



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:53 PM UTC

PDB ID : 1BIM / pdb_00001bim
Title : CRYSTALLOGRAPHIC STUDIES ON THE BINDING MODES OF P2-P3
BUTANEDIAMIDE RENIN INHIBITORS
Authors : Tong, L.
Deposited on : 1995-09-27
Resolution : 2.80 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

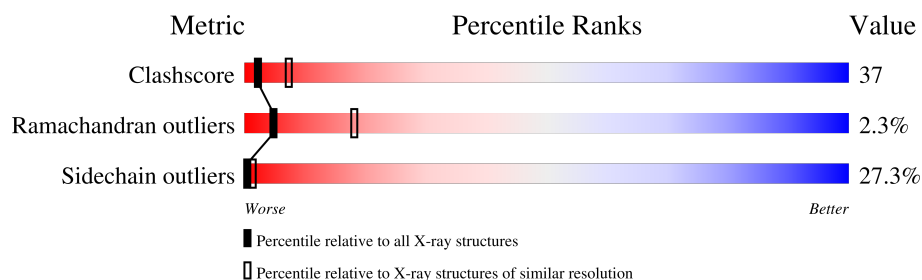
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	337	
1	B	337	

2 Entry composition [i](#)

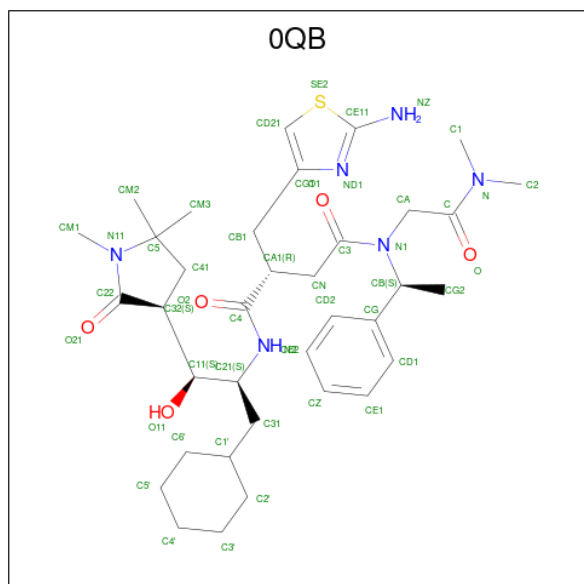
There are 2 unique types of molecules in this entry. The entry contains 5221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2575	1644	416	501	14			
1	B	333	Total	C	N	O	S	0	0	0
			2550	1630	408	498	14			

- Molecule 2 is (2S)-2-[(2-amino-1,3-thiazol-4-yl)methyl]-N 1 -{(1S,2S)-1-(cyclohexylmethyl)-2-hydroxy-2-[(3R)-1,5,5-trimethyl-2-oxopyrrolidin-3-yl]ethyl}-N 4 -[2-(dimethylamino)-2-oxoethyl]-N 4 -[(1S)-1-phenylethyl]butanediamide (CCD ID: 0QB) (formula: C₃₆H₅₄N₆O₅S).



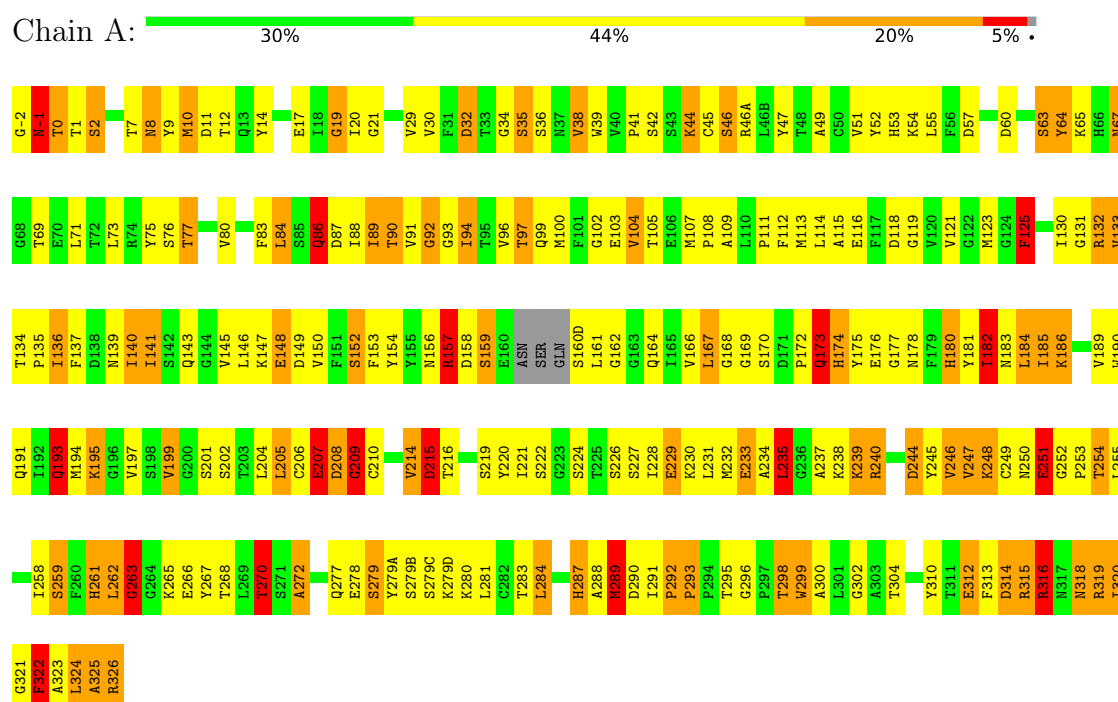
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			48	36	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			48	36	6	5	1		

3 Residue-property plots [i](#)

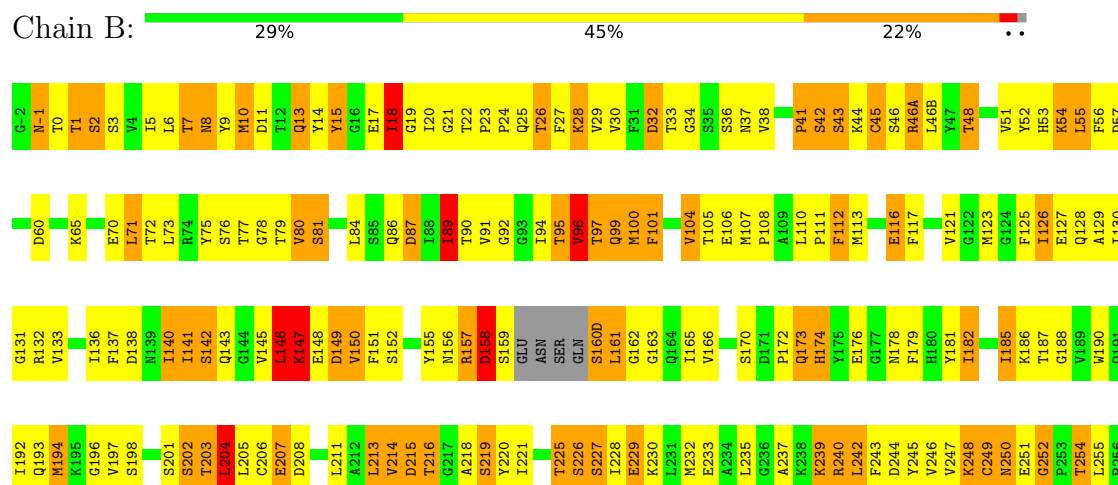
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

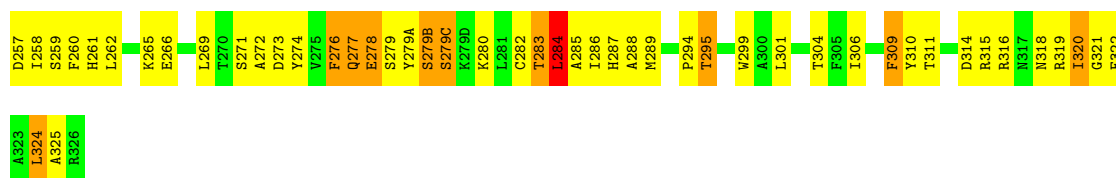
Note EDS was not executed.

• Molecule 1: Renin



• Molecule 1: Renin





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	142.90Å 142.90Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5221	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: 0QB

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	1.37	12/2634 (0.5%)	1.94	78/3570 (2.2%)
1	B	1.34	9/2609 (0.3%)	1.90	74/3540 (2.1%)
All	All	1.36	21/5243 (0.4%)	1.92	152/7110 (2.1%)

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
1	A	1	0
1	B	1	0
All	All	2	0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	GLY	CA-C	6.03	1.56	1.52
1	B	148	GLU	CD-OE1	5.97	1.36	1.25
1	A	17	GLU	CA-C	-5.90	1.45	1.52
1	B	318	ASN	CA-C	-5.88	1.46	1.53
1	A	208	ASP	CG-OD2	5.74	1.36	1.25
1	B	207	GLU	CA-C	5.65	1.60	1.52
1	A	75	TYR	CA-C	-5.54	1.46	1.52
1	B	229	GLU	CD-OE1	5.44	1.35	1.25
1	A	148	GLU	CD-OE2	5.41	1.35	1.25
1	B	278	GLU	CD-OE2	5.37	1.35	1.25
1	A	259	SER	CA-C	-5.31	1.46	1.52
1	A	251	GLU	CD-OE2	5.29	1.35	1.25
1	A	279(B)	SER	CA-C	-5.27	1.46	1.52
1	B	100	MET	C-O	5.23	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	SER	CA-C	-5.22	1.46	1.52
1	B	70	GLU	CD-OE2	5.17	1.35	1.25
1	A	60	ASP	N-CA	-5.17	1.40	1.46
1	A	207	GLU	CD-OE1	5.06	1.34	1.25
1	B	208	ASP	CG-OD1	5.05	1.34	1.25
1	B	233	GLU	CD-OE1	5.02	1.34	1.25
1	A	244	ASP	CG-OD1	5.02	1.34	1.25

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASP	CA-CB-CG	11.74	124.34	112.60
1	A	174	HIS	CA-CB-CG	-11.71	102.09	113.80
1	B	215	ASP	CA-CB-CG	11.22	123.82	112.60
1	B	60	ASP	CA-CB-CG	-10.11	102.49	112.60
1	B	259	SER	N-CA-C	10.06	124.82	108.41
1	A	180	HIS	CA-CB-CG	-9.64	104.16	113.80
1	A	199	VAL	N-CA-C	-9.20	95.33	108.58
1	A	240	ARG	N-CA-CB	8.92	119.93	108.96
1	B	43	SER	N-CA-C	-8.29	102.61	112.89
1	A	215	ASP	N-CA-C	8.26	122.71	108.76
1	B	71	LEU	N-CA-C	8.04	121.60	108.26
1	A	90	THR	N-CA-CB	8.03	123.81	110.47
1	B	129	ALA	N-CA-C	7.70	121.07	108.52
1	A	289	MET	CA-C-N	-7.62	112.28	122.42
1	A	289	MET	C-N-CA	-7.62	112.28	122.42
1	B	32	ASP	N-CA-C	7.41	120.33	108.41
1	A	64	TYR	N-CA-C	7.30	121.59	109.46
1	A	108	PRO	CA-C-N	7.29	130.78	120.28
1	A	108	PRO	C-N-CA	7.29	130.78	120.28
1	A	292	PRO	CA-C-N	7.20	124.91	119.66
1	A	292	PRO	C-N-CA	7.20	124.91	119.66
1	A	299	TRP	N-CA-C	-7.16	98.93	110.32
1	B	174	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	270	THR	N-CA-C	-7.11	99.94	110.46
1	A	295	THR	N-CA-CB	7.11	120.32	110.01
1	A	51	VAL	CB-CA-C	-7.09	102.75	112.24
1	A	278	GLU	N-CA-C	-7.08	104.65	112.72
1	B	204	LEU	N-CA-C	-7.07	103.77	113.18
1	B	202	SER	N-CA-C	7.04	120.87	109.40
1	A	208	ASP	CB-CA-C	-6.99	100.56	111.39
1	A	325	ALA	N-CA-C	6.95	119.96	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASP	CA-CB-CG	6.91	119.51	112.60
1	B	101	PHE	CA-CB-CG	6.88	120.68	113.80
1	B	65	LYS	CA-C-N	6.78	130.47	120.90
1	B	65	LYS	C-N-CA	6.78	130.47	120.90
1	B	239	LYS	N-CA-C	-6.69	100.38	110.28
1	B	249	CYS	N-CA-CB	6.63	121.70	110.49
1	B	255	LEU	CA-C-N	6.60	126.36	119.76
1	B	255	LEU	C-N-CA	6.60	126.36	119.76
1	B	104	VAL	N-CA-C	6.58	118.93	109.51
1	A	199	VAL	N-CA-CB	6.52	117.82	110.72
1	A	261	HIS	N-CA-CB	6.34	119.71	110.58
1	B	299	TRP	N-CA-C	-6.32	102.37	110.53
1	B	10	MET	N-CA-C	6.28	120.28	112.24
1	B	108	PRO	N-CA-C	6.28	122.16	111.68
1	B	149	ASP	N-CA-CB	6.28	119.04	110.57
1	B	213	LEU	CB-CA-C	-6.28	100.00	110.29
1	A	313	PHE	CA-CB-CG	-6.22	107.58	113.80
1	A	237	ALA	N-CA-C	6.17	119.17	110.23
1	B	45	CYS	CA-C-N	6.14	131.02	121.26
1	B	45	CYS	C-N-CA	6.14	131.02	121.26
1	B	8	ASN	CA-CB-CG	6.14	118.74	112.60
1	A	32	ASP	N-CA-C	6.09	120.42	107.70
1	B	99	GLN	N-CA-C	6.09	118.43	109.24
1	A	84	LEU	N-CA-C	6.07	119.54	109.46
1	A	173	GLN	N-CA-CB	6.05	119.71	110.70
1	A	322	PHE	CA-CB-CG	6.03	119.83	113.80
1	A	208	ASP	N-CA-C	-5.96	105.31	112.58
1	A	182	ILE	CB-CA-C	5.94	119.00	110.33
1	A	272	ALA	N-CA-C	-5.93	106.04	113.28
1	A	157	ARG	CB-CA-C	5.92	120.38	109.71
1	A	193	GLN	N-CA-CB	5.91	118.66	109.97
1	B	279(B)	SER	N-CA-CB	5.91	118.98	110.06
1	B	96	VAL	N-CA-C	5.89	116.12	108.35
1	B	274	TYR	N-CA-CB	5.88	120.21	110.33
1	B	257	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	97	THR	CB-CA-C	-5.85	100.53	109.89
1	A	97	THR	N-CA-C	-5.84	98.19	108.23
1	B	320	ILE	CA-C-N	-5.83	116.94	122.66
1	B	320	ILE	C-N-CA	-5.83	116.94	122.66
1	B	146	LEU	N-CA-C	5.80	118.19	108.96
1	A	86	GLN	N-CA-CB	5.80	121.51	111.13
1	B	37	ASN	CA-CB-CG	5.79	118.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LEU	N-CA-C	5.79	117.18	109.83
1	A	51	VAL	N-CA-C	-5.79	104.69	111.00
1	A	125	PHE	CA-CB-CG	5.74	119.54	113.80
1	B	133	VAL	N-CA-CB	5.73	117.87	110.99
1	A	209	GLY	CA-C-N	5.72	132.64	122.45
1	A	209	GLY	C-N-CA	5.72	132.64	122.45
1	A	199	VAL	CB-CA-C	-5.71	103.84	110.91
1	A	63	SER	CA-C-N	5.70	130.23	122.19
1	A	63	SER	C-N-CA	5.70	130.23	122.19
1	A	180	HIS	CB-CA-C	5.70	120.14	109.71
1	A	320	ILE	CA-C-N	-5.69	118.17	122.33
1	A	320	ILE	C-N-CA	-5.69	118.17	122.33
1	A	-1	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	323	ALA	N-CA-C	-5.60	100.80	109.14
1	B	208	ASP	N-CA-C	5.59	118.06	110.06
1	B	237	ALA	N-CA-C	-5.59	102.25	110.52
1	A	174	HIS	CB-CA-C	5.58	118.75	109.38
1	B	309	PHE	N-CA-C	5.58	118.61	107.62
1	B	2	SER	N-CA-C	5.55	119.30	107.70
1	B	158	ASP	N-CA-C	5.55	118.69	110.48
1	B	89	ILE	CA-C-N	-5.52	115.10	122.72
1	B	89	ILE	C-N-CA	-5.52	115.10	122.72
1	B	219	SER	N-CA-C	5.52	117.10	111.14
1	A	235	LEU	N-CA-C	5.52	119.85	113.18
1	B	259	SER	CA-CB-OG	-5.50	100.10	111.10
1	B	248	LYS	N-CA-CB	5.50	118.96	110.21
1	B	112	PHE	N-CA-C	5.49	122.50	110.80
1	A	10	MET	N-CA-C	5.48	119.55	112.86
1	B	216	THR	N-CA-C	5.43	119.63	112.89
1	A	246	VAL	N-CA-C	5.43	116.73	108.80
1	B	107	MET	CA-C-N	5.43	125.90	120.14
1	B	107	MET	C-N-CA	5.43	125.90	120.14
1	B	311	THR	N-CA-C	5.41	118.06	109.24
1	B	201	SER	CA-C-N	-5.41	114.83	122.94
1	B	201	SER	C-N-CA	-5.41	114.83	122.94
1	B	18	ILE	N-CA-CB	5.40	122.02	111.92
1	A	169	GLY	CA-C-N	5.39	130.94	122.21
1	A	169	GLY	C-N-CA	5.39	130.94	122.21
1	A	174	HIS	N-CA-CB	5.38	118.31	110.88
1	A	52	TYR	N-CA-C	5.36	119.45	113.02
1	B	252	GLY	CA-C-N	5.36	126.53	119.84
1	B	252	GLY	C-N-CA	5.36	126.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLY	CA-C-N	-5.35	117.07	123.44
1	A	263	GLY	C-N-CA	-5.35	117.07	123.44
1	A	46	SER	CB-CA-C	-5.33	101.85	109.84
1	A	140	ILE	CA-C-O	5.30	126.42	119.85
1	B	87	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	214	VAL	N-CA-C	5.26	115.20	107.15
1	B	81	SER	N-CA-C	5.25	116.39	108.46
1	B	276	PHE	CB-CA-C	-5.25	103.69	111.72
1	B	20	ILE	N-CA-C	5.25	115.52	108.17
1	A	89	ILE	CA-C-N	-5.24	115.67	123.11
1	A	89	ILE	C-N-CA	-5.24	115.67	123.11
1	A	270	THR	N-CA-CB	-5.23	102.35	110.46
1	A	45	CYS	N-CA-C	5.23	117.80	109.96
1	A	199	VAL	CA-C-O	-5.20	114.83	120.71
1	B	41	PRO	N-CA-CB	5.20	107.83	103.25
1	A	67	ASN	CA-C-N	-5.20	114.04	122.30
1	A	67	ASN	C-N-CA	-5.20	114.04	122.30
1	A	125	PHE	N-CA-C	5.19	116.63	110.19
1	A	270	THR	CA-C-O	-5.19	115.30	121.89
1	B	284	LEU	N-CA-CB	5.17	118.83	110.41
1	A	318	ASN	N-CA-C	5.16	116.95	110.91
1	A	193	GLN	CB-CG-CD	5.15	121.36	112.60
1	A	93	GLY	CA-C-N	5.15	128.07	120.91
1	A	93	GLY	C-N-CA	5.15	128.07	120.91
1	B	214	VAL	N-CA-CB	5.13	117.62	111.31
1	B	279(C)	SER	N-CA-C	-5.13	106.53	112.89
1	B	276	PHE	N-CA-CB	5.10	118.11	110.11
1	B	106	GLU	N-CA-C	-5.08	98.98	108.02
1	B	5	ILE	N-CA-CB	5.05	118.01	110.13
1	B	155	TYR	CA-C-O	-5.05	115.20	120.80
1	A	57	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	293	PRO	N-CA-C	-5.05	105.63	110.47
1	B	211	LEU	CA-C-N	-5.03	115.15	122.44
1	B	211	LEU	C-N-CA	-5.03	115.15	122.44
1	B	278	GLU	O-C-N	5.03	129.16	122.43
1	B	227	SER	N-CA-CB	5.02	117.97	110.19
1	A	67	ASN	N-CA-C	-5.01	100.12	110.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	215	ASP	CA

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Mol	Chain	Res	Type	Atom
1	B	112	PHE	CA

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	2575	0	2507	183	0
1	B	2550	0	2468	174	0
2	A	48	0	54	17	0
2	B	48	0	54	17	0
All	All	5221	0	5083	378	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 37.

All (378) 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:A:391:0QB:CD21	2:A:391:0QB:HD21	0.97	1.09
1:A:195:LYS:HB2	1:A:261:HIS:HD2	1.11	1.06
2:B:391:0QB:HD21	2:B:391:0QB:CD21	0.97	1.05
2:B:391:0QB:CG1	2:B:391:0QB:SE2	2.55	1.04
2:B:391:0QB:CD21	2:B:391:0QB:SE2	1.78	1.03
2:A:391:0QB:SE2	2:A:391:0QB:CG1	2.58	1.02
2:B:391:0QB:SE2	2:B:391:0QB:CE11	1.74	1.01
1:A:41:PRO:HB2	1:A:55:LEU:HD23	1.41	1.00
2:A:391:0QB:CD21	2:A:391:0QB:SE2	1.80	0.99
2:A:391:0QB:SE2	2:A:391:0QB:CE11	1.76	0.98
1:A:77:THR:HG22	1:A:111:PRO:HG3	1.46	0.97
1:B:48:THR:HG22	1:B:52:TYR:CE2	2.03	0.94
1:A:195:LYS:HB2	1:A:261:HIS:CD2	2.03	0.94
1:B:46(A):ARG:HA	1:B:46(A):ARG:HH11	1.34	0.92
1:A:8:ASN:ND2	1:A:11:ASP:H	1.68	0.91
2:B:391:0QB:SE2	2:B:391:0QB:ND1	2.55	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PRO:HB2	1:B:55:LEU:HD23	1.54	0.90
1:B:25:GLN:HE21	1:B:54:LYS:HZ2	0.92	0.89
1:A:8:ASN:HD21	1:A:11:ASP:H	0.89	0.88
1:A:8:ASN:HD21	1:A:11:ASP:N	1.70	0.87
2:A:391:0QB:SE2	2:A:391:0QB:ND1	2.58	0.87
2:B:391:0QB:HD21	2:B:391:0QB:CG1	2.02	0.87
1:B:205:LEU:HD13	1:B:227:SER:HB2	1.58	0.86
1:B:213:LEU:HD11	2:B:391:0QB:HM21	1.58	0.86
1:A:195:LYS:HZ1	1:A:263:GLY:N	1.74	0.85
1:B:25:GLN:NE2	1:B:54:LYS:HZ2	1.74	0.85
1:B:204:LEU:HD13	1:B:205:LEU:HG	1.59	0.85
2:A:391:0QB:HD21	2:A:391:0QB:CG1	2.05	0.85
1:B:110:LEU:HD12	1:B:111:PRO:HA	1.61	0.82
1:B:48:THR:HG22	1:B:52:TYR:HE2	1.42	0.82
1:B:-1:ASN:ND2	1:B:147:LYS:HG3	1.96	0.79
2:B:391:0QB:SE2	2:B:391:0QB:NZ	2.66	0.79
2:A:391:0QB:SE2	2:A:391:0QB:NZ	2.65	0.79
1:B:204:LEU:CD1	1:B:205:LEU:HG	2.14	0.78
1:A:195:LYS:HE2	1:A:261:HIS:CD2	2.18	0.78
1:A:-2:GLY:O	1:A:147:LYS:HA	1.84	0.77
1:B:185:ILE:HD11	1:B:193:GLN:HB3	1.65	0.77
2:B:391:0QB:ND1	2:B:391:0QB:NZ	2.26	0.77
1:B:2:SER:OG	1:B:92:GLY:HA3	1.85	0.76
1:A:252:GLY:HA3	1:A:277:GLN:OE1	1.86	0.76
2:A:391:0QB:ND1	2:A:391:0QB:NZ	2.30	0.76
1:B:7:THR:O	1:B:14:TYR:HA	1.87	0.76
1:B:32:ASP:OD2	2:B:391:0QB:H32	1.85	0.76
1:A:156:ASN:ND2	1:A:157:ARG:H	1.84	0.75
1:A:204:LEU:O	1:A:205:LEU:HG	1.87	0.75
1:B:150:VAL:HG22	1:B:314:ASP:HA	1.67	0.74
1:B:18:ILE:HG22	1:B:90:THR:O	1.87	0.74
1:B:21:GLY:HA2	1:B:87:ASP:OD1	1.86	0.74
1:B:46(A):ARG:HH11	1:B:46(A):ARG:CA	1.99	0.74
1:A:109:ALA:O	1:A:113:MET:HB2	1.86	0.74
1:B:170:SER:O	1:B:172:PRO:HD3	1.87	0.74
1:B:204:LEU:HD12	1:B:205:LEU:H	1.54	0.73
1:A:89:ILE:CD1	1:A:99:GLN:HB3	2.20	0.72
1:B:41:PRO:HG2	1:B:54:LYS:O	1.89	0.72
1:B:181:TYR:O	1:B:182:ILE:HG13	1.89	0.72
1:B:73:LEU:HD22	1:B:130:ILE:HD13	1.73	0.71
1:A:204:LEU:C	1:A:205:LEU:HG	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:HG3	1:A:245:TYR:CE2	2.26	0.71
1:B:25:GLN:HE21	1:B:54:LYS:NZ	1.80	0.71
1:B:125:PHE:HB2	1:B:188:GLY:O	1.91	0.70
1:A:181:TYR:CD1	1:A:319:ARG:HD3	2.27	0.70
1:B:196:GLY:HA2	1:B:206:CYS:HB3	1.71	0.70
1:A:65:LYS:HG3	1:A:86:GLN:HE21	1.57	0.69
1:A:199:VAL:O	1:A:204:LEU:HD12	1.92	0.69
1:B:226:SER:O	1:B:230:LYS:HD2	1.92	0.69
1:B:240:ARG:O	1:B:243:PHE:N	2.24	0.69
1:B:225:THR:O	1:B:229:GLU:HG3	1.93	0.69
1:B:279(B):SER:OG	1:B:280:LYS:HB2	1.92	0.69
1:B:252:GLY:HA3	1:B:277:GLN:HE22	1.57	0.68
1:A:39:TRP:CE3	1:A:104:VAL:HG21	2.29	0.68
1:A:42:SER:HB2	1:A:103:GLU:HB3	1.76	0.68
1:A:239:LYS:HB2	1:A:245:TYR:CZ	2.28	0.68
1:B:276:PHE:CZ	1:B:285:ALA:HB2	2.29	0.67
1:B:19:GLY:HA2	1:B:25:GLN:O	1.94	0.67
1:B:3:SER:HA	1:B:165:ILE:O	1.94	0.67
1:B:218:ALA:HA	2:B:391:0QB:HA	1.77	0.67
1:A:38:VAL:HG13	1:A:121:VAL:HG22	1.78	0.66
1:B:197:VAL:HB	1:B:205:LEU:HB2	1.77	0.66
1:B:0:THR:OG1	1:B:145:VAL:HG22	1.96	0.66
2:B:391:0QB:HD21	2:B:391:0QB:SE2	2.46	0.66
1:A:195:LYS:NZ	1:A:263:GLY:N	2.44	0.66
1:A:220:TYR:CE2	2:A:391:0QB:H23	2.30	0.65
1:A:291:ILE:O	1:A:296:GLY:HA3	1.96	0.65
1:A:173:GLN:HE22	1:A:326:ARG:HD3	1.62	0.64
1:A:246:VAL:HG21	1:A:281:LEU:HD13	1.79	0.64
1:B:111:PRO:O	1:B:113:MET:N	2.30	0.64
1:B:94:ILE:HG21	1:B:140:ILE:CD1	2.27	0.64
1:A:46:SER:HB2	1:A:47:TYR:CD2	2.33	0.64
1:B:18:ILE:HG22	1:B:91:VAL:HG22	1.80	0.64
1:A:77:THR:HG21	2:A:391:0QB:HB	1.79	0.64
1:A:46(A):ARG:HH11	1:A:46(A):ARG:HG2	1.62	0.63
1:A:153:PHE:CD2	1:A:216:THR:HG21	2.33	0.63
1:A:177:GLY:O	1:A:178:ASN:ND2	2.29	0.63
1:A:176:GLU:HG3	1:A:326:ARG:NE	2.14	0.63
1:A:94:ILE:N	1:A:94:ILE:HD13	2.13	0.63
2:A:391:0QB:HD21	2:A:391:0QB:SE2	2.48	0.63
1:B:176:GLU:HB3	1:B:324:LEU:HB3	1.80	0.63
1:A:156:ASN:OD1	1:A:160(D):SER:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:CG2	1:B:91:VAL:HG22	2.29	0.63
1:A:134:THR:HG22	1:A:139:ASN:OD1	1.99	0.62
1:B:261:HIS:ND1	1:B:266:GLU:OE1	2.33	0.62
1:B:277:GLN:HA	1:B:282:CYS:SG	2.38	0.62
1:B:127:GLU:HB2	1:B:188:GLY:HA2	1.80	0.62
1:A:221:ILE:HG13	1:A:304:THR:HB	1.79	0.62
1:A:148:GLU:HB3	1:A:168:GLY:O	2.00	0.62
1:B:213:LEU:CD1	2:B:391:OQB:HM21	2.29	0.62
1:A:190:TRP:HH2	1:A:315:ARG:HG3	1.65	0.61
1:B:149:ASP:OD1	1:B:316:ARG:HB2	2.00	0.61
1:B:32:ASP:OD1	1:B:34:GLY:N	2.34	0.61
1:A:8:ASN:HD22	1:A:9:TYR:N	1.98	0.60
1:B:28:LYS:O	1:B:117:PHE:HB2	2.01	0.60
1:A:159:SER:HG	1:A:160(D):SER:N	1.98	0.60
1:A:262:LEU:HB2	1:A:267:TYR:HD2	1.66	0.60
1:B:140:ILE:O	1:B:143:GLN:HB2	2.02	0.60
1:B:239:LYS:HG2	1:B:245:TYR:CE2	2.36	0.60
1:B:204:LEU:HD12	1:B:205:LEU:N	2.15	0.59
1:A:-1:ASN:HD21	1:A:147:LYS:HZ3	1.48	0.59
1:B:216:THR:HG22	1:B:306:ILE:CD1	2.31	0.59
1:B:239:LYS:HG2	1:B:245:TYR:CZ	2.37	0.59
1:A:-1:ASN:HD21	1:A:147:LYS:NZ	2.00	0.59
1:A:283:THR:HG22	1:A:284:LEU:O	2.02	0.59
1:A:195:LYS:NZ	1:A:263:GLY:H	2.00	0.58
1:A:261:HIS:HB2	1:A:266:GLU:OE2	2.03	0.58
1:A:298:THR:HG22	1:A:299:TRP:O	2.02	0.58
1:A:156:ASN:HB3	1:A:162:GLY:O	2.03	0.58
1:A:67:ASN:HB3	1:A:84:LEU:O	2.04	0.58
1:A:199:VAL:HG22	1:A:258:ILE:HG12	1.86	0.58
1:B:94:ILE:HD11	1:B:146:LEU:HD23	1.85	0.58
1:A:280:LYS:HG3	1:A:281:LEU:O	2.03	0.57
1:B:192:ILE:HD11	1:B:262:LEU:HD22	1.85	0.57
1:A:89:ILE:HG13	1:A:99:GLN:HB3	1.85	0.57
1:A:262:LEU:HB2	1:A:267:TYR:CD2	2.40	0.57
1:A:174:HIS:HD2	1:A:326:ARG:OXT	1.88	0.57
1:B:232:MET:HE1	1:B:284:LEU:HD12	1.87	0.57
1:B:190:TRP:HE3	1:B:320:ILE:HD11	1.69	0.57
1:B:220:TYR:HH	1:B:276:PHE:HE2	1.53	0.57
1:B:27:PHE:CD1	1:B:54:LYS:HB3	2.39	0.57
1:B:284:LEU:N	1:B:284:LEU:HD23	2.19	0.57
1:B:56:PHE:CE2	1:B:101:PHE:HZ	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ARG:C	1:B:243:PHE:H	2.13	0.56
1:A:222:SER:OG	1:A:300:ALA:HB3	2.06	0.56
1:B:116:GLU:OE1	1:B:116:GLU:HA	2.06	0.56
1:B:156:ASN:ND2	1:B:161:LEU:O	2.39	0.56
1:A:239:LYS:O	1:A:239:LYS:HG3	2.06	0.56
1:B:204:LEU:HD13	1:B:205:LEU:CG	2.33	0.55
1:A:41:PRO:CB	1:A:55:LEU:HD23	2.26	0.55
1:A:180:HIS:O	1:A:321:GLY:HA2	2.05	0.55
1:A:91:VAL:O	1:A:92:GLY:C	2.48	0.55
1:B:194:MET:SD	1:B:260:PHE:HD2	2.29	0.55
1:A:42:SER:OG	1:A:44:LYS:HG2	2.06	0.55
1:A:222:SER:HA	1:A:287:HIS:O	2.07	0.55
1:A:181:TYR:C	1:A:182:ILE:HG13	2.31	0.55
1:A:150:VAL:HB	1:A:312:GLU:OE1	2.07	0.55
1:A:252:GLY:HA2	1:A:255:LEU:HD13	1.88	0.55
1:B:246:VAL:HG12	1:B:283:THR:HA	1.88	0.55
1:A:184:LEU:HB3	1:A:191:GLN:O	2.06	0.55
1:B:196:GLY:O	1:B:261:HIS:ND1	2.39	0.55
1:A:77:THR:CG2	1:A:111:PRO:HG3	2.30	0.54
1:A:29:VAL:HG21	1:A:121:VAL:HG23	1.89	0.54
1:A:224:SER:OG	1:A:227:SER:HB2	2.07	0.54
1:A:230:LYS:O	1:A:233:GLU:HG2	2.07	0.54
1:B:26:THR:O	1:B:54:LYS:HE3	2.07	0.54
1:A:19:GLY:O	1:A:89:ILE:HA	2.08	0.54
1:A:21:GLY:HA2	1:A:87:ASP:OD1	2.08	0.54
1:B:192:ILE:CD1	1:B:262:LEU:HD22	2.38	0.54
1:A:248:LYS:O	1:A:251:GLU:HB3	2.08	0.53
1:B:198:SER:OG	1:B:261:HIS:HE1	1.90	0.53
1:B:126:ILE:HG23	1:B:127:GLU:N	2.23	0.53
1:B:248:LYS:O	1:B:249:CYS:C	2.51	0.53
1:B:151:PHE:HA	1:B:166:VAL:O	2.08	0.53
1:B:9:TYR:CE1	1:B:10:MET:HG3	2.44	0.53
1:B:34:GLY:HA3	1:B:215:ASP:OD1	2.09	0.53
1:B:-1:ASN:HD22	1:B:147:LYS:HG3	1.69	0.53
1:A:288:ALA:O	1:A:289:MET:HE3	2.08	0.53
1:A:215:ASP:O	1:A:302:GLY:HA2	2.09	0.53
1:A:8:ASN:HD22	1:A:8:ASN:C	2.16	0.52
1:B:38:VAL:HG13	1:B:121:VAL:HG22	1.92	0.52
1:A:77:THR:HG21	2:A:391:OQB:CB	2.39	0.52
1:B:249:CYS:O	1:B:251:GLU:N	2.42	0.52
1:A:67:ASN:CB	1:A:100:MET:HE1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:SER:HB3	1:A:266:GLU:HG3	1.92	0.52
1:B:251:GLU:O	1:B:254:THR:HG22	2.09	0.52
1:A:112:PHE:O	1:A:115:ALA:HB3	2.10	0.51
1:A:220:TYR:CZ	2:A:391:OQB:H23	2.45	0.51
1:A:316:ARG:HD2	1:A:316:ARG:C	2.36	0.51
1:A:69:THR:O	1:A:83:PHE:HA	2.11	0.51
1:B:279(B):SER:OG	1:B:280:LYS:HD3	2.10	0.51
1:B:73:LEU:CD2	1:B:130:ILE:HD13	2.39	0.51
1:B:46(A):ARG:HA	1:B:46(A):ARG:NH1	2.14	0.51
1:B:141:ILE:HG22	1:B:142:SER:N	2.24	0.51
1:A:89:ILE:CG1	1:A:99:GLN:HB3	2.41	0.51
1:A:270:THR:HG22	1:A:272:ALA:H	1.76	0.51
1:A:156:ASN:ND2	1:A:157:ARG:N	2.57	0.50
1:A:183:ASN:HB3	1:A:319:ARG:HB3	1.93	0.50
1:B:152:SER:HB3	1:B:310:TYR:CE1	2.46	0.50
1:B:244:ASP:HB3	1:B:287:HIS:NE2	2.25	0.50
1:A:10:MET:C	1:A:12:THR:H	2.19	0.50
1:B:94:ILE:HG21	1:B:140:ILE:HD13	1.92	0.50
1:B:99:GLN:NE2	1:B:136:ILE:HA	2.27	0.50
1:B:235:LEU:HD11	1:B:258:ILE:HD11	1.93	0.50
1:B:276:PHE:O	1:B:278:GLU:N	2.44	0.50
1:A:103:GLU:O	1:A:105:THR:HG23	2.12	0.50
1:A:248:LYS:HB2	1:A:251:GLU:HB2	1.93	0.50
1:A:53:HIS:HB3	1:A:118:ASP:OD1	2.11	0.50
1:A:175:TYR:HA	1:A:325:ALA:HA	1.94	0.50
1:B:203:THR:CG2	1:B:207:GLU:HG2	2.41	0.50
1:A:39:TRP:CD1	1:A:73:LEU:HD13	2.47	0.49
1:A:238:LYS:HE2	1:A:281:LEU:HD21	1.94	0.49
1:B:173:GLN:HA	1:B:173:GLN:OE1	2.09	0.49
1:B:136:ILE:HG23	1:B:137:PHE:N	2.27	0.49
1:A:233:GLU:HG2	1:A:234:ALA:N	2.28	0.49
1:A:149:ASP:OD1	1:A:149:ASP:O	2.30	0.49
1:B:174:HIS:O	1:B:325:ALA:HA	2.12	0.49
1:B:286:ILE:O	1:B:287:HIS:HD2	1.95	0.49
1:A:152:SER:HB3	1:A:312:GLU:HA	1.93	0.49
1:A:195:LYS:HE2	1:A:261:HIS:HD2	1.76	0.49
1:A:159:SER:HB3	1:A:160(D):SER:N	2.28	0.49
1:B:27:PHE:CE1	1:B:54:LYS:HD2	2.48	0.49
1:B:27:PHE:CE1	1:B:54:LYS:HB3	2.48	0.48
1:A:141:ILE:HD13	1:A:141:ILE:HA	1.67	0.48
1:B:42:SER:O	1:B:55:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:OD1	1:A:244:ASP:N	2.46	0.48
1:A:99:GLN:NE2	1:A:136:ILE:HA	2.28	0.48
2:B:391:0QB:H5'2	2:B:391:0QB:CD1	2.43	0.48
1:A:10:MET:O	1:A:11:ASP:HB2	2.13	0.48
1:A:133:VAL:O	1:A:135:PRO:HD3	2.14	0.48
1:A:262:LEU:O	1:A:265:LYS:N	2.45	0.48
1:B:11:ASP:OD1	1:B:158:ASP:N	2.43	0.48
1:B:75:TYR:N	1:B:78:GLY:O	2.42	0.48
1:A:233:GLU:CG	1:A:234:ALA:N	2.77	0.48
1:B:96:VAL:HG11	1:B:140:ILE:HG13	1.96	0.48
1:A:186:LYS:HA	1:A:186:LYS:HD2	1.68	0.47
1:B:225:THR:HA	1:B:288:ALA:HB1	1.96	0.47
1:A:159:SER:HB3	1:A:160(D):SER:OG	2.14	0.47
1:B:232:MET:HG3	1:B:245:TYR:CG	2.50	0.47
1:A:77:THR:HG21	2:A:391:0QB:CG2	2.45	0.47
1:A:185:ILE:HD11	1:A:193:GLN:HG2	1.97	0.47
1:B:6:LEU:HB2	1:B:163:GLY:C	2.39	0.47
1:B:110:LEU:HA	1:B:111:PRO:HA	1.63	0.47
1:B:131:GLY:O	1:B:132:ARG:C	2.57	0.47
1:A:157:ARG:HG3	1:B:160(D):SER:O	2.15	0.47
1:B:204:LEU:CD1	1:B:205:LEU:N	2.78	0.47
1:A:77:THR:HG21	2:A:391:0QB:HG21	1.97	0.47
1:A:89:ILE:HG13	1:A:99:GLN:CB	2.44	0.47
1:A:232:MET:HE3	1:A:245:TYR:CG	2.49	0.47
1:A:67:ASN:HB2	1:A:100:MET:HE1	1.96	0.47
1:B:294:PRO:HD2	1:B:295:THR:H	1.80	0.47
1:A:277:GLN:NE2	1:A:279:SER:O	2.48	0.46
1:B:248:LYS:HE3	1:B:279(C):SER:O	2.14	0.46
1:A:154:TYR:HB2	1:A:310:TYR:CE1	2.51	0.46
1:A:292:PRO:HA	1:A:293:PRO:HD2	1.66	0.46
1:B:41:PRO:CB	1:B:55:LEU:HD23	2.36	0.46
1:B:18:ILE:HD13	1:B:29:VAL:HG21	1.98	0.46
2:B:391:0QB:HN3	2:B:391:0QB:HB	1.67	0.46
1:A:194:MET:O	1:A:209:GLY:HA2	2.16	0.46
1:B:-1:ASN:CG	1:B:147:LYS:HD3	2.40	0.46
1:B:315:ARG:HD2	1:B:315:ARG:HA	1.56	0.46
1:B:53:HIS:O	1:B:55:LEU:HG	2.16	0.46
1:A:181:TYR:CD1	1:A:319:ARG:CD	2.98	0.46
1:B:7:THR:HG22	1:B:15:TYR:CE1	2.51	0.46
1:A:2:SER:O	1:A:166:VAL:HA	2.16	0.46
1:B:42:SER:HB2	1:B:104:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ILE:O	1:B:95:THR:HA	2.16	0.46
1:B:150:VAL:CG2	1:B:314:ASP:HA	2.43	0.46
1:A:125:PHE:H	1:A:125:PHE:HD1	1.64	0.45
1:A:279(D):LYS:HD2	1:A:279(D):LYS:N	2.31	0.45
2:A:391:0QB:HB	2:A:391:0QB:HN3	1.62	0.45
1:B:232:MET:CE	1:B:245:TYR:HB2	2.46	0.45
1:B:239:LYS:HD2	1:B:243:PHE:O	2.16	0.45
1:A:232:MET:HG3	1:A:245:TYR:CZ	2.52	0.45
1:A:280:LYS:HG3	1:A:281:LEU:N	2.30	0.45
1:B:244:ASP:CB	1:B:287:HIS:NE2	2.80	0.45
2:B:391:0QB:HD2	2:B:391:0QB:HG22	1.76	0.45
1:A:141:ILE:C	1:A:143:GLN:H	2.25	0.45
1:A:235:LEU:HD21	1:A:255:LEU:HD23	1.99	0.45
1:B:43:SER:OG	1:B:57:ASP:HA	2.16	0.45
1:A:235:LEU:HD23	1:A:284:LEU:HD21	1.99	0.45
1:A:39:TRP:HA	1:A:102:GLY:O	2.17	0.45
1:A:34:GLY:O	2:A:391:0QB:HM21	2.16	0.45
1:A:7:THR:O	1:A:14:TYR:HA	2.17	0.45
1:B:-1:ASN:ND2	1:B:147:LYS:CG	2.75	0.45
1:B:248:LYS:HB3	1:B:250:ASN:OD1	2.17	0.45
1:A:46(A):ARG:HG2	1:A:46(A):ARG:NH1	2.30	0.44
1:A:104:VAL:O	1:A:104:VAL:HG12	2.16	0.44
1:B:235:LEU:N	1:B:235:LEU:CD1	2.78	0.44
1:B:271:SER:O	1:B:272:ALA:C	2.61	0.44
1:A:131:GLY:O	1:A:132:ARG:C	2.58	0.44
1:B:156:ASN:HB3	1:B:162:GLY:HA2	1.99	0.44
1:B:221:ILE:HG13	1:B:304:THR:HB	1.99	0.44
1:A:249:CYS:HB3	1:A:279:SER:O	2.17	0.44
1:B:21:GLY:O	1:B:24:PRO:HA	2.17	0.44
1:B:126:ILE:CG2	1:B:127:GLU:N	2.80	0.44
1:A:150:VAL:HG12	1:A:314:ASP:HA	1.99	0.44
1:A:190:TRP:CH2	1:A:315:ARG:HG3	2.49	0.44
1:A:229:GLU:O	1:A:233:GLU:HB3	2.17	0.44
1:B:15:TYR:N	1:B:15:TYR:CD1	2.85	0.44
1:B:94:ILE:HG21	1:B:140:ILE:HD11	1.97	0.44
1:B:179:PHE:HA	1:B:322:PHE:O	2.17	0.44
1:A:96:VAL:HG21	1:A:136:ILE:HG13	1.99	0.44
1:A:29:VAL:HA	1:A:119:GLY:O	2.18	0.44
1:B:73:LEU:O	1:B:79:THR:HG23	2.17	0.44
1:B:126:ILE:O	1:B:127:GLU:C	2.61	0.44
1:A:279(D):LYS:HD2	1:A:279(D):LYS:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:ND2	1:A:8:ASN:C	2.74	0.43
1:B:242:LEU:C	1:B:243:PHE:CD2	2.96	0.43
1:A:247:VAL:O	1:A:248:LYS:C	2.60	0.43
1:B:13:GLN:HE21	1:B:13:GLN:HB3	1.64	0.43
1:B:204:LEU:HD13	1:B:205:LEU:CD2	2.48	0.43
1:A:-2:GLY:C	1:A:147:LYS:HA	2.42	0.43
1:A:41:PRO:HG3	1:A:107:MET:SD	2.58	0.43
1:A:238:LYS:HB2	1:A:246:VAL:HG23	2.00	0.43
1:B:232:MET:HG3	1:B:245:TYR:CD2	2.54	0.43
1:A:250:ASN:OD1	1:A:250:ASN:N	2.50	0.43
1:A:233:GLU:HG2	1:A:234:ALA:H	1.84	0.43
1:A:315:ARG:O	1:A:316:ARG:C	2.60	0.43
1:B:18:ILE:CD1	1:B:29:VAL:HG21	2.48	0.43
1:A:49:ALA:CB	1:A:107:MET:HG2	2.49	0.42
1:A:250:ASN:OD1	1:A:279(C):SER:HA	2.19	0.42
1:A:279(A):TYR:N	1:A:279(A):TYR:CD1	2.87	0.42
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.88	0.42
1:B:157:ARG:H	1:B:157:ARG:HG2	1.59	0.42
2:B:391:0QB:H5'2	2:B:391:0QB:HD1	1.99	0.42
1:A:12:THR:O	1:A:219:SER:OG	2.31	0.42
1:A:191:GLN:OE1	1:A:298:THR:HG23	2.19	0.42
1:A:206:CYS:O	1:A:206:CYS:SG	2.77	0.42
1:B:22:THR:HA	1:B:23:PRO:HA	1.92	0.42
1:B:48:THR:O	1:B:51:VAL:HB	2.18	0.42
1:B:250:ASN:CG	1:B:279(C):SER:HA	2.45	0.42
1:A:176:GLU:CG	1:A:326:ARG:NE	2.82	0.42
1:A:0:THR:OG1	1:A:145:VAL:HB	2.19	0.42
1:A:315:ARG:O	1:A:316:ARG:O	2.38	0.42
1:B:45:CYS:O	1:B:46(A):ARG:NH1	2.49	0.42
1:B:248:LYS:HE2	1:B:250:ASN:OD1	2.20	0.42
1:A:20:ILE:HA	1:A:88:ILE:O	2.20	0.42
1:B:147:LYS:HB2	1:B:147:LYS:HE2	1.60	0.42
1:B:149:ASP:OD1	1:B:149:ASP:O	2.37	0.42
1:A:84:LEU:HB3	1:A:100:MET:HE3	2.02	0.42
1:A:252:GLY:C	1:A:254:THR:H	2.28	0.42
1:A:326:ARG:HH12	1:B:1:THR:HG22	1.85	0.42
1:A:207:GLU:O	1:A:208:ASP:HB2	2.20	0.42
1:A:2:SER:HB3	1:A:92:GLY:O	2.19	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.74	0.41
1:B:181:TYR:HA	1:B:321:GLY:HA2	2.02	0.41
1:B:203:THR:HG22	1:B:207:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:CE2	1:A:216:THR:HG21	2.56	0.41
1:A:32:ASP:OD2	1:A:35:SER:OG	2.29	0.41
1:A:94:ILE:HG13	1:A:140:ILE:HD13	2.01	0.41
1:B:8:ASN:ND2	1:B:156:ASN:O	2.54	0.41
1:B:220:TYR:OH	1:B:276:PHE:HE2	2.04	0.41
1:A:137:PHE:HE1	1:A:167:LEU:HB3	1.86	0.41
1:A:182:ILE:HD13	1:A:322:PHE:CE2	2.55	0.41
1:B:309:PHE:O	1:B:310:TYR:C	2.63	0.41
1:A:153:PHE:CD2	1:A:216:THR:CG2	3.03	0.41
1:A:232:MET:CG	1:A:245:TYR:CE2	2.99	0.41
1:B:314:ASP:O	1:B:315:ARG:C	2.61	0.41
1:A:46:SER:HB2	1:A:47:TYR:CE2	2.55	0.41
1:B:33:THR:HG22	1:B:123:MET:HB2	2.03	0.41
1:A:42:SER:HB3	1:A:105:THR:HG22	2.02	0.41
1:A:89:ILE:HD11	1:A:99:GLN:HB3	2.02	0.41
1:B:7:THR:CG2	1:B:8:ASN:N	2.83	0.41
1:B:33:THR:HG23	1:B:216:THR:OG1	2.21	0.41
1:B:80:VAL:O	1:B:81:SER:HB3	2.20	0.41
1:B:215:ASP:OD2	1:B:218:ALA:HB2	2.21	0.41
1:B:232:MET:HE3	1:B:245:TYR:CB	2.51	0.41
1:B:242:LEU:HB3	1:B:243:PHE:CE2	2.56	0.41
1:A:249:CYS:O	1:A:250:ASN:C	2.64	0.41
1:A:283:THR:C	1:A:284:LEU:O	2.59	0.41
1:B:1:THR:HG22	1:B:1:THR:O	2.20	0.41
1:A:148:GLU:O	1:A:168:GLY:HA2	2.21	0.40
1:B:8:ASN:HA	1:B:13:GLN:O	2.21	0.40
1:A:64:TYR:CD1	1:A:64:TYR:C	2.99	0.40
1:B:249:CYS:C	1:B:251:GLU:N	2.79	0.40
1:A:194:MET:HB3	1:A:210:CYS:SG	2.60	0.40
1:B:-1:ASN:ND2	1:B:147:LYS:HD3	2.35	0.40
1:B:73:LEU:HA	1:B:73:LEU:HD23	1.65	0.40
1:B:279:SER:O	1:B:279(A):TYR:HD1	2.04	0.40
1:B:190:TRP:CE3	1:B:320:ILE:HD11	2.54	0.40
1:A:174:HIS:O	1:A:325:ALA:HB1	2.21	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	330/337 (98%)	288 (87%)	33 (10%)	9 (3%)	4	15
1	B	329/337 (98%)	284 (86%)	39 (12%)	6 (2%)	6	23
All	All	659/674 (98%)	572 (87%)	72 (11%)	15 (2%)	5	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	316	ARG
1	B	112	PHE
1	B	242	LEU
1	A	92	GLY
1	B	250	ASN
1	B	277	GLN
1	A	209	GLY
1	A	279	SER
1	A	253	PRO
1	B	147	LYS
1	B	182	ILE
1	A	263	GLY
1	A	172	PRO
1	A	136	ILE

5.3.2 Protein sidechains [i](#)

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	284/287 (99%)	204 (72%)	80 (28%)	0	1
1	B	280/287 (98%)	206 (74%)	74 (26%)	0	2
All	All	564/574 (98%)	410 (73%)	154 (27%)	0	1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	0	THR
1	A	1	THR
1	A	8	ASN
1	A	30	VAL
1	A	35	SER
1	A	36	SER
1	A	38	VAL
1	A	44	LYS
1	A	54	LYS
1	A	63	SER
1	A	71	LEU
1	A	76	SER
1	A	77	THR
1	A	80	VAL
1	A	86	GLN
1	A	90	THR
1	A	94	ILE
1	A	97	THR
1	A	104	VAL
1	A	114	LEU
1	A	116	GLU
1	A	123	MET
1	A	125	PHE
1	A	130	ILE
1	A	132	ARG
1	A	133	VAL
1	A	141	ILE
1	A	146	LEU
1	A	152	SER
1	A	157	ARG
1	A	158	ASP
1	A	159	SER
1	A	161	LEU
1	A	164	GLN

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	170	SER
1	A	173	GLN
1	A	182	ILE
1	A	184	LEU
1	A	186	LYS
1	A	189	VAL
1	A	193	GLN
1	A	195	LYS
1	A	197	VAL
1	A	201	SER
1	A	202	SER
1	A	205	LEU
1	A	207	GLU
1	A	214	VAL
1	A	215	ASP
1	A	226	SER
1	A	228	ILE
1	A	229	GLU
1	A	231	LEU
1	A	233	GLU
1	A	235	LEU
1	A	239	LYS
1	A	240	ARG
1	A	247	VAL
1	A	248	LYS
1	A	251	GLU
1	A	254	THR
1	A	262	LEU
1	A	268	THR
1	A	270	THR
1	A	284	LEU
1	A	287	HIS
1	A	289	MET
1	A	290	ASP
1	A	298	THR
1	A	312	GLU
1	A	315	ARG
1	A	316	ARG
1	A	318	ASN
1	A	319	ARG
1	A	320	ILE

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Mol	Chain	Res	Type
1	A	322	PHE
1	A	324	LEU
1	A	326	ARG
1	B	-1	ASN
1	B	1	THR
1	B	7	THR
1	B	13	GLN
1	B	15	TYR
1	B	17	GLU
1	B	18	ILE
1	B	26	THR
1	B	28	LYS
1	B	30	VAL
1	B	36	SER
1	B	42	SER
1	B	44	LYS
1	B	46	SER
1	B	46(A)	ARG
1	B	46(B)	LEU
1	B	48	THR
1	B	54	LYS
1	B	55	LEU
1	B	71	LEU
1	B	72	THR
1	B	76	SER
1	B	77	THR
1	B	80	VAL
1	B	84	LEU
1	B	86	GLN
1	B	89	ILE
1	B	95	THR
1	B	96	VAL
1	B	97	THR
1	B	100	MET
1	B	105	THR
1	B	116	GLU
1	B	126	ILE
1	B	128	GLN
1	B	138	ASP
1	B	140	ILE
1	B	141	ILE
1	B	142	SER

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Mol	Chain	Res	Type
1	B	146	LEU
1	B	147	LYS
1	B	150	VAL
1	B	157	ARG
1	B	158	ASP
1	B	159	SER
1	B	160(D)	SER
1	B	161	LEU
1	B	173	GLN
1	B	178	ASN
1	B	185	ILE
1	B	186	LYS
1	B	187	THR
1	B	194	MET
1	B	202	SER
1	B	203	THR
1	B	204	LEU
1	B	214	VAL
1	B	219	SER
1	B	225	THR
1	B	226	SER
1	B	228	ILE
1	B	240	ARG
1	B	247	VAL
1	B	254	THR
1	B	265	LYS
1	B	269	LEU
1	B	273	ASP
1	B	283	THR
1	B	284	LEU
1	B	289	MET
1	B	295	THR
1	B	301	LEU
1	B	319	ARG
1	B	324	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	8	ASN
1	A	25	GLN

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Mol	Chain	Res	Type
1	A	86	GLN
1	A	99	GLN
1	A	143	GLN
1	A	156	ASN
1	A	164	GLN
1	A	173	GLN
1	A	174	HIS
1	A	178	ASN
1	A	193	GLN
1	A	261	HIS
1	B	-1	ASN
1	B	25	GLN
1	B	66	HIS
1	B	139	ASN
1	B	173	GLN
1	B	261	HIS
1	B	277	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](#)

2 ligands are 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
2	0QB	A	391	-	51,51,51	1.96	18 (35%)	62,73,73	2.17	18 (29%)
2	0QB	B	391	-	51,51,51	1.83	15 (29%)	62,73,73	2.36	15 (24%)

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
2	0QB	A	391	-	-	6/48/75/75	0/4/4/4
2	0QB	B	391	-	-	9/48/75/75	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	391	0QB	C5-N11	-5.57	1.42	1.48
2	B	391	0QB	O21-C22	4.16	1.29	1.22
2	B	391	0QB	C5-N11	-3.88	1.44	1.48
2	B	391	0QB	CE11-ND1	-3.64	1.26	1.31
2	A	391	0QB	O21-C22	3.49	1.28	1.22
2	A	391	0QB	CD21-SE2	3.26	1.80	1.71
2	B	391	0QB	CE1-CD1	-3.20	1.33	1.38
2	A	391	0QB	CD2-CG	-3.15	1.34	1.39
2	B	391	0QB	CE2-CD2	-3.12	1.33	1.38
2	A	391	0QB	CD1-CG	-3.11	1.34	1.39
2	B	391	0QB	CD1-CG	-2.97	1.34	1.39
2	A	391	0QB	C31-C21	2.94	1.57	1.53
2	B	391	0QB	CD2-CG	-2.87	1.34	1.39
2	B	391	0QB	C-N	2.61	1.37	1.34
2	B	391	0QB	C4-N2	2.61	1.39	1.34
2	B	391	0QB	CG1-ND1	-2.56	1.33	1.38
2	B	391	0QB	CD21-SE2	2.51	1.78	1.71
2	A	391	0QB	CB-N1	-2.48	1.45	1.48
2	A	391	0QB	CE2-CD2	-2.47	1.34	1.38
2	A	391	0QB	O-C	-2.43	1.17	1.23
2	A	391	0QB	CZ-CE2	-2.40	1.33	1.38
2	A	391	0QB	CE11-NZ	-2.40	1.30	1.34
2	A	391	0QB	CE1-CD1	-2.39	1.34	1.38
2	A	391	0QB	C41-C32	2.36	1.58	1.54
2	A	391	0QB	CA-C	-2.30	1.49	1.53
2	A	391	0QB	C21-N2	2.27	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	391	0QB	CD21-CG1	-2.22	1.31	1.35
2	B	391	0QB	CE11-NZ	-2.19	1.30	1.34
2	A	391	0QB	C4-N2	2.16	1.38	1.34
2	A	391	0QB	CE11-ND1	-2.16	1.28	1.31
2	B	391	0QB	C11-C21	2.09	1.57	1.53
2	A	391	0QB	C11-C21	2.09	1.57	1.53
2	B	391	0QB	C31-C21	2.06	1.56	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	0QB	CG2-CB-CG	-9.86	88.83	113.36
2	B	391	0QB	CD21-SE2-CE11	-7.60	85.57	88.84
2	A	391	0QB	CM2-C5-N11	-6.23	104.29	111.00
2	A	391	0QB	CD21-SE2-CE11	-5.81	86.34	88.84
2	A	391	0QB	CA-C-N	4.95	122.25	116.69
2	B	391	0QB	CA-N1-CB	4.91	125.16	117.99
2	A	391	0QB	CG2-CB-N1	-4.55	105.61	110.39
2	A	391	0QB	O2-C4-CA1	-4.47	115.28	122.19
2	B	391	0QB	CN-CA1-C4	-4.34	103.54	109.71
2	A	391	0QB	CN-CA1-C4	-4.33	103.55	109.71
2	A	391	0QB	O21-C22-C32	-4.16	123.17	127.36
2	A	391	0QB	C32-C22-N11	4.08	112.64	108.02
2	B	391	0QB	CG2-CB-N1	3.82	114.40	110.39
2	A	391	0QB	CA1-C4-N2	3.70	122.55	116.19
2	B	391	0QB	CM1-N11-C5	3.46	124.12	121.62
2	B	391	0QB	CM3-C5-N11	-3.25	107.50	111.00
2	B	391	0QB	O2-C4-CA1	-3.14	117.34	122.19
2	A	391	0QB	C41-C5-N11	3.01	104.40	100.53
2	B	391	0QB	O21-C22-C32	-2.94	124.40	127.36
2	B	391	0QB	C32-C22-N11	2.80	111.19	108.02
2	A	391	0QB	C-CA-N1	-2.79	108.80	112.06
2	A	391	0QB	CM3-C5-N11	2.77	113.99	111.00
2	A	391	0QB	C41-C32-C22	-2.75	101.11	103.57
2	B	391	0QB	CM2-C5-N11	2.73	113.95	111.00
2	B	391	0QB	C41-C32-C22	-2.65	101.20	103.57
2	B	391	0QB	C31-C21-C11	-2.64	107.95	112.18
2	A	391	0QB	O-C-N	-2.55	117.84	121.89
2	B	391	0QB	C31-C1'-C6'	-2.51	105.86	111.71
2	B	391	0QB	CB1-CA1-C4	-2.28	106.47	109.71
2	A	391	0QB	C31-C1'-C6'	-2.24	106.50	111.71
2	A	391	0QB	CG-CB-N1	-2.23	107.52	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	391	0QB	C31-C21-C11	-2.21	108.64	112.18
2	A	391	0QB	CA-N1-CB	2.16	121.14	117.99

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	391	0QB	C21-C11-C32-C41
2	A	391	0QB	O11-C11-C32-C22
2	B	391	0QB	O11-C11-C32-C22
2	B	391	0QB	C6'-C1'-C31-C21
2	A	391	0QB	C2'-C1'-C31-C21
2	A	391	0QB	C6'-C1'-C31-C21
2	B	391	0QB	C2'-C1'-C31-C21
2	B	391	0QB	N2-C21-C31-C1'
2	A	391	0QB	O11-C11-C32-C41
2	B	391	0QB	O11-C11-C32-C41
2	A	391	0QB	C4-CA1-CB1-CG1
2	B	391	0QB	C21-C11-C32-C41
2	B	391	0QB	CG2-CB-N1-CA
2	B	391	0QB	CG2-CB-N1-C3
2	B	391	0QB	C4-CA1-CB1-CG1

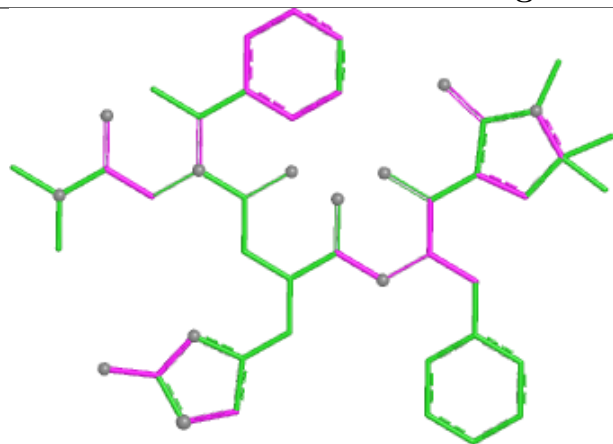
There are no ring outliers.

2 monomers are involved in 34 short contacts:

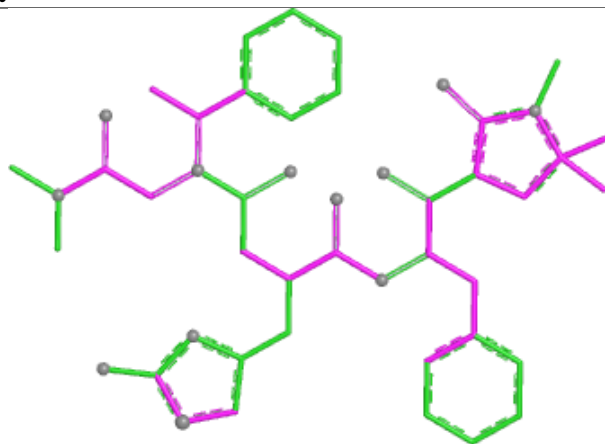
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	391	0QB	17	0
2	B	391	0QB	17	0

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.

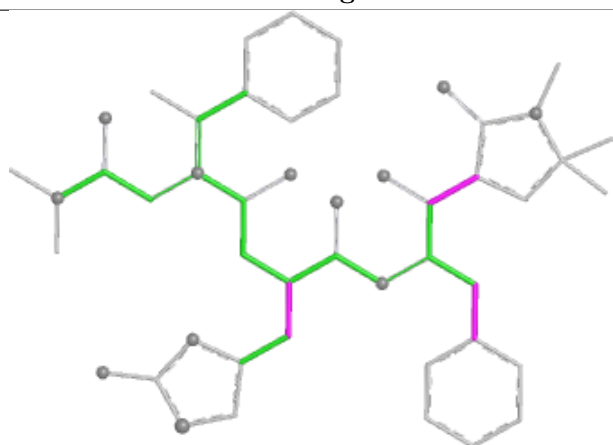
Ligand 0QB A 391



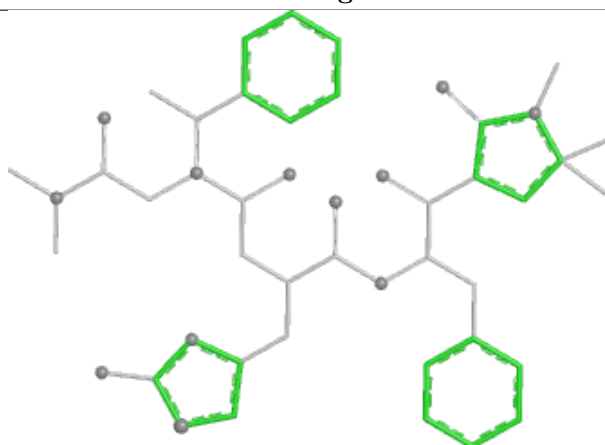
Bond lengths



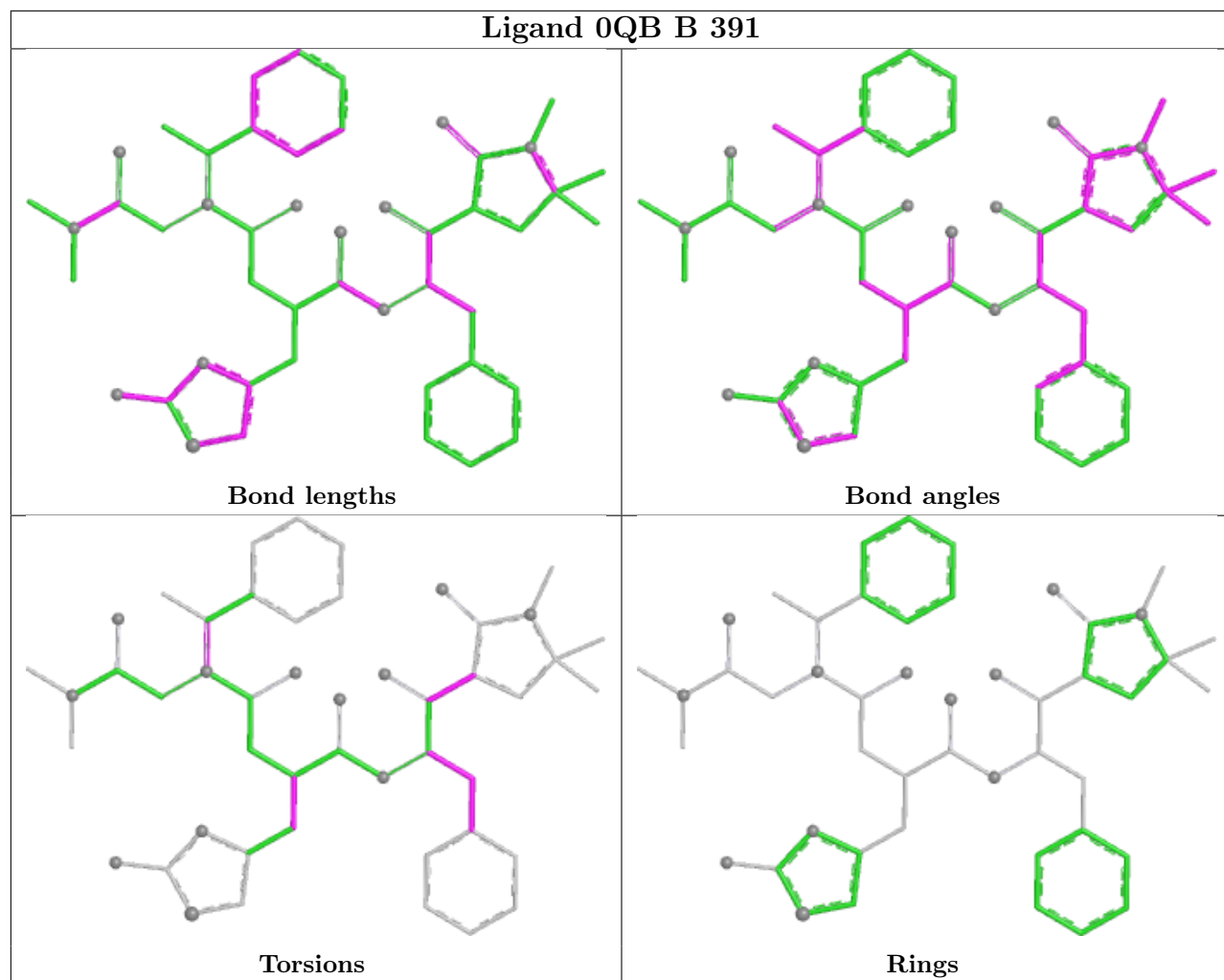
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.