



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:33 AM UTC

PDB ID : 1BAV / pdb_00001bav
Title : CARBOXYPEPTIDASE A COMPLEXED WITH 2-BENZYL-3-iodo-PRO
PANOIC ACID (BIP)
Authors : Martin, P.; Edwards, B.
Deposited on : 1996-11-14
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

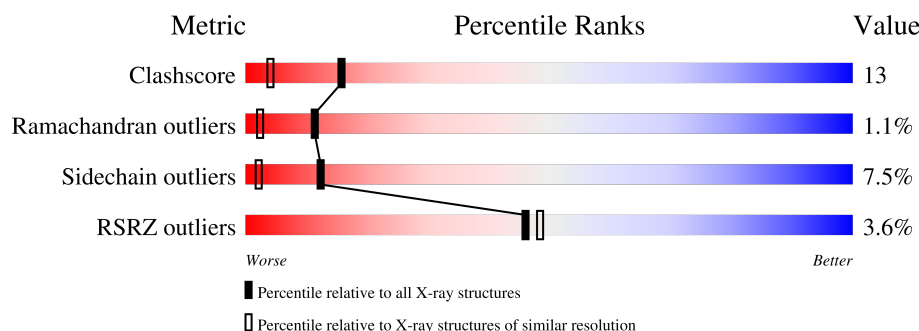
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	3% 77% 18% • •
1	B	309	3% 70% 24% 5% •
1	C	309	5% 75% 20% 5% •
1	D	309	3% 64% 29% 6% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10371 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2436	1561	406	464	5			
1	B	307	Total	C	N	O	S	0	0	0
			2436	1561	406	464	5			
1	C	307	Total	C	N	O	S	0	0	0
			2436	1561	406	464	5			
1	D	307	Total	C	N	O	S	0	0	0
			2436	1561	406	464	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLN	GLU	conflict	UNP P00730
A	31	GLU	GLN	conflict	UNP P00730
A	89	ASN	ASP	conflict	UNP P00730
A	93	ASN	ASP	conflict	UNP P00730
A	114	ASN	ASP	conflict	UNP P00730
A	122	GLU	GLN	conflict	UNP P00730
A	185	ASN	ASP	conflict	UNP P00730
A	228	ALA	GLU	conflict	UNP P00730
A	305	VAL	LEU	conflict	UNP P00730
B	28	GLN	GLU	conflict	UNP P00730
B	31	GLU	GLN	conflict	UNP P00730
B	89	ASN	ASP	conflict	UNP P00730
B	93	ASN	ASP	conflict	UNP P00730
B	114	ASN	ASP	conflict	UNP P00730
B	122	GLU	GLN	conflict	UNP P00730
B	185	ASN	ASP	conflict	UNP P00730
B	228	ALA	GLU	conflict	UNP P00730
B	305	VAL	LEU	conflict	UNP P00730
C	28	GLN	GLU	conflict	UNP P00730
C	31	GLU	GLN	conflict	UNP P00730
C	89	ASN	ASP	conflict	UNP P00730

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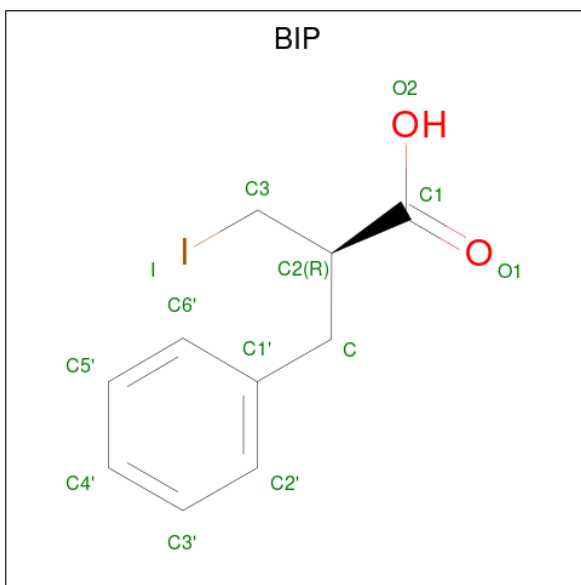
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Chain	Residue	Modelled	Actual	Comment	Reference
C	93	ASN	ASP	conflict	UNP P00730
C	114	ASN	ASP	conflict	UNP P00730
C	122	GLU	GLN	conflict	UNP P00730
C	185	ASN	ASP	conflict	UNP P00730
C	228	ALA	GLU	conflict	UNP P00730
C	305	VAL	LEU	conflict	UNP P00730
D	28	GLN	GLU	conflict	UNP P00730
D	31	GLU	GLN	conflict	UNP P00730
D	89	ASN	ASP	conflict	UNP P00730
D	93	ASN	ASP	conflict	UNP P00730
D	114	ASN	ASP	conflict	UNP P00730
D	122	GLU	GLN	conflict	UNP P00730
D	185	ASN	ASP	conflict	UNP P00730
D	228	ALA	GLU	conflict	UNP P00730
D	305	VAL	LEU	conflict	UNP P00730

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is 2-BENZYL-3-IODOPROPANOIC ACID (CCD ID: BIP) (formula: C₁₀H₁₁IO₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			12	10	2		
3	C	1	Total	C	O	0	0
			12	10	2		
3	D	1	Total	C	O	0	0
			12	10	2		

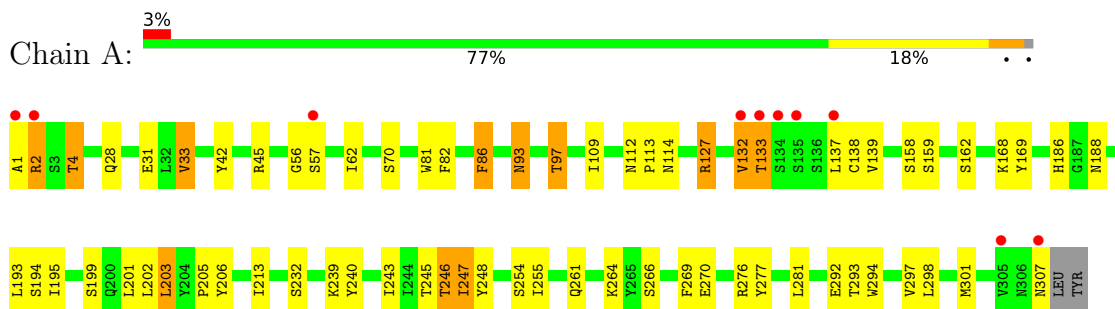
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	155	Total	O	0	0
			155	155		
4	C	129	Total	O	0	0
			129	129		
4	D	137	Total	O	0	0
			137	137		

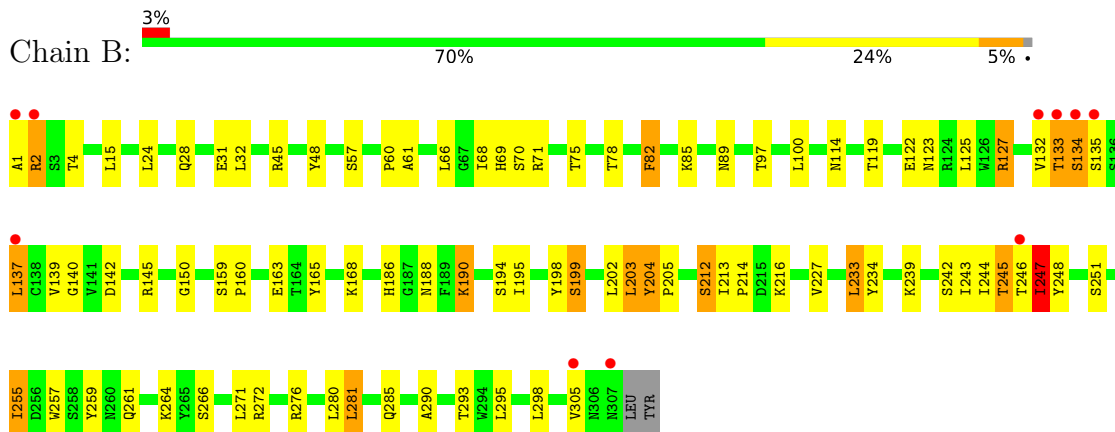
3 Residue-property plots

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.

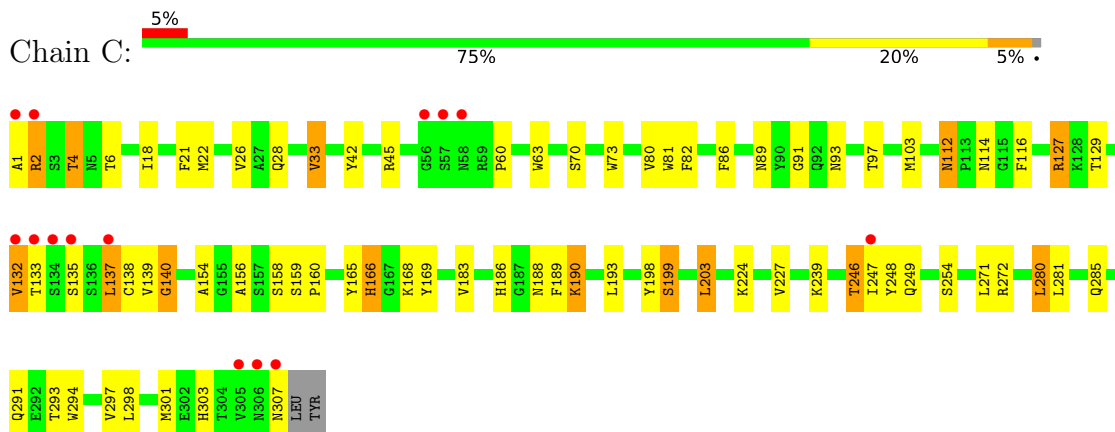
• Molecule 1: CARBOXYPEPTIDASE A



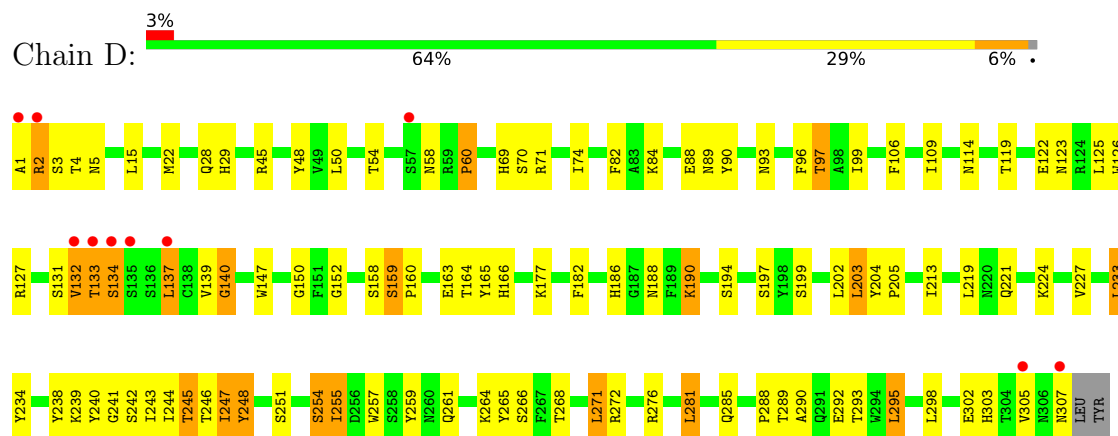
• Molecule 1: CARBOXYPEPTIDASE A



• Molecule 1: CARBOXYPEPTIDASE A



● Molecule 1: CARBOXYPEPTIDASE A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.70Å 60.50Å 91.80Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.60 104.87 – 1.62	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.60) 44.6 (104.87-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.16 (at 1.62Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , 0.213 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.5	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10371	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 98.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4415e-11. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BIP, ZN

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	0.61	0/2502	1.07	18/3402 (0.5%)
1	B	0.59	0/2502	1.09	14/3402 (0.4%)
1	C	0.58	0/2502	1.04	12/3402 (0.4%)
1	D	0.58	0/2502	1.06	15/3402 (0.4%)
All	All	0.59	0/10008	1.07	59/13608 (0.4%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	SER	N-CA-C	8.36	121.32	111.71
1	C	70	SER	N-CA-C	7.93	120.62	111.11
1	B	82	PHE	CB-CG-CD2	-7.78	107.48	120.70
1	D	244	ILE	N-CA-C	7.30	118.02	110.36
1	D	70	SER	N-CA-C	7.23	120.03	111.71
1	C	246	THR	N-CA-C	7.04	122.87	113.72
1	A	264	LYS	N-CA-C	6.92	119.46	111.02
1	C	254	SER	N-CA-C	6.78	118.67	111.28
1	D	140	GLY	N-CA-C	6.71	121.13	112.68
1	A	93	ASN	CA-C-N	6.58	126.08	119.24
1	A	93	ASN	C-N-CA	6.58	126.08	119.24
1	B	82	PHE	CB-CG-CD1	6.56	131.86	120.70
1	A	33	VAL	N-CA-C	6.50	118.15	108.46
1	C	159	SER	CA-C-N	6.49	127.00	119.47
1	C	159	SER	C-N-CA	6.49	127.00	119.47
1	C	140	GLY	N-CA-C	6.45	120.29	112.48
1	B	244	ILE	N-CA-C	6.44	117.19	110.62
1	A	232	SER	N-CA-C	6.44	120.23	112.38
1	D	264	LYS	N-CA-C	6.28	118.12	111.28
1	D	159	SER	CA-C-N	6.24	125.93	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	159	SER	C-N-CA	6.24	125.93	119.56
1	A	109	ILE	N-CA-C	6.21	117.00	110.72
1	C	135	SER	N-CA-C	-6.19	102.85	110.65
1	D	60	PRO	N-CA-C	-6.16	101.59	111.38
1	A	246	THR	N-CA-C	6.12	122.79	113.61
1	D	109	ILE	N-CA-C	6.06	116.84	110.72
1	D	122	GLU	N-CA-C	6.03	121.14	113.55
1	B	204	TYR	CA-C-N	6.01	125.97	119.78
1	B	204	TYR	C-N-CA	6.01	125.97	119.78
1	C	89	ASN	N-CA-C	5.92	120.23	112.89
1	A	261	GLN	N-CA-C	-5.86	105.62	112.89
1	B	145	ARG	N-CA-C	-5.79	105.59	114.16
1	A	56	GLY	N-CA-C	5.78	122.98	112.58
1	A	4	THR	N-CA-C	-5.75	105.76	112.89
1	B	70	SER	N-CA-C	5.71	120.78	111.37
1	B	61	ALA	N-CA-C	5.69	117.72	109.07
1	B	195	ILE	N-CA-C	5.68	116.48	108.36
1	D	89	ASN	N-CA-C	5.66	118.39	111.82
1	A	270	GLU	N-CA-C	-5.65	97.99	107.99
1	A	292	GLU	N-CA-C	5.60	117.46	111.36
1	B	140	GLY	N-CA-C	5.57	119.64	112.18
1	B	264	LYS	N-CA-C	5.51	116.97	111.07
1	A	254	SER	N-CA-C	5.37	117.22	111.36
1	A	239	LYS	N-CA-C	-5.34	101.47	109.95
1	A	112	ASN	CA-C-N	5.33	124.51	118.97
1	A	112	ASN	C-N-CA	5.33	124.51	118.97
1	D	29	HIS	CA-C-N	5.30	125.62	119.47
1	D	29	HIS	C-N-CA	5.30	125.62	119.47
1	B	48	TYR	N-CA-C	5.26	117.82	109.24
1	C	166	HIS	N-CA-C	5.16	119.42	113.18
1	C	4	THR	N-CA-C	-5.14	106.27	112.54
1	B	247	ILE	CB-CA-C	-5.13	102.88	111.29
1	C	73	TRP	N-CA-C	5.12	118.31	111.75
1	C	33	VAL	N-CA-C	5.10	116.05	108.46
1	A	86	PHE	CB-CG-CD1	5.09	129.35	120.70
1	D	271	LEU	N-CA-C	5.09	117.38	109.60
1	D	197	SER	N-CA-C	-5.08	101.57	109.24
1	D	82	PHE	CB-CG-CD2	-5.02	112.17	120.70
1	B	122	GLU	N-CA-C	5.01	121.48	110.80

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	2436	0	2352	50	0
1	B	2436	0	2352	68	0
1	C	2436	0	2352	61	0
1	D	2436	0	2352	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	8	2	0
3	B	12	0	8	0	0
3	C	12	0	8	1	0
3	D	12	0	8	1	0
4	A	154	0	0	15	0
4	B	155	0	0	16	0
4	C	129	0	0	6	0
4	D	137	0	0	12	0
All	All	10371	0	9440	256	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 13.

All (256) 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:C:293:THR:HB	4:C:380:HOH:O	1.45	1.17
1:B:97:THR:HB	4:B:423:HOH:O	1.48	1.11
1:D:246:THR:HB	4:D:396:HOH:O	1.55	1.04
1:B:293:THR:HB	4:B:378:HOH:O	1.55	1.03
1:A:293:THR:HB	4:A:397:HOH:O	1.59	1.01
1:A:132:VAL:HG23	1:A:133:THR:H	1.28	0.97
1:D:255:ILE:HG21	4:D:409:HOH:O	1.65	0.95
1:C:132:VAL:HG23	1:C:133:THR:H	1.36	0.90
1:D:243:ILE:HG23	1:D:247:ILE:HD11	1.53	0.89
1:D:221:GLN:HB2	4:D:432:HOH:O	1.73	0.89
1:B:255:ILE:HG21	4:B:419:HOH:O	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:HIS:HD2	1:C:188:ASN:H	1.22	0.86
1:C:60:PRO:HB3	1:C:190:LYS:HD2	1.57	0.86
1:C:203:LEU:HG	1:C:247:ILE:HD11	1.60	0.84
1:B:242:SER:O	1:B:246:THR:HG23	1.78	0.83
1:A:186:HIS:HD2	1:A:188:ASN:H	1.27	0.83
1:D:4:THR:H	1:D:28:GLN:HE22	1.28	0.81
1:D:22:MET:HE3	1:D:50:LEU:HG	1.65	0.79
1:C:93:ASN:O	1:C:97:THR:HG23	1.83	0.79
1:A:93:ASN:O	1:A:97:THR:HG22	1.82	0.78
1:C:42:TYR:OH	1:C:132:VAL:HG22	1.85	0.77
1:B:85:LYS:HD2	1:B:89:ASN:ND2	2.00	0.77
1:A:86:PHE:HE1	1:A:294:TRP:HZ3	1.34	0.76
1:C:137:LEU:HD13	1:C:137:LEU:H	1.50	0.75
1:A:1:ALA:HB1	1:A:2:ARG:HH21	1.50	0.75
1:A:168:LYS:HG2	4:A:370:HOH:O	1.87	0.74
1:C:246:THR:HB	4:C:362:HOH:O	1.86	0.74
1:B:255:ILE:HG12	4:B:419:HOH:O	1.86	0.74
1:A:42:TYR:OH	1:A:132:VAL:HG22	1.87	0.73
1:A:243:ILE:HG23	1:A:247:ILE:HD12	1.70	0.72
1:C:186:HIS:CD2	1:C:188:ASN:H	2.07	0.72
1:B:186:HIS:HD2	1:B:188:ASN:H	1.36	0.72
1:D:190:LYS:HE3	1:D:190:LYS:HA	1.71	0.72
1:A:31:GLU:HB2	4:A:362:HOH:O	1.89	0.71
1:C:132:VAL:HG23	1:C:133:THR:N	2.03	0.71
1:B:45:ARG:HH11	1:B:114:ASN:ND2	1.89	0.71
1:C:91:GLY:H	1:C:97:THR:HG22	1.56	0.71
1:C:4:THR:H	1:C:28:GLN:HE22	1.37	0.70
1:B:160:PRO:HA	1:B:165:TYR:CD2	2.26	0.70
1:A:4:THR:H	1:A:28:GLN:HE22	1.40	0.70
1:A:82:PHE:HZ	1:A:293:THR:HG23	1.57	0.70
1:A:82:PHE:CZ	1:A:293:THR:HG23	2.28	0.69
1:C:82:PHE:HZ	1:C:293:THR:HG23	1.59	0.67
1:A:205:PRO:HG3	1:A:255:ILE:HG22	1.77	0.67
1:D:119:THR:HA	1:D:123:ASN:O	1.96	0.66
1:D:247:ILE:HD12	1:D:248:TYR:H	1.60	0.66
1:B:4:THR:H	1:B:28:GLN:HE22	1.42	0.66
1:B:150:GLY:O	1:B:251:SER:HB2	1.96	0.66
1:C:82:PHE:CZ	1:C:293:THR:HG23	2.31	0.66
1:B:203:LEU:HD12	1:B:246:THR:HG21	1.77	0.65
1:C:272:ARG:HH11	1:C:285:GLN:HE21	1.43	0.65
1:D:281:LEU:HD13	1:D:285:GLN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG23	1:A:133:THR:N	2.09	0.63
1:B:272:ARG:HH11	1:B:285:GLN:HE21	1.46	0.63
1:D:245:THR:HB	4:D:410:HOH:O	1.98	0.62
1:C:280:LEU:HD12	1:C:280:LEU:N	2.15	0.61
1:D:137:LEU:HD13	1:D:137:LEU:H	1.65	0.61
1:A:186:HIS:HD2	1:A:188:ASN:N	1.96	0.60
1:B:194:SER:HB3	4:B:403:HOH:O	2.02	0.60
1:D:194:SER:CB	4:D:395:HOH:O	2.49	0.60
1:B:190:LYS:HE3	1:B:190:LYS:HA	1.84	0.60
1:D:257:TRP:O	1:D:261:GLN:HG2	2.01	0.60
1:A:245:THR:HG22	1:A:246:THR:HG23	1.84	0.59
1:D:152:GLY:HA2	1:D:166:HIS:CD2	2.38	0.59
1:B:186:HIS:CD2	1:B:188:ASN:H	2.20	0.59
1:C:186:HIS:HD2	1:C:188:ASN:N	1.98	0.59
1:B:32:LEU:HD11	1:B:100:LEU:HD13	1.85	0.58
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.02	0.58
1:B:214:PRO:HD3	4:B:459:HOH:O	2.04	0.57
1:D:2:ARG:N	1:D:2:ARG:NE	2.52	0.57
1:A:246:THR:HB	4:A:371:HOH:O	2.03	0.57
1:D:255:ILE:HG12	4:D:409:HOH:O	2.04	0.57
1:C:45:ARG:HH11	1:C:114:ASN:ND2	2.03	0.57
1:D:255:ILE:HG13	1:D:266:SER:HB3	1.86	0.57
1:D:302:GLU:O	1:D:305:VAL:HG12	2.05	0.57
1:D:204:TYR:O	1:D:242:SER:HA	2.04	0.57
1:D:303:HIS:HB2	4:D:426:HOH:O	2.04	0.57
1:A:86:PHE:CE1	1:A:294:TRP:HZ3	2.20	0.56
1:A:243:ILE:HG23	1:A:247:ILE:CD1	2.35	0.56
1:D:194:SER:HB3	4:D:395:HOH:O	2.05	0.56
1:A:132:VAL:CG2	1:A:133:THR:H	2.09	0.56
1:B:246:THR:HB	4:B:402:HOH:O	2.05	0.56
1:B:255:ILE:HG13	1:B:266:SER:HB3	1.87	0.56
1:D:289:THR:O	1:D:293:THR:HG22	2.06	0.56
1:C:198:TYR:O	1:C:199:SER:CB	2.55	0.55
1:A:247:ILE:HD13	3:A:311:BIP:H2A	1.88	0.55
1:C:272:ARG:HH11	1:C:285:GLN:NE2	2.05	0.54
1:A:62:ILE:HD13	1:A:301:MET:HG2	1.89	0.54
1:B:233:LEU:HD13	1:B:234:TYR:CE2	2.42	0.54
1:D:71:ARG:HD3	1:D:125:LEU:O	2.08	0.54
1:B:132:VAL:O	1:B:133:THR:HB	2.08	0.54
1:B:257:TRP:O	1:B:261:GLN:HG2	2.07	0.54
1:A:297:VAL:HG12	1:A:301:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ARG:N	1:D:2:ARG:HE	2.05	0.54
1:B:194:SER:CB	4:B:403:HOH:O	2.56	0.53
1:B:205:PRO:HB2	1:B:213:ILE:HG21	1.90	0.53
1:A:194:SER:HB3	4:A:366:HOH:O	2.08	0.53
1:D:233:LEU:HD13	1:D:234:TYR:CE2	2.43	0.53
1:A:276:ARG:HD3	1:A:277:TYR:CZ	2.42	0.53
1:C:137:LEU:H	1:C:137:LEU:CD1	2.20	0.53
1:D:241:GLY:HA3	1:D:246:THR:HG21	1.91	0.53
1:D:290:ALA:HA	1:D:293:THR:HG22	1.91	0.53
1:C:127:ARG:NH2	4:C:385:HOH:O	2.42	0.52
1:D:186:HIS:HD2	1:D:188:ASN:H	1.57	0.52
1:C:291:GLN:O	1:C:294:TRP:HB3	2.09	0.52
1:B:45:ARG:HH11	1:B:114:ASN:HD22	1.53	0.52
1:C:203:LEU:CG	1:C:247:ILE:HD11	2.37	0.52
1:D:45:ARG:HH11	1:D:114:ASN:ND2	2.07	0.52
1:B:119:THR:HA	1:B:123:ASN:O	2.10	0.52
1:D:127:ARG:HD2	1:D:163:GLU:HB3	1.92	0.52
1:C:22:MET:O	1:C:26:VAL:HG23	2.10	0.52
1:D:133:THR:O	1:D:134:SER:CB	2.58	0.52
1:A:168:LYS:HG3	1:A:169:TYR:CD2	2.46	0.51
1:D:22:MET:HE1	1:D:48:TYR:HB3	1.92	0.51
1:A:159:SER:O	1:A:162:SER:HB3	2.10	0.51
1:A:194:SER:CB	4:A:366:HOH:O	2.58	0.51
1:C:45:ARG:HD2	1:C:114:ASN:HD22	1.75	0.51
1:B:243:ILE:HA	1:B:246:THR:OG1	2.11	0.51
1:C:203:LEU:N	1:C:203:LEU:HD22	2.25	0.51
1:A:205:PRO:HG3	1:A:255:ILE:CG2	2.39	0.51
1:C:2:ARG:N	1:C:2:ARG:NE	2.59	0.51
1:D:241:GLY:CA	1:D:246:THR:HG21	2.41	0.50
1:D:74:ILE:HD13	1:D:281:LEU:HD12	1.93	0.50
1:D:254:SER:CB	4:D:402:HOH:O	2.60	0.50
1:A:203:LEU:CD2	1:A:247:ILE:HD11	2.40	0.50
1:C:60:PRO:HB3	1:C:190:LYS:CD	2.36	0.50
1:B:168:LYS:HG2	4:B:401:HOH:O	2.12	0.50
1:B:246:THR:CB	4:B:402:HOH:O	2.60	0.50
1:B:281:LEU:HD11	1:B:285:GLN:HB2	1.93	0.50
1:C:91:GLY:H	1:C:97:THR:CG2	2.24	0.50
1:B:66:LEU:HD22	1:B:75:THR:O	2.11	0.49
1:B:78:THR:HG21	1:B:293:THR:HG21	1.93	0.49
1:A:255:ILE:HG23	1:A:266:SER:HB3	1.93	0.49
1:B:137:LEU:HD13	1:B:137:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ALA:HA	1:B:293:THR:HG22	1.93	0.49
1:B:2:ARG:HB2	1:B:2:ARG:NH1	2.27	0.49
1:B:160:PRO:HA	1:B:165:TYR:CG	2.48	0.48
1:D:54:THR:HG21	1:D:90:TYR:CZ	2.48	0.48
1:A:243:ILE:O	1:A:247:ILE:HG13	2.13	0.48
1:A:113:PRO:HD2	4:A:394:HOH:O	2.12	0.48
1:A:127:ARG:NH2	4:A:399:HOH:O	2.46	0.48
1:D:303:HIS:O	1:D:307:ASN:ND2	2.46	0.48
1:C:183:VAL:HG13	1:C:189:PHE:CD2	2.48	0.48
1:D:150:GLY:O	1:D:251:SER:HB2	2.13	0.48
1:B:186:HIS:HD2	1:B:188:ASN:N	2.09	0.48
1:C:247:ILE:CD1	3:C:311:BIP:H2A	2.44	0.48
1:D:268:THR:HG21	3:D:311:BIP:H6'	1.96	0.48
1:D:1:ALA:C	1:D:2:ARG:HE	2.21	0.48
1:D:227:VAL:HG13	1:D:238:TYR:HB2	1.96	0.47
1:D:126:TRP:CH2	1:D:139:VAL:HG13	2.49	0.47
1:C:224:LYS:HE2	4:C:351:HOH:O	2.15	0.47
1:D:245:THR:CB	4:D:410:HOH:O	2.58	0.47
1:A:138:CYS:HB3	4:A:421:HOH:O	2.15	0.47
1:C:160:PRO:HA	1:C:165:TYR:CD2	2.50	0.47
1:D:265:TYR:CE1	1:D:303:HIS:HD2	2.33	0.46
1:B:127:ARG:HD2	1:B:163:GLU:HB3	1.97	0.46
1:C:2:ARG:HB2	1:C:2:ARG:CZ	2.46	0.46
1:D:133:THR:O	1:D:134:SER:HB2	2.16	0.46
1:B:212:SER:HB3	4:B:460:HOH:O	2.16	0.46
1:A:203:LEU:HD21	1:A:247:ILE:HD11	1.96	0.46
1:B:276:ARG:O	1:B:276:ARG:HD3	2.16	0.46
1:D:132:VAL:O	1:D:133:THR:HB	2.15	0.46
1:A:294:TRP:HZ2	4:A:363:HOH:O	1.98	0.45
1:C:138:CYS:HB3	4:C:412:HOH:O	2.15	0.45
1:C:154:ALA:HB3	1:C:249:GLN:NE2	2.30	0.45
1:D:160:PRO:HA	1:D:165:TYR:CD2	2.51	0.45
1:B:2:ARG:HB2	1:B:2:ARG:CZ	2.45	0.45
1:B:127:ARG:CD	1:B:163:GLU:HB3	2.47	0.45
1:B:281:LEU:CD1	1:B:285:GLN:HB2	2.46	0.45
1:D:69:HIS:CE1	4:D:372:HOH:O	2.70	0.45
1:B:186:HIS:CE1	4:B:451:HOH:O	2.69	0.45
1:D:84:LYS:O	1:D:88:GLU:HG2	2.17	0.45
1:B:127:ARG:HD3	1:B:163:GLU:O	2.16	0.45
1:C:132:VAL:CG2	1:C:133:THR:N	2.74	0.45
1:C:63:TRP:HB2	1:C:189:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:VAL:CG1	1:C:301:MET:HE3	2.47	0.45
1:D:303:HIS:O	1:D:307:ASN:HB2	2.17	0.45
1:B:32:LEU:HD11	1:B:100:LEU:CD1	2.46	0.44
1:B:242:SER:O	1:B:246:THR:CG2	2.59	0.44
1:D:213:ILE:HB	1:D:259:TYR:CZ	2.52	0.44
1:C:198:TYR:O	1:C:199:SER:HB3	2.17	0.44
1:B:243:ILE:HG23	1:B:247:ILE:HD11	1.97	0.44
1:C:112:ASN:C	1:C:112:ASN:HD22	2.26	0.44
1:C:303:HIS:O	1:C:307:ASN:N	2.51	0.44
1:D:3:SER:C	1:D:5:ASN:H	2.26	0.44
1:D:106:PHE:CE2	1:D:182:PHE:HZ	2.35	0.44
1:A:1:ALA:N	4:A:451:HOH:O	2.50	0.44
1:C:129:THR:O	1:C:140:GLY:HA3	2.17	0.44
1:D:127:ARG:HG2	1:D:163:GLU:OE1	2.17	0.44
1:D:4:THR:N	1:D:28:GLN:HE22	2.06	0.44
1:C:21:PHE:CE2	1:C:80:VAL:HG13	2.53	0.44
1:C:168:LYS:HE3	1:C:169:TYR:CE2	2.53	0.44
1:A:247:ILE:HD13	3:A:311:BIP:C	2.48	0.44
1:C:186:HIS:HE1	4:C:324:HOH:O	2.01	0.44
1:B:69:HIS:NE2	1:B:142:ASP:OD1	2.51	0.43
1:B:4:THR:N	1:B:28:GLN:HE22	2.14	0.43
1:B:272:ARG:HH11	1:B:285:GLN:NE2	2.14	0.43
1:D:96:PHE:HA	1:D:99:ILE:HD12	2.00	0.43
1:C:81:TRP:HE3	1:C:82:PHE:HD1	1.66	0.43
1:B:204:TYR:O	1:B:242:SER:HA	2.18	0.43
1:D:159:SER:HA	1:D:160:PRO:HD3	1.90	0.43
1:B:82:PHE:CE1	1:B:293:THR:HG23	2.54	0.43
1:A:201:LEU:HD22	4:A:371:HOH:O	2.17	0.43
1:A:293:THR:CB	4:A:397:HOH:O	2.40	0.43
1:B:243:ILE:HD11	1:B:255:ILE:HG21	1.99	0.43
1:C:18:ILE:HD12	1:C:116:PHE:CE2	2.54	0.43
1:B:68:ILE:HG22	4:B:393:HOH:O	2.19	0.43
1:B:82:PHE:HE1	1:B:293:THR:HG23	1.83	0.43
1:B:198:TYR:O	1:B:199:SER:CB	2.67	0.43
1:C:60:PRO:O	1:C:103:MET:HB3	2.18	0.43
1:B:71:ARG:HD3	1:B:125:LEU:O	2.19	0.43
1:B:245:THR:CB	4:B:421:HOH:O	2.67	0.42
1:A:81:TRP:HE3	1:A:82:PHE:HD1	1.67	0.42
1:D:205:PRO:HG3	1:D:255:ILE:HG23	2.01	0.42
1:B:255:ILE:CG2	4:B:419:HOH:O	2.51	0.42
1:B:60:PRO:HB3	1:B:190:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PRO:HA	1:B:165:TYR:CE2	2.54	0.42
1:C:239:LYS:N	1:C:239:LYS:HD2	2.35	0.42
1:D:60:PRO:HA	1:D:188:ASN:O	2.20	0.42
1:D:147:TRP:CE2	1:D:254:SER:HB3	2.55	0.42
1:D:203:LEU:HG	1:D:243:ILE:HA	2.01	0.42
1:D:213:ILE:CD1	1:D:219:LEU:HD22	2.50	0.42
1:C:168:LYS:HG3	1:C:169:TYR:CD2	2.55	0.42
1:D:93:ASN:O	1:D:97:THR:CG2	2.68	0.42
1:B:214:PRO:HD2	1:B:259:TYR:OH	2.19	0.42
1:C:160:PRO:HA	1:C:165:TYR:CG	2.54	0.42
1:D:45:ARG:HH11	1:D:114:ASN:HD22	1.67	0.41
1:A:206:TYR:CE2	1:A:213:ILE:HG22	2.54	0.41
1:B:186:HIS:HE1	4:B:451:HOH:O	2.04	0.41
1:D:147:TRP:CD2	1:D:254:SER:HB3	2.55	0.41
1:D:272:ARG:HH21	1:D:292:GLU:CD	2.28	0.41
1:A:195:ILE:HD12	1:A:269:PHE:HB2	2.01	0.41
1:A:186:HIS:HE1	4:A:324:HOH:O	2.02	0.41
1:C:280:LEU:N	1:C:280:LEU:CD1	2.83	0.41
1:A:246:THR:CB	4:A:371:HOH:O	2.64	0.41
1:C:1:ALA:HB1	1:C:6:THR:HB	2.01	0.41
1:C:91:GLY:N	1:C:97:THR:HG22	2.28	0.41
1:C:137:LEU:HD22	1:C:138:CYS:SG	2.61	0.41
1:D:139:VAL:HG22	1:D:140:GLY:N	2.36	0.41
1:D:243:ILE:HG23	1:D:247:ILE:CD1	2.38	0.41
1:B:134:SER:OG	1:B:135:SER:N	2.53	0.41
1:B:243:ILE:C	1:B:246:THR:HG1	2.27	0.41
1:C:2:ARG:N	1:C:2:ARG:HE	2.19	0.41
1:D:224:LYS:HE2	1:D:240:TYR:OH	2.21	0.41
1:D:285:GLN:C	1:D:288:PRO:HD2	2.46	0.41
1:D:295:LEU:HD12	1:D:295:LEU:HA	1.87	0.41
1:A:202:LEU:O	1:A:240:TYR:HA	2.21	0.41
1:D:254:SER:HB2	4:D:402:HOH:O	2.21	0.41
1:B:1:ALA:O	1:B:24:LEU:HD11	2.22	0.40
1:C:156:ALA:HB1	1:C:166:HIS:HB3	2.02	0.40
1:D:290:ALA:HA	1:D:293:THR:CG2	2.51	0.40
1:C:86:PHE:HE1	1:C:294:TRP:HZ3	1.68	0.40
1:D:22:MET:HE1	1:D:48:TYR:CB	2.50	0.40
1:D:131:SER:O	1:D:139:VAL:HG23	2.20	0.40
1:A:127:ARG:C	1:A:127:ARG:HD3	2.47	0.40
1:D:3:SER:C	1:D:5:ASN:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	305/309 (99%)	283 (93%)	19 (6%)	3 (1%)	12	3
1	B	305/309 (99%)	284 (93%)	18 (6%)	3 (1%)	12	3
1	C	305/309 (99%)	289 (95%)	14 (5%)	2 (1%)	18	6
1	D	305/309 (99%)	280 (92%)	20 (7%)	5 (2%)	7	1
All	All	1220/1236 (99%)	1136 (93%)	71 (6%)	13 (1%)	11	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	THR
1	B	134	SER
1	B	199	SER
1	C	199	SER
1	D	134	SER
1	D	199	SER
1	A	199	SER
1	C	132	VAL
1	D	58	ASN
1	A	57	SER
1	D	133	THR
1	A	132	VAL
1	D	132	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	263/265 (99%)	248 (94%)	15 (6%)	18	4
1	B	263/265 (99%)	237 (90%)	26 (10%)	7	1
1	C	263/265 (99%)	247 (94%)	16 (6%)	17	3
1	D	263/265 (99%)	241 (92%)	22 (8%)	10	1
All	All	1052/1060 (99%)	973 (92%)	79 (8%)	12	2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	33	VAL
1	A	97	THR
1	A	127	ARG
1	A	133	THR
1	A	137	LEU
1	A	139	VAL
1	A	158	SER
1	A	193	LEU
1	A	203	LEU
1	A	247	ILE
1	A	248	TYR
1	A	281	LEU
1	A	298	LEU
1	A	307	ASN
1	B	2	ARG
1	B	15	LEU
1	B	31	GLU
1	B	57	SER
1	B	127	ARG
1	B	137	LEU
1	B	139	VAL
1	B	159	SER
1	B	190	LYS
1	B	202	LEU
1	B	203	LEU
1	B	212	SER
1	B	216	LYS
1	B	227	VAL
1	B	233	LEU
1	B	239	LYS
1	B	245	THR
1	B	247	ILE

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Mol	Chain	Res	Type
1	B	248	TYR
1	B	255	ILE
1	B	271	LEU
1	B	280	LEU
1	B	281	LEU
1	B	295	LEU
1	B	298	LEU
1	B	305	VAL
1	C	2	ARG
1	C	33	VAL
1	C	112	ASN
1	C	127	ARG
1	C	137	LEU
1	C	139	VAL
1	C	158	SER
1	C	190	LYS
1	C	193	LEU
1	C	203	LEU
1	C	227	VAL
1	C	248	TYR
1	C	271	LEU
1	C	280	LEU
1	C	281	LEU
1	C	298	LEU
1	D	2	ARG
1	D	15	LEU
1	D	97	THR
1	D	137	LEU
1	D	158	SER
1	D	164	THR
1	D	177	LYS
1	D	190	LYS
1	D	202	LEU
1	D	203	LEU
1	D	233	LEU
1	D	239	LYS
1	D	245	THR
1	D	247	ILE
1	D	248	TYR
1	D	254	SER
1	D	255	ILE
1	D	271	LEU

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Mol	Chain	Res	Type
1	D	276	ARG
1	D	281	LEU
1	D	295	LEU
1	D	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	28	GLN
1	A	37	GLN
1	A	112	ASN
1	A	114	ASN
1	A	171	ASN
1	A	186	HIS
1	A	285	GLN
1	B	5	ASN
1	B	8	ASN
1	B	28	GLN
1	B	29	HIS
1	B	58	ASN
1	B	89	ASN
1	B	92	GLN
1	B	112	ASN
1	B	114	ASN
1	B	186	HIS
1	B	249	GLN
1	B	285	GLN
1	C	28	GLN
1	C	37	GLN
1	C	92	GLN
1	C	112	ASN
1	C	114	ASN
1	C	171	ASN
1	C	186	HIS
1	C	249	GLN
1	C	285	GLN
1	C	307	ASN
1	D	5	ASN
1	D	28	GLN
1	D	29	HIS
1	D	112	ASN

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Mol	Chain	Res	Type
1	D	114	ASN
1	D	186	HIS
1	D	249	GLN
1	D	285	GLN
1	D	307	ASN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	BIP	D	311	1	12,12,13	0.90	0	15,15,16	0.34	0
3	BIP	C	311	1	12,12,13	0.79	0	15,15,16	0.93	1 (6%)
3	BIP	A	311	1	12,12,13	0.77	0	15,15,16	0.80	0
3	BIP	B	311	1	12,12,13	0.84	0	15,15,16	0.55	0

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	BIP	D	311	1	-	0/8/8/10	0/1/1/1
3	BIP	C	311	1	-	3/8/8/10	0/1/1/1
3	BIP	A	311	1	-	4/8/8/10	0/1/1/1
3	BIP	B	311	1	-	0/8/8/10	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	BIP	O1-C1-C2	-2.42	114.90	122.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	311	BIP	O1-C1-C2-C3
3	C	311	BIP	O1-C1-C2-C3
3	C	311	BIP	O2-C1-C2-C3
3	A	311	BIP	O2-C1-C2-C3
3	A	311	BIP	O1-C1-C2-C
3	A	311	BIP	O2-C1-C2-C
3	C	311	BIP	O2-C1-C2-C

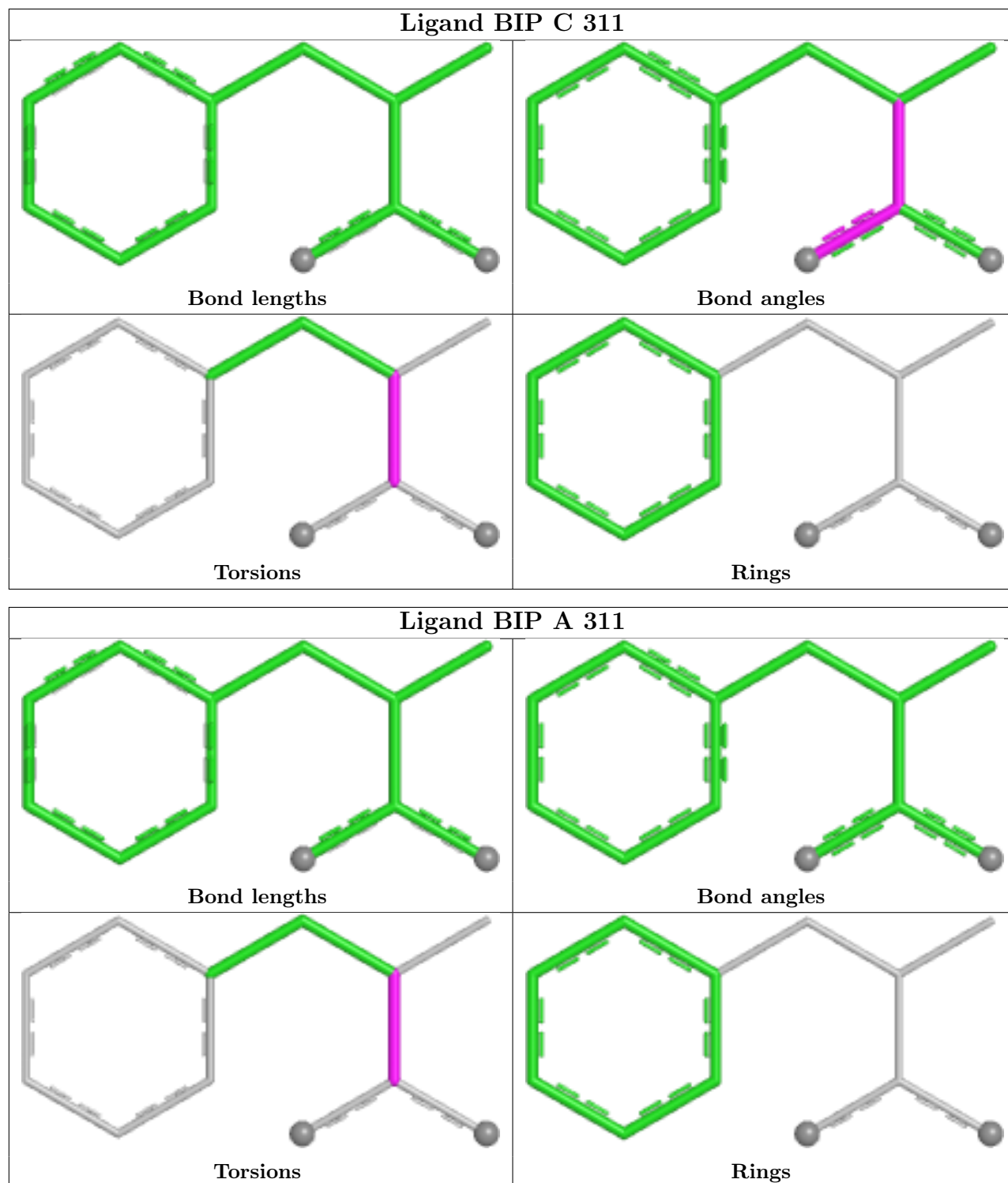
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	311	BIP	1	0
3	C	311	BIP	1	0
3	A	311	BIP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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 ⓘ

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	307/309 (99%)	-0.30	10 (3%)	49	52	3, 10, 23, 49	0
1	B	307/309 (99%)	-0.31	10 (3%)	49	52	4, 10, 21, 47	0
1	C	307/309 (99%)	-0.20	14 (4%)	37	39	2, 11, 25, 47	0
1	D	307/309 (99%)	-0.20	10 (3%)	49	52	3, 11, 26, 50	0
All	All	1228/1236 (99%)	-0.25	44 (3%)	46	48	2, 10, 25, 50	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	133	THR	7.7
1	A	133	THR	6.6
1	D	133	THR	5.8
1	B	1	ALA	5.3
1	B	133	THR	4.9
1	C	137	LEU	4.6
1	C	134	SER	4.6
1	A	2	ARG	4.1
1	D	137	LEU	3.9
1	C	132	VAL	3.9
1	B	246	THR	3.8
1	A	134	SER	3.8
1	A	1	ALA	3.7
1	A	137	LEU	3.7
1	C	2	ARG	3.5
1	D	2	ARG	3.5
1	C	307	ASN	3.5
1	D	57	SER	3.5
1	C	58	ASN	3.4
1	D	134	SER	3.3
1	B	137	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	135	SER	3.2
1	C	306	ASN	3.2
1	B	2	ARG	3.1
1	B	132	VAL	3.0
1	D	305	VAL	3.0
1	A	132	VAL	2.9
1	C	1	ALA	2.9
1	C	57	SER	2.8
1	B	305	VAL	2.8
1	C	135	SER	2.7
1	C	247	ILE	2.7
1	B	307	ASN	2.7
1	B	134	SER	2.7
1	A	307	ASN	2.6
1	D	307	ASN	2.6
1	A	57	SER	2.6
1	D	132	VAL	2.5
1	B	135	SER	2.5
1	D	1	ALA	2.4
1	A	305	VAL	2.3
1	C	56	GLY	2.3
1	C	305	VAL	2.1
1	A	135	SER	2.1

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.

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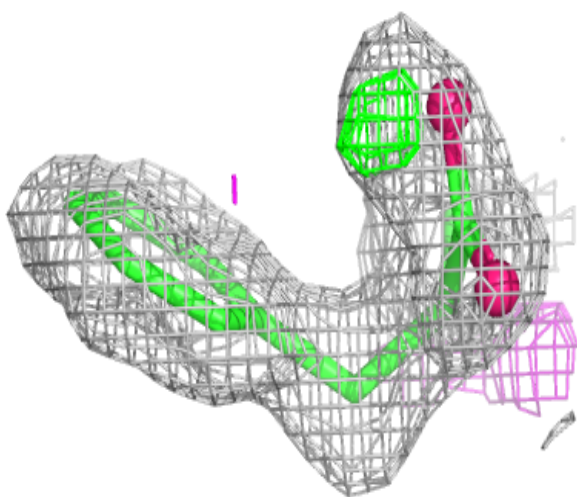
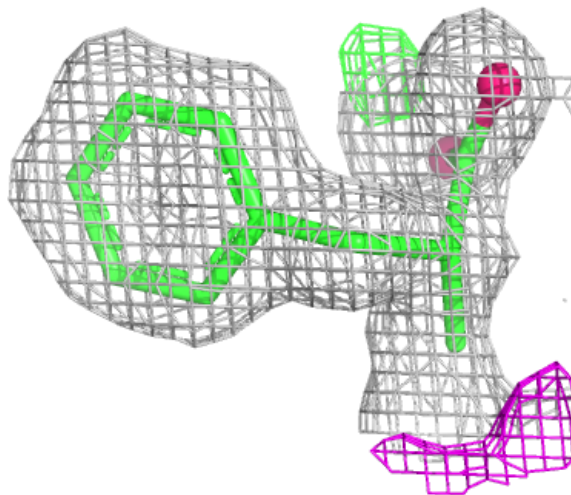
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BIP	D	311	12/13	0.90	0.08	6,8,11,12	0
3	BIP	C	311	12/13	0.93	0.12	25,29,36,37	0
3	BIP	A	311	12/13	0.95	0.06	6,9,11,11	0
3	BIP	B	311	12/13	0.95	0.07	12,14,15,22	0
2	ZN	A	310	1/1	1.00	0.01	8,8,8,8	0
2	ZN	B	310	1/1	1.00	0.01	12,12,12,12	0
2	ZN	C	310	1/1	1.00	0.02	6,6,6,6	0
2	ZN	D	310	1/1	1.00	0.01	12,12,12,12	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.

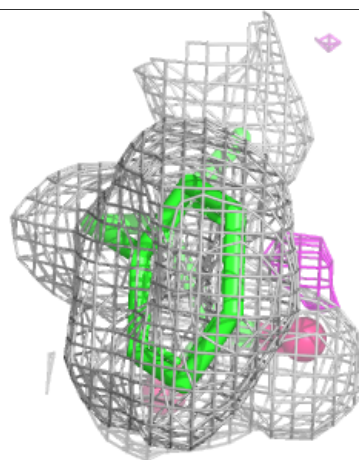
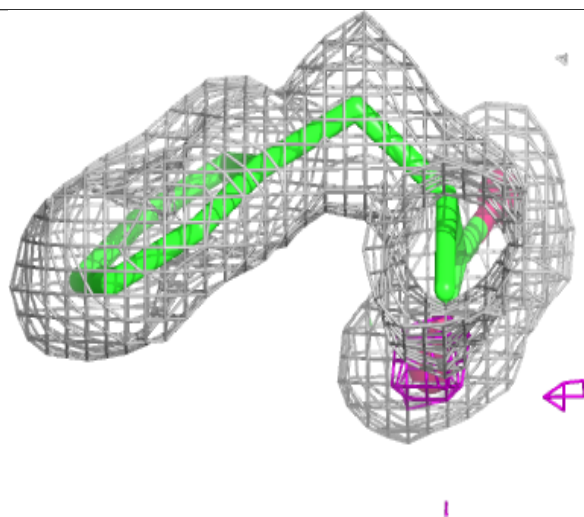
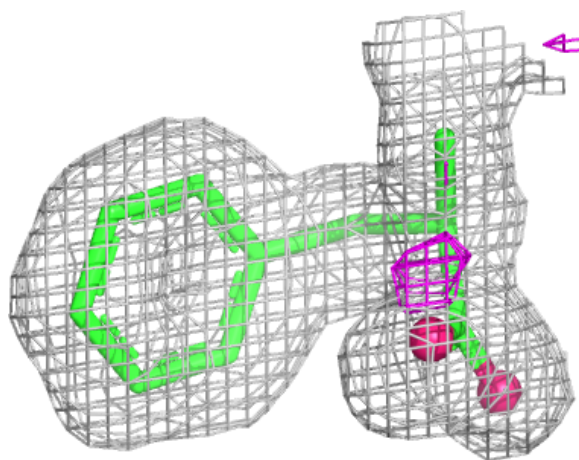
Electron density around BIP C 311:

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



Electron density around BIP A 311:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.