



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:35 PM UTC

PDB ID : 1BQM / pdb_00001bqm
Title : HIV-1 RT/HBY 097
Authors : Hsiou, Y.; Das, K.; Ding, J.; Arnold, E.
Deposited on : 1998-08-17
Resolution : 3.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

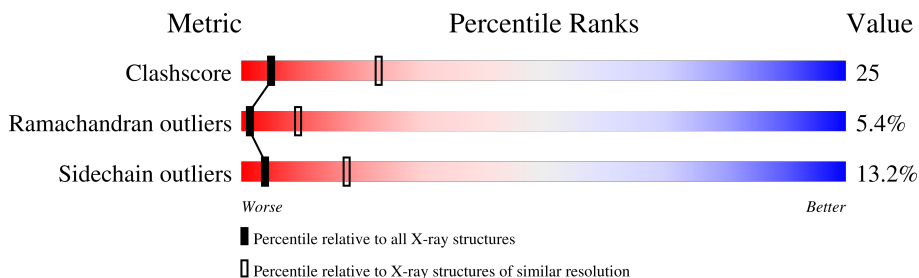
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	
2	B	430	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HBV	A	557	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7799 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	0	0
			4338	2804	719	808	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

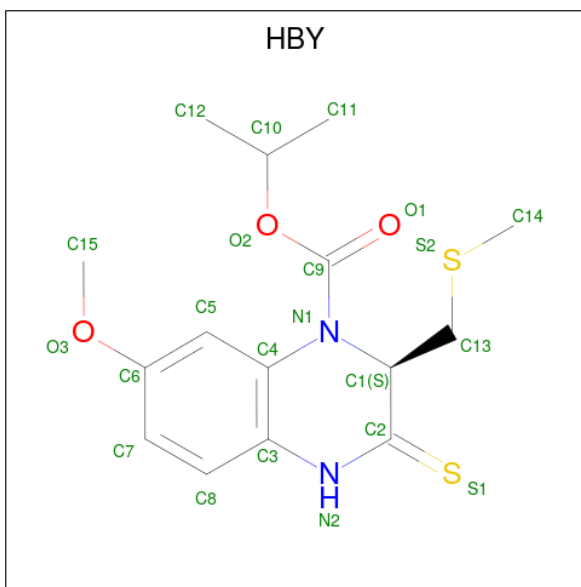
- Molecule 2 is a protein called REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3439	2240	567	627	5			

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 (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMETHYL-3,4-DIHYDROQUINOXALIN-2(1H)-THIONE (CCD ID: HBY) (formula: C₁₅H₂₀N₂O₃S₂).



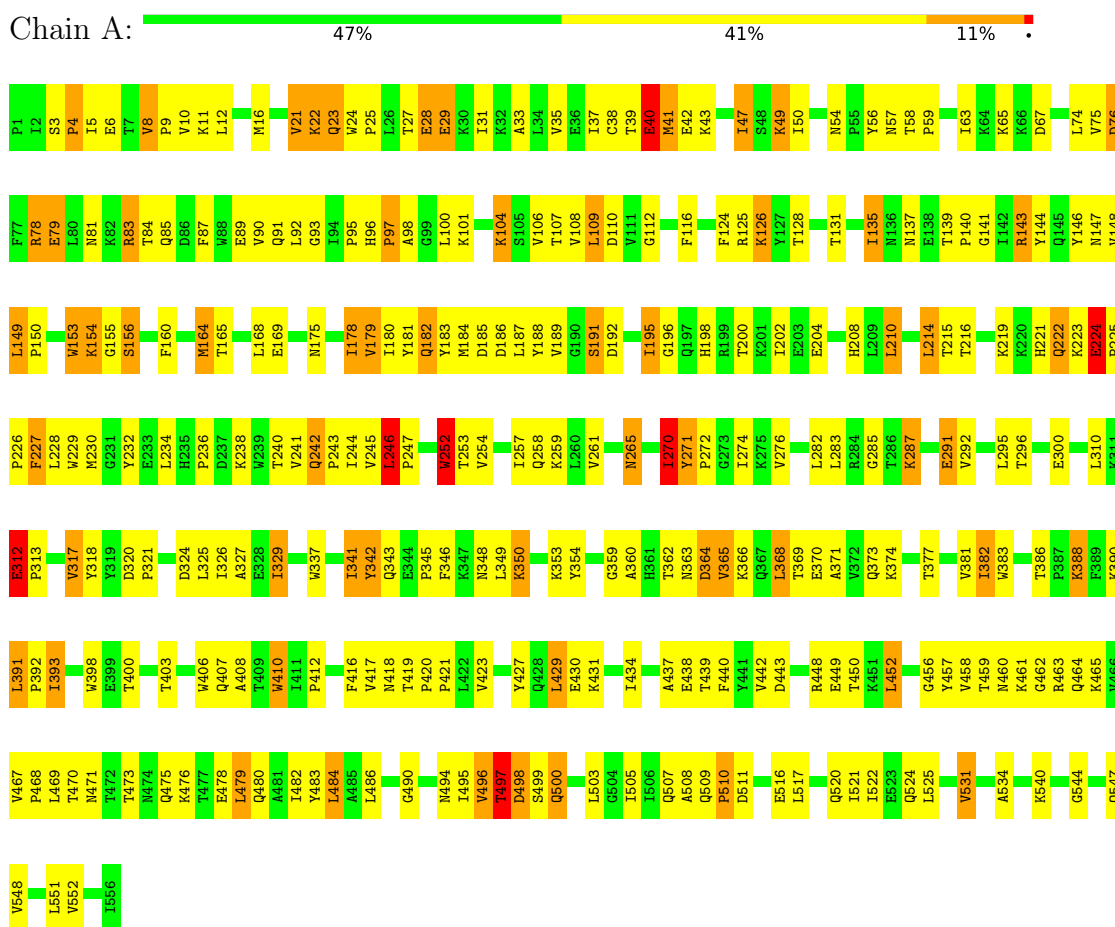
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	22	15	2	3	2	0	0

3 Residue-property plots

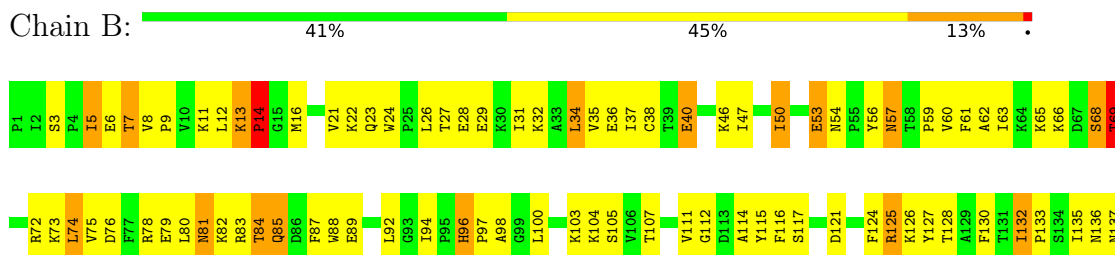
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: REVERSE TRANSCRIPTASE



• Molecule 2: REVERSE TRANSCRIPTASE



E370	E298	T216	E138
A371	E298	P217	T142
A372	L303	D218	R143
A373	A304	K219	Y144
I375	E305	Q222	Q145
T376	N306	K223	N147
T377	R307	E224	V148
	E308	P225	L149
I380	I309	P226	P150
I381	L310	W230	Q151
I382	K311		G152
W383	V314	E233	W153
	R315	H315	K154
T386	G316	P236	G155
F389	V317		S156
K390	Y318	W239	P157
L391	Y319	T240	
I393	D324	V241	S163
K394		Q242	M164
K395	A327	P243	T165
E396	A327	T244	K166
	E328	V245	L167
I397	I329	L246	L168
W398	Q330	P247	E169
E399	K331		P170
T400	Q332	D250	
W401		S251	Q174
W402	Q336	W252	N175
T403	W337	T253	
E404	T338	V254	Y181
Y405	Y339		Y182
W406	Q340	T257	Y183
Q407		Q258	M184
A408	Q343	K259	D186
T409	E344	L260	L187
W410	P345	V261	Y188
I411	F346		
A412	K347	W266	L195
E413	K348	A267	G196
W414	L349	S268	Q197
	K350	Q269	H198
N418	T351	T270	
T419	G352	V271	K201
A420	K353	P272	I202
A421	Y354	G273	E203
L422	A355	T274	E204
	R356		
L425	W357	L279	L205
W426	R358		R206
		L282	Q207
Q428			H208
L429	T362	L289	L209
E430	K363	T290	L210
	D364	E291	R211
	V365	V292	G212
	K366	T293	G213
	Q367	L294	L214
	L368	T295	T215
	T260		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.20 Å 69.40 Å 104.60 Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10	Depositor
% Data completeness (in resolution range)	99.1 (10.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.258 , 0.362	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7799	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.63	0/4451	1.23	64/6070 (1.1%)
2	B	0.66	0/3538	1.36	66/4821 (1.4%)
All	All	0.65	0/7989	1.29	130/10891 (1.2%)

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	380	ILE	N-CA-C	-11.54	100.24	110.74
2	B	89	GLU	N-CA-C	-10.96	99.47	113.72
2	B	401	TRP	N-CA-C	10.12	125.44	113.20
2	B	241	VAL	N-CA-C	9.50	121.94	107.78
2	B	87	PHE	N-CA-C	-9.44	102.13	114.31
2	B	84	THR	N-CA-C	8.77	120.45	111.07
2	B	81	ASN	N-CA-C	-8.54	101.66	110.97
2	B	344	GLU	CA-C-N	8.35	130.27	119.84
2	B	344	GLU	C-N-CA	8.35	130.27	119.84
1	A	8	VAL	CA-C-N	8.34	131.63	120.79
1	A	8	VAL	C-N-CA	8.34	131.63	120.79
2	B	132	ILE	CA-C-N	8.06	128.01	120.03
2	B	132	ILE	C-N-CA	8.06	128.01	120.03
1	A	224	GLU	N-CA-C	8.06	119.92	109.93
1	A	270	ILE	N-CA-C	8.05	119.05	111.48
2	B	175	ASN	CA-C-N	8.02	129.86	119.84
2	B	175	ASN	C-N-CA	8.02	129.86	119.84
1	A	41	MET	N-CA-C	-7.97	103.69	113.41
1	A	342	TYR	N-CA-C	7.91	121.78	109.52
2	B	121	ASP	N-CA-C	7.91	121.75	109.96
2	B	293	ILE	N-CA-C	7.90	116.50	107.89
1	A	497	THR	N-CA-C	7.83	122.60	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	PHE	N-CA-C	7.54	121.74	109.59
2	B	382	ILE	N-CA-C	7.51	118.43	111.45
1	A	386	THR	CA-C-N	7.41	127.39	119.76
1	A	386	THR	C-N-CA	7.41	127.39	119.76
2	B	391	LEU	N-CA-C	7.38	119.08	109.93
2	B	7	THR	N-CA-C	7.25	121.22	109.40
2	B	419	THR	CA-C-N	7.24	127.84	120.38
2	B	419	THR	C-N-CA	7.24	127.84	120.38
2	B	85	GLN	N-CA-C	7.22	123.34	113.37
1	A	63	ILE	N-CA-C	7.21	124.33	109.34
1	A	270	ILE	CB-CA-C	-7.19	105.60	111.71
1	A	224	GLU	CA-C-N	7.16	127.75	120.38
1	A	224	GLU	C-N-CA	7.16	127.75	120.38
2	B	348	ASN	N-CA-C	7.10	119.37	109.15
2	B	12	LEU	N-CA-C	7.09	121.60	110.32
2	B	376	THR	N-CA-C	6.98	119.91	111.40
2	B	366	LYS	N-CA-C	-6.87	103.54	112.68
2	B	143	ARG	N-CA-C	6.85	120.49	107.75
2	B	8	VAL	CB-CA-C	-6.84	103.01	110.95
1	A	225	PRO	N-CA-C	6.82	119.02	110.70
2	B	414	TRP	N-CA-C	6.80	119.51	109.24
1	A	143	ARG	N-CA-C	6.76	119.42	108.34
1	A	521	ILE	N-CA-C	-6.75	103.64	111.00
1	A	208	HIS	N-CA-C	-6.73	104.02	111.36
1	A	500	GLN	N-CA-C	-6.69	103.46	111.69
2	B	310	LEU	N-CA-C	-6.64	105.07	112.57
1	A	391	LEU	N-CA-C	6.57	121.14	108.45
2	B	36	GLU	N-CA-C	-6.55	104.22	111.36
2	B	3	SER	CA-C-N	6.44	128.15	120.23
2	B	3	SER	C-N-CA	6.44	128.15	120.23
2	B	215	THR	N-CA-C	-6.41	100.35	109.96
1	A	312	GLU	CA-C-N	6.40	127.84	119.84
1	A	312	GLU	C-N-CA	6.40	127.84	119.84
1	A	365	VAL	N-CA-C	-6.40	104.27	110.42
1	A	38	CYS	N-CA-C	6.38	118.23	111.28
2	B	408	ALA	N-CA-C	6.33	118.76	108.76
1	A	498	ASP	N-CA-C	-6.26	104.08	111.03
1	A	456	GLY	N-CA-C	6.24	118.81	111.63
2	B	309	ILE	N-CA-C	-6.22	104.55	113.07
1	A	343	GLN	N-CA-C	-6.21	101.57	111.02
2	B	68	SER	N-CA-C	6.20	119.20	109.96
2	B	314	VAL	N-CA-C	6.16	122.16	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	GLU	N-CA-C	-6.12	103.34	111.24
1	A	191	SER	N-CA-C	6.12	116.17	108.45
1	A	204	GLU	N-CA-C	-6.12	104.53	111.14
1	A	484	LEU	N-CA-C	-6.11	103.56	111.02
2	B	203	GLU	N-CA-C	-6.11	104.62	111.28
1	A	165	THR	N-CA-C	-6.11	105.65	113.23
1	A	49	LYS	N-CA-C	6.11	119.14	108.52
1	A	388	LYS	N-CA-C	-6.10	99.92	109.25
2	B	94	ILE	CA-C-N	6.09	126.03	119.76
2	B	94	ILE	C-N-CA	6.09	126.03	119.76
2	B	57	ASN	N-CA-C	6.07	116.44	107.88
2	B	149	LEU	CA-C-N	6.06	125.82	119.76
2	B	149	LEU	C-N-CA	6.06	125.82	119.76
1	A	252	TRP	N-CA-C	6.05	119.94	110.32
2	B	169	GLU	N-CA-C	6.04	121.74	113.77
2	B	40	GLU	N-CA-C	-6.02	104.72	111.28
1	A	29	GLU	N-CA-C	5.99	117.81	111.28
2	B	96	HIS	CA-C-N	5.98	127.31	119.84
2	B	96	HIS	C-N-CA	5.98	127.31	119.84
2	B	386	THR	CA-C-N	5.94	125.91	120.03
2	B	386	THR	C-N-CA	5.94	125.91	120.03
2	B	174	GLN	N-CA-C	-5.93	105.53	112.89
2	B	224	GLU	N-CA-C	-5.92	103.20	110.31
1	A	195	ILE	N-CA-C	5.86	121.53	109.34
1	A	83	ARG	N-CA-C	5.84	118.60	111.82
1	A	214	LEU	N-CA-C	5.81	118.22	108.23
1	A	348	ASN	N-CA-C	5.81	119.72	109.96
1	A	179	VAL	N-CA-C	5.79	121.37	109.34
1	A	499	SER	N-CA-C	5.75	118.79	110.28
2	B	396	GLU	N-CA-C	5.69	119.49	112.54
1	A	23	GLN	N-CA-C	5.64	118.77	110.59
1	A	259	LYS	N-CA-C	-5.63	105.13	112.23
1	A	391	LEU	CA-C-N	5.62	126.87	119.84
1	A	391	LEU	C-N-CA	5.62	126.87	119.84
2	B	16	MET	N-CA-C	5.62	118.74	110.59
2	B	233	GLU	N-CA-C	5.61	117.60	108.63
2	B	358	ARG	N-CA-C	-5.60	105.56	112.90
1	A	410	TRP	N-CA-C	5.57	117.17	107.49
2	B	184	MET	CB-CA-C	-5.57	110.17	116.63
1	A	22	LYS	N-CA-C	-5.56	98.96	110.80
1	A	329	ILE	N-CA-C	5.55	115.98	107.77
1	A	40	GLU	N-CA-C	-5.54	105.13	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	MET	N-CA-C	5.54	118.53	110.17
2	B	324	ASP	N-CA-C	5.53	118.24	109.50
1	A	92	LEU	N-CA-C	-5.52	106.75	112.93
1	A	110	ASP	N-CA-C	5.48	117.66	108.23
1	A	189	VAL	CB-CA-C	-5.46	104.14	110.91
1	A	76	ASP	N-CA-C	5.44	117.11	108.67
2	B	344	GLU	N-CA-C	-5.41	97.85	109.81
2	B	13	LYS	CA-C-N	5.40	126.59	119.84
2	B	13	LYS	C-N-CA	5.40	126.59	119.84
2	B	422	LEU	N-CA-C	-5.39	106.38	113.17
1	A	169	GLU	N-CA-C	5.36	120.85	113.77
1	A	96	HIS	CA-C-N	5.35	126.53	119.84
1	A	96	HIS	C-N-CA	5.35	126.53	119.84
2	B	372	VAL	CB-CA-C	-5.33	104.95	112.14
1	A	245	VAL	N-CA-C	5.30	115.26	107.15
2	B	371	ALA	N-CA-C	-5.30	105.08	112.45
1	A	149	LEU	CA-C-N	5.21	125.42	120.31
1	A	149	LEU	C-N-CA	5.21	125.42	120.31
2	B	142	ILE	N-CA-C	-5.13	99.30	107.15
1	A	382	ILE	N-CA-C	5.12	120.00	109.34
1	A	246	LEU	CA-C-N	5.11	126.23	119.84
1	A	246	LEU	C-N-CA	5.11	126.23	119.84
2	B	428	GLN	N-CA-C	5.11	116.35	107.93
1	A	416	PHE	N-CA-C	5.02	117.58	110.10

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	4338	0	4229	219	0
2	B	3439	0	3390	177	0
3	A	22	0	20	25	0
All	All	7799	0	7639	390	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 25.

All (390) 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)
2:B:26:LEU:HD12	2:B:133:PRO:HG3	1.41	1.03
1:A:327:ALA:HB2	1:A:341:ILE:HG23	1.46	0.97
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.50	0.92
1:A:234:LEU:HB3	3:A:557:HBY:H153	1.53	0.90
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.55	0.89
2:B:38:CYS:HB3	2:B:144:TYR:HE2	1.36	0.88
2:B:210:LEU:HD11	2:B:216:THR:HG23	1.56	0.87
2:B:183:TYR:CE2	2:B:380:ILE:HD12	2.10	0.87
1:A:227:PHE:HD2	3:A:557:HBY:H151	1.40	0.86
1:A:188:TYR:O	3:A:557:HBY:C14	2.24	0.85
1:A:9:PRO:HG2	2:B:53:GLU:HG2	1.59	0.84
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.08	0.83
1:A:98:ALA:HB2	1:A:350:LYS:HG3	1.62	0.82
1:A:419:THR:HG22	1:A:421:PRO:HD2	1.62	0.82
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.15	0.81
2:B:63:ILE:HD11	2:B:74:LEU:HD22	1.59	0.81
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.15	0.81
1:A:240:THR:HG22	1:A:241:VAL:H	1.43	0.81
2:B:339:TYR:CD2	2:B:375:ILE:HD12	2.15	0.81
2:B:305:GLU:O	2:B:309:ILE:HG13	1.79	0.80
1:A:257:ILE:O	1:A:261:VAL:HG23	1.81	0.80
1:A:188:TYR:CE2	3:A:557:HBY:H121	2.18	0.78
2:B:368:LEU:O	2:B:372:VAL:HG23	1.84	0.78
1:A:100:LEU:HD11	3:A:557:HBY:H111	1.66	0.78
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.48	0.78
1:A:430:GLU:HG2	1:A:531:VAL:O	1.83	0.77
1:A:476:LYS:HG3	1:A:517:LEU:HD22	1.64	0.77
1:A:417:VAL:HG12	1:A:418:ASN:H	1.50	0.77
2:B:369:THR:HG23	2:B:406:TRP:HE3	1.49	0.76
1:A:483:TYR:HE1	1:A:524:GLN:HE21	1.33	0.75
2:B:13:LYS:HG2	2:B:14:PRO:HD2	1.68	0.75
1:A:12:LEU:HD23	1:A:84:THR:HA	1.69	0.74
2:B:425:LEU:HD23	2:B:426:TRP:H	1.52	0.74
1:A:459:THR:OG1	1:A:463:ARG:HB3	1.86	0.73
2:B:27:THR:O	2:B:31:ILE:HG13	1.88	0.73
2:B:197:GLN:O	2:B:201:LYS:HE2	1.88	0.73
2:B:319:TYR:HD1	2:B:343:GLN:HE22	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD13	3:A:557:HBY:C4	2.19	0.72
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.70	0.72
1:A:100:LEU:HD13	3:A:557:HBY:N1	2.04	0.72
1:A:101:LYS:HE2	1:A:321:PRO:HD3	1.69	0.72
1:A:326:ILE:HG22	1:A:342:TYR:O	1.90	0.71
2:B:368:LEU:HD21	2:B:391:LEU:HD22	1.71	0.71
1:A:382:ILE:O	2:B:136:ASN:HB2	1.90	0.71
2:B:125:ARG:HG2	2:B:146:TYR:O	1.90	0.71
1:A:98:ALA:CB	1:A:350:LYS:HG3	2.21	0.71
2:B:13:LYS:HD2	2:B:83:ARG:O	1.90	0.70
2:B:27:THR:HG22	2:B:28:GLU:N	2.06	0.70
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.21	0.70
1:A:420:PRO:HG2	1:A:421:PRO:HD3	1.74	0.70
1:A:21:VAL:HG12	1:A:22:LYS:H	1.56	0.69
1:A:483:TYR:HE1	1:A:524:GLN:NE2	1.91	0.69
2:B:310:LEU:O	2:B:311:LYS:HD2	1.92	0.69
1:A:366:LYS:O	1:A:370:GLU:HG3	1.92	0.69
2:B:5:ILE:HG22	2:B:6:GLU:H	1.58	0.69
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.07	0.69
1:A:79:GLU:O	1:A:83:ARG:HD2	1.93	0.68
1:A:188:TYR:O	3:A:557:HBY:H141	1.92	0.68
1:A:439:THR:H	1:A:460:ASN:ND2	1.90	0.68
2:B:351:THR:HG21	2:B:429:LEU:HB3	1.74	0.68
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.75	0.68
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.24	0.68
1:A:227:PHE:CD2	3:A:557:HBY:H151	2.28	0.68
1:A:229:TRP:NE1	3:A:557:HBY:H113	2.09	0.68
2:B:13:LYS:CG	2:B:14:PRO:HD2	2.23	0.67
1:A:382:ILE:HG23	2:B:136:ASN:OD1	1.94	0.67
1:A:31:ILE:O	1:A:35:VAL:HG23	1.95	0.67
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.59	0.67
1:A:188:TYR:O	3:A:557:HBY:H142	1.95	0.67
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.60	0.67
1:A:229:TRP:CD2	3:A:557:HBY:H122	2.29	0.66
1:A:240:THR:HG22	1:A:241:VAL:N	2.11	0.66
1:A:253:THR:HA	1:A:292:VAL:HA	1.78	0.66
2:B:395:LYS:HG2	2:B:399:GLU:OE2	1.96	0.66
2:B:79:GLU:O	2:B:83:ARG:HG2	1.96	0.66
2:B:31:ILE:O	2:B:35:VAL:HG23	1.97	0.65
1:A:496:VAL:HA	1:A:534:ALA:HB3	1.78	0.64
2:B:303:LEU:O	2:B:307:ARG:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD22	3:A:557:HBX:H1	1.79	0.64
1:A:377:THR:O	1:A:381:VAL:HG23	1.98	0.64
2:B:21:VAL:HG12	2:B:22:LYS:H	1.63	0.64
1:A:149:LEU:HD13	1:A:156:SER:HA	1.81	0.63
1:A:282:LEU:H	1:A:282:LEU:HD23	1.64	0.63
2:B:405:TYR:CD1	2:B:405:TYR:N	2.66	0.63
1:A:8:VAL:HG13	1:A:9:PRO:HD2	1.79	0.63
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.80	0.63
2:B:224:GLU:HG2	2:B:225:PRO:HD2	1.80	0.63
1:A:417:VAL:HG12	1:A:418:ASN:N	2.14	0.63
2:B:61:PHE:CZ	2:B:402:TRP:CZ2	2.87	0.63
1:A:479:LEU:HB3	1:A:517:LEU:HD21	1.81	0.62
2:B:405:TYR:HD1	2:B:405:TYR:H	1.46	0.62
1:A:33:ALA:O	1:A:37:ILE:HD13	1.99	0.62
1:A:318:TYR:CE2	3:A:557:HBX:H8	2.34	0.62
2:B:183:TYR:CD2	2:B:380:ILE:HD12	2.33	0.62
2:B:183:TYR:HE2	2:B:380:ILE:HD12	1.63	0.62
1:A:191:SER:OG	1:A:198:HIS:CD2	2.53	0.62
2:B:339:TYR:CG	2:B:375:ILE:HD12	2.34	0.62
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.65	0.62
1:A:10:VAL:HG12	1:A:124:PHE:CE2	2.35	0.61
2:B:54:ASN:OD1	2:B:56:TYR:HD1	1.81	0.61
2:B:167:ILE:O	2:B:208:HIS:HE1	1.83	0.61
2:B:304:ALA:HA	2:B:307:ARG:HB3	1.82	0.61
1:A:108:VAL:HA	1:A:187:LEU:O	2.00	0.61
2:B:164:MET:HE3	2:B:182:GLN:NE2	2.16	0.61
2:B:63:ILE:CD1	2:B:74:LEU:HD22	2.31	0.61
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.20	0.60
1:A:438:GLU:HG3	1:A:460:ASN:ND2	2.16	0.60
2:B:181:TYR:CD1	2:B:182:GLN:N	2.69	0.60
2:B:279:LEU:O	2:B:282:LEU:HB3	2.01	0.60
2:B:270:ILE:O	2:B:272:PRO:HD3	2.02	0.60
1:A:116:PHE:O	1:A:148:VAL:HG11	2.01	0.60
1:A:544:GLY:O	1:A:548:VAL:HG23	2.02	0.59
1:A:551:LEU:HD12	1:A:552:VAL:HG13	1.84	0.59
1:A:188:TYR:CD2	3:A:557:HBX:H121	2.36	0.59
1:A:198:HIS:O	1:A:202:ILE:HG12	2.02	0.59
2:B:207:GLN:O	2:B:211:ARG:HG3	2.03	0.59
2:B:266:TRP:C	2:B:268:SER:H	2.08	0.59
1:A:224:GLU:HB2	1:A:226:PRO:HD2	1.85	0.59
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.49	0.59
1:A:49:LYS:HA	1:A:144:TYR:HA	1.84	0.59
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.84	0.58
1:A:108:VAL:O	1:A:223:LYS:HG3	2.02	0.58
2:B:291:GLU:O	2:B:293:ILE:HG23	2.04	0.58
2:B:96:HIS:HD2	2:B:181:TYR:CE2	2.22	0.58
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.29	0.57
2:B:27:THR:CG2	2:B:28:GLU:N	2.68	0.57
2:B:21:VAL:HG12	2:B:22:LYS:N	2.20	0.57
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.86	0.57
2:B:181:TYR:HD1	2:B:182:GLN:N	2.02	0.57
1:A:101:LYS:NZ	1:A:321:PRO:HG3	2.20	0.56
1:A:141:GLY:O	1:A:143:ARG:HG2	2.05	0.56
1:A:393:ILE:HD11	1:A:398:TRP:HB2	1.87	0.56
1:A:438:GLU:HB3	1:A:440:PHE:HE1	1.70	0.56
1:A:270:ILE:HD12	1:A:270:ILE:H	1.69	0.56
2:B:7:THR:O	2:B:9:PRO:HD3	2.05	0.56
2:B:63:ILE:HD13	2:B:406:TRP:O	2.05	0.56
2:B:345:PRO:O	2:B:346:PHE:HB2	2.04	0.56
1:A:168:LEU:HD22	1:A:180:ILE:CD1	2.36	0.56
1:A:95:PRO:HD2	1:A:229:TRP:HZ2	1.71	0.56
1:A:350:LYS:NZ	1:A:350:LYS:HB3	2.21	0.56
1:A:3:SER:OG	1:A:5:ILE:HG22	2.06	0.55
1:A:508:ALA:C	1:A:509:GLN:HG2	2.30	0.55
1:A:131:THR:OG1	1:A:143:ARG:HB3	2.06	0.55
1:A:261:VAL:HG13	1:A:276:VAL:HG12	1.88	0.55
2:B:154:LYS:HG3	2:B:184:MET:SD	2.47	0.55
1:A:475:GLN:HA	1:A:478:GLU:OE1	2.07	0.55
1:A:229:TRP:HB3	1:A:234:LEU:HD12	1.89	0.55
2:B:239:TRP:NE1	2:B:382:ILE:HD11	2.22	0.54
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.42	0.54
1:A:196:GLY:O	1:A:200:THR:HG23	2.06	0.54
2:B:112:GLY:HA3	2:B:185:ASP:HB3	1.87	0.54
2:B:183:TYR:CD2	2:B:380:ILE:HG23	2.43	0.54
1:A:252:TRP:H	1:A:252:TRP:CD1	2.24	0.54
2:B:239:TRP:HE1	2:B:382:ILE:HD11	1.73	0.54
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.38	0.53
2:B:181:TYR:HD1	2:B:182:GLN:H	1.56	0.53
1:A:139:THR:N	1:A:140:PRO:HD3	2.23	0.53
2:B:37:ILE:HG22	2:B:38:CYS:N	2.23	0.53
1:A:100:LEU:HD22	3:A:557:HBX:C2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG12	2:B:258:GLN:HE21	1.74	0.53
2:B:310:LEU:C	2:B:311:LYS:HD2	2.33	0.53
2:B:151:GLN:HG2	2:B:185:ASP:OD2	2.09	0.53
1:A:59:PRO:HG3	1:A:78:ARG:HH21	1.74	0.53
1:A:100:LEU:HD22	3:A:557:HBY:C1	2.39	0.52
2:B:126:LYS:HE3	2:B:127:TYR:CE1	2.44	0.52
2:B:293:ILE:HG13	2:B:293:ILE:O	2.08	0.52
2:B:253:THR:HG22	2:B:292:VAL:HA	1.90	0.52
2:B:354:TYR:CD2	2:B:371:ALA:HB2	2.44	0.52
2:B:373:GLN:HE22	2:B:407:GLN:N	2.06	0.52
3:A:557:HBY:O2	3:A:557:HBY:H5	2.10	0.52
1:A:125:ARG:HH11	1:A:147:ASN:HD22	1.58	0.52
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.91	0.52
1:A:101:LYS:HZ3	1:A:321:PRO:HG3	1.73	0.52
2:B:225:PRO:N	2:B:226:PRO:HD2	2.23	0.52
2:B:195:ILE:HD13	2:B:195:ILE:H	1.75	0.51
1:A:41:MET:HB3	1:A:47:ILE:HD11	1.93	0.51
1:A:520:GLN:O	1:A:524:GLN:HG2	2.10	0.51
2:B:27:THR:HG22	2:B:28:GLU:H	1.76	0.51
2:B:124:PHE:CE1	2:B:127:TYR:HD2	2.29	0.51
2:B:340:GLN:NE2	2:B:429:LEU:HA	2.25	0.51
1:A:56:TYR:N	1:A:56:TYR:CD1	2.78	0.51
1:A:393:ILE:HD13	1:A:398:TRP:HE3	1.76	0.51
1:A:210:LEU:HD22	1:A:215:THR:HA	1.93	0.51
2:B:112:GLY:CA	2:B:185:ASP:HB3	2.41	0.51
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.46	0.51
2:B:356:ARG:HA	2:B:356:ARG:NE	2.26	0.51
2:B:63:ILE:HD12	2:B:74:LEU:HD13	1.93	0.50
2:B:251:SER:HB2	2:B:295:LEU:HD21	1.93	0.50
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.93	0.50
1:A:11:LYS:N	1:A:85:GLN:OE1	2.44	0.50
1:A:106:VAL:HG12	1:A:107:THR:N	2.27	0.50
1:A:508:ALA:O	1:A:509:GLN:HG2	2.12	0.50
2:B:257:ILE:O	2:B:261:VAL:HG23	2.11	0.50
1:A:10:VAL:CG1	1:A:124:PHE:CE2	2.94	0.50
1:A:23:GLN:O	1:A:25:PRO:HD3	2.11	0.50
1:A:108:VAL:HG22	1:A:188:TYR:CD1	2.46	0.50
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.94	0.50
1:A:350:LYS:HB3	1:A:350:LYS:HZ2	1.76	0.50
2:B:336:GLN:HA	2:B:355:ALA:HA	1.93	0.50
1:A:392:PRO:O	1:A:423:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TYR:C	2:B:117:SER:H	2.20	0.49
1:A:182:GLN:HE21	1:A:183:TYR:N	2.11	0.49
1:A:191:SER:OG	1:A:198:HIS:HD2	1.95	0.49
1:A:56:TYR:O	1:A:57:ASN:HB2	2.11	0.49
2:B:315:HIS:O	2:B:316:GLY:C	2.55	0.49
2:B:369:THR:HG23	2:B:406:TRP:CE3	2.38	0.49
1:A:285:GLY:C	1:A:287:LYS:H	2.20	0.49
1:A:8:VAL:CG1	1:A:9:PRO:HD2	2.43	0.49
2:B:34:LEU:HD21	2:B:61:PHE:O	2.11	0.49
2:B:65:LYS:HB2	2:B:72:ARG:HG3	1.93	0.48
1:A:182:GLN:O	1:A:182:GLN:HG3	2.12	0.48
2:B:156:SER:H	2:B:157:PRO:HD2	1.78	0.48
1:A:470:THR:O	1:A:471:ASN:HB2	2.13	0.48
2:B:210:LEU:O	2:B:213:GLY:O	2.31	0.48
1:A:160:PHE:CE2	1:A:182:GLN:OE1	2.67	0.48
2:B:349:LEU:HD22	2:B:383:TRP:HZ2	1.79	0.48
2:B:371:ALA:O	2:B:375:ILE:HG12	2.13	0.48
2:B:239:TRP:CD1	2:B:382:ILE:HD11	2.48	0.48
1:A:229:TRP:CE2	3:A:557:HBY:H122	2.49	0.48
1:A:258:GLN:HE21	1:A:283:LEU:HD21	1.77	0.48
1:A:100:LEU:HB3	3:A:557:HBY:N2	2.29	0.48
2:B:5:ILE:HG22	2:B:6:GLU:N	2.27	0.48
2:B:135:ILE:HD12	2:B:135:ILE:H	1.78	0.48
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.79	0.48
1:A:224:GLU:OE1	1:A:226:PRO:HG2	2.13	0.48
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.49	0.48
2:B:344:GLU:HA	2:B:345:PRO:HD2	1.61	0.48
2:B:206:ARG:HH12	2:B:219:LYS:HA	1.79	0.47
1:A:39:THR:HG22	1:A:39:THR:O	2.14	0.47
1:A:483:TYR:CE1	1:A:524:GLN:NE2	2.76	0.47
2:B:27:THR:CG2	2:B:28:GLU:H	2.26	0.47
1:A:410:TRP:HB2	2:B:365:VAL:HG23	1.96	0.47
1:A:87:PHE:CE2	1:A:155:GLY:HA3	2.49	0.47
1:A:291:GLU:HG3	1:A:291:GLU:O	2.13	0.47
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.49	0.47
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.78	0.47
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.44	0.47
2:B:107:THR:OG1	2:B:198:HIS:HE1	1.98	0.47
1:A:420:PRO:HG2	1:A:421:PRO:CD	2.44	0.47
1:A:246:LEU:HA	1:A:247:PRO:HD2	1.76	0.47
2:B:267:ALA:O	2:B:271:TYR:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:C	2:B:268:SER:N	2.73	0.46
1:A:282:LEU:HD13	1:A:296:THR:HG23	1.98	0.46
1:A:398:TRP:C	1:A:400:THR:H	2.23	0.46
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.73	0.46
2:B:103:LYS:O	2:B:105:SER:N	2.48	0.46
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.15	0.46
2:B:100:LEU:HD22	2:B:181:TYR:HB2	1.96	0.46
1:A:178:ILE:HA	1:A:191:SER:HB3	1.97	0.46
1:A:407:GLN:HG3	2:B:393:ILE:HA	1.97	0.46
2:B:210:LEU:CD1	2:B:216:THR:HG23	2.37	0.46
1:A:326:ILE:HD11	1:A:390:LYS:HG2	1.97	0.46
2:B:50:ILE:HG12	2:B:145:GLN:HB2	1.98	0.46
2:B:31:ILE:O	2:B:31:ILE:HG22	2.16	0.46
2:B:214:LEU:HD12	2:B:214:LEU:HA	1.66	0.46
2:B:247:PRO:HB2	2:B:250:ASP:CB	2.46	0.46
2:B:402:TRP:O	2:B:404:GLU:N	2.49	0.46
2:B:425:LEU:HD23	2:B:427:TYR:H	1.81	0.46
1:A:40:GLU:HG2	1:A:43:LYS:HD2	1.97	0.46
1:A:312:GLU:HA	1:A:313:PRO:HD2	1.65	0.45
2:B:47:ILE:HD12	2:B:130:PHE:HZ	1.81	0.45
2:B:400:THR:HG22	2:B:401:TRP:CD1	2.50	0.45
1:A:112:GLY:HA2	1:A:185:ASP:HB3	1.98	0.45
2:B:78:ARG:HD3	2:B:411:ILE:O	2.15	0.45
2:B:244:ILE:O	2:B:244:ILE:HG22	2.14	0.45
2:B:254:VAL:HG23	2:B:291:GLU:O	2.16	0.45
2:B:398:TRP:O	2:B:402:TRP:HD1	1.99	0.45
1:A:398:TRP:C	1:A:398:TRP:CD1	2.92	0.45
1:A:227:PHE:HD2	3:A:557:HBX:C15	2.21	0.45
1:A:329:ILE:CD1	1:A:391:LEU:HD21	2.47	0.45
1:A:443:ASP:HB2	1:A:548:VAL:CG1	2.47	0.45
2:B:111:VAL:HG12	2:B:111:VAL:O	2.17	0.45
1:A:109:LEU:HD23	1:A:216:THR:CG2	2.47	0.45
1:A:500:GLN:O	1:A:503:LEU:HB3	2.16	0.45
2:B:354:TYR:CE2	2:B:371:ALA:HB2	2.52	0.45
1:A:175:ASN:O	1:A:178:ILE:HG22	2.17	0.45
1:A:406:TRP:O	2:B:331:LYS:NZ	2.50	0.45
2:B:46:LYS:O	2:B:147:ASN:HB2	2.16	0.45
2:B:365:VAL:HG12	2:B:365:VAL:O	2.17	0.45
2:B:46:LYS:C	2:B:147:ASN:HD22	2.26	0.44
1:A:90:VAL:HG23	1:A:91:GLN:N	2.32	0.44
1:A:180:ILE:HG22	1:A:181:TYR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:THR:HA	2:B:420:PRO:HD3	1.80	0.44
1:A:100:LEU:HD13	3:A:557:HBY:C3	2.47	0.44
2:B:339:TYR:CD1	2:B:352:GLY:O	2.71	0.44
1:A:452:LEU:HD12	1:A:452:LEU:O	2.18	0.44
2:B:376:THR:O	2:B:380:ILE:HG12	2.17	0.44
2:B:400:THR:CG2	2:B:401:TRP:CD1	3.01	0.44
2:B:224:GLU:O	2:B:225:PRO:C	2.60	0.44
1:A:443:ASP:HB2	1:A:548:VAL:HG12	1.99	0.44
2:B:274:ILE:HG12	2:B:306:ASN:OD1	2.18	0.44
2:B:314:VAL:HG23	2:B:315:HIS:H	1.82	0.44
1:A:240:THR:CG2	1:A:241:VAL:H	2.21	0.44
1:A:337:TRP:CZ3	1:A:368:LEU:HD12	2.52	0.44
2:B:114:ALA:CB	2:B:215:THR:HG22	2.48	0.44
1:A:168:LEU:HD22	1:A:180:ILE:HD13	2.00	0.44
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.99	0.44
2:B:132:ILE:HB	2:B:142:ILE:HB	2.00	0.44
1:A:224:GLU:C	1:A:226:PRO:HD2	2.43	0.43
1:A:254:VAL:HG23	1:A:291:GLU:HG3	2.00	0.43
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.35	0.43
2:B:327:ALA:O	2:B:389:PHE:HA	2.18	0.43
1:A:54:ASN:HD22	1:A:143:ARG:HH21	1.65	0.43
1:A:59:PRO:O	1:A:75:VAL:HG13	2.18	0.43
1:A:246:LEU:O	1:A:246:LEU:HD12	2.18	0.43
1:A:365:VAL:O	1:A:368:LEU:HB3	2.17	0.43
1:A:393:ILE:CD1	1:A:398:TRP:HB2	2.48	0.43
2:B:80:LEU:O	2:B:84:THR:N	2.52	0.43
1:A:482:ILE:HG23	1:A:495:ILE:HG21	2.00	0.43
1:A:164:MET:HE2	1:A:164:MET:HB3	1.86	0.43
1:A:178:ILE:O	1:A:178:ILE:HG23	2.19	0.43
2:B:111:VAL:HG21	2:B:187:LEU:HD22	2.00	0.43
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.64	0.43
1:A:497:THR:HG22	1:A:498:ASP:N	2.34	0.43
2:B:355:ALA:O	2:B:356:ARG:HB2	2.18	0.43
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.74	0.43
1:A:511:ASP:O	1:A:522:ILE:HD13	2.19	0.43
1:A:229:TRP:CE3	1:A:230:MET:HG2	2.54	0.43
1:A:406:TRP:CG	1:A:407:GLN:H	2.37	0.43
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.53	0.43
2:B:210:LEU:HD12	2:B:210:LEU:HA	1.71	0.43
1:A:390:LYS:HA	1:A:390:LYS:HD3	1.72	0.43
1:A:317:VAL:HG12	1:A:349:LEU:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:HA	2:B:88:TRP:HB2	2.01	0.42
1:A:246:LEU:H	1:A:246:LEU:HG	1.52	0.42
1:A:363:ASN:OD1	1:A:364:ASP:N	2.53	0.42
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.33	0.42
1:A:438:GLU:HA	1:A:460:ASN:HD21	1.84	0.42
1:A:509:GLN:N	1:A:510:PRO:HD3	2.33	0.42
2:B:259:LYS:HD3	2:B:426:TRP:HH2	1.84	0.42
2:B:274:ILE:HG23	2:B:306:ASN:HD21	1.84	0.42
2:B:337:TRP:HB2	2:B:354:TYR:HB3	2.02	0.42
1:A:222:GLN:O	1:A:223:LYS:HG2	2.20	0.42
1:A:229:TRP:CD1	1:A:234:LEU:HD11	2.54	0.42
1:A:458:VAL:HG22	1:A:464:GLN:HG2	2.00	0.42
2:B:81:ASN:O	2:B:82:LYS:C	2.62	0.42
1:A:91:GLN:C	1:A:93:GLY:H	2.27	0.42
1:A:265:ASN:HD21	1:A:353:LYS:NZ	2.18	0.42
2:B:366:LYS:O	2:B:370:GLU:HG3	2.20	0.42
2:B:402:TRP:C	2:B:404:GLU:H	2.28	0.42
1:A:234:LEU:CB	3:A:557:HBY:H153	2.37	0.42
1:A:5:ILE:HG13	1:A:6:GLU:N	2.35	0.42
1:A:160:PHE:HE2	1:A:182:GLN:OE1	2.03	0.42
2:B:115:TYR:N	2:B:115:TYR:CD1	2.85	0.42
2:B:242:GLN:N	2:B:243:PRO:HD3	2.35	0.42
1:A:467:VAL:HA	1:A:468:PRO:HD2	1.81	0.42
1:A:482:ILE:O	1:A:486:LEU:N	2.52	0.42
2:B:316:GLY:O	2:B:318:TYR:N	2.52	0.42
2:B:368:LEU:HG	2:B:398:TRP:CZ3	2.55	0.42
1:A:271:TYR:HA	1:A:272:PRO:HD2	1.79	0.42
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.55	0.42
2:B:368:LEU:HD23	2:B:398:TRP:CZ3	2.55	0.42
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.49	0.41
2:B:73:LYS:HG2	2:B:74:LEU:N	2.34	0.41
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.85	0.41
1:A:369:THR:O	1:A:369:THR:HG22	2.19	0.41
2:B:65:LYS:HB2	2:B:72:ARG:CG	2.50	0.41
1:A:221:HIS:O	1:A:223:LYS:N	2.53	0.41
2:B:339:TYR:CG	2:B:375:ILE:CD1	3.03	0.41
1:A:54:ASN:HD22	1:A:143:ARG:NH2	2.19	0.41
1:A:429:LEU:N	1:A:429:LEU:HD23	2.35	0.41
3:A:557:HBY:O1	3:A:557:HBY:H112	2.19	0.41
2:B:28:GLU:O	2:B:29:GLU:C	2.64	0.41
2:B:34:LEU:HD21	2:B:62:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:SER:O	2:B:69:THR:HG23	2.20	0.41
1:A:128:THR:OG1	1:A:146:TYR:HB2	2.20	0.41
2:B:205:LEU:O	2:B:205:LEU:HD12	2.20	0.41
2:B:34:LEU:HD12	2:B:132:ILE:HG23	2.02	0.41
1:A:188:TYR:CZ	3:A:557:HBX:H121	2.55	0.41
2:B:50:ILE:HD12	2:B:143:ARG:HG2	2.02	0.41
2:B:188:TYR:CE1	2:B:380:ILE:HG21	2.55	0.41
1:A:326:ILE:HG13	1:A:388:LYS:O	2.19	0.41
1:A:373:GLN:O	1:A:374:LYS:C	2.64	0.41
2:B:136:ASN:O	2:B:136:ASN:ND2	2.54	0.41
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.82	0.41
1:A:37:ILE:HD12	1:A:37:ILE:N	2.35	0.41
1:A:126:LYS:HE3	1:A:126:LYS:HB3	1.85	0.41
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.77	0.41
1:A:229:TRP:HD1	1:A:234:LEU:HD11	1.85	0.41
1:A:326:ILE:CG2	1:A:342:TYR:O	2.62	0.41
2:B:82:LYS:HD2	2:B:413:GLU:OE2	2.21	0.41
1:A:27:THR:HA	1:A:135:ILE:HG23	2.03	0.41
1:A:341:ILE:CD1	1:A:383:TRP:HH2	2.34	0.40
2:B:23:GLN:NE2	2:B:24:TRP:O	2.52	0.40
1:A:56:TYR:H	1:A:56:TYR:HD1	1.69	0.40
1:A:403:THR:HG22	1:A:403:THR:O	2.21	0.40
1:A:265:ASN:HD22	1:A:265:ASN:HA	1.53	0.40
2:B:38:CYS:SG	2:B:73:LYS:NZ	2.85	0.40
1:A:341:ILE:HD13	1:A:383:TRP:CH2	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	554/556 (100%)	453 (82%)	75 (14%)	26 (5%)	2 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	428/430 (100%)	342 (80%)	59 (14%)	27 (6%)	1	6
All	All	982/986 (100%)	795 (81%)	134 (14%)	53 (5%)	1	9

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	67	ASP
1	A	104	LYS
1	A	195	ILE
1	A	222	GLN
1	A	324	ASP
1	A	412	PRO
2	B	14	PRO
2	B	104	LYS
2	B	316	GLY
2	B	317	VAL
1	A	179	VAL
1	A	219	LYS
1	A	345	PRO
2	B	116	PHE
2	B	125	ARG
2	B	212	TRP
2	B	244	ILE
2	B	251	SER
2	B	356	ARG
2	B	427	TYR
1	A	153	TRP
1	A	184	MET
1	A	287	LYS
2	B	69	THR
2	B	98	ALA
2	B	138	GLU
2	B	153	TRP
2	B	230	MET
2	B	345	PRO
2	B	403	THR
1	A	154	LYS
1	A	236	PRO
1	A	360	ALA
2	B	66	LYS
2	B	222	GLN

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Mol	Chain	Res	Type
1	A	244	ILE
2	B	5	ILE
2	B	195	ILE
2	B	267	ALA
1	A	271	TYR
1	A	359	GLY
1	A	4	PRO
1	A	490	GLY
2	B	236	PRO
1	A	21	VAL
2	B	156	SER
1	A	24	TRP
1	A	510	PRO
2	B	148	VAL
2	B	292	VAL
1	A	156	SER
1	A	462	GLY

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	450/496 (91%)	384 (85%)	66 (15%)	3	14
2	B	363/392 (93%)	322 (89%)	41 (11%)	5	23
All	All	813/888 (92%)	706 (87%)	107 (13%)	4	17

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	28	GLU
1	A	29	GLU
1	A	40	GLU
1	A	42	GLU
1	A	47	ILE

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Mol	Chain	Res	Type
1	A	50	ILE
1	A	65	LYS
1	A	74	LEU
1	A	76	ASP
1	A	78	ARG
1	A	79	GLU
1	A	81	ASN
1	A	89	GLU
1	A	97	PRO
1	A	109	LEU
1	A	126	LYS
1	A	135	ILE
1	A	137	ASN
1	A	154	LYS
1	A	164	MET
1	A	178	ILE
1	A	182	GLN
1	A	210	LEU
1	A	214	LEU
1	A	224	GLU
1	A	228	LEU
1	A	238	LYS
1	A	242	GLN
1	A	246	LEU
1	A	252	TRP
1	A	265	ASN
1	A	270	ILE
1	A	274	ILE
1	A	291	GLU
1	A	295	LEU
1	A	300	GLU
1	A	310	LEU
1	A	312	GLU
1	A	317	VAL
1	A	341	ILE
1	A	346	PHE
1	A	350	LYS
1	A	362	THR
1	A	364	ASP
1	A	368	LEU
1	A	393	ILE
1	A	429	LEU

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Mol	Chain	Res	Type
1	A	431	LYS
1	A	442	VAL
1	A	448	ARG
1	A	449	GLU
1	A	450	THR
1	A	452	LEU
1	A	461	LYS
1	A	473	THR
1	A	479	LEU
1	A	484	LEU
1	A	496	VAL
1	A	497	THR
1	A	505	ILE
1	A	507	GLN
1	A	516	GLU
1	A	531	VAL
1	A	540	LYS
1	A	547	GLN
2	B	11	LYS
2	B	14	PRO
2	B	32	LYS
2	B	34	LEU
2	B	40	GLU
2	B	50	ILE
2	B	53	GLU
2	B	60	VAL
2	B	69	THR
2	B	74	LEU
2	B	75	VAL
2	B	92	LEU
2	B	137	ASN
2	B	163	SER
2	B	166	LYS
2	B	185	ASP
2	B	195	ILE
2	B	203	GLU
2	B	210	LEU
2	B	218	ASP
2	B	239	TRP
2	B	246	LEU
2	B	252	TRP
2	B	266	TRP

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Mol	Chain	Res	Type
2	B	274	ILE
2	B	290	THR
2	B	298	GLU
2	B	318	TYR
2	B	324	ASP
2	B	328	GLU
2	B	330	GLN
2	B	332	GLN
2	B	356	ARG
2	B	362	THR
2	B	377	THR
2	B	405	TYR
2	B	409	THR
2	B	414	TRP
2	B	418	ASN
2	B	425	LEU
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	81	ASN
1	A	174	GLN
1	A	175	ASN
1	A	182	GLN
1	A	198	HIS
1	A	258	GLN
1	A	265	ASN
1	A	340	GLN
1	A	361	HIS
1	A	367	GLN
1	A	428	GLN
1	A	460	ASN
1	A	494	ASN
2	B	57	ASN
2	B	91	GLN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	198	HIS
2	B	208	HIS

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Mol	Chain	Res	Type
2	B	330	GLN
2	B	343	GLN
2	B	373	GLN
2	B	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HBV	A	557	-	22,23,23	6.62	18 (81%)	24,32,32	1.95	5 (20%)

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	HBV	A	557	-	-	5/13/29/29	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	HBY	C9-N1	14.00	1.57	1.37
3	A	557	HBY	C3-C4	12.35	1.54	1.40
3	A	557	HBY	C2-S1	10.48	1.82	1.66
3	A	557	HBY	O3-C6	8.79	1.55	1.37
3	A	557	HBY	C7-C6	8.73	1.55	1.38
3	A	557	HBY	C1-N1	8.22	1.58	1.47
3	A	557	HBY	C8-C7	7.65	1.51	1.38
3	A	557	HBY	O1-C9	7.15	1.31	1.21
3	A	557	HBY	C2-N2	6.87	1.45	1.36
3	A	557	HBY	O2-C9	4.81	1.43	1.34
3	A	557	HBY	O2-C10	4.78	1.58	1.47
3	A	557	HBY	C3-N2	3.80	1.46	1.39
3	A	557	HBY	C13-C1	3.65	1.60	1.52
3	A	557	HBY	C8-C3	3.61	1.45	1.39
3	A	557	HBY	C13-S2	3.36	1.89	1.81
3	A	557	HBY	O3-C15	3.18	1.51	1.42
3	A	557	HBY	C4-N1	2.35	1.45	1.42
3	A	557	HBY	C5-C4	2.29	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	HBY	O2-C9-N1	5.42	118.10	110.93
3	A	557	HBY	C3-N2-C2	-4.94	120.51	124.76
3	A	557	HBY	O1-C9-N1	-2.88	119.29	123.99
3	A	557	HBY	O2-C10-C12	2.45	113.65	107.13
3	A	557	HBY	C5-C4-N1	-2.10	118.50	121.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

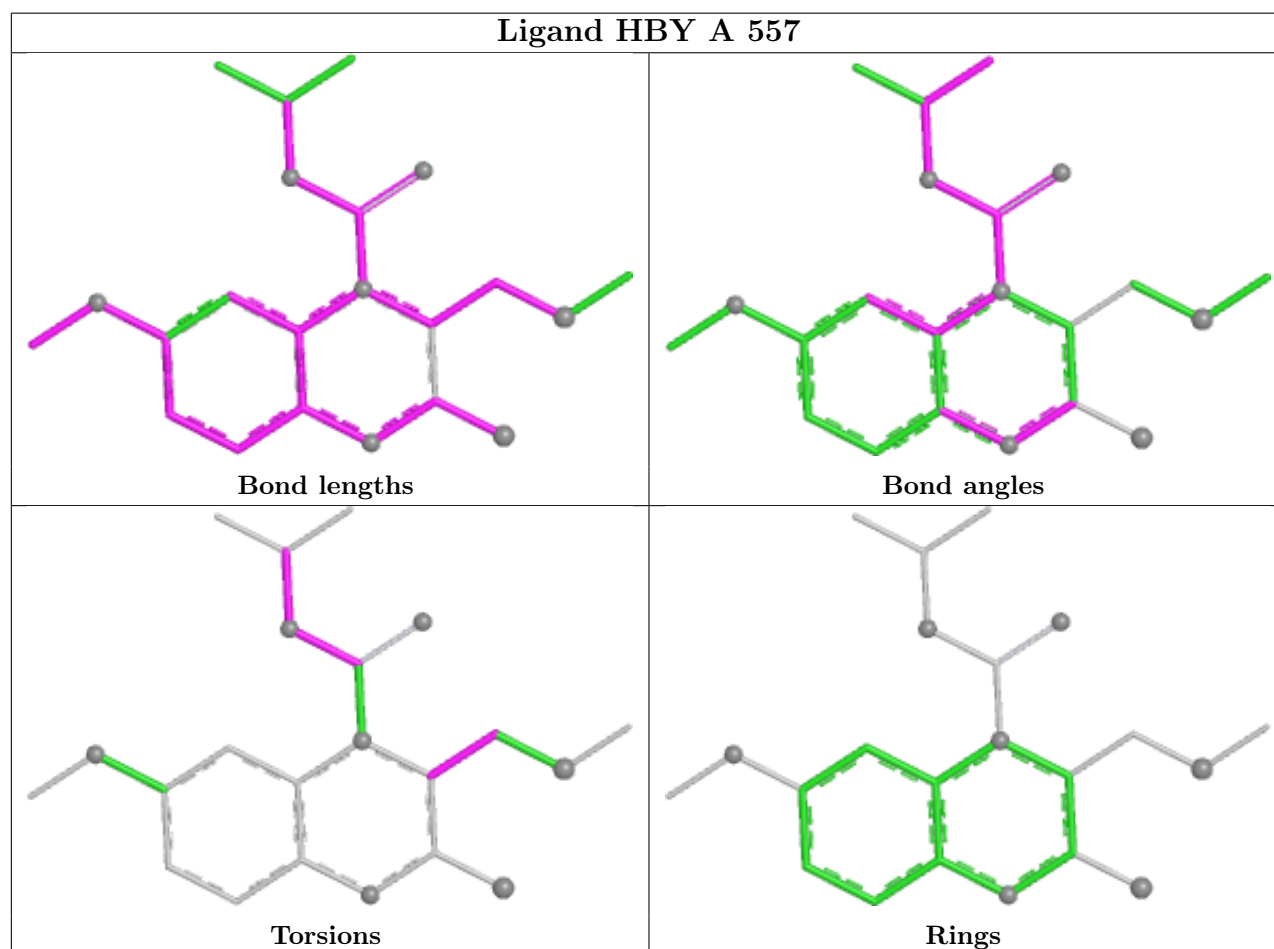
Mol	Chain	Res	Type	Atoms
3	A	557	HBY	C2-C1-C13-S2
3	A	557	HBY	N1-C1-C13-S2
3	A	557	HBY	N1-C9-O2-C10
3	A	557	HBY	O1-C9-O2-C10
3	A	557	HBY	C11-C10-O2-C9

There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	HBV	25	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.