



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:36 PM UTC

PDB ID : 2BAN / pdb_00002ban
Title : Crystal structure of HIV-1 reverse transcriptase (RT) in complex with JANSSEN-R157208
Authors : Das, K.; Arnold, E.
Deposited on : 2005-10-14
Resolution : 2.95 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

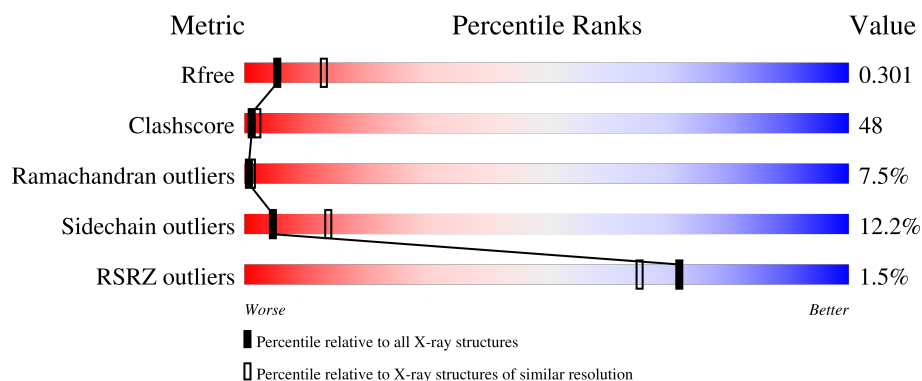
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	560	
2	B	430	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7922 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 P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4431	2864	733	827	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3465	2256	570	633	6			

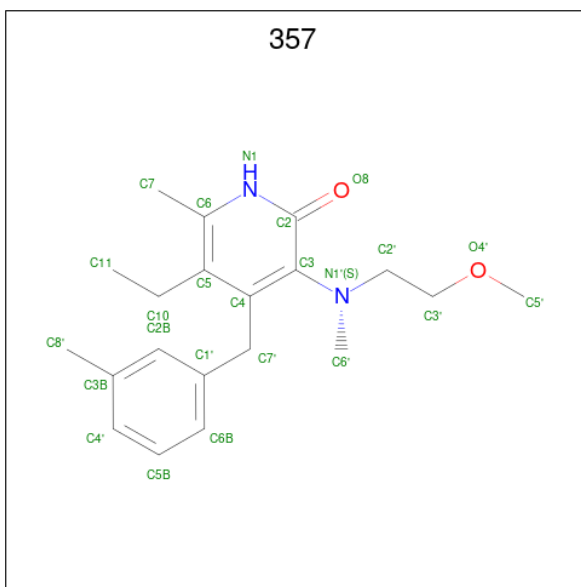
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-ETHYL-3-[(2-METHOXYETHYL)METHYLAMINO]-6-METHYL-4-(3-METHYLBENZYL)PYRIDIN-2(1H)-ONE (CCD ID: 357) (formula: C₂₀H₂₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	20	2	2		

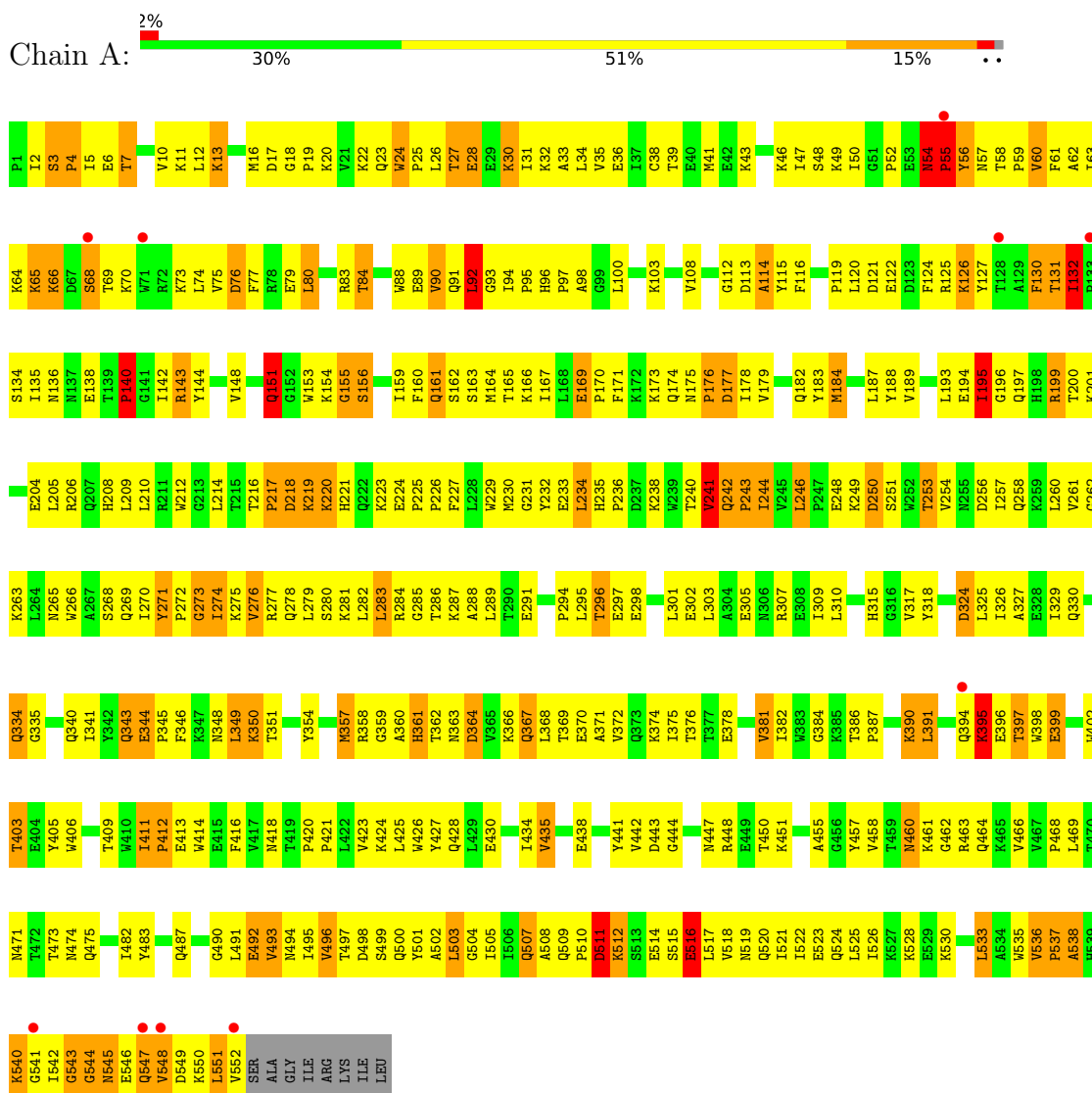
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

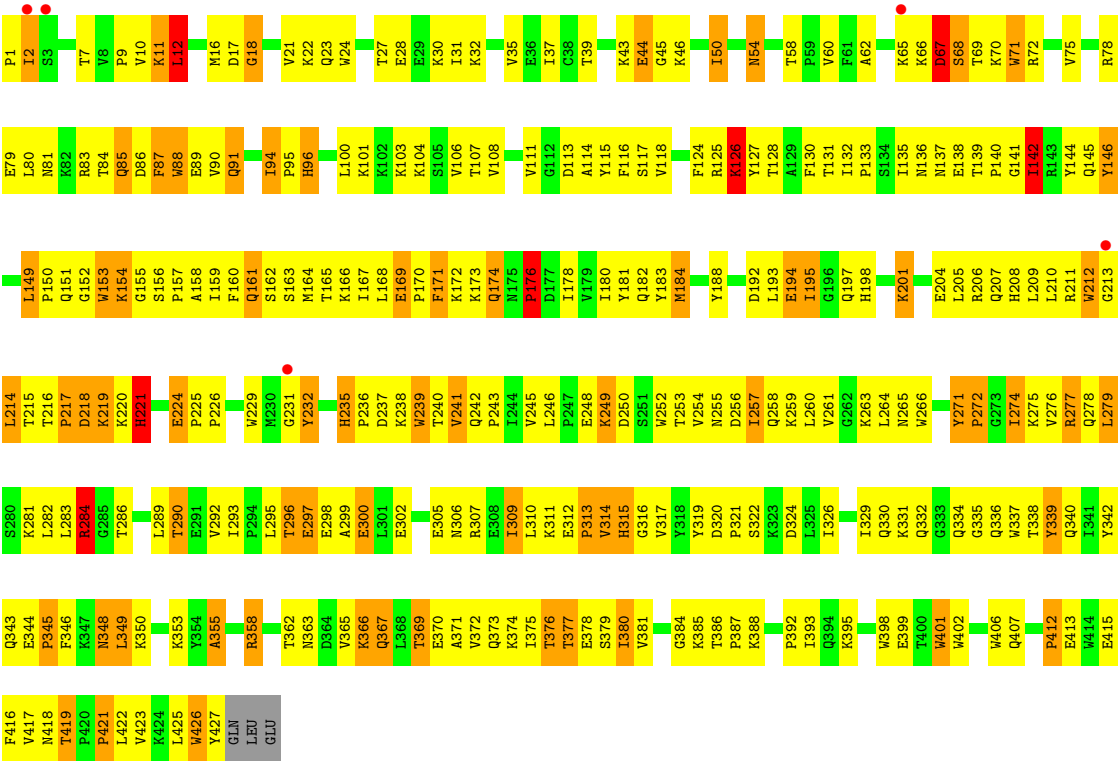
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 P66 subunit



• Molecule 2: Reverse transcriptase P51 subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.24Å 69.43Å 104.45Å 90.00° 106.49° 90.00°	Depositor
Resolution (Å)	19.86 – 2.95 19.86 – 2.95	Depositor EDS
% Data completeness (in resolution range)	91.9 (19.86-2.95) 93.4 (19.86-2.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.243 , 0.305 0.243 , 0.301	Depositor DCC
R_{free} test set	1533 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: MN, 357

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	0.54	0/4546	1.21	51/6185 (0.8%)
2	B	0.60	0/3566	1.22	45/4856 (0.9%)
All	All	0.57	0/8112	1.21	96/11041 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	PRO	N-CA-C	13.59	140.47	112.47
2	B	89	GLU	N-CA-C	-11.82	97.25	114.39
2	B	426	TRP	N-CA-C	-11.66	98.36	112.59
1	A	540	LYS	N-CA-C	-10.08	100.12	111.71
1	A	26	LEU	N-CA-C	9.78	131.63	110.80
2	B	239	TRP	N-CA-C	9.54	124.44	109.07
2	B	94	ILE	CA-C-N	9.45	130.04	119.93
2	B	94	ILE	C-N-CA	9.45	130.04	119.93
1	A	343	GLN	N-CA-C	-8.83	101.85	114.12
1	A	54	ASN	CA-C-N	8.56	130.54	119.84
1	A	54	ASN	C-N-CA	8.56	130.54	119.84
2	B	277	ARG	N-CA-C	7.79	122.47	112.34
2	B	87	PHE	N-CA-C	-7.70	101.83	112.30
2	B	153	TRP	N-CA-C	7.69	120.60	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	71	TRP	N-CA-C	7.68	120.44	110.53
1	A	551	LEU	N-CA-C	-7.63	103.07	112.38
1	A	544	GLY	N-CA-C	-7.62	105.86	115.31
1	A	24	TRP	CA-C-N	7.51	129.23	119.84
1	A	24	TRP	C-N-CA	7.51	129.23	119.84
1	A	132	ILE	CA-C-N	7.50	129.22	119.84
1	A	132	ILE	C-N-CA	7.50	129.22	119.84
2	B	401	TRP	N-CA-C	7.48	122.70	113.50
2	B	133	PRO	N-CA-C	7.35	121.84	111.33
2	B	172	LYS	N-CA-C	-7.32	103.81	112.89
1	A	169	GLU	CA-C-N	-7.14	110.92	119.84
1	A	169	GLU	C-N-CA	-7.14	110.92	119.84
1	A	273	GLY	N-CA-C	7.05	122.04	113.79
1	A	54	ASN	N-CA-C	7.03	125.35	109.81
1	A	135	ILE	N-CA-C	-6.97	103.51	110.62
1	A	511	ASP	N-CA-C	-6.97	103.76	112.90
2	B	58	THR	CA-C-N	6.95	127.36	119.92
2	B	58	THR	C-N-CA	6.95	127.36	119.92
2	B	271	TYR	CA-C-N	6.93	128.50	119.84
2	B	271	TYR	C-N-CA	6.93	128.50	119.84
2	B	208	HIS	N-CA-C	-6.79	103.57	110.97
2	B	88	TRP	N-CA-C	-6.70	102.20	112.99
2	B	70	LYS	N-CA-C	6.69	120.36	110.46
1	A	271	TYR	CA-C-N	6.64	128.14	119.84
1	A	271	TYR	C-N-CA	6.64	128.14	119.84
2	B	96	HIS	CA-C-N	6.53	128.00	119.84
2	B	96	HIS	C-N-CA	6.53	128.00	119.84
1	A	234	LEU	N-CA-C	6.52	119.88	107.75
1	A	68	SER	N-CA-C	6.51	120.23	111.24
1	A	151	GLN	N-CA-C	6.51	124.68	110.80
1	A	493	VAL	N-CA-C	6.40	116.84	107.75
1	A	357	MET	N-CA-C	6.35	124.32	110.80
1	A	32	LYS	N-CA-C	-6.28	105.52	113.43
1	A	140	PRO	N-CA-C	-6.14	99.81	112.47
2	B	54	ASN	CA-C-N	6.09	126.99	120.47
2	B	54	ASN	C-N-CA	6.09	126.99	120.47
2	B	235	HIS	CA-C-N	6.05	126.49	119.47
2	B	235	HIS	C-N-CA	6.05	126.49	119.47
1	A	411	ILE	CB-CA-C	-6.05	104.24	110.71
2	B	173	LYS	N-CA-C	-5.99	104.44	110.97
2	B	21	VAL	N-CA-C	5.95	117.16	108.53
1	A	512	LYS	N-CA-C	5.93	117.98	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	TYR	N-CA-C	5.92	118.84	110.50
1	A	283	LEU	N-CA-C	5.91	123.39	110.80
1	A	538	ALA	N-CA-C	5.89	123.34	110.80
1	A	549	ASP	N-CA-C	5.89	117.78	111.36
2	B	44	GLU	N-CA-C	-5.88	106.15	113.15
2	B	224	GLU	CA-C-N	5.87	126.43	120.38
2	B	224	GLU	C-N-CA	5.87	126.43	120.38
1	A	219	LYS	N-CA-C	-5.86	98.33	110.80
1	A	349	LEU	N-CA-C	-5.83	104.34	112.45
1	A	390	LYS	N-CA-C	-5.79	98.44	108.69
1	A	7	THR	N-CA-C	5.73	118.29	110.55
2	B	339	TYR	N-CA-C	5.68	117.73	108.76
1	A	361	HIS	N-CA-C	5.65	122.83	110.80
1	A	391	LEU	CA-C-N	5.51	126.73	119.84
1	A	391	LEU	C-N-CA	5.51	126.73	119.84
2	B	184	MET	CB-CA-C	-5.51	109.74	117.23
1	A	3	SER	N-CA-C	5.47	119.12	110.58
2	B	142	ILE	N-CA-C	-5.43	100.61	108.87
1	A	30	LYS	N-CA-C	-5.40	105.95	112.54
1	A	80	LEU	N-CA-C	-5.35	104.42	111.96
2	B	279	LEU	N-CA-C	-5.34	105.63	111.82
1	A	357	MET	CA-C-N	5.32	129.30	120.94
1	A	357	MET	C-N-CA	5.32	129.30	120.94
2	B	221	HIS	N-CA-C	-5.31	102.66	110.52
2	B	309	ILE	N-CA-C	-5.28	106.39	112.98
1	A	136	ASN	N-CA-C	5.25	121.98	110.80
1	A	536	VAL	CA-C-N	5.21	125.22	119.90
1	A	536	VAL	C-N-CA	5.21	125.22	119.90
1	A	27	THR	N-CA-C	5.19	118.11	107.37
2	B	358	ARG	N-CA-C	5.14	120.03	113.55
2	B	216	THR	N-CA-C	5.12	119.06	108.71
2	B	312	GLU	CA-C-N	5.11	126.22	119.84
2	B	312	GLU	C-N-CA	5.11	126.22	119.84
2	B	416	PHE	N-CA-C	5.10	118.12	109.76
1	A	381	VAL	CB-CA-C	-5.10	105.19	112.22
2	B	107	THR	N-CA-C	-5.05	103.00	110.48
1	A	327	ALA	N-CA-C	-5.04	100.50	109.06
2	B	171	PHE	N-CA-C	-5.02	106.50	113.18
1	A	48	SER	N-CA-C	5.01	117.32	108.75
2	B	37	ILE	CB-CA-C	-5.00	105.29	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	232	TYR	Sidechain

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	4431	0	4413	460	0
2	B	3465	0	3456	316	0
3	A	1	0	0	0	0
4	A	24	0	28	5	0
5	A	1	0	0	0	0
All	All	7922	0	7897	761	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 48.

All (761) 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:362:THR:HG22	1:A:363:ASN:H	1.08	1.18
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.06	1.15
1:A:132:ILE:HG13	1:A:142:ILE:HB	1.30	1.13
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.31	1.11
1:A:54:ASN:HB2	1:A:55:PRO:HD3	1.32	1.07
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.14	1.06
1:A:241:VAL:HG11	1:A:266:TRP:NE1	1.71	1.02
1:A:242:GLN:HB2	1:A:243:PRO:HD3	1.34	1.02
1:A:131:THR:HG23	1:A:143:ARG:HD2	1.39	1.02
1:A:241:VAL:CG1	1:A:266:TRP:HE1	1.78	0.97
1:A:362:THR:HG22	1:A:363:ASN:N	1.79	0.97
1:A:362:THR:CG2	1:A:363:ASN:H	1.80	0.94
2:B:276:VAL:H	2:B:277:ARG:HH11	0.96	0.94
1:A:35:VAL:HG22	1:A:132:ILE:HD12	1.50	0.94
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.47	0.93
1:A:161:GLN:HG2	1:A:182:GLN:HE21	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:C	1:A:220:LYS:H	1.63	0.92
2:B:11:LYS:HD3	2:B:11:LYS:H	1.35	0.92
2:B:87:PHE:O	2:B:91:GLN:HB2	1.70	0.90
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.16	0.90
2:B:149:LEU:HD22	2:B:156:SER:HA	1.51	0.89
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.38	0.89
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.54	0.88
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.54	0.87
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.71	0.87
1:A:240:THR:HG22	1:A:241:VAL:H	1.38	0.87
2:B:277:ARG:O	2:B:281:LYS:HG3	1.75	0.86
1:A:460:ASN:ND2	1:A:461:LYS:H	1.73	0.86
1:A:233:GLU:CD	1:A:242:GLN:HE21	1.83	0.86
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.10	0.86
1:A:270:ILE:O	1:A:272:PRO:HD3	1.76	0.85
1:A:460:ASN:HD22	1:A:461:LYS:H	1.22	0.85
1:A:249:LYS:HG3	1:A:250:ASP:H	1.40	0.85
2:B:276:VAL:N	2:B:277:ARG:HH11	1.74	0.85
1:A:195:ILE:HD12	1:A:195:ILE:H	1.40	0.84
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.59	0.84
2:B:277:ARG:CD	2:B:277:ARG:H	1.90	0.84
1:A:54:ASN:HB2	1:A:55:PRO:CD	2.08	0.84
1:A:90:VAL:HG23	1:A:91:GLN:H	1.44	0.83
1:A:231:GLY:O	1:A:241:VAL:HG13	1.78	0.82
2:B:241:VAL:HG13	2:B:243:PRO:HD3	1.62	0.82
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.15	0.82
1:A:64:LYS:HE2	1:A:68:SER:HA	1.62	0.82
1:A:450:THR:O	1:A:451:LYS:HG2	1.79	0.82
1:A:27:THR:CG2	1:A:30:LYS:HB2	2.09	0.81
2:B:78:ARG:HD3	2:B:412:PRO:O	1.79	0.81
1:A:74:LEU:HD12	1:A:75:VAL:H	1.45	0.81
1:A:132:ILE:CG1	1:A:142:ILE:HB	2.10	0.81
2:B:139:THR:HB	2:B:140:PRO:HD2	1.63	0.80
1:A:66:LYS:C	1:A:68:SER:H	1.89	0.80
2:B:276:VAL:H	2:B:277:ARG:NH1	1.78	0.80
2:B:306:ASN:ND2	2:B:309:ILE:HD12	1.97	0.79
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.63	0.79
2:B:350:LYS:HE3	2:B:378:GLU:OE1	1.82	0.79
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.12	0.79
2:B:235:HIS:HB2	2:B:238:LYS:HE3	1.64	0.79
2:B:275:LYS:HA	2:B:277:ARG:NH1	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ARG:O	2:B:127:TYR:N	2.16	0.79
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.48	0.78
2:B:241:VAL:HG22	2:B:242:GLN:H	1.48	0.78
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.65	0.78
1:A:74:LEU:HD12	1:A:75:VAL:N	1.98	0.78
2:B:156:SER:N	2:B:157:PRO:HD2	1.99	0.78
2:B:224:GLU:O	2:B:226:PRO:HD3	1.84	0.78
1:A:279:LEU:HD12	1:A:279:LEU:H	1.49	0.78
2:B:66:LYS:C	2:B:68:SER:H	1.90	0.78
2:B:31:ILE:O	2:B:35:VAL:HG23	1.83	0.77
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.66	0.77
2:B:284:ARG:HG3	2:B:284:ARG:NH1	1.90	0.77
2:B:206:ARG:HE	2:B:217:PRO:HB2	1.48	0.77
2:B:296:THR:HG22	2:B:297:GLU:N	2.00	0.77
2:B:11:LYS:HD3	2:B:11:LYS:N	1.97	0.77
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.15	0.76
2:B:156:SER:H	2:B:157:PRO:HD2	1.50	0.76
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.21	0.76
2:B:128:THR:OG1	2:B:146:TYR:HB2	1.86	0.76
1:A:23:GLN:O	1:A:25:PRO:HD3	1.86	0.75
1:A:460:ASN:ND2	1:A:461:LYS:N	2.34	0.75
2:B:296:THR:CG2	2:B:297:GLU:H	1.99	0.75
2:B:314:VAL:HG12	2:B:315:HIS:H	1.49	0.75
1:A:195:ILE:H	1:A:195:ILE:CD1	2.00	0.74
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.22	0.74
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.69	0.74
1:A:511:ASP:OD1	1:A:512:LYS:HG2	1.87	0.74
2:B:278:GLN:NE2	2:B:281:LYS:HD2	2.02	0.74
2:B:101:LYS:O	2:B:236:PRO:HB2	1.87	0.74
1:A:100:LEU:HD11	4:A:562:357:H8'1	1.69	0.73
1:A:164:MET:HE3	1:A:187:LEU:HD11	1.71	0.73
2:B:277:ARG:H	2:B:277:ARG:HD3	1.53	0.73
2:B:149:LEU:CD2	2:B:156:SER:HA	2.19	0.72
1:A:92:LEU:HG	1:A:93:GLY:N	2.05	0.72
1:A:278:GLN:HG2	1:A:302:GLU:OE2	1.89	0.72
1:A:317:VAL:HG12	1:A:348:ASN:O	1.90	0.72
1:A:242:GLN:HB2	1:A:243:PRO:CD	2.16	0.71
2:B:28:GLU:HG2	2:B:32:LYS:HE3	1.72	0.71
2:B:174:GLN:O	2:B:176:PRO:HD3	1.89	0.71
2:B:340:GLN:HG2	2:B:426:TRP:CZ2	2.24	0.71
2:B:281:LYS:HA	2:B:284:ARG:NH1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:O	2:B:257:ILE:HG22	1.90	0.70
2:B:166:LYS:HE2	2:B:212:TRP:HH2	1.57	0.70
1:A:60:VAL:C	1:A:61:PHE:HD1	2.00	0.69
1:A:240:THR:HG22	1:A:241:VAL:N	2.07	0.69
2:B:253:THR:H	2:B:256:ASP:HB2	1.57	0.69
1:A:298:GLU:H	1:A:298:GLU:CD	2.00	0.69
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.74	0.69
1:A:161:GLN:HG2	1:A:182:GLN:NE2	2.05	0.69
1:A:163:SER:HA	1:A:166:LYS:HE3	1.74	0.69
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.58	0.69
2:B:241:VAL:HG22	2:B:242:GLN:N	2.06	0.68
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.19	0.68
2:B:296:THR:CG2	2:B:297:GLU:N	2.55	0.68
1:A:28:GLU:H	1:A:28:GLU:CD	2.02	0.68
1:A:487:GLN:HG3	1:A:524:GLN:HE22	1.58	0.68
2:B:7:THR:O	2:B:9:PRO:HD3	1.94	0.68
1:A:64:LYS:HE2	1:A:68:SER:CA	2.24	0.68
1:A:242:GLN:O	1:A:244:ILE:HG13	1.94	0.68
1:A:358:ARG:C	1:A:360:ALA:H	2.02	0.68
1:A:195:ILE:HD12	1:A:195:ILE:N	2.08	0.67
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.95	0.67
2:B:306:ASN:HD22	2:B:309:ILE:HD12	1.60	0.67
2:B:279:LEU:HD12	2:B:299:ALA:HB1	1.77	0.67
2:B:314:VAL:HG12	2:B:315:HIS:N	2.09	0.67
2:B:380:ILE:O	2:B:384:GLY:HA2	1.95	0.67
4:A:562:357:H5'1	2:B:138:GLU:HB3	1.77	0.67
2:B:12:LEU:HA	2:B:84:THR:HG22	1.75	0.67
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.77	0.67
2:B:66:LYS:HZ1	2:B:218:ASP:HB2	1.59	0.66
1:A:430:GLU:CD	1:A:530:LYS:HE3	2.20	0.66
1:A:210:LEU:HA	1:A:214:LEU:O	1.96	0.66
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.76	0.66
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.90	0.66
1:A:59:PRO:HB2	1:A:61:PHE:CE1	2.31	0.65
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.78	0.65
1:A:20:LYS:HG2	1:A:56:TYR:HB3	1.77	0.65
1:A:493:VAL:HG22	1:A:494:ASN:N	2.11	0.65
1:A:296:THR:HG22	1:A:297:GLU:N	2.11	0.65
1:A:65:LYS:HE2	1:A:66:LYS:HA	1.79	0.65
1:A:65:LYS:HE2	1:A:66:LYS:CA	2.26	0.65
1:A:297:GLU:N	1:A:297:GLU:OE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:THR:HG22	2:B:297:GLU:H	1.58	0.65
2:B:213:GLY:C	2:B:215:THR:H	2.05	0.65
2:B:219:LYS:NZ	2:B:219:LYS:HB3	2.12	0.65
2:B:349:LEU:HD23	2:B:349:LEU:N	2.11	0.65
1:A:164:MET:HE3	1:A:187:LEU:HD21	1.79	0.65
1:A:41:MET:HB2	1:A:47:ILE:HD11	1.79	0.64
1:A:138:GLU:O	1:A:138:GLU:HG3	1.98	0.64
1:A:398:TRP:CH2	1:A:411:ILE:HD11	2.32	0.64
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.80	0.64
1:A:521:ILE:O	1:A:525:LEU:HG	1.97	0.64
2:B:275:LYS:O	2:B:302:GLU:CD	2.41	0.64
1:A:265:ASN:O	1:A:268:SER:N	2.31	0.64
1:A:543:GLY:O	2:B:284:ARG:HA	1.97	0.64
2:B:366:LYS:O	2:B:370:GLU:HG3	1.98	0.63
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.32	0.63
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.29	0.63
2:B:277:ARG:CD	2:B:277:ARG:N	2.58	0.63
1:A:286:THR:HG22	1:A:288:ALA:H	1.64	0.63
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.80	0.63
1:A:324:ASP:O	1:A:326:ILE:HD12	1.98	0.63
1:A:537:PRO:HB2	1:A:541:GLY:HA3	1.81	0.63
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.81	0.63
2:B:373:GLN:HE22	2:B:407:GLN:H	1.45	0.63
1:A:276:VAL:HG12	1:A:276:VAL:O	1.98	0.63
1:A:96:HIS:CE1	1:A:350:LYS:HD2	2.34	0.62
1:A:277:ARG:HD2	1:A:334:GLN:HB2	1.81	0.62
1:A:509:GLN:N	1:A:510:PRO:HD3	2.14	0.62
2:B:66:LYS:O	2:B:68:SER:N	2.33	0.62
2:B:1:PRO:HD2	2:B:117:SER:HA	1.82	0.62
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.81	0.62
1:A:17:ASP:O	1:A:83:ARG:HD3	1.98	0.62
1:A:420:PRO:HA	1:A:421:PRO:C	2.24	0.62
2:B:17:ASP:O	2:B:83:ARG:NH1	2.33	0.62
2:B:146:TYR:CG	2:B:150:PRO:HG3	2.35	0.62
2:B:1:PRO:CD	2:B:117:SER:HA	2.29	0.61
2:B:66:LYS:C	2:B:68:SER:N	2.57	0.61
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.82	0.61
1:A:235:HIS:CD2	1:A:238:LYS:HG3	2.35	0.61
1:A:286:THR:HG21	1:A:291:GLU:OE1	2.00	0.61
1:A:434:ILE:H	1:A:494:ASN:HD21	1.48	0.61
2:B:91:GLN:HE21	2:B:91:GLN:C	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.35	0.61
1:A:218:ASP:C	1:A:220:LYS:N	2.38	0.61
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.35	0.61
2:B:335:GLY:O	2:B:355:ALA:HA	2.01	0.61
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.81	0.61
1:A:457:TYR:C	1:A:457:TYR:CD2	2.79	0.61
1:A:503:LEU:HD11	1:A:507:GLN:OE1	2.00	0.61
2:B:421:PRO:HG2	2:B:422:LEU:H	1.65	0.60
1:A:126:LYS:NZ	1:A:126:LYS:HB3	2.16	0.60
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.83	0.60
1:A:108:VAL:HG23	1:A:108:VAL:O	2.00	0.60
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.83	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
1:A:219:LYS:HD2	1:A:219:LYS:N	2.16	0.60
1:A:441:TYR:O	1:A:548:VAL:HG11	2.01	0.60
1:A:49:LYS:HA	1:A:143:ARG:O	2.01	0.60
1:A:219:LYS:C	1:A:221:HIS:H	2.09	0.60
1:A:495:ILE:HB	1:A:533:LEU:HD22	1.83	0.60
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.37	0.60
1:A:170:PRO:HB2	1:A:174:GLN:NE2	2.16	0.60
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.84	0.60
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.32	0.60
2:B:348:ASN:C	2:B:349:LEU:HD23	2.26	0.60
2:B:100:LEU:HD11	2:B:106:VAL:CG1	2.32	0.60
1:A:132:ILE:HG13	1:A:142:ILE:CB	2.20	0.59
2:B:371:ALA:O	2:B:375:ILE:HG13	2.02	0.59
1:A:19:PRO:O	1:A:56:TYR:HB2	2.02	0.59
2:B:281:LYS:HG2	2:B:284:ARG:CZ	2.32	0.59
2:B:365:VAL:HG12	2:B:366:LYS:N	2.17	0.59
2:B:277:ARG:N	2:B:277:ARG:HD2	2.17	0.59
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.37	0.59
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.32	0.59
1:A:124:PHE:CD2	1:A:124:PHE:O	2.55	0.59
1:A:426:TRP:O	1:A:427:TYR:HB3	2.03	0.59
1:A:451:LYS:HE3	1:A:471:ASN:ND2	2.17	0.59
1:A:460:ASN:HD22	1:A:460:ASN:N	2.00	0.59
1:A:540:LYS:HE3	2:B:265:ASN:HD21	1.68	0.59
1:A:164:MET:CE	1:A:187:LEU:HD11	2.32	0.58
1:A:238:LYS:HE2	1:A:315:HIS:HB2	1.85	0.58
2:B:154:LYS:HG2	2:B:184:MET:HG2	1.83	0.58
1:A:57:ASN:ND2	1:A:58:THR:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:SER:OG	1:A:502:ALA:HB3	2.02	0.58
1:A:298:GLU:CD	1:A:298:GLU:N	2.60	0.58
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.04	0.58
1:A:201:LYS:HA	1:A:204:GLU:HG3	1.85	0.58
1:A:244:ILE:HD13	1:A:310:LEU:HD22	1.86	0.58
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.39	0.58
2:B:315:HIS:C	2:B:317:VAL:H	2.11	0.58
1:A:46:LYS:HE2	1:A:116:PHE:O	2.03	0.58
2:B:166:LYS:HE2	2:B:212:TRP:CH2	2.38	0.58
1:A:19:PRO:O	1:A:56:TYR:CB	2.52	0.58
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.39	0.58
2:B:206:ARG:NE	2:B:217:PRO:HB2	2.19	0.58
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.39	0.57
1:A:34:LEU:CD1	1:A:132:ILE:HG22	2.35	0.57
1:A:188:TYR:CD2	4:A:562:357:H6'	2.39	0.57
1:A:517:LEU:O	1:A:520:GLN:HB2	2.04	0.57
1:A:34:LEU:HD12	1:A:132:ILE:HG22	1.86	0.57
1:A:242:GLN:O	1:A:244:ILE:N	2.35	0.57
1:A:33:ALA:O	1:A:36:GLU:HB3	2.04	0.57
1:A:545:ASN:HA	1:A:548:VAL:HG23	1.85	0.57
1:A:112:GLY:C	1:A:114:ALA:H	2.13	0.57
2:B:266:TRP:HH2	2:B:426:TRP:CZ3	2.22	0.57
1:A:490:GLY:O	1:A:492:GLU:N	2.37	0.57
1:A:296:THR:HG22	1:A:298:GLU:OE1	2.05	0.57
1:A:460:ASN:HD22	1:A:461:LYS:N	1.92	0.57
2:B:297:GLU:HA	2:B:297:GLU:OE1	2.04	0.56
2:B:373:GLN:NE2	2:B:407:GLN:H	2.02	0.56
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.86	0.56
1:A:94:ILE:HD13	1:A:230:MET:HG3	1.87	0.56
1:A:284:ARG:HG3	1:A:285:GLY:N	2.19	0.56
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.39	0.56
2:B:125:ARG:C	2:B:127:TYR:H	2.13	0.56
1:A:394:GLN:HG2	1:A:397:THR:OG1	2.04	0.56
2:B:156:SER:N	2:B:157:PRO:CD	2.68	0.56
2:B:194:GLU:O	2:B:195:ILE:C	2.48	0.56
2:B:423:VAL:HG12	2:B:423:VAL:O	2.06	0.56
1:A:350:LYS:NZ	1:A:350:LYS:HB3	2.21	0.56
2:B:279:LEU:HA	2:B:299:ALA:HB1	1.88	0.56
2:B:385:LYS:O	2:B:385:LYS:HG3	2.05	0.56
1:A:131:THR:OG1	1:A:143:ARG:NE	2.35	0.56
1:A:254:VAL:O	1:A:258:GLN:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CZ2	2:B:418:ASN:O	2.59	0.56
1:A:537:PRO:O	1:A:541:GLY:O	2.24	0.56
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.36	0.56
2:B:248:GLU:HA	2:B:307:ARG:NH2	2.20	0.56
1:A:223:LYS:O	1:A:223:LYS:HG3	2.06	0.56
1:A:542:ILE:CG1	1:A:546:GLU:HA	2.36	0.56
2:B:419:THR:O	2:B:421:PRO:HD3	2.06	0.56
1:A:487:GLN:HG3	1:A:524:GLN:NE2	2.21	0.55
2:B:201:LYS:O	2:B:204:GLU:HB3	2.06	0.55
2:B:259:LYS:O	2:B:263:LYS:HD3	2.06	0.55
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.88	0.55
2:B:419:THR:O	2:B:419:THR:HG23	2.06	0.55
2:B:252:TRP:O	2:B:292:VAL:HG13	2.07	0.55
2:B:311:LYS:O	2:B:313:PRO:HD3	2.07	0.55
1:A:376:THR:HG23	1:A:386:THR:HG22	1.88	0.55
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.37	0.55
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.88	0.55
2:B:249:LYS:HE2	2:B:252:TRP:CZ3	2.42	0.55
1:A:41:MET:HB2	1:A:47:ILE:CD1	2.37	0.55
1:A:210:LEU:O	1:A:210:LEU:HD12	2.06	0.55
1:A:382:ILE:O	2:B:136:ASN:HB2	2.05	0.55
1:A:402:TRP:CE3	1:A:403:THR:HA	2.42	0.55
2:B:278:GLN:HE22	2:B:281:LYS:HD2	1.71	0.55
2:B:296:THR:O	2:B:300:GLU:HB2	2.07	0.55
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.72	0.55
1:A:235:HIS:HD2	1:A:238:LYS:HG3	1.70	0.55
1:A:460:ASN:C	1:A:462:GLY:H	2.14	0.55
2:B:282:LEU:HD13	2:B:296:THR:OG1	2.06	0.55
2:B:23:GLN:NE2	2:B:24:TRP:O	2.40	0.55
2:B:213:GLY:O	2:B:215:THR:N	2.40	0.55
1:A:113:ASP:O	1:A:114:ALA:C	2.50	0.55
1:A:183:TYR:C	1:A:183:TYR:CD2	2.85	0.55
1:A:84:THR:HG23	1:A:124:PHE:CZ	2.42	0.54
1:A:399:GLU:OE1	1:A:402:TRP:NE1	2.39	0.54
1:A:457:TYR:C	1:A:457:TYR:HD2	2.15	0.54
1:A:496:VAL:HG12	1:A:496:VAL:O	2.06	0.54
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.33	0.54
1:A:57:ASN:CG	1:A:58:THR:H	2.13	0.54
1:A:344:GLU:HG3	1:A:345:PRO:HD2	1.88	0.54
1:A:66:LYS:C	1:A:68:SER:N	2.61	0.54
1:A:96:HIS:NE2	1:A:350:LYS:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HH11	1:A:334:GLN:HB2	1.73	0.54
2:B:115:TYR:C	2:B:117:SER:H	2.15	0.54
1:A:194:GLU:O	1:A:196:GLY:N	2.41	0.54
1:A:317:VAL:HG13	1:A:349:LEU:HD23	1.90	0.54
1:A:325:LEU:HD22	1:A:341:ILE:CG2	2.38	0.54
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.43	0.54
2:B:16:MET:HE3	2:B:16:MET:HA	1.90	0.54
1:A:515:SER:O	1:A:517:LEU:N	2.41	0.54
2:B:66:LYS:NZ	2:B:218:ASP:HB2	2.23	0.54
1:A:162:SER:O	1:A:166:LYS:HG3	2.08	0.54
1:A:368:LEU:O	1:A:372:VAL:HG23	2.07	0.54
1:A:427:TYR:OH	1:A:509:GLN:HA	2.09	0.54
2:B:261:VAL:HG21	2:B:283:LEU:HD11	1.90	0.53
2:B:274:ILE:HG22	2:B:274:ILE:O	2.07	0.53
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.90	0.53
1:A:73:LYS:HG2	1:A:74:LEU:N	2.23	0.53
1:A:482:ILE:O	1:A:483:TYR:C	2.50	0.53
2:B:80:LEU:HD12	2:B:80:LEU:O	2.08	0.53
2:B:209:LEU:HB3	2:B:215:THR:OG1	2.08	0.53
2:B:241:VAL:CG2	2:B:242:GLN:H	2.19	0.53
2:B:337:TRP:HE1	2:B:367:GLN:HG2	1.73	0.53
1:A:23:GLN:HE21	1:A:24:TRP:H	1.57	0.53
1:A:234:LEU:HD22	4:A:562:357:H111	1.90	0.53
1:A:301:LEU:O	1:A:305:GLU:HG3	2.09	0.53
1:A:362:THR:CG2	1:A:363:ASN:N	2.49	0.53
1:A:398:TRP:CZ3	1:A:411:ILE:HD11	2.43	0.53
2:B:22:LYS:HD3	2:B:24:TRP:CZ3	2.42	0.53
2:B:343:GLN:O	2:B:344:GLU:HG2	2.08	0.53
2:B:329:ILE:HD11	2:B:375:ILE:HD12	1.91	0.53
1:A:223:LYS:C	1:A:225:PRO:HD3	2.34	0.53
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.44	0.52
2:B:277:ARG:H	2:B:277:ARG:HD2	1.67	0.52
1:A:115:TYR:HD1	1:A:115:TYR:H	1.57	0.52
1:A:54:ASN:CB	1:A:55:PRO:CD	2.77	0.52
2:B:10:VAL:HG13	2:B:88:TRP:CZ2	2.43	0.52
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.44	0.52
1:A:233:GLU:CD	1:A:242:GLN:NE2	2.61	0.52
1:A:277:ARG:HH11	1:A:334:GLN:CB	2.22	0.52
2:B:183:TYR:HE2	2:B:184:MET:SD	2.32	0.52
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.92	0.52
1:A:269:GLN:O	1:A:351:THR:N	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HD13	1:A:428:GLN:OE1	2.10	0.52
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.39	0.52
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.43	0.52
2:B:168:LEU:HD13	2:B:180:ILE:HD12	1.91	0.52
2:B:395:LYS:O	2:B:399:GLU:HG3	2.10	0.52
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.44	0.52
1:A:233:GLU:OE1	1:A:235:HIS:NE2	2.41	0.52
1:A:517:LEU:O	1:A:520:GLN:N	2.43	0.52
2:B:326:ILE:CG2	2:B:342:TYR:CE1	2.93	0.52
1:A:296:THR:CG2	1:A:297:GLU:N	2.73	0.51
2:B:276:VAL:HG22	2:B:276:VAL:O	2.09	0.51
2:B:90:VAL:HG12	2:B:91:GLN:N	2.25	0.51
2:B:50:ILE:HG21	2:B:54:ASN:HD22	1.75	0.51
2:B:314:VAL:HB	2:B:317:VAL:HG21	1.92	0.51
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.74	0.51
1:A:62:ALA:O	1:A:63:ILE:HD13	2.10	0.51
1:A:411:ILE:O	1:A:412:PRO:O	2.27	0.51
2:B:115:TYR:O	2:B:117:SER:N	2.43	0.51
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.46	0.51
2:B:278:GLN:HE21	2:B:278:GLN:HA	1.75	0.51
1:A:12:LEU:O	1:A:13:LYS:C	2.54	0.51
1:A:542:ILE:HG12	1:A:546:GLU:HA	1.93	0.51
1:A:54:ASN:CB	1:A:55:PRO:HD3	2.19	0.51
1:A:161:GLN:NE2	1:A:161:GLN:C	2.69	0.51
1:A:424:LYS:HD3	1:A:426:TRP:CH2	2.46	0.51
2:B:320:ASP:OD1	2:B:322:SER:OG	2.20	0.51
1:A:134:SER:CB	1:A:140:PRO:HD3	2.41	0.51
2:B:276:VAL:N	2:B:277:ARG:NH1	2.48	0.51
1:A:153:TRP:O	1:A:156:SER:HB2	2.11	0.50
1:A:283:LEU:O	1:A:284:ARG:C	2.54	0.50
1:A:358:ARG:O	1:A:360:ALA:N	2.43	0.50
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.93	0.50
1:A:116:PHE:O	1:A:148:VAL:HG11	2.11	0.50
1:A:233:GLU:OE2	1:A:242:GLN:HG3	2.11	0.50
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.92	0.50
2:B:245:VAL:HG22	2:B:246:LEU:O	2.11	0.50
1:A:3:SER:CB	1:A:5:ILE:HG13	2.37	0.50
1:A:276:VAL:O	1:A:276:VAL:CG1	2.60	0.50
2:B:174:GLN:O	2:B:176:PRO:CD	2.57	0.50
2:B:332:GLN:HB3	2:B:336:GLN:O	2.11	0.50
2:B:94:ILE:HD11	2:B:158:ALA:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:PHE:O	2:B:161:GLN:C	2.54	0.50
2:B:314:VAL:HB	2:B:317:VAL:CG2	2.42	0.50
1:A:175:ASN:C	1:A:177:ASP:H	2.20	0.50
1:A:279:LEU:HD12	1:A:279:LEU:N	2.24	0.50
2:B:151:GLN:O	2:B:153:TRP:N	2.45	0.50
1:A:77:PHE:O	1:A:80:LEU:HB3	2.12	0.50
1:A:108:VAL:HG13	1:A:227:PHE:CE1	2.47	0.50
1:A:167:ILE:O	1:A:170:PRO:HD2	2.12	0.50
1:A:240:THR:CG2	1:A:241:VAL:H	2.08	0.50
2:B:376:THR:O	2:B:379:SER:N	2.45	0.50
1:A:275:LYS:O	1:A:276:VAL:HG23	2.12	0.50
2:B:213:GLY:C	2:B:215:THR:N	2.67	0.50
2:B:249:LYS:HB3	2:B:249:LYS:NZ	2.27	0.50
2:B:66:LYS:NZ	2:B:218:ASP:CB	2.75	0.50
2:B:274:ILE:HG23	2:B:306:ASN:OD1	2.11	0.50
2:B:406:TRP:CZ2	2:B:412:PRO:HD2	2.47	0.50
1:A:434:ILE:HG21	1:A:492:GLU:CG	2.41	0.49
1:A:511:ASP:CG	1:A:512:LYS:HG2	2.37	0.49
2:B:132:ILE:HB	2:B:142:ILE:HG13	1.94	0.49
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.47	0.49
2:B:315:HIS:O	2:B:317:VAL:N	2.45	0.49
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.46	0.49
1:A:98:ALA:HB2	1:A:350:LYS:HG3	1.93	0.49
2:B:118:VAL:HB	2:B:149:LEU:HD13	1.93	0.49
1:A:2:ILE:HG22	1:A:3:SER:N	2.27	0.49
1:A:65:LYS:HE2	1:A:66:LYS:N	2.28	0.49
1:A:195:ILE:O	1:A:199:ARG:HD3	2.11	0.49
1:A:226:PRO:HB3	1:A:235:HIS:ND1	2.27	0.49
1:A:238:LYS:HE2	1:A:315:HIS:CB	2.43	0.49
1:A:286:THR:HG22	1:A:287:LYS:N	2.28	0.49
1:A:138:GLU:O	1:A:140:PRO:HD3	2.13	0.49
1:A:17:ASP:CG	1:A:18:GLY:N	2.70	0.49
1:A:92:LEU:CG	1:A:93:GLY:N	2.70	0.49
2:B:71:TRP:H	2:B:71:TRP:CD1	2.29	0.49
2:B:198:HIS:O	2:B:201:LYS:N	2.46	0.49
2:B:235:HIS:O	2:B:238:LYS:HG2	2.13	0.49
2:B:28:GLU:HA	2:B:31:ILE:HD12	1.94	0.49
1:A:58:THR:HG22	1:A:76:ASP:O	2.12	0.49
1:A:460:ASN:HA	2:B:286:THR:O	2.13	0.49
1:A:246:LEU:HD23	1:A:246:LEU:H	1.78	0.49
2:B:401:TRP:O	2:B:402:TRP:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:PRO:C	1:A:469:LEU:HG	2.37	0.49
2:B:124:PHE:O	2:B:125:ARG:C	2.56	0.49
2:B:282:LEU:HG	2:B:293:ILE:HD11	1.94	0.49
1:A:175:ASN:N	1:A:176:PRO:HD3	2.27	0.48
1:A:317:VAL:HG22	1:A:318:TYR:H	1.77	0.48
2:B:183:TYR:CD2	2:B:183:TYR:C	2.91	0.48
1:A:413:GLU:OE2	1:A:413:GLU:HA	2.12	0.48
1:A:542:ILE:O	1:A:543:GLY:O	2.31	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.95	0.48
1:A:542:ILE:O	1:A:542:ILE:HG23	2.13	0.48
2:B:84:THR:O	2:B:86:ASP:N	2.46	0.48
2:B:139:THR:HB	2:B:140:PRO:CD	2.34	0.48
1:A:242:GLN:CB	1:A:243:PRO:CD	2.87	0.48
1:A:273:GLY:O	1:A:274:ILE:C	2.55	0.48
2:B:100:LEU:HD11	2:B:106:VAL:HG13	1.93	0.48
2:B:164:MET:C	2:B:166:LYS:N	2.70	0.48
1:A:358:ARG:C	1:A:360:ALA:N	2.67	0.48
1:A:366:LYS:O	1:A:370:GLU:HG3	2.13	0.48
2:B:65:LYS:HD2	2:B:72:ARG:HG3	1.95	0.48
2:B:279:LEU:HA	2:B:299:ALA:CB	2.42	0.48
1:A:249:LYS:HG3	1:A:250:ASP:OD2	2.14	0.48
1:A:253:THR:HG23	1:A:256:ASP:H	1.79	0.48
1:A:340:GLN:HA	1:A:351:THR:HA	1.96	0.48
1:A:402:TRP:CD2	1:A:403:THR:N	2.81	0.48
1:A:543:GLY:C	1:A:545:ASN:H	2.19	0.48
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.44	0.48
1:A:296:THR:HG22	1:A:297:GLU:H	1.76	0.48
2:B:279:LEU:CD1	2:B:299:ALA:HB1	2.43	0.48
1:A:90:VAL:HG23	1:A:91:GLN:N	2.22	0.48
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.95	0.48
2:B:1:PRO:C	2:B:2:ILE:HG13	2.38	0.48
2:B:260:LEU:HG	2:B:264:LEU:HD12	1.94	0.48
1:A:163:SER:HA	1:A:166:LYS:CE	2.42	0.48
2:B:28:GLU:O	2:B:32:LYS:HG3	2.13	0.48
2:B:425:LEU:HA	2:B:427:TYR:HD1	1.79	0.48
1:A:178:ILE:HD11	1:A:201:LYS:HG3	1.96	0.47
1:A:345:PRO:HB2	1:A:346:PHE:CD1	2.49	0.47
1:A:451:LYS:HE3	1:A:471:ASN:HD22	1.78	0.47
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.49	0.47
2:B:284:ARG:NH1	2:B:284:ARG:CG	2.67	0.47
1:A:234:LEU:HB3	4:A:562:357:H111	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ILE:O	1:A:270:ILE:HG13	2.14	0.47
1:A:521:ILE:O	1:A:521:ILE:HG22	2.14	0.47
2:B:151:GLN:C	2:B:153:TRP:N	2.71	0.47
2:B:281:LYS:HG2	2:B:284:ARG:NH2	2.29	0.47
1:A:179:VAL:HG23	1:A:179:VAL:O	2.15	0.47
1:A:384:GLY:O	2:B:27:THR:HG23	2.14	0.47
2:B:167:ILE:O	2:B:170:PRO:HD2	2.14	0.47
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.96	0.47
1:A:178:ILE:CG2	1:A:189:VAL:HG13	2.44	0.47
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.96	0.47
1:A:406:TRP:CZ2	2:B:419:THR:HB	2.49	0.47
2:B:210:LEU:HA	2:B:215:THR:O	2.15	0.47
1:A:10:VAL:HG12	1:A:11:LYS:N	2.29	0.47
1:A:95:PRO:HA	2:B:136:ASN:O	2.13	0.47
1:A:108:VAL:CG1	1:A:227:PHE:CE1	2.98	0.47
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.80	0.47
1:A:543:GLY:C	1:A:545:ASN:N	2.73	0.47
1:A:493:VAL:CG2	1:A:494:ASN:N	2.77	0.47
2:B:194:GLU:O	2:B:197:GLN:N	2.47	0.47
2:B:376:THR:O	2:B:377:THR:C	2.57	0.47
2:B:131:THR:CG2	2:B:141:GLY:HA3	2.45	0.47
1:A:46:LYS:HD2	1:A:46:LYS:N	2.29	0.47
1:A:56:TYR:CD1	1:A:56:TYR:N	2.72	0.47
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.50	0.47
1:A:130:PHE:HE1	1:A:144:TYR:HB2	1.74	0.47
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.96	0.47
1:A:92:LEU:HG	1:A:93:GLY:H	1.80	0.47
1:A:171:PHE:C	1:A:173:LYS:N	2.73	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.50	0.47
1:A:277:ARG:O	1:A:281:LYS:HB2	2.14	0.46
1:A:296:THR:CG2	1:A:297:GLU:H	2.27	0.46
1:A:326:ILE:HD12	1:A:326:ILE:N	2.30	0.46
2:B:296:THR:HG23	2:B:297:GLU:H	1.80	0.46
1:A:2:ILE:CG2	1:A:3:SER:N	2.78	0.46
1:A:91:GLN:O	1:A:92:LEU:C	2.58	0.46
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.97	0.46
2:B:43:LYS:C	2:B:45:GLY:H	2.20	0.46
1:A:115:TYR:HE2	1:A:156:SER:HB3	1.80	0.46
1:A:122:GLU:CD	1:A:125:ARG:HH11	2.24	0.46
1:A:294:PRO:O	1:A:296:THR:N	2.48	0.46
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:VAL:CG1	2:B:315:HIS:N	2.78	0.46
1:A:59:PRO:HB2	1:A:61:PHE:HE1	1.80	0.46
1:A:79:GLU:O	1:A:83:ARG:NH1	2.49	0.46
1:A:120:LEU:O	1:A:121:ASP:C	2.58	0.46
1:A:515:SER:O	1:A:516:GLU:C	2.59	0.46
1:A:3:SER:OG	1:A:212:TRP:O	2.34	0.46
1:A:175:ASN:O	1:A:177:ASP:N	2.46	0.46
1:A:270:ILE:HD11	1:A:315:HIS:O	2.16	0.46
1:A:547:GLN:CA	1:A:547:GLN:HE21	2.28	0.46
2:B:11:LYS:N	2:B:11:LYS:CD	2.75	0.46
2:B:326:ILE:HG21	2:B:342:TYR:HE1	1.81	0.46
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.28	0.46
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.16	0.46
1:A:381:VAL:O	2:B:136:ASN:HA	2.16	0.46
1:A:277:ARG:NH2	1:A:281:LYS:HE2	2.31	0.46
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.39	0.46
2:B:149:LEU:HB3	2:B:156:SER:HB3	1.98	0.46
1:A:27:THR:O	1:A:31:ILE:N	2.47	0.46
1:A:261:VAL:O	1:A:262:GLY:C	2.59	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.46
2:B:30:LYS:HB3	2:B:62:ALA:HB3	1.98	0.46
1:A:279:LEU:HD21	1:A:303:LEU:HD13	1.98	0.46
2:B:339:TYR:C	2:B:340:GLN:OE1	2.59	0.46
2:B:365:VAL:O	2:B:367:GLN:N	2.49	0.46
1:A:253:THR:O	1:A:257:ILE:HG13	2.16	0.45
2:B:314:VAL:CG1	2:B:315:HIS:H	2.24	0.45
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.16	0.45
1:A:170:PRO:HG2	1:A:171:PHE:H	1.80	0.45
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.34	0.45
2:B:345:PRO:C	2:B:346:PHE:CD1	2.95	0.45
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.97	0.45
1:A:280:SER:C	1:A:282:LEU:N	2.74	0.45
1:A:402:TRP:CE3	1:A:402:TRP:C	2.94	0.45
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.80	0.45
1:A:88:TRP:O	1:A:89:GLU:C	2.59	0.45
2:B:100:LEU:HD11	2:B:106:VAL:HG11	1.98	0.45
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.79	0.45
2:B:295:LEU:CB	2:B:300:GLU:HG2	2.46	0.45
2:B:374:LYS:HE2	2:B:378:GLU:OE2	2.15	0.45
1:A:12:LEU:O	1:A:13:LYS:O	2.34	0.45
1:A:164:MET:HB3	1:A:182:GLN:HE22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD12	1:A:303:LEU:HD11	1.99	0.45
1:A:398:TRP:CD1	1:A:399:GLU:N	2.84	0.45
1:A:493:VAL:HG22	1:A:494:ASN:H	1.80	0.45
1:A:3:SER:HB3	1:A:4:PRO:HD2	1.98	0.45
2:B:94:ILE:HA	2:B:95:PRO:HD2	1.75	0.45
2:B:151:GLN:C	2:B:153:TRP:H	2.24	0.45
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.51	0.45
2:B:205:LEU:O	2:B:206:ARG:C	2.58	0.45
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.98	0.45
2:B:128:THR:CB	2:B:146:TYR:HB2	2.47	0.45
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.99	0.45
1:A:5:ILE:HD13	1:A:167:ILE:HD11	1.99	0.45
1:A:34:LEU:CB	1:A:132:ILE:HG21	2.47	0.45
1:A:155:GLY:O	1:A:159:ILE:HD12	2.17	0.45
2:B:39:THR:O	2:B:43:LYS:HG3	2.16	0.45
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.97	0.45
2:B:23:GLN:HG3	2:B:131:THR:O	2.17	0.45
1:A:19:PRO:O	1:A:56:TYR:HB3	2.17	0.45
1:A:216:THR:HB	1:A:217:PRO:HD2	1.99	0.45
1:A:249:LYS:HG3	1:A:250:ASP:N	2.21	0.45
1:A:250:ASP:OD2	1:A:250:ASP:N	2.50	0.45
1:A:394:GLN:O	1:A:396:GLU:N	2.50	0.45
2:B:315:HIS:C	2:B:317:VAL:N	2.75	0.45
1:A:406:TRP:CE3	1:A:406:TRP:C	2.95	0.44
1:A:473:THR:O	1:A:474:ASN:C	2.60	0.44
2:B:162:SER:O	2:B:164:MET:N	2.49	0.44
1:A:12:LEU:CD1	1:A:127:TYR:CE2	3.01	0.44
2:B:164:MET:C	2:B:166:LYS:H	2.25	0.44
2:B:345:PRO:C	2:B:346:PHE:HD1	2.26	0.44
1:A:122:GLU:O	1:A:125:ARG:HG3	2.18	0.44
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.52	0.44
1:A:134:SER:CB	1:A:140:PRO:CD	2.96	0.44
1:A:151:GLN:HA	1:A:151:GLN:HE21	1.82	0.44
1:A:405:TYR:O	2:B:331:LYS:HD3	2.18	0.44
1:A:17:ASP:CG	1:A:18:GLY:H	2.26	0.44
1:A:130:PHE:CD1	1:A:130:PHE:N	2.86	0.44
1:A:265:ASN:O	1:A:266:TRP:C	2.60	0.44
1:A:350:LYS:HB3	1:A:350:LYS:HZ2	1.81	0.44
1:A:371:ALA:O	1:A:372:VAL:C	2.60	0.44
1:A:537:PRO:O	1:A:541:GLY:HA3	2.18	0.44
2:B:68:SER:O	2:B:69:THR:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:THR:HA	2:B:398:TRP:HH2	1.83	0.44
1:A:94:ILE:CG2	1:A:229:TRP:CH2	3.01	0.44
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.48	0.44
1:A:522:ILE:O	1:A:525:LEU:N	2.50	0.44
1:A:12:LEU:HD11	1:A:127:TYR:CD2	2.53	0.44
1:A:369:THR:HG1	1:A:398:TRP:HZ3	1.65	0.44
2:B:1:PRO:HB2	2:B:2:ILE:H	1.62	0.44
2:B:151:GLN:O	2:B:152:GLY:C	2.60	0.44
1:A:303:LEU:O	1:A:307:ARG:HG3	2.19	0.43
2:B:66:LYS:HZ2	2:B:218:ASP:HB3	1.82	0.43
2:B:295:LEU:HB2	2:B:300:GLU:HG2	2.00	0.43
2:B:363:ASN:HB3	2:B:366:LYS:HB3	2.00	0.43
1:A:430:GLU:OE1	1:A:530:LYS:HE3	2.18	0.43
2:B:214:LEU:HG	2:B:214:LEU:O	2.18	0.43
2:B:249:LYS:HE2	2:B:252:TRP:CE3	2.53	0.43
1:A:508:ALA:C	1:A:510:PRO:HD3	2.44	0.43
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	0.43
2:B:423:VAL:HG13	2:B:426:TRP:HE3	1.83	0.43
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.28	0.43
1:A:116:PHE:HA	1:A:148:VAL:HG21	2.00	0.43
1:A:350:LYS:HE3	1:A:378:GLU:OE2	2.18	0.43
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.52	0.43
2:B:91:GLN:HE21	2:B:91:GLN:CA	2.32	0.43
2:B:257:ILE:O	2:B:260:LEU:HB3	2.18	0.43
2:B:305:GLU:OE2	2:B:309:ILE:HD11	2.18	0.43
1:A:193:LEU:HB3	1:A:197:GLN:HG3	2.01	0.43
1:A:399:GLU:HG3	1:A:402:TRP:HE1	1.83	0.43
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.53	0.43
1:A:280:SER:O	1:A:281:LYS:C	2.60	0.43
2:B:241:VAL:CG2	2:B:242:GLN:N	2.76	0.43
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.54	0.43
1:A:297:GLU:H	1:A:297:GLU:CD	2.27	0.43
1:A:402:TRP:CZ3	1:A:403:THR:HA	2.54	0.43
2:B:87:PHE:C	2:B:88:TRP:CD1	2.97	0.43
2:B:153:TRP:O	2:B:155:GLY:N	2.43	0.43
2:B:342:TYR:CD1	2:B:342:TYR:C	2.97	0.43
2:B:358:ARG:O	2:B:362:THR:CB	2.67	0.43
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.43
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.54	0.43
1:A:126:LYS:HB3	1:A:126:LYS:HZ3	1.81	0.43
1:A:154:LYS:O	1:A:156:SER:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.54	0.43
1:A:334:GLN:HE21	1:A:334:GLN:HB3	1.68	0.43
2:B:90:VAL:O	2:B:91:GLN:C	2.62	0.43
1:A:22:LYS:HD2	1:A:22:LYS:HA	1.69	0.43
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.49	0.43
1:A:154:LYS:C	1:A:156:SER:H	2.26	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.43
1:A:277:ARG:HH21	1:A:281:LYS:HE2	1.84	0.43
1:A:507:GLN:C	1:A:509:GLN:H	2.26	0.43
2:B:426:TRP:O	2:B:426:TRP:HD1	2.01	0.43
1:A:390:LYS:C	1:A:391:LEU:HG	2.44	0.42
1:A:460:ASN:C	1:A:462:GLY:N	2.77	0.42
1:A:514:GLU:OE1	1:A:514:GLU:N	2.51	0.42
2:B:219:LYS:HB3	2:B:219:LYS:HZ3	1.84	0.42
2:B:340:GLN:N	2:B:340:GLN:CD	2.76	0.42
2:B:349:LEU:O	2:B:350:LYS:HB2	2.19	0.42
1:A:248:GLU:HB3	1:A:307:ARG:NH2	2.34	0.42
2:B:365:VAL:C	2:B:367:GLN:N	2.77	0.42
2:B:398:TRP:O	2:B:402:TRP:HD1	2.01	0.42
1:A:27:THR:O	1:A:28:GLU:C	2.62	0.42
1:A:138:GLU:O	1:A:138:GLU:CG	2.64	0.42
1:A:171:PHE:C	1:A:173:LYS:H	2.26	0.42
1:A:240:THR:C	1:A:241:VAL:CG2	2.92	0.42
1:A:524:GLN:O	1:A:525:LEU:C	2.63	0.42
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.54	0.42
2:B:125:ARG:O	2:B:126:LYS:C	2.61	0.42
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
1:A:69:THR:O	1:A:69:THR:HG22	2.19	0.42
1:A:201:LYS:CA	1:A:204:GLU:HG3	2.50	0.42
2:B:24:TRP:CD1	2:B:24:TRP:H	2.37	0.42
2:B:249:LYS:HG2	2:B:252:TRP:CZ2	2.54	0.42
2:B:418:ASN:O	2:B:419:THR:HB	2.18	0.42
1:A:540:LYS:HE3	2:B:265:ASN:ND2	2.32	0.42
2:B:306:ASN:HD22	2:B:309:ILE:CD1	2.28	0.42
2:B:332:GLN:CB	2:B:336:GLN:O	2.67	0.42
2:B:346:PHE:CD1	2:B:346:PHE:N	2.87	0.42
1:A:3:SER:HB2	1:A:5:ILE:HD12	2.00	0.42
1:A:34:LEU:HB2	1:A:132:ILE:HG21	2.01	0.42
1:A:507:GLN:O	1:A:509:GLN:HG3	2.19	0.42
2:B:171:PHE:CD1	2:B:171:PHE:C	2.98	0.42
2:B:353:LYS:O	2:B:353:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.42
1:A:169:GLU:O	1:A:170:PRO:C	2.58	0.42
1:A:208:HIS:O	1:A:209:LEU:C	2.62	0.42
1:A:218:ASP:O	1:A:220:LYS:N	2.47	0.42
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.53	0.42
1:A:443:ASP:CG	1:A:444:GLY:H	2.27	0.42
2:B:388:LYS:HA	2:B:413:GLU:O	2.19	0.42
1:A:94:ILE:HG23	1:A:229:TRP:CZ2	2.55	0.42
1:A:112:GLY:C	1:A:114:ALA:N	2.78	0.42
1:A:411:ILE:C	1:A:412:PRO:O	2.62	0.42
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.55	0.42
1:A:233:GLU:OE2	1:A:242:GLN:CG	2.68	0.42
1:A:443:ASP:CG	1:A:444:GLY:N	2.78	0.42
1:A:325:LEU:HD22	1:A:341:ILE:HG21	2.02	0.41
2:B:23:GLN:NE2	2:B:23:GLN:C	2.78	0.41
2:B:181:TYR:CD1	2:B:182:GLN:N	2.88	0.41
1:A:275:LYS:C	1:A:276:VAL:HG23	2.45	0.41
1:A:550:LYS:C	1:A:552:VAL:N	2.77	0.41
2:B:278:GLN:HE21	2:B:278:GLN:CA	2.32	0.41
2:B:340:GLN:CG	2:B:426:TRP:CZ2	3.00	0.41
1:A:260:LEU:HD11	1:A:303:LEU:HD11	2.01	0.41
1:A:277:ARG:NH1	1:A:334:GLN:HB2	2.35	0.41
1:A:394:GLN:O	1:A:395:LYS:C	2.62	0.41
1:A:394:GLN:C	1:A:396:GLU:N	2.78	0.41
2:B:28:GLU:HG3	2:B:135:ILE:HD11	2.02	0.41
2:B:118:VAL:O	2:B:149:LEU:HD12	2.19	0.41
2:B:206:ARG:HG3	2:B:206:ARG:HH11	1.85	0.41
2:B:275:LYS:HG2	2:B:277:ARG:HD3	2.02	0.41
1:A:50:ILE:O	1:A:143:ARG:HB3	2.21	0.41
1:A:83:ARG:NH1	1:A:83:ARG:CG	2.83	0.41
1:A:334:GLN:H	1:A:334:GLN:HG2	1.65	0.41
2:B:165:THR:O	2:B:169:GLU:HB2	2.20	0.41
2:B:178:ILE:HD11	2:B:201:LYS:CG	2.50	0.41
2:B:254:VAL:O	2:B:258:GLN:HG3	2.20	0.41
1:A:249:LYS:HG2	1:A:251:SER:OG	2.21	0.41
2:B:44:GLU:OE1	2:B:46:LYS:HE3	2.20	0.41
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.87	0.41
2:B:241:VAL:CG1	2:B:243:PRO:HD3	2.43	0.41
2:B:253:THR:OG1	2:B:256:ASP:OD2	2.24	0.41
1:A:55:PRO:HB2	1:A:56:TYR:H	1.54	0.41
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:PRO:HA	2:B:417:VAL:HG22	2.03	0.41
1:A:66:LYS:O	1:A:68:SER:N	2.54	0.41
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.55	0.41
1:A:183:TYR:CE1	1:A:229:TRP:NE1	2.89	0.41
2:B:188:TYR:CD1	2:B:188:TYR:N	2.88	0.41
1:A:503:LEU:O	1:A:504:GLY:C	2.64	0.41
2:B:164:MET:O	2:B:166:LYS:N	2.53	0.41
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.51	0.41
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.84	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.81	0.41
1:A:516:GLU:HG2	1:A:517:LEU:N	2.35	0.41
2:B:67:ASP:O	2:B:68:SER:C	2.64	0.41
2:B:135:ILE:C	2:B:137:ASN:N	2.79	0.41
2:B:214:LEU:C	2:B:215:THR:O	2.60	0.41
2:B:246:LEU:HD12	2:B:307:ARG:HG2	2.02	0.41
1:A:132:ILE:HD11	1:A:142:ILE:HG21	2.02	0.41
1:A:200:THR:O	1:A:201:LYS:C	2.64	0.41
1:A:219:LYS:C	1:A:221:HIS:N	2.77	0.41
1:A:416:PHE:CZ	1:A:418:ASN:HA	2.56	0.41
2:B:160:PHE:O	2:B:162:SER:N	2.54	0.41
1:A:56:TYR:O	1:A:143:ARG:NH2	2.53	0.40
1:A:173:LYS:O	1:A:176:PRO:HD3	2.20	0.40
1:A:253:THR:O	1:A:254:VAL:C	2.63	0.40
2:B:319:TYR:O	2:B:321:PRO:HD3	2.22	0.40
1:A:92:LEU:C	1:A:92:LEU:HD12	2.46	0.40
1:A:197:GLN:HA	1:A:200:THR:OG1	2.21	0.40
1:A:402:TRP:CE3	1:A:403:THR:N	2.89	0.40
1:A:547:GLN:HE21	1:A:547:GLN:C	2.29	0.40
2:B:2:ILE:O	2:B:2:ILE:HG22	2.21	0.40
2:B:183:TYR:CD1	2:B:380:ILE:HG23	2.57	0.40
1:A:27:THR:HG23	1:A:27:THR:O	2.21	0.40
1:A:263:LYS:HB2	1:A:263:LYS:HE3	1.80	0.40
1:A:275:LYS:O	1:A:276:VAL:CG2	2.69	0.40
1:A:317:VAL:HG22	1:A:318:TYR:N	2.36	0.40
2:B:221:HIS:HD2	2:B:229:TRP:CB	2.34	0.40
2:B:253:THR:CG2	2:B:292:VAL:HG22	2.44	0.40
2:B:255:ASN:O	2:B:259:LYS:HG3	2.21	0.40
2:B:426:TRP:O	2:B:426:TRP:CD1	2.74	0.40
1:A:103:LYS:HE2	1:A:179:VAL:HG21	2.02	0.40
1:A:161:GLN:C	1:A:161:GLN:HE21	2.28	0.40
1:A:344:GLU:HG3	1:A:345:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:GLY:O	2:B:159:ILE:HG13	2.21	0.40
2:B:340:GLN:HB3	2:B:348:ASN:HD22	1.87	0.40
2:B:423:VAL:HG13	2:B:426:TRP:CE3	2.55	0.40
1:A:60:VAL:O	1:A:61:PHE:HD1	2.02	0.40
1:A:458:VAL:HG13	1:A:464:GLN:HG2	2.02	0.40
2:B:79:GLU:C	2:B:81:ASN:N	2.78	0.40
2:B:167:ILE:HA	2:B:212:TRP:CE3	2.57	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	550/560 (98%)	414 (75%)	100 (18%)	36 (6%)	1	1
2	B	425/430 (99%)	313 (74%)	75 (18%)	37 (9%)	0	1
All	All	975/990 (98%)	727 (75%)	175 (18%)	73 (8%)	1	1

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	90	VAL
1	A	114	ALA
1	A	242	GLN
1	A	357	MET
1	A	491	LEU
1	A	516	GLU
2	B	116	PHE
2	B	126	LYS
2	B	195	ILE
2	B	220	LYS

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Mol	Chain	Res	Type
2	B	421	PRO
1	A	66	LYS
1	A	195	ILE
1	A	276	VAL
1	A	295	LEU
1	A	296	THR
1	A	412	PRO
1	A	543	GLY
2	B	12	LEU
2	B	18	GLY
2	B	67	ASP
2	B	85	GLN
2	B	103	LYS
2	B	154	LYS
2	B	163	SER
2	B	174	GLN
2	B	214	LEU
2	B	284	ARG
2	B	296	THR
2	B	314	VAL
2	B	316	GLY
2	B	366	LYS
2	B	376	THR
2	B	377	THR
1	A	92	LEU
1	A	151	GLN
1	A	220	LYS
1	A	289	LEU
1	A	395	LYS
1	A	528	LYS
2	B	161	GLN
2	B	240	THR
2	B	272	PRO
2	B	355	ALA
1	A	16	MET
1	A	54	ASN
1	A	70	LYS
1	A	503	LEU
1	A	538	ALA
2	B	2	ILE
2	B	68	SER
1	A	140	PRO

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Mol	Chain	Res	Type
1	A	241	VAL
1	A	359	GLY
2	B	176	PRO
2	B	345	PRO
1	A	176	PRO
1	A	309	ILE
2	B	111	VAL
2	B	313	PRO
2	B	412	PRO
2	B	419	THR
1	A	52	PRO
1	A	155	GLY
1	A	243	PRO
1	A	274	ILE
2	B	231	GLY
1	A	4	PRO
1	A	13	LYS
2	B	217	PRO
2	B	225	PRO
2	B	241	VAL

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	477/500 (95%)	414 (87%)	63 (13%)	4	12
2	B	375/392 (96%)	334 (89%)	41 (11%)	6	18
All	All	852/892 (96%)	748 (88%)	104 (12%)	5	14

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	39	THR
1	A	43	LYS

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Mol	Chain	Res	Type
1	A	55	PRO
1	A	56	TYR
1	A	60	VAL
1	A	65	LYS
1	A	76	ASP
1	A	84	THR
1	A	92	LEU
1	A	126	LYS
1	A	130	PHE
1	A	131	THR
1	A	132	ILE
1	A	143	ARG
1	A	156	SER
1	A	161	GLN
1	A	165	THR
1	A	177	ASP
1	A	184	MET
1	A	195	ILE
1	A	199	ARG
1	A	217	PRO
1	A	218	ASP
1	A	224	GLU
1	A	241	VAL
1	A	244	ILE
1	A	246	LEU
1	A	250	ASP
1	A	253	THR
1	A	324	ASP
1	A	334	GLN
1	A	344	GLU
1	A	350	LYS
1	A	361	HIS
1	A	364	ASP
1	A	367	GLN
1	A	387	PRO
1	A	395	LYS
1	A	397	THR
1	A	399	GLU
1	A	403	THR
1	A	409	THR
1	A	414	TRP
1	A	435	VAL

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Mol	Chain	Res	Type
1	A	448	ARG
1	A	460	ASN
1	A	466	VAL
1	A	492	GLU
1	A	496	VAL
1	A	497	THR
1	A	500	GLN
1	A	507	GLN
1	A	511	ASP
1	A	516	GLU
1	A	523	GLU
1	A	526	ILE
1	A	533	LEU
1	A	537	PRO
1	A	545	ASN
1	A	547	GLN
1	A	548	VAL
1	A	551	LEU
2	B	11	LYS
2	B	12	LEU
2	B	50	ILE
2	B	67	ASP
2	B	91	GLN
2	B	113	ASP
2	B	126	LYS
2	B	142	ILE
2	B	145	GLN
2	B	149	LEU
2	B	169	GLU
2	B	176	PRO
2	B	194	GLU
2	B	201	LYS
2	B	207	GLN
2	B	211	ARG
2	B	212	TRP
2	B	218	ASP
2	B	219	LYS
2	B	221	HIS
2	B	232	TYR
2	B	249	LYS
2	B	250	ASP
2	B	257	ILE

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Mol	Chain	Res	Type
2	B	274	ILE
2	B	284	ARG
2	B	290	THR
2	B	297	GLU
2	B	298	GLU
2	B	300	GLU
2	B	310	LEU
2	B	315	HIS
2	B	324	ASP
2	B	334	GLN
2	B	348	ASN
2	B	349	LEU
2	B	367	GLN
2	B	369	THR
2	B	372	VAL
2	B	380	ILE
2	B	386	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	151	GLN
1	A	161	GLN
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	242	GLN
1	A	330	GLN
1	A	332	GLN
1	A	334	GLN
1	A	367	GLN
1	A	418	ASN
1	A	460	ASN
1	A	471	ASN
1	A	474	ASN
1	A	494	ASN
1	A	509	GLN
1	A	519	ASN
1	A	545	ASN
1	A	547	GLN
2	B	54	ASN

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Mol	Chain	Res	Type
2	B	91	GLN
2	B	96	HIS
2	B	145	GLN
2	B	207	GLN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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$
4	357	A	562	-	24,25,25	1.96	6 (25%)	28,34,34	2.25	8 (28%)

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
4	357	A	562	-	-	1/14/14/14	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	562	357	C6-C5	4.82	1.43	1.36
4	A	562	357	C7'-C4	2.79	1.55	1.51
4	A	562	357	C2B-C1'	2.70	1.43	1.39
4	A	562	357	O8-C2	2.68	1.28	1.23
4	A	562	357	C2B-C3B	2.44	1.42	1.39
4	A	562	357	C7'-C1'	2.41	1.55	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	562	357	C6'-N1'-C2'	-5.60	104.74	115.90
4	A	562	357	C3-C2-N1	5.26	120.20	110.94
4	A	562	357	C2-N1-C6	-4.41	123.04	126.25
4	A	562	357	C7-C6-N1	3.59	117.59	113.42
4	A	562	357	C5'-O4'-C3'	2.91	130.44	112.90
4	A	562	357	C10-C5-C4	2.76	121.33	116.90
4	A	562	357	O8-C2-C3	-2.73	120.92	127.62
4	A	562	357	C7-C6-C5	-2.32	121.93	126.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	562	357	C3'-C2'-N1'-C6'

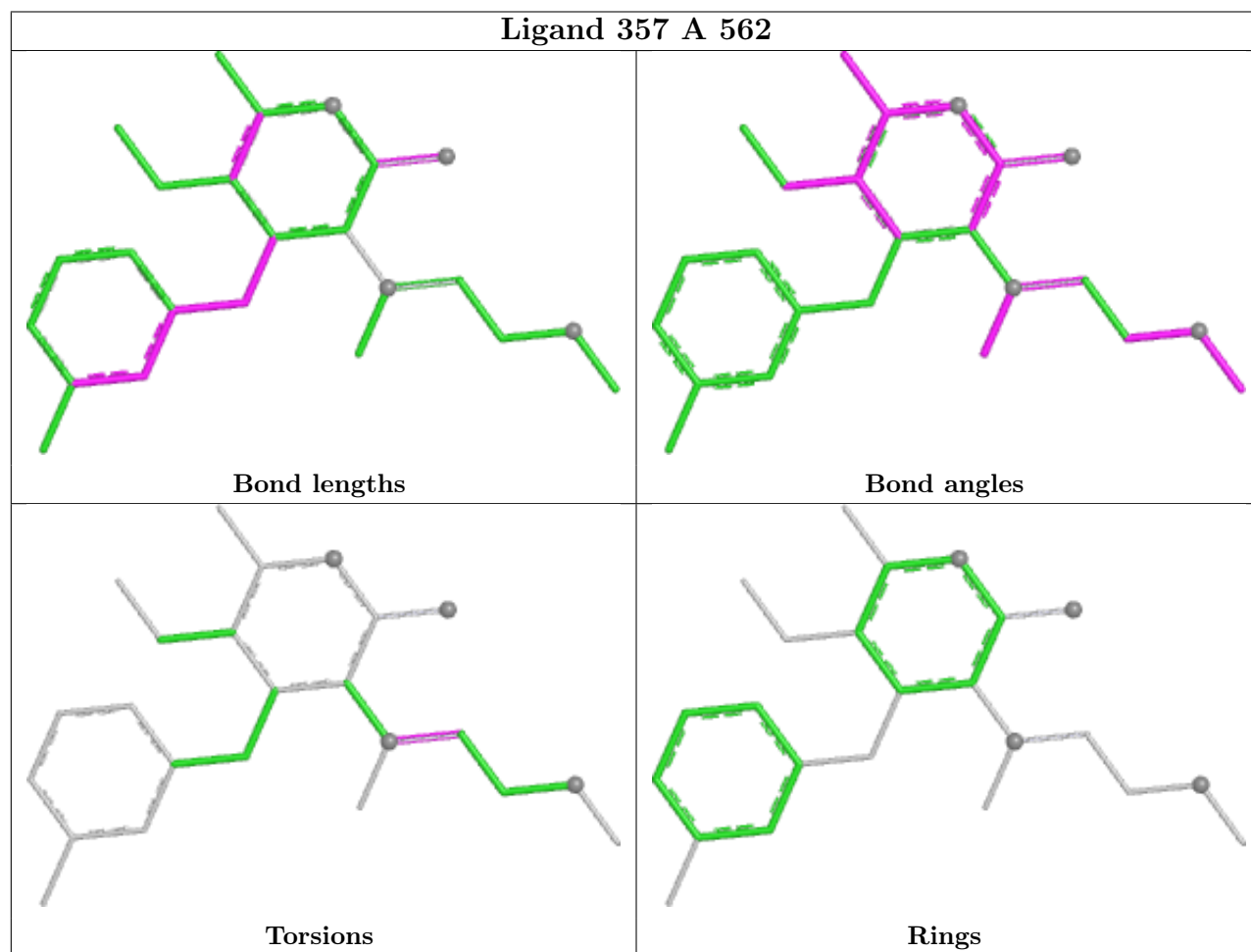
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	562	357	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	552/560 (98%)	-0.18	10 (1%) 67 59	46, 94, 118, 126	0
2	B	427/430 (99%)	-0.34	5 (1%) 76 71	38, 80, 120, 127	0
All	All	979/990 (98%)	-0.25	15 (1%) 72 65	38, 90, 119, 127	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ILE	4.8
1	A	133	PRO	3.2
1	A	71	TRP	3.2
1	A	548	VAL	3.1
2	B	231	GLY	2.7
2	B	3	SER	2.7
1	A	547	GLN	2.7
1	A	55	PRO	2.6
2	B	65	LYS	2.5
1	A	541	GLY	2.3
1	A	128	THR	2.3
1	A	552	VAL	2.2
2	B	213	GLY	2.2
1	A	394	GLN	2.2
1	A	68	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

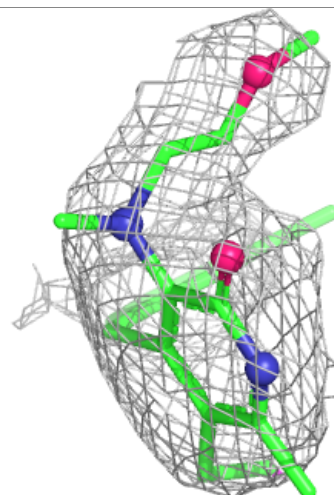
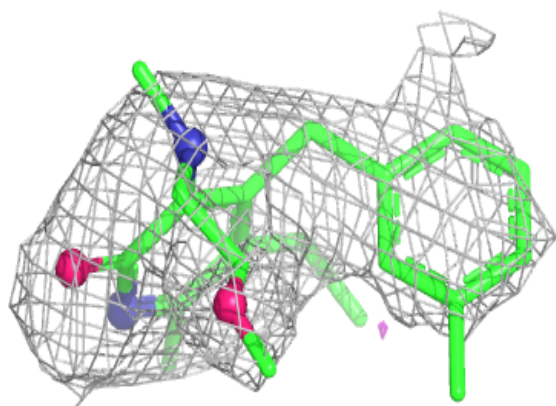
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	357	A	562	24/24	0.96	0.10	72,79,87,89	0
3	MN	A	561	1/1	0.98	0.02	85,85,85,85	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 357 A 562:

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.