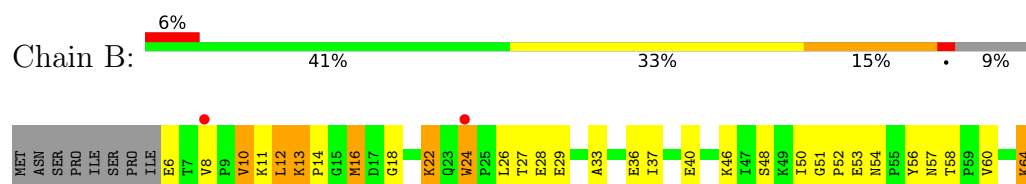
3 Residue-property plots

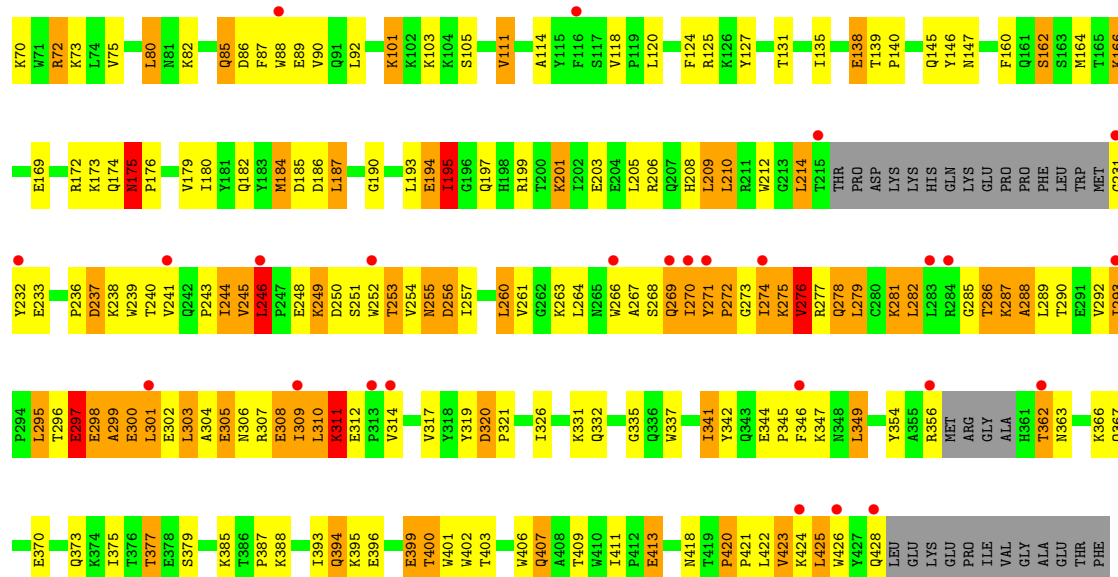
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	118.86Å 155.03Å 155.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.49 – 2.60 94.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (94.49-2.60) 99.8 (94.33-2.60)	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 , 80.8	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	0.96	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

5.1 Standard geometry

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	0.82	1/4659 (0.0%)	1.31	63/6330 (1.0%)
2	B	0.80	0/3438	1.32	35/4671 (0.7%)
All	All	0.81	1/8097 (0.0%)	1.31	98/11001 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	VAL	CA-CB	5.48	1.60	1.54

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	ASP	CA-C-N	17.23	137.13	119.56
2	B	320	ASP	C-N-CA	17.23	137.13	119.56
1	A	320	ASP	CA-C-N	14.15	134.00	119.56
1	A	320	ASP	C-N-CA	14.15	134.00	119.56
1	A	224	GLU	CA-C-N	13.36	129.41	119.66
1	A	224	GLU	C-N-CA	13.36	129.41	119.66
1	A	118	VAL	CA-C-N	11.61	131.73	119.89
1	A	118	VAL	C-N-CA	11.61	131.73	119.89
2	B	51	GLY	CA-C-N	10.92	133.50	119.84
2	B	51	GLY	C-N-CA	10.92	133.50	119.84
2	B	139	THR	CA-C-N	-10.60	108.91	120.14
2	B	139	THR	C-N-CA	-10.60	108.91	120.14
2	B	175	ASN	CA-C-N	10.42	132.87	119.84
2	B	175	ASN	C-N-CA	10.42	132.87	119.84
1	A	175	ASN	CA-C-N	10.23	130.99	119.32
1	A	175	ASN	C-N-CA	10.23	130.99	119.32
2	B	270	ILE	N-CA-C	-9.85	103.34	111.81
1	A	312	GLU	CA-C-N	-9.76	107.64	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	C-N-CA	-9.76	107.64	119.84
2	B	233	GLU	N-CA-C	9.66	124.47	108.73
1	A	509	GLN	CA-C-N	-8.73	111.03	119.85
1	A	509	GLN	C-N-CA	-8.73	111.03	119.85
2	B	401	TRP	N-CA-C	8.29	123.52	113.41
1	A	432	GLU	CA-C-N	8.23	128.74	119.93
1	A	432	GLU	C-N-CA	8.23	128.74	119.93
1	A	461	ARG	N-CA-C	-7.92	103.69	112.72
1	A	536	VAL	CA-C-N	-7.78	112.33	120.03
1	A	536	VAL	C-N-CA	-7.78	112.33	120.03
2	B	18	GLY	CA-C-N	7.49	127.76	119.90
2	B	18	GLY	C-N-CA	7.49	127.76	119.90
2	B	271	TYR	CA-C-N	7.49	129.20	119.84
2	B	271	TYR	C-N-CA	7.49	129.20	119.84
1	A	3	SER	CA-C-N	7.47	127.11	119.56
1	A	3	SER	C-N-CA	7.47	127.11	119.56
1	A	382	ILE	N-CA-C	7.20	118.00	110.72
1	A	419	THR	CA-C-N	-7.19	112.97	120.38
1	A	419	THR	C-N-CA	-7.19	112.97	120.38
2	B	244	ILE	N-CA-C	-7.08	99.81	109.37
2	B	402	TRP	N-CA-C	7.01	119.81	111.33
1	A	68	SER	N-CA-C	6.85	119.37	110.53
1	A	319	TYR	N-CA-C	6.81	120.33	109.24
2	B	186	ASP	N-CA-C	6.64	120.50	109.95
1	A	94	ILE	CA-C-N	-6.61	113.17	119.85
1	A	94	ILE	C-N-CA	-6.61	113.17	119.85
2	B	299	ALA	N-CA-C	-6.55	104.14	111.28
2	B	118	VAL	CA-C-N	-6.46	113.30	120.14
2	B	118	VAL	C-N-CA	-6.46	113.30	120.14
1	A	13	LYS	CA-C-N	6.41	127.85	119.84
1	A	13	LYS	C-N-CA	6.41	127.85	119.84
2	B	297	GLU	N-CA-C	6.36	120.30	112.54
1	A	470	THR	N-CA-C	6.34	120.90	111.96
2	B	147	ASN	N-CA-C	-6.34	105.85	113.97
1	A	343	GLN	N-CA-C	-6.33	106.19	114.04
1	A	235	HIS	CA-C-N	-6.16	113.39	120.04
1	A	235	HIS	C-N-CA	-6.16	113.39	120.04
2	B	195	ILE	N-CA-C	6.14	119.64	111.17
2	B	420	PRO	CA-C-N	6.07	127.43	119.84
2	B	420	PRO	C-N-CA	6.07	127.43	119.84
1	A	246	LEU	CA-C-N	6.05	126.40	119.93
1	A	246	LEU	C-N-CA	6.05	126.40	119.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	LEU	N-CA-C	5.97	123.52	110.80
1	A	154	LYS	N-CA-C	5.95	118.53	111.33
1	A	147	ASN	N-CA-C	-5.92	106.69	114.04
1	A	349	LEU	N-CA-C	-5.92	104.40	111.69
1	A	175	ASN	C-N-CD	-5.92	100.73	125.00
1	A	348	ASN	N-CA-C	5.86	118.85	110.24
1	A	0	SER	CA-C-N	-5.80	113.79	119.76
1	A	0	SER	C-N-CA	-5.80	113.79	119.76
1	A	350	LYS	N-CA-C	5.75	116.14	108.38
2	B	240	THR	N-CA-C	5.72	117.92	109.69
1	A	132	ILE	N-CA-C	-5.72	102.36	107.56
2	B	411	ILE	CA-C-N	-5.72	114.86	120.52
2	B	411	ILE	C-N-CA	-5.72	114.86	120.52
2	B	285	GLY	N-CA-C	-5.71	103.12	112.83
1	A	249	LYS	N-CA-C	5.70	118.50	108.75
1	A	139	THR	CA-C-N	5.60	125.53	119.76
1	A	139	THR	C-N-CA	5.60	125.53	119.76
1	A	131	THR	CA-C-N	-5.59	118.80	122.60
1	A	131	THR	C-N-CA	-5.59	118.80	122.60
1	A	470	THR	CA-C-N	-5.59	114.21	123.37
1	A	470	THR	C-N-CA	-5.59	114.21	123.37
2	B	65	LYS	CB-CA-C	-5.51	108.62	115.89
1	A	194	GLU	N-CA-C	-5.48	100.75	109.96
1	A	548	VAL	N-CA-C	-5.45	104.14	111.44
1	A	366	LYS	N-CA-C	-5.42	105.02	111.69
1	A	199	ARG	N-CA-C	-5.41	105.78	112.38
1	A	8	VAL	CA-C-N	-5.33	114.27	119.76
1	A	8	VAL	C-N-CA	-5.33	114.27	119.76
1	A	108	VAL	CB-CA-C	5.32	118.27	110.98
1	A	540	LYS	N-CA-C	-5.28	98.64	107.99
2	B	194	GLU	N-CA-C	-5.28	103.17	110.35
1	A	388	LYS	N-CA-C	-5.28	100.64	109.24
2	B	246	LEU	CA-C-N	-5.25	114.83	120.03
2	B	246	LEU	C-N-CA	-5.25	114.83	120.03
1	A	65	LYS	N-CA-C	5.13	117.18	109.23
1	A	5	ILE	N-CA-C	5.11	119.96	109.34
1	A	500	GLN	N-CA-C	-5.09	105.92	111.82
2	B	210	LEU	N-CA-C	5.08	118.58	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4542	0	4595	366	0
2	B	3344	0	3369	228	0
3	A	29	0	13	2	0
4	A	232	0	0	13	0
4	B	193	0	0	8	0
All	All	8340	0	7977	565	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 36.

All (565) 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:HG3	1:A:143:ARG:HH11	1.30	0.95
1:A:175:ASN:HD21	1:A:201:LYS:HZ1	0.94	0.94
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:ND2	1:A:201:LYS:HZ1	1.67	0.91
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:13:LYS:CB	2:B:16:MET:HE3	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:173:LYS:HA	1:A:173:LYS:HZ2	1.37	0.85
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:HA	1:A:173:LYS:NZ	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: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
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.25	0.82
2:B:298:GLU:CD	2:B:298:GLU:H	1.86	0.82
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
2:B:13:LYS:HB3	2:B:16:MET:HE3	1.63	0.79
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:108:VAL:HG22	1:A:223:LYS:HD2	1.69	0.73
1:A:360:ALA:HA	1:A:514:GLU:OE1	1.89	0.73
1:A:230:MET:HA	1:A:230:MET:HE2	1.70	0.72
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:102:LYS:O	1:A:103:LYS:NZ	2.26	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:194:GLU:CD	1:A:194:GLU:H	2.00	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:LYS:HB2	2:B:16:MET:HE3	1.76	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
2:B:52:PRO:HD2	2:B:53:GLU:OE1	1.94	0.68
1:A:65:LYS:CE	1:A:72:ARG:HH11	2.07	0.67
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
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
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:91:GLN:HG3	1:A:93:GLY:O	1.95	0.65
1:A:181:TYR:HE1	2:B:138:GLU:HG3	1.61	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:79:GLU:HG3	1:A:83:ARG:HE	1.62	0.65
1:A:326:ILE:CD1	1:A:388:LYS:HE3	2.26	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
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:63:ILE:HG13	1:A:72:ARG:HG3	1.79	0.64
1:A:424:LYS:HE3	1:A:426:TRP:CD2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLN:HE21	1:A:524:GLN:CA	2.09	0.64
1:A:13:LYS:O	1:A:16:MET:HB2	1.97	0.64
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.79	0.63
1:A:555:GLY:O	1:A:556:ILE:HD13	1.97	0.63
2:B:66:LYS:HG2	2:B:407:GLN:HE21	1.63	0.63
1:A:1:PRO:C	1:A:2:ILE:HD13	2.22	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:268:SER:C	2:B:270:ILE:H	2.07	0.62
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
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:65:LYS:HG2	1:A:68:SER:HB3	1.82	0.62
1:A:500:GLN:OE1	2:B:422:LEU:HG	2.00	0.62
1:A:497:THR:O	1:A:535:TRP:HA	2.00	0.62
2:B:273:GLY:O	2:B:275:LYS:NZ	2.29	0.62
2:B:344:GLU:CB	2:B:347:LYS:HD3	2.24	0.62
1:A:298:GLU:H	1:A:298:GLU:CD	2.07	0.62
1:A:230:MET:HE2	1:A:230:MET:CA	2.30	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:HD12	2:B:210:LEU:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:244:ILE:HD12	1:A:244:ILE:H	1.65	0.58
1:A:356:ARG:NH2	1:A:358:ARG:HD2	2.19	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:362:THR:CG2	2:B:366:LYS:HG2	2.30	0.57
1:A:26:LEU:HD22	1:A:133:PRO:HG3	1.86	0.57
1:A:171:PHE:HA	1:A:174:GLN:NE2	2.19	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
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:66:LYS:O	1:A:67:ASP:HB2	2.05	0.57
1:A:171:PHE:O	1:A:175:ASN:HB2	2.04	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
1:A:40:GLU:HA	1:A:40:GLU:OE1	2.02	0.56
1:A:277:ARG:HE	1:A:336:GLN:CD	2.13	0.56
2:B:296:THR:HB	2:B:298:GLU:OE2	2.06	0.56
1:A:3:SER:HB3	1:A:5:ILE:HD13	1.86	0.56
1:A:325:LEU:C	1:A:326:ILE:HD13	2.31	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
1:A:373:GLN:OE1	2:B:400:THR:HG21	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:ARG:HH12	1:A:218:ASP:CB	2.19	0.55
2:B:184:MET:HE1	4:B:451:HOH:O	2.06	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
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:406:TRP:CZ3	2:B:418:ASN:HA	2.39	0.54
1:A:500:GLN:CG	2:B:422:LEU:HG	2.38	0.54
1:A:2:ILE:HD13	1:A:2:ILE:N	2.23	0.54
2:B:209:LEU:CG	2:B:214:LEU:HD12	2.26	0.54
1:A:284:ARG:C	1:A:286:THR:H	2.14	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:102:LYS:HZ3	1:A:237:ASP:HB3	1.74	0.52
1:A:365:VAL:O	1:A:369:THR:HG23	2.09	0.52
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:CA	1:A:230:MET:CE	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:194:GLU:CD	1:A:194:GLU:N	2.67	0.50
1:A:312:GLU:OE2	1:A:312:GLU:O	2.30	0.50
2:B:208:HIS:O	2:B:212:TRP:HE3	1.93	0.50
1:A:457:TYR:CD1	1:A:457:TYR:C	2.89	0.50
1:A:277:ARG:HH12	1:A:278:GLN:HG2	1.74	0.50
1:A:296:THR:HG23	1:A:298:GLU:CD	2.36	0.50
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.93	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
2:B:292:VAL:HG12	2:B:293:ILE:N	2.26	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
2:B:268:SER:C	2:B:269:GLN:HG3	2.36	0.49
2:B:298:GLU:CD	2:B:298:GLU:N	2.64	0.49
1:A:122:GLU:HB2	4:A:622:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:60:VAL:HG23	2:B:75:VAL:HG22	1.93	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
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:68:SER:OG	1:A:69:THR:N	2.46	0.49
1:A:135:ILE:O	1:A:138:GLU:OE2	2.30	0.49
1:A:555:GLY:C	1:A:556:ILE:HD13	2.38	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
1:A:116:PHE:O	1:A:148:VAL:HG11	2.13	0.48
1:A:51:GLY:HA3	1:A:53:GLU:OE2	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
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
1:A:460:ASN:HB2	2:B:286:THR:O	2.13	0.48
1:A:468:THR:C	1:A:469:LEU:HG	2.38	0.48
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.95	0.48
2:B:66:LYS:HA	2:B:407:GLN:NE2	2.28	0.48
2:B:268:SER:O	2:B:270:ILE:HG22	2.14	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:56:TYR:O	2:B:57:ASN:HB2	2.13	0.48
1:A:64:LYS:C	1:A:65:LYS:HD2	2.38	0.48
1:A:89:GLU:O	1:A:90:VAL:O	2.32	0.47
1:A:417:VAL:HG13	1:A:419:THR:HG23	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:SER:C	2:B:270:ILE:N	2.72	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:21:VAL:HG22	1:A:59:PRO:HD3	1.97	0.47
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.49	0.47
1:A:63:ILE:HG23	1:A:74:LEU:HD11	1.95	0.47
1:A:65:LYS:HZ1	1:A:72:ARG:NH1	2.13	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
2:B:174:GLN:C	2:B:176:PRO:HD3	2.40	0.47
1:A:3:SER:HA	1:A:4:PRO:HD2	1.68	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: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:101:LYS:HD3	1:A:321:PRO:CG	2.44	0.46
1:A:410:TRP:CZ3	2:B:363:ASN:HB3	2.51	0.46
2:B:22:LYS:HE3	2:B:22:LYS:HB2	1.48	0.46
2:B:65:LYS:HD3	2:B:72:ARG:HB2	1.98	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
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: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: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
2:B:103:LYS:HG3	2:B:190:GLY:C	2.40	0.46
1:A:63:ILE:HG23	1:A:74:LEU:CD1	2.46	0.45
1:A:356:ARG:NH2	1:A:358:ARG:CD	2.78	0.45
2:B:249:LYS:CG	2:B:250:ASP:N	2.79	0.45
1:A:64:LYS:HZ3	1:A:69:THR:HA	1.81	0.45
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.80	0.45
2:B:57:ASN:OD1	2:B:131:THR:OG1	2.30	0.45
2:B:175:ASN:N	2:B:176:PRO:HD3	2.31	0.45
1:A:181:TYR:HD2	3:A:601:R8E:CL29	2.37	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
2:B:236:PRO:C	2:B:238:LYS:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:6:GLU:N	4:B:572:HOH:O	2.49	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
1:A:164:MET:O	1:A:164:MET:HG3	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:278:GLN:HA	2:B:278:GLN:NE2	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:274:ILE:C	2:B:275:LYS:HD3	2.42	0.45
2:B:422:LEU:CD1	2:B:426:TRP:CH2	3.00	0.45
1:A:63:ILE:HG12	1:A:74:LEU:HG	1.99	0.45
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.43	0.45
1:A:546:GLU:HG3	1:A:546:GLU:H	1.36	0.45
2:B:292:VAL:O	2:B:293:ILE:HG22	2.17	0.45
1:A:219:LYS:O	1:A:220:LYS:HG2	2.18	0.44
1:A:346:PHE:N	1:A:346:PHE:CD1	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:296:THR:OG1	2:B:298:GLU:OE1	2.31	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
1:A:88:TRP:NE1	4:A:720:HOH:O	2.50	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:20:LYS:HG2	1:A:55:PRO:O	2.17	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:549:ASP:O	1:A:553:SER:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:A:326:ILE:N	2.33	0.44
1:A:529:GLU:C	1:A:530:LYS:HG2	2.42	0.44
1:A:228:LEU:HD12	1:A:228:LEU:N	2.32	0.44
1:A:337:TRP:NE1	1:A:367:GLN:OE1	2.43	0.44
1:A:13:LYS:HE3	1:A:84:THR:O	2.18	0.44
1:A:60:VAL:CG1	1:A:75:VAL:HG22	2.42	0.44
1:A:175:ASN:ND2	1:A:178:ILE:CD1	2.80	0.44
1:A:61:PHE:HB2	4:A:623:HOH: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:438:GLU:OE1	1:A:459:THR:OG1	2.27	0.44
2:B:310:LEU:C	2:B:312:GLU:H	2.25	0.44
1:A:198:HIS:C	1:A:200:THR:N	2.75	0.43
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
1:A:175:ASN:CG	1:A:201:LYS:NZ	2.76	0.43
1:A:194:GLU:C	1:A:196:GLY:N	2.76	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:443:ASP:CB	1:A:548:VAL:HB	2.48	0.43
1:A:457:TYR:CD1	1:A:457:TYR:O	2.71	0.43
1:A:472:THR:HB	1:A:473:THR:H	1.61	0.43
2:B:257:ILE:HG23	2:B:279:LEU:HD12	2.00	0.43
1:A:434:ILE:HG21	1:A:492:GLU:OE1	2.19	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.87	0.43
2:B:6:GLU:O	2:B:6:GLU:HG2	2.16	0.43
2:B:249:LYS:HE2	2:B:249:LYS:HB3	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:82:LYS:O	1:A:82:LYS:HG3	2.17	0.43
1:A:424:LYS:CE	1:A:426:TRP:CE3	3.01	0.43
1:A:433:PRO:HB2	2:B:290:THR:CG2	2.49	0.43
1:A:527:LYS:HZ2	1:A:527:LYS:HG3	1.62	0.43
2:B:260:LEU:HD23	2:B:260:LEU:HA	1.70	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:O	2:B:268:SER:O	2.36	0.43
2:B:342:TYR:CD2	2:B:342:TYR:C	2.96	0.43
1:A:63:ILE:HD13	1:A:74:LEU:HD21	1.94	0.43
1:A:380:ILE:HD13	2:B:27:THR:HG22	2.00	0.43
1:A:404:GLU:HG3	1:A:404:GLU:H	1.63	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:CG	1:A:557:ARG:NH1	2.81	0.42
2:B:80:LEU:O	2:B:80:LEU:HD22	2.19	0.42
2:B:271:TYR:CB	2:B:274:ILE:HD11	2.48	0.42
1:A:4:PRO:HD2	1:A:212:TRP:C	2.44	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:402:TRP:CZ3	1:A:403:THR:OG1	2.73	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
2:B:406:TRP:C	2:B:407:GLN:HG2	2.40	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: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:72:ARG:HH22	2:B:409:THR:HG21	1.81	0.42
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.55	0.42
1:A:88:TRP:HB2	2:B:54:ASN:O	2.20	0.42
1:A:384:GLY:O	2:B:27:THR:HB	2.19	0.42
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.30	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
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:546:GLU:CD	1:A:547:GLN:NE2	2.78	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:105:SER:O	2:B:190:GLY:HA2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:CE	1:A:426:TRP:CH2	3.00	0.41
2:B:82:LYS:HE3	2:B:413:GLU:OE2	2.20	0.41
2:B:319:TYR:O	2:B:321:PRO:HD3	2.20	0.41
1:A:65:LYS:HE2	1:A:72:ARG:HD2	2.00	0.41
1:A:388:LYS:HE3	1:A:388:LYS:HB2	1.82	0.41
2:B:345:PRO:O	2:B:346:PHE:HB2	2.19	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
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:3:SER:OG	1:A:5:ILE:HD12	2.20	0.41
1:A:104:LYS:HG3	1:A:192:ASP:OD2	2.20	0.41
1:A:194:GLU:O	1:A:195:ILE:C	2.63	0.41
1:A:550:LYS:H	1:A:550:LYS:HG3	1.56	0.41
2:B:88:TRP:CZ3	2:B:89:GLU:HB2	2.56	0.41
2:B:90:VAL:O	2:B:90:VAL:HG23	2.20	0.41
2:B:236:PRO:C	2:B:238:LYS:N	2.79	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
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
1:A:500:GLN:CD	2:B:422:LEU:HG	2.45	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:OE1	1:A:516:GLU:HA	2.20	0.41
2:B:253:THR:HG23	2:B:254:VAL:N	2.36	0.41
1:A:21:VAL:HG22	1:A:59:PRO:HG3	2.01	0.40
1:A:102:LYS:NZ	1:A:237:ASP:HB3	2.36	0.40
1:A:249:LYS:HB2	1:A:249:LYS:HE2	1.32	0.40
1:A:286:THR:HG23	1:A:287:LYS:O	2.20	0.40
1:A:460:ASN:HD21	2:B:288:ALA:HB2	1.86	0.40
2:B:271:TYR:CD1	2:B:310:LEU:CD1	3.00	0.40
1:A:41:MET:HE2	1:A:47:ILE:HG23	2.04	0.40
1:A:210:LEU:C	1:A:212:TRP:H	2.30	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
1:A:210:LEU:C	1:A:212:TRP:N	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:NZ	1:A:426:TRP:CE3	2.89	0.40
2:B:85:GLN:O	2:B:89:GLU:HB3	2.21	0.40
2:B:296:THR:HB	2:B:298:GLU:CD	2.46	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
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	4
2	B	398/443 (90%)	369 (93%)	21 (5%)	8 (2%)	6	12
All	All	954/1006 (95%)	855 (90%)	72 (8%)	27 (3%)	4	6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	372 (75%)	126 (25%)	0	1
2	B	368/403 (91%)	282 (77%)	86 (23%)	1	1
All	All	866/906 (96%)	654 (76%)	212 (24%)	1	1

All (212) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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
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	108	VAL
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	151	GLN
1	A	161	GLN
1	A	162	SER
1	A	166	LYS
1	A	173	LYS
1	A	179	VAL
1	A	193	LEU
1	A	194	GLU
1	A	195	ILE
1	A	197	GLN
1	A	200	THR
1	A	202	ILE
1	A	205	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	ARG
1	A	215	THR
1	A	219	LYS
1	A	220	LYS
1	A	230	MET
1	A	242	GLN
1	A	244	ILE
1	A	245	VAL
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	291	GLU
1	A	292	VAL
1	A	293	ILE
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	312	GLU
1	A	326	ILE
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	374	LYS
1	A	380	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	388	LYS
1	A	395	LYS
1	A	399	GLU
1	A	400	THR
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	431	LYS
1	A	435	VAL
1	A	452	LEU
1	A	454	LYS
1	A	459	THR
1	A	476	LYS
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	528	LYS
1	A	530	LYS
1	A	542	ILE
1	A	546	GLU
1	A	547	GLN
1	A	548	VAL
1	A	550	LYS
1	A	551	LEU
1	A	552	VAL
1	A	553	SER
1	A	557	ARG
2	B	8	VAL
2	B	10	VAL
2	B	11	LYS
2	B	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	13	LYS
2	B	16	MET
2	B	22	LYS
2	B	24	TRP
2	B	26	LEU
2	B	29	GLU
2	B	40	GLU
2	B	46	LYS
2	B	48	SER
2	B	58	THR
2	B	64	LYS
2	B	65	LYS
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	101	LYS
2	B	111	VAL
2	B	120	LEU
2	B	138	GLU
2	B	162	SER
2	B	166	LYS
2	B	169	GLU
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	201	LYS
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	245	VAL
2	B	246	LEU
2	B	248	GLU
2	B	249	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	251	SER
2	B	253	THR
2	B	255	ASN
2	B	256	ASP
2	B	260	LEU
2	B	261	VAL
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
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	301	LEU
2	B	303	LEU
2	B	305	GLU
2	B	308	GLU
2	B	309	ILE
2	B	310	LEU
2	B	311	LYS
2	B	314	VAL
2	B	341	ILE
2	B	349	LEU
2	B	362	THR
2	B	377	THR
2	B	394	GLN
2	B	399	GLU
2	B	400	THR
2	B	403	THR
2	B	407	GLN
2	B	413	GLU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	147	ASN
1	A	151	GLN
1	A	161	GLN
1	A	175	ASN
1	A	198	HIS
1	A	207	GLN
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
1	A	394	GLN
1	A	418	ASN
1	A	428	GLN
1	A	460	ASN
1	A	480	GLN
1	A	487	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
2	B	96	HIS
2	B	137	ASN
2	B	174	GLN
2	B	175	ASN
2	B	182	GLN
2	B	258	GLN
2	B	265	ASN
2	B	278	GLN
2	B	306	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	R8E	A	601	-	31,32,32	2.67	10 (32%)	41,45,45	2.73	15 (36%)

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	-	-	3/11/11/11	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8E	C2-C26	-7.38	1.29	1.44
3	A	601	R8E	C18-N19	-5.81	1.30	1.35
3	A	601	R8E	C23-N25	4.66	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	R8E	C8-C13	-4.64	1.31	1.39
3	A	601	R8E	C17-C16	3.43	1.53	1.45
3	A	601	R8E	C17-C18	-3.15	1.38	1.41
3	A	601	R8E	C5-C6	2.90	1.43	1.38
3	A	601	R8E	C11-C10	-2.73	1.33	1.38
3	A	601	R8E	C16-N20	2.64	1.34	1.29
3	A	601	R8E	C9-C10	-2.50	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	R8E	N19-C18-N24	7.65	131.94	125.64
3	A	601	R8E	C8-C13-CL29	-6.21	112.33	119.44
3	A	601	R8E	C18-N19-N20	5.85	114.42	111.18
3	A	601	R8E	C11-C12-C13	-4.84	113.29	119.98
3	A	601	R8E	C15-O14-C10	4.61	125.89	117.63
3	A	601	R8E	C1-C6-CL28	-4.49	113.54	119.17
3	A	601	R8E	C12-C11-C10	4.36	124.71	119.73
3	A	601	R8E	O14-C15-C16	-4.11	99.26	109.50
3	A	601	R8E	O7-C8-C13	-3.48	111.73	119.51
3	A	601	R8E	C5-C6-CL28	3.02	122.96	119.17
3	A	601	R8E	C12-C13-CL29	2.89	124.12	118.42
3	A	601	R8E	C21-C17-C18	2.43	119.58	117.16
3	A	601	R8E	C8-C9-C10	-2.26	115.25	119.13
3	A	601	R8E	C9-C8-C13	2.15	122.19	119.29
3	A	601	R8E	C12-C13-C8	2.04	123.52	120.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

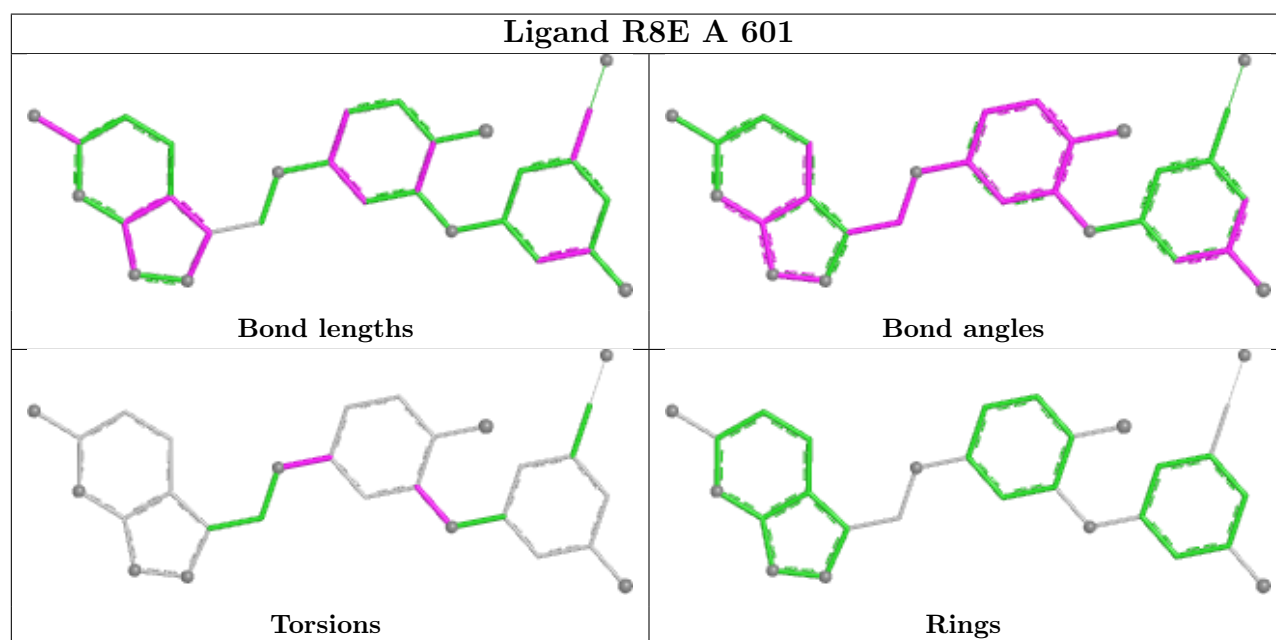
Mol	Chain	Res	Type	Atoms
3	A	601	R8E	C9-C10-O14-C15
3	A	601	R8E	C11-C10-O14-C15
3	A	601	R8E	C13-C8-O7-C4

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	21 (3%)	44 38	28, 55, 93, 125	0
2	B	404/443 (91%)	0.17	28 (6%)	23 18	27, 50, 108, 126	0
All	All	962/1006 (95%)	0.12	49 (5%)	33 28	27, 54, 102, 126	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	215	THR	4.2
2	B	270	ILE	4.1
1	A	286	THR	3.8
2	B	266	TRP	3.4
2	B	24	TRP	3.3
1	A	136	ASN	3.3
1	A	554	ALA	3.2
1	A	543	GLY	3.1
2	B	283	LEU	3.1
1	A	402	TRP	2.9
1	A	553	SER	2.9
2	B	116	PHE	2.9
2	B	252	TRP	2.9
2	B	346	PHE	2.9
1	A	138	GLU	2.8
1	A	291	GLU	2.8
1	A	137	ASN	2.7
1	A	63	ILE	2.7
1	A	288	ALA	2.7
2	B	232	TYR	2.6
2	B	293	ILE	2.6
1	A	549	ASP	2.6
2	B	428	GLN	2.6
2	B	424	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	357	MET	2.5
2	B	241	VAL	2.5
2	B	314	VAL	2.5
1	A	22	LYS	2.4
2	B	231	GLY	2.4
2	B	271	TYR	2.4
2	B	274	ILE	2.4
2	B	301	LEU	2.4
2	B	313	PRO	2.4
1	A	66	LYS	2.3
1	A	542	ILE	2.3
1	A	5	ILE	2.3
2	B	356	ARG	2.3
2	B	269	GLN	2.3
1	A	551	LEU	2.3
1	A	139	THR	2.2
1	A	539	HIS	2.2
2	B	246	LEU	2.2
2	B	88	TRP	2.2
1	A	287	LYS	2.2
2	B	426	TRP	2.1
2	B	8	VAL	2.1
2	B	362	THR	2.0
2	B	309	ILE	2.0
2	B	284	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

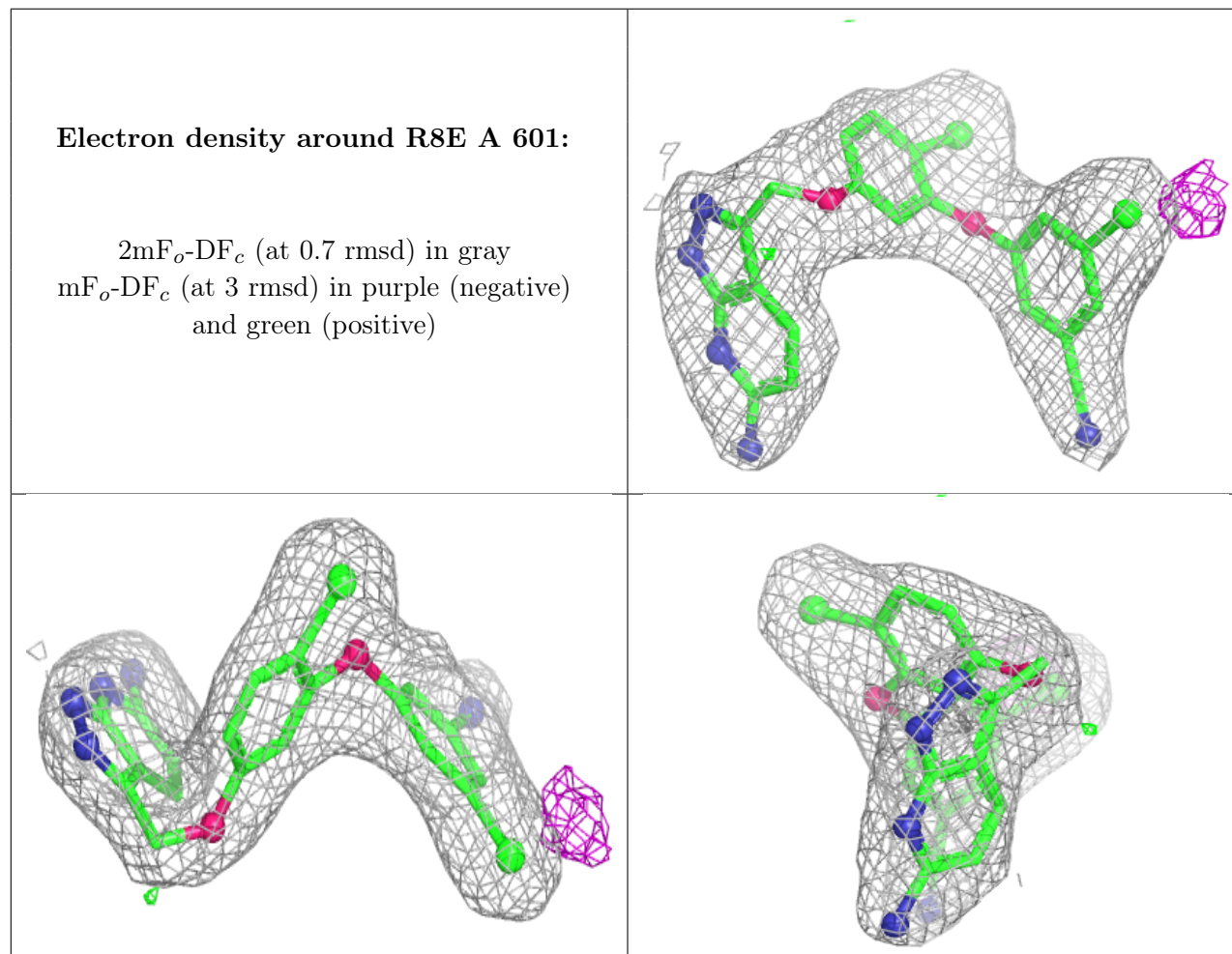
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	R8E	A	601	29/29	0.97	0.07	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.