



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:50 PM UTC

PDB ID : 6PVS / pdb_00006pvs
Title : Structure of Nicotinamide N-Methyltransferase (NNMT) in complex with inhibitor LL320
Authors : Noinaj, N.; Huang, R.; Chen, D.; Yadav, R.
Deposited on : 2019-07-21
Resolution : 2.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

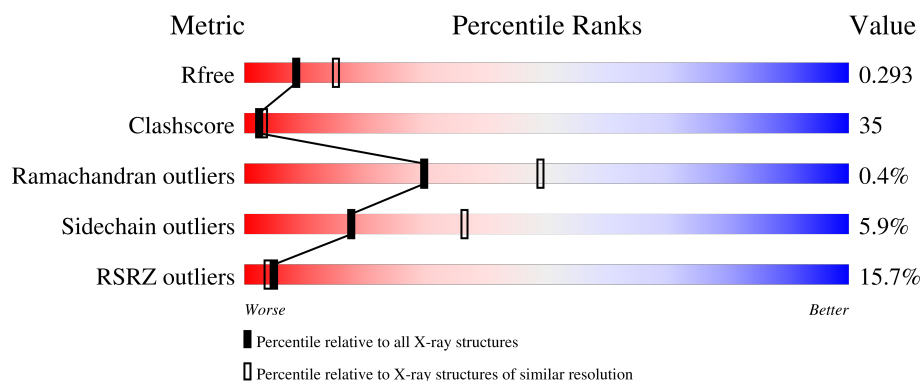
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	283	14% 51% 42% 5%
1	B	283	16% 53% 39% 5%
1	C	283	14% 42% 43% 6% 9%
1	D	283	15% 50% 37% 9%

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
2	P0V	D	301	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8506 atoms, of which 104 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 NNMT protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2076	1327	338	399	12			
1	B	270	Total	C	N	O	S	0	0	0
			2083	1335	337	399	12			
1	C	257	Total	C	N	O	S	0	0	0
			1997	1284	322	380	11			
1	D	258	Total	C	N	O	S	0	0	0
			1988	1276	319	382	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q6FH49
A	-17	GLY	-	expression tag	UNP Q6FH49
A	-16	SER	-	expression tag	UNP Q6FH49
A	-15	SER	-	expression tag	UNP Q6FH49
A	-14	HIS	-	expression tag	UNP Q6FH49
A	-13	HIS	-	expression tag	UNP Q6FH49
A	-12	HIS	-	expression tag	UNP Q6FH49
A	-11	HIS	-	expression tag	UNP Q6FH49
A	-10	HIS	-	expression tag	UNP Q6FH49
A	-9	HIS	-	expression tag	UNP Q6FH49
A	-8	SER	-	expression tag	UNP Q6FH49
A	-7	SER	-	expression tag	UNP Q6FH49
A	-6	GLY	-	expression tag	UNP Q6FH49
A	-5	LEU	-	expression tag	UNP Q6FH49
A	-4	VAL	-	expression tag	UNP Q6FH49
A	-3	PRO	-	expression tag	UNP Q6FH49
A	-2	ARG	-	expression tag	UNP Q6FH49
A	-1	GLY	-	expression tag	UNP Q6FH49
A	0	SER	-	expression tag	UNP Q6FH49
A	100	ALA	LYS	engineered mutation	UNP Q6FH49
A	101	ALA	GLU	engineered mutation	UNP Q6FH49

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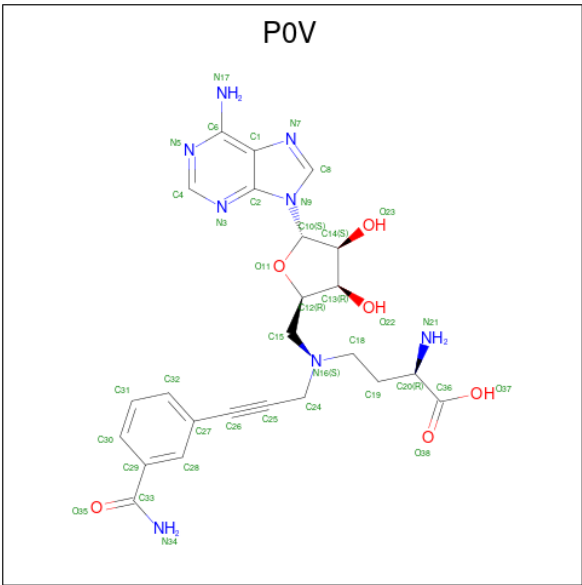
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	GLU	engineered mutation	UNP Q6FH49
B	-18	MET	-	expression tag	UNP Q6FH49
B	-17	GLY	-	expression tag	UNP Q6FH49
B	-16	SER	-	expression tag	UNP Q6FH49
B	-15	SER	-	expression tag	UNP Q6FH49
B	-14	HIS	-	expression tag	UNP Q6FH49
B	-13	HIS	-	expression tag	UNP Q6FH49
B	-12	HIS	-	expression tag	UNP Q6FH49
B	-11	HIS	-	expression tag	UNP Q6FH49
B	-10	HIS	-	expression tag	UNP Q6FH49
B	-9	HIS	-	expression tag	UNP Q6FH49
B	-8	SER	-	expression tag	UNP Q6FH49
B	-7	SER	-	expression tag	UNP Q6FH49
B	-6	GLY	-	expression tag	UNP Q6FH49
B	-5	LEU	-	expression tag	UNP Q6FH49
B	-4	VAL	-	expression tag	UNP Q6FH49
B	-3	PRO	-	expression tag	UNP Q6FH49
B	-2	ARG	-	expression tag	UNP Q6FH49
B	-1	GLY	-	expression tag	UNP Q6FH49
B	0	SER	-	expression tag	UNP Q6FH49
B	100	ALA	LYS	engineered mutation	UNP Q6FH49
B	101	ALA	GLU	engineered mutation	UNP Q6FH49
B	103	ALA	GLU	engineered mutation	UNP Q6FH49
C	-18	MET	-	expression tag	UNP Q6FH49
C	-17	GLY	-	expression tag	UNP Q6FH49
C	-16	SER	-	expression tag	UNP Q6FH49
C	-15	SER	-	expression tag	UNP Q6FH49
C	-14	HIS	-	expression tag	UNP Q6FH49
C	-13	HIS	-	expression tag	UNP Q6FH49
C	-12	HIS	-	expression tag	UNP Q6FH49
C	-11	HIS	-	expression tag	UNP Q6FH49
C	-10	HIS	-	expression tag	UNP Q6FH49
C	-9	HIS	-	expression tag	UNP Q6FH49
C	-8	SER	-	expression tag	UNP Q6FH49
C	-7	SER	-	expression tag	UNP Q6FH49
C	-6	GLY	-	expression tag	UNP Q6FH49
C	-5	LEU	-	expression tag	UNP Q6FH49
C	-4	VAL	-	expression tag	UNP Q6FH49
C	-3	PRO	-	expression tag	UNP Q6FH49
C	-2	ARG	-	expression tag	UNP Q6FH49
C	-1	GLY	-	expression tag	UNP Q6FH49
C	0	SER	-	expression tag	UNP Q6FH49

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	ALA	LYS	engineered mutation	UNP Q6FH49
C	101	ALA	GLU	engineered mutation	UNP Q6FH49
C	103	ALA	GLU	engineered mutation	UNP Q6FH49
D	-18	MET	-	expression tag	UNP Q6FH49
D	-17	GLY	-	expression tag	UNP Q6FH49
D	-16	SER	-	expression tag	UNP Q6FH49
D	-15	SER	-	expression tag	UNP Q6FH49
D	-14	HIS	-	expression tag	UNP Q6FH49
D	-13	HIS	-	expression tag	UNP Q6FH49
D	-12	HIS	-	expression tag	UNP Q6FH49
D	-11	HIS	-	expression tag	UNP Q6FH49
D	-10	HIS	-	expression tag	UNP Q6FH49
D	-9	HIS	-	expression tag	UNP Q6FH49
D	-8	SER	-	expression tag	UNP Q6FH49
D	-7	SER	-	expression tag	UNP Q6FH49
D	-6	GLY	-	expression tag	UNP Q6FH49
D	-5	LEU	-	expression tag	UNP Q6FH49
D	-4	VAL	-	expression tag	UNP Q6FH49
D	-3	PRO	-	expression tag	UNP Q6FH49
D	-2	ARG	-	expression tag	UNP Q6FH49
D	-1	GLY	-	expression tag	UNP Q6FH49
D	0	SER	-	expression tag	UNP Q6FH49
D	100	ALA	LYS	engineered mutation	UNP Q6FH49
D	101	ALA	GLU	engineered mutation	UNP Q6FH49
D	103	ALA	GLU	engineered mutation	UNP Q6FH49

- Molecule 2 is 9-(5-([(3R)-3-amino-3-carboxypropyl][3-(3-carbamoylphenyl)prop-2-yn-1-yl]amino}-5-deoxy-alpha-D-lyxofuranosyl)-9H-purin-6-amine (CCD ID: P0V) (formula: C₂₄H₂₈N₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			64	24	26	8	6		
2	B	1	Total	C	H	N	O	0	0
			64	24	26	8	6		
2	C	1	Total	C	H	N	O	0	0
			64	24	26	8	6		
2	D	1	Total	C	H	N	O	0	0
			64	24	26	8	6		

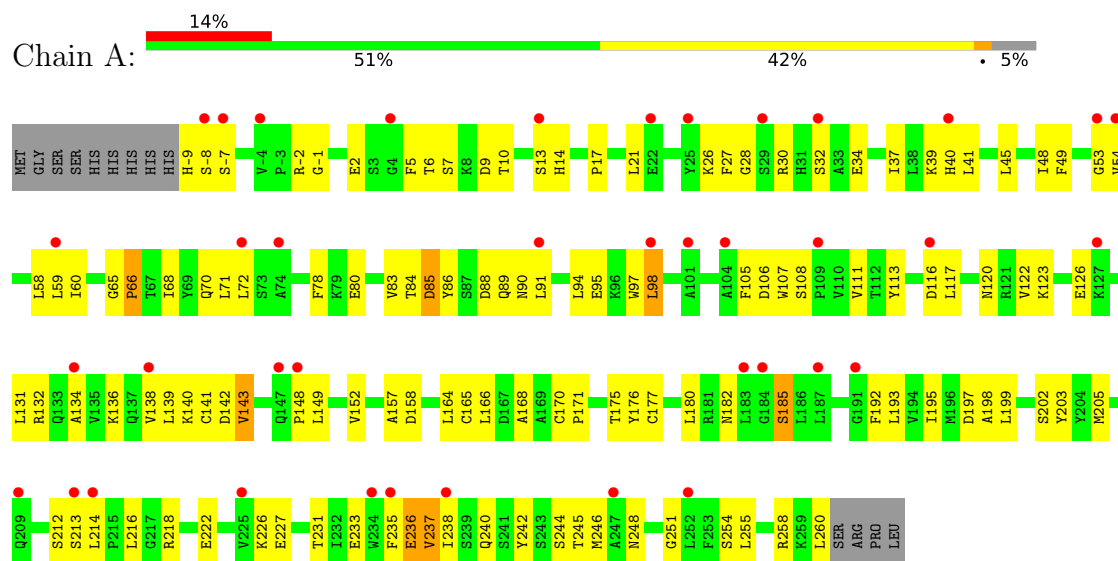
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	31	Total	O	0	0
			31	31		
3	C	29	Total	O	0	0
			29	29		
3	D	18	Total	O	0	0
			18	18		

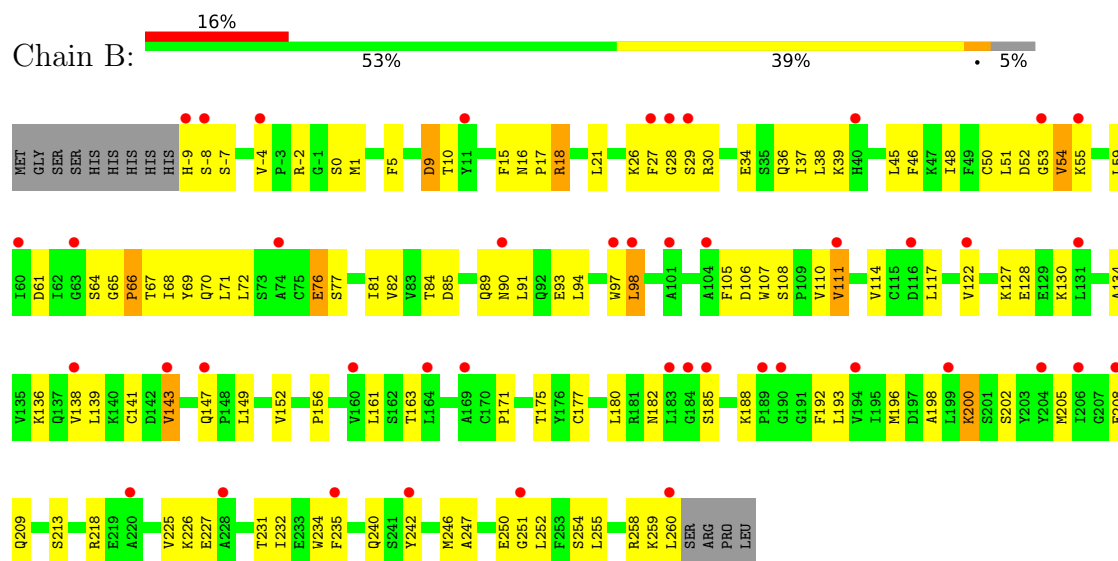
3 Residue-property plots [i](#)

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 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.

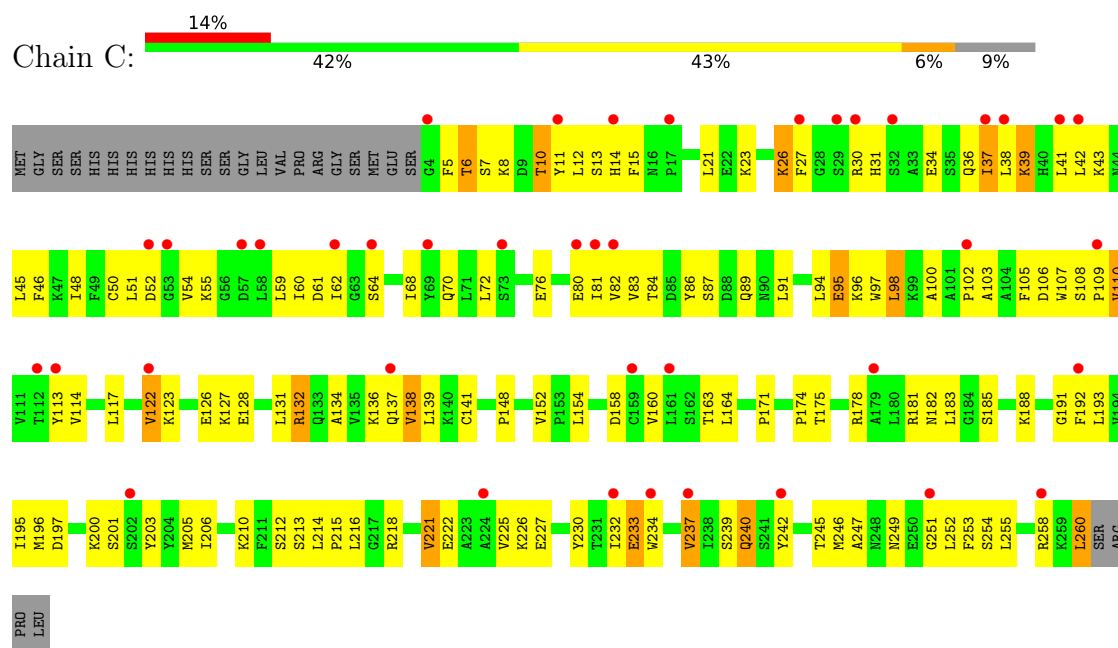
• Molecule 1: NNMT protein



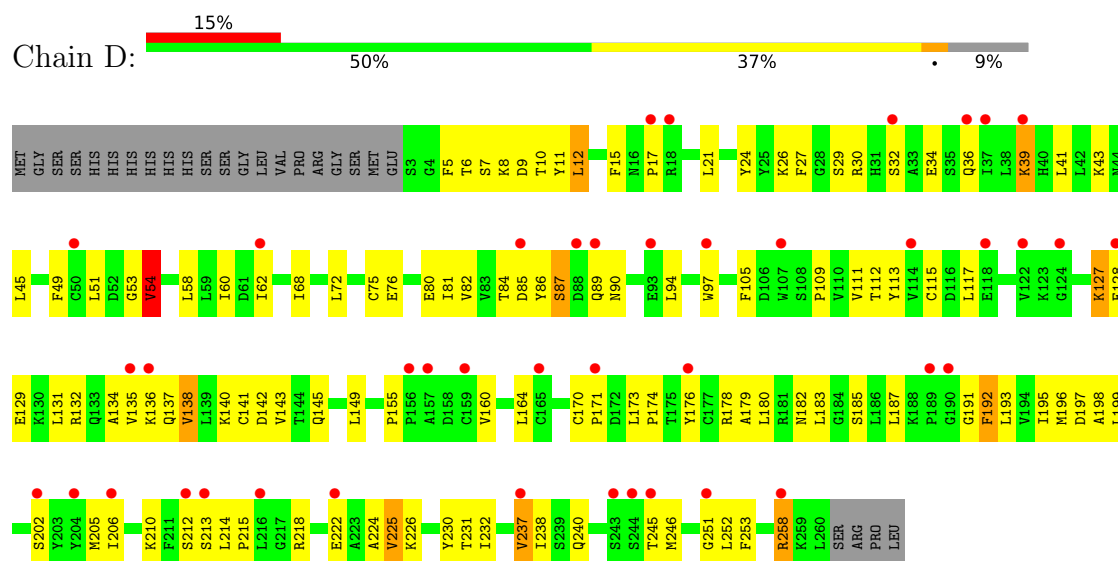
• Molecule 1: NNMT protein



• Molecule 1: NNMT protein



• Molecule 1: NNMT protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.23Å 62.53Å 108.36Å 82.72° 82.48° 68.34°	Depositor
Resolution (Å)	52.84 – 2.58 52.84 – 2.58	Depositor EDS
% Data completeness (in resolution range)	73.0 (52.84-2.58) 57.5 (52.84-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.233 , 0.292 0.236 , 0.293	Depositor DCC
R_{free} test set	1554 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8506	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P0V

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	0.23	0/2120	0.52	0/2874
1	B	0.21	0/2129	0.53	0/2887
1	C	0.43	3/2041 (0.1%)	0.67	4/2768 (0.1%)
1	D	0.44	4/2030 (0.2%)	0.62	3/2753 (0.1%)
All	All	0.34	7/8320 (0.1%)	0.59	7/11282 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	258	ARG	CZ-NH2	-9.06	1.21	1.33
1	D	192	PHE	CE2-CZ	-8.77	1.12	1.38
1	D	192	PHE	CD1-CE1	-8.13	1.14	1.38
1	C	240	GLN	CG-CD	-7.61	1.33	1.52
1	C	240	GLN	CD-NE2	5.39	1.44	1.33
1	D	192	PHE	CG-CD1	-5.36	1.27	1.38
1	C	39	LYS	CD-CE	-5.10	1.37	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	ILE	CB-CG1-CD1	14.15	143.52	113.80
1	C	39	LYS	CD-CE-NZ	6.17	131.64	111.90
1	D	39	LYS	CA-CB-CG	5.62	125.34	114.10
1	D	258	ARG	CD-NE-CZ	5.43	132.01	124.40
1	C	37	ILE	CB-CA-C	-5.04	105.51	111.97
1	D	192	PHE	CZ-CE2-CD2	-5.04	110.93	120.00
1	C	240	GLN	OE1-CD-NE2	5.03	127.63	122.60

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	2076	0	2058	132	0
1	B	2083	0	2066	129	0
1	C	1997	0	1986	182	0
1	D	1988	0	1972	151	0
2	A	38	26	0	3	0
2	B	38	26	0	6	0
2	C	38	26	0	1	0
2	D	38	26	0	6	0
3	A	28	0	0	13	0
3	B	31	0	0	12	0
3	C	29	0	0	7	0
3	D	18	0	0	9	0
All	All	8402	104	8082	576	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 35.

All (576) 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:23:LYS:HE2	1:C:246:MET:SD	1.91	1.09
1:D:90:ASN:ND2	2:D:301:P0V:O22	1.89	1.03
1:D:143:VAL:HG12	1:D:179:ALA:HB1	1.42	1.01
1:A:91:LEU:HB2	1:B:208:GLU:CD	1.86	1.01
1:A:91:LEU:HB2	1:B:208:GLU:OE2	1.61	0.98
1:B:61:ASP:OD2	1:B:64:SER:OG	1.82	0.97
1:A:171:PRO:HD2	1:A:175:THR:HG21	1.47	0.96
1:A:58:LEU:HD21	1:A:60:ILE:HG13	1.45	0.96
1:C:37:ILE:HG13	1:C:240:GLN:HE22	1.30	0.95
1:A:26:LYS:HG3	1:A:28:GLY:H	1.31	0.95
1:B:231:THR:HB	1:B:260:LEU:HD21	1.49	0.94
1:D:222:GLU:O	3:D:401:HOH:O	1.84	0.94
1:A:113:TYR:O	3:A:401:HOH:O	1.85	0.93
1:D:226:LYS:HZ3	1:D:232:ILE:H	1.17	0.93
1:C:80:GLU:HG3	1:C:136:LYS:CE	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:SER:HB2	2:D:301:P0V:O23	1.69	0.91
1:D:11:TYR:O	1:D:89:GLN:NE2	2.04	0.90
1:D:192:PHE:HE1	1:D:258:ARG:HE	1.13	0.90
1:A:177:CYS:HA	3:A:409:HOH:O	1.72	0.90
1:A:180:LEU:HB2	3:A:409:HOH:O	1.70	0.89
1:A:231:THR:HB	1:A:260:LEU:HD21	1.55	0.89
1:D:29:SER:OG	3:D:402:HOH:O	1.90	0.89
1:A:122:VAL:CG2	1:A:126:GLU:HB3	2.03	0.89
1:A:21:LEU:HD11	1:A:66:PRO:HG2	1.53	0.89
1:C:233:GLU:OE2	1:C:258:ARG:NE	2.06	0.88
1:C:37:ILE:HG13	1:C:240:GLN:NE2	1.89	0.88
1:B:26:LYS:HG3	1:B:28:GLY:H	1.38	0.88
1:B:26:LYS:HE3	1:B:28:GLY:HA3	1.52	0.88
1:C:23:LYS:NZ	1:C:246:MET:HG2	1.88	0.88
1:B:17:PRO:HD3	3:B:403:HOH:O	1.76	0.86
1:C:122:VAL:CG2	1:C:126:GLU:HB3	2.06	0.85
1:A:58:LEU:HD21	1:A:60:ILE:CG1	2.05	0.85
1:A:80:GLU:HG2	1:A:136:LYS:HD2	1.58	0.85
1:A:86:TYR:O	1:A:140:LYS:NZ	2.10	0.85
1:D:199:LEU:HD11	1:D:237:VAL:HG22	1.57	0.84
1:C:100:ALA:HB2	1:C:132:ARG:NH2	1.92	0.84
1:B:180:LEU:HB2	3:B:413:HOH:O	1.76	0.84
1:C:11:TYR:O	1:C:89:GLN:NE2	2.09	0.84
1:C:107:TRP:HE3	1:C:110:VAL:HG11	1.43	0.83
1:D:84:THR:HB	1:D:141:CYS:HB2	1.59	0.82
1:B:21:LEU:CD1	1:B:66:PRO:HG2	2.10	0.82
1:C:158:ASP:OD2	3:C:401:HOH:O	1.98	0.81
1:D:58:LEU:HD22	1:D:155:PRO:HG2	1.60	0.81
1:C:37:ILE:HG12	1:C:240:GLN:OE1	1.80	0.81
1:A:91:LEU:HD23	1:A:94:LEU:HD12	1.61	0.81
1:C:34:GLU:HG2	1:C:246:MET:HE1	1.61	0.81
1:A:95:GLU:HG2	1:B:-7:SER:HB3	1.62	0.81
1:C:83:VAL:HG23	1:C:138:VAL:HG13	1.60	0.81
1:A:122:VAL:HG21	1:A:126:GLU:HB3	1.62	0.81
1:C:80:GLU:HG3	1:C:136:LYS:NZ	1.96	0.81
1:B:68:ILE:CG2	1:B:94:LEU:HD11	2.11	0.81
1:B:177:CYS:HA	3:B:413:HOH:O	1.81	0.80
1:C:127:LYS:HD2	3:C:407:HOH:O	1.80	0.80
1:D:72:LEU:O	3:D:403:HOH:O	1.99	0.80
1:C:8:LYS:HD2	1:C:86:TYR:CZ	2.17	0.79
1:D:143:VAL:CG1	1:D:179:ALA:HB1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:CD1	1:A:66:PRO:HG2	2.12	0.78
1:C:91:LEU:HD22	1:C:138:VAL:HG12	1.66	0.78
1:A:48:ILE:O	1:A:54:VAL:HG12	1.83	0.78
1:A:58:LEU:CD2	1:A:60:ILE:HG13	2.14	0.77
1:B:177:CYS:SG	3:B:408:HOH:O	2.42	0.77
1:B:107:TRP:O	1:B:111:VAL:HG13	1.84	0.77
1:C:100:ALA:HB2	1:C:132:ARG:HH22	1.50	0.77
1:B:34:GLU:HG2	1:B:246:MET:HE1	1.67	0.76
1:B:259:LYS:HD3	3:B:409:HOH:O	1.85	0.76
1:D:21:LEU:HD13	1:D:105:PHE:CG	2.20	0.76
1:B:143:VAL:HG13	2:B:301:P0V:N5	2.00	0.76
1:C:21:LEU:HD13	1:C:105:PHE:CG	2.20	0.76
1:A:116:ASP:N	3:A:401:HOH:O	2.19	0.75
1:C:6:THR:HG22	1:C:212:SER:CB	2.17	0.75
1:C:96:LYS:HE2	1:C:103:ALA:HB3	1.68	0.75
1:C:6:THR:HG22	1:C:212:SER:OG	1.86	0.75
1:B:-9:HIS:NE2	1:B:-2:ARG:HG2	2.02	0.75
1:C:91:LEU:HD22	1:C:138:VAL:CG1	2.17	0.75
1:B:67:THR:HG21	2:B:301:P0V:O38	1.86	0.75
1:B:242:TYR:HB2	1:B:247:ALA:HB3	1.68	0.74
1:C:102:PRO:HD2	3:C:419:HOH:O	1.85	0.74
1:D:192:PHE:CE1	1:D:258:ARG:NE	2.55	0.74
1:A:199:LEU:HD11	1:A:237:VAL:HG22	1.69	0.73
1:D:182:ASN:O	1:D:185:SER:HB3	1.88	0.73
1:C:68:ILE:CG2	1:C:94:LEU:HD11	2.18	0.73
1:B:16:ASN:OD1	1:B:18:ARG:HG2	1.88	0.73
1:C:182:ASN:O	1:C:185:SER:HB3	1.88	0.73
1:C:34:GLU:HG3	3:C:412:HOH:O	1.89	0.73
1:D:54:VAL:HG22	1:D:192:PHE:CD2	2.23	0.73
1:A:98:LEU:O	1:C:178:ARG:HD3	1.88	0.73
1:B:30:ARG:O	1:B:39:LYS:NZ	2.19	0.73
1:C:60:ILE:HG12	1:C:82:VAL:HG21	1.69	0.73
1:D:87:SER:HB3	1:D:89:GLN:CD	2.13	0.73
1:C:39:LYS:HE3	1:C:113:TYR:CE1	2.22	0.73
1:B:52:ASP:OD1	1:D:43:LYS:NZ	2.20	0.72
1:C:136:LYS:O	1:C:137:GLN:HG3	1.90	0.72
1:D:212:SER:O	3:D:404:HOH:O	2.08	0.72
1:C:55:LYS:O	3:C:402:HOH:O	2.08	0.71
1:D:226:LYS:NZ	1:D:232:ILE:H	1.86	0.71
1:B:108:SER:O	1:B:111:VAL:HG22	1.90	0.71
1:C:60:ILE:HA	1:C:82:VAL:CG2	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LEU:HD23	1:D:197:ASP:HA	1.73	0.71
1:A:91:LEU:HB2	1:B:208:GLU:OE1	1.89	0.71
1:D:30:ARG:HH21	1:D:113:TYR:HE2	1.39	0.71
1:A:48:ILE:HG22	1:A:54:VAL:HG11	1.71	0.71
1:B:21:LEU:HD11	1:B:66:PRO:HG2	1.72	0.71
1:D:76:GLU:OE2	1:D:127:LYS:NZ	2.23	0.70
1:A:5:PHE:CD2	1:A:171:PRO:HA	2.26	0.70
1:A:6:THR:HG23	1:A:212:SER:OG	1.91	0.70
1:C:80:GLU:HG3	1:C:136:LYS:HE3	1.72	0.70
1:D:191:GLY:O	1:D:258:ARG:HA	1.91	0.70
1:A:5:PHE:CE2	1:A:171:PRO:HA	2.27	0.69
1:D:86:TYR:HA	1:D:141:CYS:O	1.93	0.69
1:C:26:LYS:NZ	3:C:405:HOH:O	2.26	0.69
1:D:226:LYS:HZ3	1:D:232:ILE:N	1.89	0.69
1:A:86:TYR:OH	3:A:402:HOH:O	2.05	0.69
1:B:26:LYS:HE3	1:B:28:GLY:CA	2.22	0.69
1:D:192:PHE:HZ	1:D:258:ARG:HH11	1.39	0.69
1:C:221:VAL:HG21	1:C:253:PHE:CE2	2.27	0.69
1:B:9:HIS:CE1	1:B:2:ARG:HG2	2.27	0.68
1:C:84:THR:HB	1:C:141:CYS:HB2	1.73	0.68
1:C:122:VAL:HG23	1:C:126:GLU:HB3	1.76	0.68
1:D:111:VAL:HG11	1:D:128:GLU:HG3	1.75	0.68
1:A:2:ARG:O	1:A:6:THR:HG22	1.94	0.68
1:C:23:LYS:HZ3	1:C:246:MET:HG2	1.56	0.68
1:C:39:LYS:HE3	1:C:113:TYR:CZ	2.28	0.68
1:B:65:GLY:N	1:B:85:ASP:OD1	2.22	0.68
1:B:94:LEU:O	1:B:98:LEU:HD23	1.93	0.68
1:C:37:ILE:CG1	1:C:240:GLN:HE22	2.07	0.68
1:D:226:LYS:N	3:D:401:HOH:O	2.01	0.68
1:C:148:PRO:HG3	1:C:182:ASN:HB3	1.76	0.67
1:D:68:ILE:CG2	1:D:94:LEU:HD11	2.23	0.67
1:D:193:LEU:HD21	1:D:195:ILE:HD11	1.76	0.67
1:C:54:VAL:HG22	1:C:192:PHE:CD1	2.29	0.67
1:D:199:LEU:HD11	1:D:237:VAL:CG2	2.24	0.67
1:C:80:GLU:CG	1:C:136:LYS:NZ	2.56	0.67
1:B:26:LYS:HG3	1:B:28:GLY:N	2.10	0.67
1:B:147:GLN:OE1	3:B:402:HOH:O	2.13	0.67
1:C:27:PHE:HD2	1:C:109:PRO:HB2	1.59	0.67
1:A:84:THR:HB	1:A:141:CYS:HB2	1.77	0.67
1:B:5:PHE:CD2	1:B:171:PRO:HA	2.30	0.67
1:D:68:ILE:HG23	1:D:94:LEU:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD12	3:A:409:HOH:O	1.95	0.66
1:D:7:SER:O	1:D:10:THR:OG1	2.14	0.66
1:D:36:GLN:O	1:D:39:LYS:HB2	1.96	0.66
1:B:15:PHE:O	3:B:403:HOH:O	2.13	0.66
1:A:192:PHE:CE1	1:A:258:ARG:HD2	2.31	0.66
1:B:200:LYS:HD2	1:B:250:GLU:CD	2.21	0.66
1:C:31:HIS:HA	1:C:36:GLN:HE21	1.60	0.66
1:D:5:PHE:CE2	1:D:171:PRO:HA	2.31	0.66
1:B:-2:ARG:NH2	1:B:209:GLN:OE1	2.30	0.65
1:C:191:GLY:O	1:C:258:ARG:HA	1.96	0.65
1:D:185:SER:OG	3:D:406:HOH:O	2.12	0.65
1:A:88:ASP:HB3	1:B:208:GLU:HG3	1.78	0.65
1:B:198:ALA:HB3	2:B:301:P0V:N34	2.11	0.65
1:A:88:ASP:HA	1:B:208:GLU:OE2	1.96	0.65
1:C:197:ASP:HB3	1:C:253:PHE:HE1	1.62	0.65
1:D:198:ALA:HB3	2:D:301:P0V:N34	2.12	0.65
1:A:26:LYS:HE2	3:A:412:HOH:O	1.95	0.65
1:A:72:LEU:HD23	1:A:131:LEU:HD22	1.77	0.65
1:D:192:PHE:HZ	1:D:258:ARG:NH1	1.95	0.65
1:C:39:LYS:CE	1:C:113:TYR:CZ	2.80	0.65
1:C:96:LYS:CE	1:C:103:ALA:HB3	2.27	0.64
1:B:84:THR:HG21	1:B:149:LEU:HD21	1.79	0.64
1:C:8:LYS:HD2	1:C:86:TYR:CE2	2.31	0.64
1:C:30:ARG:HD3	1:C:31:HIS:CD2	2.33	0.64
1:A:21:LEU:HD23	1:A:105:PHE:CG	2.32	0.63
1:B:21:LEU:HD23	1:B:105:PHE:CG	2.32	0.63
1:B:34:GLU:CG	1:B:246:MET:HE1	2.27	0.63
1:D:86:TYR:O	1:D:140:LYS:NZ	2.25	0.63
1:C:80:GLU:HG3	1:C:136:LYS:HZ1	1.63	0.63
1:C:34:GLU:CG	1:C:246:MET:HE1	2.30	0.62
1:A:40:HIS:HE1	1:A:236:GLU:OE1	1.83	0.62
1:A:48:ILE:CG2	1:A:54:VAL:HG11	2.29	0.62
1:C:214:LEU:CD2	1:C:216:LEU:HD21	2.29	0.62
1:D:87:SER:CB	1:D:89:GLN:NE2	2.63	0.62
1:B:182:ASN:O	1:B:185:SER:HB3	1.99	0.62
1:D:87:SER:OG	1:D:89:GLN:NE2	2.33	0.62
1:D:87:SER:HB3	1:D:89:GLN:NE2	2.14	0.61
1:C:68:ILE:HG23	1:C:94:LEU:HD11	1.82	0.61
1:C:122:VAL:HG21	1:C:126:GLU:HB3	1.81	0.61
1:D:8:LYS:HD2	1:D:86:TYR:CZ	2.35	0.61
1:B:89:GLN:HB2	3:B:403:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ALA:O	1:B:136:LYS:HG2	2.00	0.61
1:D:45:LEU:HD21	1:D:196:MET:HE2	1.82	0.61
1:B:72:LEU:CD2	1:B:111:VAL:HA	2.31	0.61
1:C:26:LYS:HG2	1:C:27:PHE:N	2.15	0.61
1:C:39:LYS:CE	1:C:113:TYR:CE1	2.83	0.61
1:A:106:ASP:OD2	1:A:108:SER:HB3	2.01	0.61
1:A:107:TRP:O	1:A:111:VAL:HG23	2.00	0.61
1:C:6:THR:HG21	1:C:212:SER:H	1.65	0.61
1:C:50:CYS:C	1:C:51:LEU:HD12	2.26	0.61
1:C:225:VAL:HG11	1:C:232:ILE:HD11	1.82	0.61
1:C:113:TYR:CZ	1:C:117:LEU:HD21	2.35	0.61
1:D:21:LEU:HD13	1:D:105:PHE:CB	2.31	0.61
1:C:60:ILE:HG12	1:C:82:VAL:CG2	2.30	0.60
1:A:182:ASN:O	1:A:185:SER:HB3	2.00	0.60
1:C:39:LYS:HE3	1:C:113:TYR:CD1	2.35	0.60
1:A:134:ALA:O	1:A:136:LYS:HG3	2.01	0.60
1:B:1:MET:HE3	1:C:215:PRO:O	2.02	0.60
1:C:8:LYS:CE	1:C:86:TYR:OH	2.49	0.60
1:C:30:ARG:HD3	1:C:31:HIS:HD2	1.66	0.60
1:D:36:GLN:HB2	1:D:240:GLN:NE2	2.17	0.60
1:D:160:VAL:HG13	1:D:187:LEU:CD2	2.32	0.59
1:A:2:GLU:OE2	1:A:2:GLU:HA	2.01	0.59
1:B:198:ALA:HA	1:B:252:LEU:HD13	1.84	0.59
1:C:6:THR:CG2	1:C:212:SER:H	2.16	0.59
1:C:21:LEU:HB3	1:C:105:PHE:CE1	2.37	0.59
1:C:38:LEU:O	1:C:42:LEU:HG	2.03	0.59
1:C:122:VAL:HG22	1:C:123:LYS:O	2.03	0.59
1:C:253:PHE:HE2	1:C:255:LEU:HD23	1.68	0.59
1:C:46:PHE:CZ	1:C:51:LEU:HD11	2.37	0.58
1:C:23:LYS:HZ1	1:C:246:MET:HG2	1.63	0.58
1:D:60:ILE:HG12	1:D:82:VAL:HG21	1.84	0.58
1:A:34:GLU:CG	1:A:246:MET:HE1	2.32	0.58
1:B:26:LYS:HG3	1:B:27:PHE:N	2.18	0.58
1:B:29:SER:O	3:B:404:HOH:O	2.17	0.58
1:C:60:ILE:HG23	1:C:82:VAL:HG23	1.85	0.58
1:A:122:VAL:HG23	1:A:126:GLU:OE1	2.03	0.58
1:C:60:ILE:HA	1:C:82:VAL:HG23	1.85	0.58
1:C:83:VAL:CG2	1:C:138:VAL:HG13	2.30	0.58
1:C:54:VAL:HG22	1:C:192:PHE:CE1	2.39	0.58
1:C:222:GLU:O	1:C:225:VAL:HG12	2.03	0.58
1:D:41:LEU:O	1:D:45:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:CD1	1:C:240:GLN:HE22	2.16	0.58
1:A:139:LEU:HD22	1:A:152:VAL:HG21	1.86	0.57
1:D:27:PHE:HD2	1:D:109:PRO:HB2	1.68	0.57
1:A:236:GLU:HG2	1:A:254:SER:HB3	1.85	0.57
1:B:84:THR:HB	1:B:141:CYS:HB2	1.87	0.57
1:B:48:ILE:CG1	1:B:234:TRP:HZ2	2.18	0.57
1:C:96:LYS:HE2	1:C:103:ALA:CB	2.35	0.57
1:D:81:ILE:HB	1:D:135:VAL:HA	1.87	0.57
1:A:72:LEU:CD2	1:A:131:LEU:HD22	2.34	0.57
1:D:8:LYS:HD2	1:D:86:TYR:CE2	2.39	0.57
1:C:80:GLU:CG	1:C:136:LYS:HZ1	2.16	0.57
1:D:8:LYS:NZ	1:D:142:ASP:OD2	2.37	0.57
1:B:69:TYR:OH	2:B:301:P0V:O37	2.21	0.57
1:C:128:GLU:O	1:C:132:ARG:HD3	2.04	0.57
1:C:37:ILE:CG1	1:C:240:GLN:OE1	2.52	0.56
1:C:23:LYS:NZ	1:C:246:MET:CG	2.65	0.56
1:D:34:GLU:HG2	1:D:246:MET:HE1	1.87	0.56
1:A:6:THR:CG2	1:A:212:SER:H	2.18	0.56
1:A:34:GLU:HG3	1:A:246:MET:HE1	1.88	0.56
1:D:17:PRO:HG3	1:D:89:GLN:O	2.05	0.56
1:D:58:LEU:CD2	1:D:155:PRO:HG2	2.33	0.56
1:D:60:ILE:O	1:D:160:VAL:HA	2.06	0.56
1:A:6:THR:HG21	1:A:212:SER:H	1.71	0.56
1:B:91:LEU:HD22	1:B:138:VAL:CG1	2.35	0.56
1:D:45:LEU:HD21	1:D:196:MET:CE	2.35	0.56
1:B:163:THR:CG2	1:B:196:MET:HE2	2.36	0.56
1:C:8:LYS:NZ	1:C:86:TYR:OH	2.38	0.56
1:A:-9:HIS:NE2	1:A:-7:SER:OG	2.39	0.56
1:A:88:ASP:HA	1:B:208:GLU:CD	2.30	0.56
1:D:75:CYS:N	3:D:403:HOH:O	2.37	0.56
1:A:13:SER:HB2	1:A:14:HIS:ND1	2.20	0.55
1:A:30:ARG:HG3	1:A:39:LYS:NZ	2.21	0.55
1:C:68:ILE:HG22	1:C:94:LEU:HD11	1.88	0.55
1:B:-9:HIS:NE2	1:B:-2:ARG:HA	2.21	0.55
1:C:6:THR:HG22	1:C:212:SER:HB2	1.86	0.55
1:D:81:ILE:HD12	1:D:134:ALA:HB3	1.89	0.55
1:D:128:GLU:HB3	1:D:132:ARG:HH12	1.72	0.55
1:C:260:LEU:C	1:C:260:LEU:HD12	2.31	0.55
1:D:111:VAL:HG21	1:D:128:GLU:CG	2.37	0.55
1:A:236:GLU:CG	1:A:254:SER:HB3	2.37	0.55
1:A:98:LEU:HD11	1:A:132:ARG:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:VAL:HG21	1:B:128:GLU:OE2	2.07	0.54
1:C:197:ASP:HB3	1:C:253:PHE:CE1	2.43	0.54
1:D:24:TYR:CZ	1:D:246:MET:HE3	2.41	0.54
1:C:251:GLY:C	1:C:252:LEU:HD12	2.32	0.54
1:D:9:ASP:HA	1:D:12:LEU:HD23	1.90	0.54
1:A:193:LEU:HD21	1:A:195:ILE:HD11	1.88	0.54
1:D:164:LEU:HA	1:D:197:ASP:OD1	2.06	0.54
1:B:156:PRO:HB2	1:B:188:LYS:HG2	1.90	0.54
1:B:59:LEU:C	1:B:59:LEU:HD23	2.33	0.54
1:A:218:ARG:HG3	1:A:235:PHE:CE1	2.43	0.54
1:C:26:LYS:HE2	1:C:34:GLU:OE1	2.07	0.54
1:A:-8:SER:O	1:A:-7:SER:HB2	2.07	0.54
1:C:34:GLU:CD	1:C:34:GLU:H	2.15	0.54
1:D:226:LYS:CE	1:D:232:ILE:H	2.21	0.54
1:B:-9:HIS:CG	1:B:-8:SER:H	2.25	0.53
1:D:34:GLU:CD	1:D:34:GLU:H	2.17	0.53
1:C:23:LYS:HZ1	1:C:246:MET:CG	2.21	0.53
1:D:226:LYS:HE2	1:D:232:ILE:HG13	1.90	0.53
1:A:84:THR:HB	1:A:141:CYS:CB	2.39	0.53
1:A:148:PRO:HG3	1:A:182:ASN:HB3	1.90	0.53
1:C:68:ILE:HG23	1:C:94:LEU:CD1	2.39	0.53
1:C:160:VAL:HG23	1:C:193:LEU:HD12	1.90	0.53
1:D:60:ILE:HA	1:D:82:VAL:CG2	2.39	0.53
1:B:231:THR:HB	1:B:260:LEU:CD2	2.31	0.53
1:C:8:LYS:CD	1:C:86:TYR:CZ	2.90	0.53
1:D:226:LYS:HD3	1:D:230:TYR:O	2.09	0.52
1:A:7:SER:O	1:A:10:THR:HB	2.09	0.52
1:C:8:LYS:HE3	1:C:86:TYR:OH	2.09	0.52
1:C:15:PHE:CE2	1:C:206:ILE:HD11	2.45	0.52
1:A:71:LEU:HD11	1:A:83:VAL:HG11	1.91	0.52
1:B:17:PRO:HB3	1:B:66:PRO:HG3	1.91	0.52
1:B:68:ILE:HG22	1:B:94:LEU:HD11	1.89	0.52
1:B:180:LEU:HD22	1:B:193:LEU:HD21	1.90	0.52
1:C:60:ILE:HG23	1:C:82:VAL:CG2	2.39	0.52
1:D:6:THR:H	1:D:212:SER:CB	2.22	0.52
1:B:9:ASP:HB3	3:B:426:HOH:O	2.09	0.52
1:C:95:GLU:HA	1:C:98:LEU:HD23	1.92	0.52
1:A:40:HIS:CE1	1:A:238:ILE:HG21	2.45	0.52
1:C:51:LEU:HD12	1:C:51:LEU:N	2.25	0.52
1:D:75:CYS:HB3	1:D:131:LEU:HD13	1.91	0.52
1:C:12:LEU:HA	1:C:89:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ASP:O	1:D:141:CYS:N	2.42	0.51
1:B:68:ILE:HG23	1:B:94:LEU:HD11	1.89	0.51
1:C:134:ALA:O	1:C:136:LYS:HG3	2.09	0.51
1:D:62:ILE:HG13	1:D:183:LEU:HD22	1.91	0.51
1:A:240:GLN:O	1:A:251:GLY:HA2	2.10	0.51
1:B:17:PRO:CB	1:B:66:PRO:HG3	2.41	0.51
1:A:91:LEU:HD12	1:B:208:GLU:OE1	2.09	0.51
1:A:198:ALA:O	3:A:403:HOH:O	2.18	0.51
1:D:5:PHE:CD2	1:D:171:PRO:HA	2.46	0.51
1:D:213:SER:O	1:D:215:PRO:HD3	2.11	0.51
1:B:51:LEU:HD22	1:D:117:LEU:HD22	1.93	0.51
1:A:84:THR:HG21	1:A:149:LEU:HD21	1.91	0.51
1:A:117:LEU:N	3:A:401:HOH:O	1.95	0.51
1:D:75:CYS:HB3	1:D:131:LEU:CD1	2.41	0.51
1:A:32:SER:HB2	1:A:34:GLU:OE1	2.11	0.51
1:C:171:PRO:HD2	1:C:175:THR:HG21	1.92	0.51
1:D:87:SER:CB	1:D:89:GLN:HE22	2.23	0.51
1:C:5:PHE:CD2	1:C:171:PRO:HA	2.46	0.51
1:C:62:ILE:HG13	1:C:183:LEU:HD22	1.93	0.51
1:A:59:LEU:HD23	1:A:59:LEU:C	2.36	0.50
1:A:59:LEU:HB2	1:A:78:PHE:CD2	2.45	0.50
1:B:27:PHE:CD1	1:B:38:LEU:HD23	2.45	0.50
1:B:48:ILE:HG12	1:B:234:TRP:HZ2	1.74	0.50
1:D:226:LYS:NZ	1:D:231:THR:HA	2.26	0.50
1:A:65:GLY:N	1:A:85:ASP:OD1	2.33	0.50
1:C:37:ILE:HG13	1:C:240:GLN:CD	2.36	0.50
1:C:60:ILE:HA	1:C:82:VAL:HG22	1.91	0.50
1:D:32:SER:O	1:D:36:GLN:HG2	2.11	0.50
1:A:34:GLU:H	1:A:34:GLU:CD	2.20	0.50
1:A:80:GLU:HG2	1:A:136:LYS:CD	2.34	0.50
1:A:142:ASP:O	1:A:148:PRO:HA	2.11	0.50
1:C:106:ASP:OD1	1:C:108:SER:HB3	2.11	0.50
1:D:60:ILE:HG12	1:D:82:VAL:CG2	2.41	0.50
1:B:45:LEU:HG	1:B:196:MET:HE1	1.93	0.50
1:C:21:LEU:HD13	1:C:105:PHE:CB	2.41	0.50
1:A:17:PRO:HB3	1:A:90:ASN:OD1	2.12	0.50
1:C:181:ARG:NH2	1:C:227:GLU:OE2	2.45	0.50
1:D:21:LEU:HD13	1:D:105:PHE:HB2	1.94	0.50
1:C:203:TYR:CD2	1:C:210:LYS:HE2	2.46	0.50
1:D:192:PHE:CZ	1:D:258:ARG:NH1	2.76	0.50
1:B:93:GLU:O	1:B:93:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TRP:HE3	1:B:98:LEU:HD22	1.77	0.49
1:C:7:SER:O	1:C:10:THR:OG1	2.30	0.49
1:B:202:SER:HA	1:B:213:SER:O	2.12	0.49
1:C:97:TRP:CH2	1:C:132:ARG:HD2	2.47	0.49
1:A:122:VAL:HG22	1:A:123:LYS:N	2.27	0.49
1:D:60:ILE:HA	1:D:82:VAL:HG23	1.93	0.49
1:D:143:VAL:HG12	1:D:179:ALA:CB	2.27	0.49
1:A:21:LEU:HB3	1:A:105:PHE:CE1	2.47	0.49
1:A:34:GLU:HG2	1:A:246:MET:HE1	1.94	0.49
1:B:45:LEU:CD1	1:B:70:GLN:HA	2.43	0.49
1:C:213:SER:O	1:C:215:PRO:HD3	2.11	0.49
1:B:251:GLY:C	1:B:252:LEU:HD22	2.38	0.49
1:D:36:GLN:HB2	1:D:240:GLN:HE22	1.76	0.49
1:D:68:ILE:HG23	1:D:94:LEU:CD1	2.40	0.49
1:B:36:GLN:HA	1:B:39:LYS:HE3	1.95	0.49
1:B:106:ASP:OD2	1:B:108:SER:HB3	2.13	0.49
1:D:138:VAL:CG2	1:D:138:VAL:O	2.60	0.49
1:C:174:PRO:O	1:C:178:ARG:HG3	2.12	0.49
1:D:85:ASP:OD2	2:D:301:P0V:O23	2.30	0.49
1:D:192:PHE:CD1	1:D:258:ARG:HG2	2.47	0.49
1:C:37:ILE:CG1	1:C:240:GLN:NE2	2.68	0.48
1:C:82:VAL:HG23	1:C:82:VAL:O	2.13	0.48
1:D:54:VAL:HG22	1:D:192:PHE:CE2	2.48	0.48
1:D:87:SER:CB	1:D:89:GLN:CD	2.83	0.48
1:D:176:TYR:HD1	1:D:224:ALA:HB1	1.78	0.48
1:D:145:GLN:HA	3:D:405:HOH:O	2.12	0.48
1:A:49:PHE:HD1	1:A:54:VAL:HG13	1.78	0.48
1:B:117:LEU:HD22	1:D:51:LEU:HD22	1.95	0.48
1:C:94:LEU:O	1:C:98:LEU:HD23	2.13	0.48
1:C:205:MET:SD	1:C:210:LYS:HB2	2.53	0.48
1:D:15:PHE:CE2	1:D:206:ILE:HD11	2.49	0.48
1:A:122:VAL:HG22	1:A:126:GLU:HB3	1.94	0.48
1:B:45:LEU:HD21	1:B:196:MET:HE2	1.96	0.48
1:A:17:PRO:HB3	1:A:66:PRO:HG3	1.95	0.48
1:B:76:GLU:OE1	1:B:130:LYS:HE2	2.14	0.48
1:B:82:VAL:HG11	1:B:139:LEU:HD12	1.94	0.48
1:B:192:PHE:HE1	1:B:258:ARG:HE	1.62	0.48
1:C:39:LYS:NZ	1:C:113:TYR:CE1	2.82	0.48
1:C:61:ASP:OD2	1:C:64:SER:OG	2.17	0.48
1:C:107:TRP:CE3	1:C:110:VAL:HG11	2.35	0.48
1:D:136:LYS:O	1:D:137:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HA	1:A:94:LEU:HG	1.95	0.48
1:A:255:LEU:HD12	1:A:255:LEU:C	2.39	0.48
1:C:80:GLU:CG	1:C:136:LYS:HD2	2.44	0.48
1:C:225:VAL:CG1	1:C:232:ILE:HD11	2.43	0.48
1:D:82:VAL:HG23	1:D:82:VAL:O	2.13	0.48
1:D:90:ASN:HD22	2:D:301:P0V:C13	2.26	0.48
1:C:98:LEU:HA	1:C:132:ARG:HG2	1.95	0.48
1:C:242:TYR:HB2	1:C:247:ALA:HB3	1.95	0.48
1:C:255:LEU:C	1:C:255:LEU:HD12	2.38	0.48
1:D:112:THR:O	1:D:115:CYS:HB2	2.14	0.48
1:D:226:LYS:HZ2	1:D:231:THR:HA	1.79	0.48
1:A:143:VAL:HG13	2:A:301:P0V:N5	2.28	0.47
1:C:240:GLN:O	1:C:251:GLY:HA2	2.14	0.47
1:C:233:GLU:OE2	1:C:258:ARG:CZ	2.62	0.47
1:C:27:PHE:CD1	1:C:38:LEU:HD23	2.50	0.47
1:C:72:LEU:HD23	1:C:131:LEU:HD22	1.96	0.47
1:C:48:ILE:O	1:C:52:ASP:HB2	2.14	0.47
1:C:59:LEU:C	1:C:59:LEU:HD23	2.40	0.47
1:B:171:PRO:HD2	1:B:175:THR:HG21	1.95	0.47
1:A:91:LEU:HD22	1:A:138:VAL:HG13	1.96	0.47
1:C:214:LEU:HD23	1:C:216:LEU:HD21	1.94	0.47
1:B:72:LEU:O	1:B:127:LYS:NZ	2.43	0.47
1:A:49:PHE:CD1	1:A:54:VAL:HG13	2.50	0.47
1:B:-9:HIS:CG	1:B:-8:SER:N	2.82	0.46
1:D:85:ASP:N	1:D:141:CYS:HB3	2.29	0.46
1:B:55:LYS:CB	1:B:77:SER:HB3	2.45	0.46
1:C:8:LYS:NZ	1:C:86:TYR:CE1	2.83	0.46
1:C:226:LYS:HB3	1:C:226:LYS:HE2	1.54	0.46
1:D:134:ALA:O	1:D:136:LYS:HG3	2.15	0.46
1:C:21:LEU:HB3	1:C:105:PHE:CD1	2.51	0.46
1:C:37:ILE:CG1	1:C:240:GLN:CD	2.88	0.46
1:C:39:LYS:HE2	1:C:113:TYR:CZ	2.50	0.46
1:A:89:GLN:H	1:A:89:GLN:CD	2.23	0.46
1:C:106:ASP:OD2	3:C:404:HOH:O	2.21	0.46
1:D:24:TYR:CE1	1:D:246:MET:HE3	2.51	0.46
1:B:218:ARG:HG3	1:B:235:PHE:CE1	2.51	0.46
1:B:5:PHE:CE2	1:B:171:PRO:HA	2.51	0.45
1:C:84:THR:HB	1:C:141:CYS:CB	2.43	0.45
1:D:128:GLU:HB3	1:D:132:ARG:NH1	2.31	0.45
1:D:89:GLN:HG2	1:D:90:ASN:N	2.30	0.45
1:D:173:LEU:HB3	1:D:174:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:CYS:SG	1:A:176:TYR:HA	2.57	0.45
1:B:240:GLN:O	1:B:251:GLY:HA2	2.16	0.45
1:C:113:TYR:CE1	1:C:117:LEU:HD21	2.50	0.45
1:A:199:LEU:HD11	1:A:237:VAL:CG2	2.42	0.45
1:B:45:LEU:HD13	1:B:70:GLN:HA	1.98	0.45
1:C:30:ARG:O	1:C:36:GLN:NE2	2.50	0.45
1:C:39:LYS:HA	1:C:42:LEU:HB2	1.98	0.45
1:C:80:GLU:CD	1:C:136:LYS:HZ1	2.25	0.45
1:A:41:LEU:O	1:A:45:LEU:HG	2.16	0.45
1:C:163:THR:HG22	1:C:196:MET:HE2	1.98	0.45
1:C:253:PHE:CE2	1:C:255:LEU:HD23	2.49	0.45
1:A:107:TRP:NE1	3:A:404:HOH:O	2.19	0.45
1:B:-9:HIS:HD1	1:B:-7:SER:H	1.64	0.45
1:B:70:GLN:HB2	1:B:161:LEU:HD21	1.98	0.45
1:C:122:VAL:HG22	1:C:123:LYS:N	2.30	0.45
1:D:87:SER:HB3	1:D:89:GLN:OE1	2.17	0.45
1:D:87:SER:CB	1:D:89:GLN:OE1	2.65	0.45
1:A:-2:ARG:NH2	1:A:-1:GLY:H	2.15	0.45
1:A:122:VAL:HG21	1:A:126:GLU:CB	2.39	0.45
1:B:69:TYR:HA	1:B:72:LEU:HD13	1.99	0.45
1:C:38:LEU:O	1:C:41:LEU:HB2	2.17	0.45
1:A:37:ILE:HD12	1:A:242:TYR:CD1	2.52	0.44
1:A:97:TRP:CZ3	1:A:98:LEU:HD22	2.53	0.44
1:A:233:GLU:OE2	1:A:258:ARG:HD3	2.17	0.44
1:D:160:VAL:HG23	1:D:193:LEU:HD12	1.99	0.44
1:D:226:LYS:HE2	1:D:232:ILE:H	1.82	0.44
1:B:226:LYS:NZ	1:B:232:ILE:H	2.16	0.44
1:D:39:LYS:HB3	1:D:39:LYS:HE3	1.51	0.44
1:D:21:LEU:HB3	1:D:105:PHE:CE1	2.52	0.44
1:D:84:THR:HG21	1:D:149:LEU:HD21	1.99	0.44
1:A:98:LEU:O	1:A:132:ARG:HD3	2.17	0.44
1:D:39:LYS:HB2	1:D:39:LYS:HE2	1.53	0.44
1:D:193:LEU:CD2	1:D:195:ILE:HD11	2.46	0.44
1:C:39:LYS:HE3	1:C:113:TYR:CE2	2.52	0.44
1:A:142:ASP:HA	2:A:301:P0V:N5	2.32	0.44
1:B:91:LEU:HD22	1:B:138:VAL:HG13	2.00	0.44
1:B:94:LEU:HD12	1:B:94:LEU:HA	1.78	0.44
1:C:21:LEU:HD13	1:C:105:PHE:CD1	2.52	0.44
1:C:45:LEU:HD13	1:C:70:GLN:HA	1.99	0.44
1:D:80:GLU:HG2	1:D:136:LYS:CE	2.48	0.44
1:A:198:ALA:HB3	3:A:406:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:O	1:B:81:ILE:HA	2.18	0.44
1:B:205:MET:N	1:B:246:MET:O	2.44	0.44
1:B:255:LEU:C	1:B:255:LEU:HD12	2.43	0.44
1:C:163:THR:CG2	1:C:196:MET:HE2	2.48	0.44
1:D:49:PHE:CE1	1:D:54:VAL:HG11	2.53	0.44
1:B:84:THR:HB	1:B:141:CYS:CB	2.48	0.44
1:B:110:VAL:O	1:B:114:VAL:HG23	2.17	0.44
1:A:164:LEU:HD13	2:A:301:P0V:C32	2.48	0.43
1:B:163:THR:HG21	1:B:196:MET:HE2	1.99	0.43
1:C:8:LYS:NZ	1:C:86:TYR:CZ	2.86	0.43
1:C:46:PHE:CE2	1:C:51:LEU:HD11	2.54	0.43
1:B:156:PRO:HB2	1:B:188:LYS:CG	2.49	0.43
1:C:87:SER:HB2	1:C:89:GLN:OE1	2.17	0.43
1:C:201:SER:HB2	1:C:249:ASN:HB3	2.01	0.43
1:D:21:LEU:HD13	1:D:105:PHE:CD1	2.53	0.43
1:A:88:ASP:O	1:B:208:GLU:OE2	2.37	0.43
1:A:91:LEU:CB	1:B:208:GLU:OE1	2.63	0.43
1:B:45:LEU:HD21	1:B:196:MET:CE	2.48	0.43
1:B:64:SER:O	2:B:301:P0V:N21	2.52	0.43
1:C:234:TRP:HH2	1:C:254:SER:HG	1.61	0.43
1:D:205:MET:SD	1:D:210:LYS:HB2	2.58	0.43
1:C:76:GLU:CD	1:C:127:LYS:HZ3	2.24	0.43
1:C:113:TYR:CE2	1:C:117:LEU:HD11	2.53	0.43
1:C:193:LEU:HD22	1:C:230:TYR:CZ	2.54	0.43
1:D:72:LEU:HD23	1:D:72:LEU:HA	1.73	0.43
1:D:160:VAL:HG13	1:D:187:LEU:HD21	2.00	0.43
1:A:58:LEU:HD22	1:A:157:ALA:HA	2.01	0.43
1:C:193:LEU:HD11	1:C:195:ILE:HD11	2.01	0.43
1:D:12:LEU:HD21	1:D:86:TYR:CE2	2.53	0.43
1:A:53:GLY:O	1:A:54:VAL:C	2.61	0.43
1:A:68:ILE:HD11	1:A:107:TRP:CG	2.54	0.43
1:A:203:TYR:CZ	1:A:248:ASN:HB3	2.53	0.43
1:B:65:GLY:C	1:B:90:ASN:HB3	2.43	0.43
1:A:68:ILE:C	1:A:68:ILE:HD12	2.44	0.43
1:C:12:LEU:CD2	1:C:87:SER:HA	2.49	0.43
1:C:218:ARG:HG2	1:C:237:VAL:HG11	2.01	0.43
1:C:205:MET:HE3	1:C:205:MET:HB3	1.92	0.43
1:D:49:PHE:HD1	1:D:54:VAL:HG12	1.84	0.43
1:D:170:CYS:O	1:D:214:LEU:HB2	2.19	0.43
1:A:158:ASP:HB3	3:A:405:HOH:O	2.19	0.43
1:C:59:LEU:HD22	1:C:81:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PHE:CE1	1:C:212:SER:HB2	2.53	0.42
1:C:39:LYS:HG2	1:C:113:TYR:CE2	2.55	0.42
1:A:45:LEU:HD13	1:A:70:GLN:HA	2.00	0.42
1:B:1:MET:HE2	1:B:1:MET:HB3	1.87	0.42
1:D:53:GLY:O	1:D:54:VAL:C	2.62	0.42
1:A:54:VAL:HG13	1:A:54:VAL:O	2.19	0.42
1:C:252:LEU:HD12	1:C:252:LEU:N	2.35	0.42
1:D:253:PHE:CD1	1:D:253:PHE:C	2.96	0.42
1:C:110:VAL:O	1:C:114:VAL:HG23	2.19	0.42
1:D:174:PRO:O	1:D:178:ARG:HG3	2.18	0.42
1:A:205:MET:HE3	1:A:205:MET:HB3	1.94	0.42
1:C:39:LYS:O	1:C:43:LYS:N	2.40	0.42
1:C:200:LYS:N	1:C:216:LEU:O	2.40	0.42
1:A:5:PHE:CG	1:A:171:PRO:HB3	2.55	0.42
1:A:214:LEU:HG	1:A:216:LEU:HD21	2.02	0.42
1:D:81:ILE:CD1	1:D:131:LEU:HD12	2.49	0.42
1:A:26:LYS:HG3	1:A:27:PHE:N	2.34	0.42
1:B:65:GLY:HA2	1:B:90:ASN:ND2	2.34	0.42
1:B:234:TRP:HB2	1:D:238:ILE:HG22	2.01	0.42
1:C:139:LEU:HD22	1:C:152:VAL:HG21	2.01	0.42
1:A:166:LEU:CD1	1:A:180:LEU:HD21	2.50	0.42
1:D:21:LEU:HB3	1:D:105:PHE:CD1	2.54	0.42
1:D:160:VAL:HG13	1:D:187:LEU:HD23	2.01	0.42
1:B:27:PHE:HA	3:B:410:HOH:O	2.19	0.41
1:A:165:CYS:O	1:A:168:ALA:N	2.53	0.41
1:C:164:LEU:HD12	2:C:301:P0V:O38	2.20	0.41
1:A:32:SER:HB2	1:A:34:GLU:CD	2.46	0.41
1:A:88:ASP:CB	1:B:208:GLU:HG3	2.48	0.41
1:B:26:LYS:CG	1:B:27:PHE:N	2.83	0.41
1:B:37:ILE:HD12	1:B:242:TYR:CD1	2.56	0.41
1:D:85:ASP:OD2	2:D:301:P0V:C14	2.68	0.41
1:D:97:TRP:CE2	1:D:132:ARG:NH2	2.88	0.41
1:A:-2:ARG:HA	1:A:-2:ARG:HD2	1.79	0.41
1:B:53:GLY:O	1:B:54:VAL:C	2.63	0.41
1:B:163:THR:HG22	1:B:196:MET:HE2	2.00	0.41
1:C:122:VAL:CG2	1:C:123:LYS:N	2.83	0.41
1:D:164:LEU:HA	1:D:197:ASP:CG	2.45	0.41
1:D:225:VAL:N	3:D:401:HOH:O	2.52	0.41
1:A:202:SER:HA	1:A:213:SER:O	2.21	0.41
1:C:13:SER:HB2	1:C:14:HIS:ND1	2.36	0.41
1:D:24:TYR:CE2	1:D:246:MET:CE	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:PHE:CD1	1:D:54:VAL:HG12	2.56	0.41
1:D:193:LEU:HD22	1:D:230:TYR:CE2	2.56	0.41
1:A:214:LEU:HG	1:A:216:LEU:CD2	2.51	0.41
1:B:68:ILE:HG23	1:B:94:LEU:CD1	2.50	0.41
1:B:139:LEU:CD2	1:B:152:VAL:HG11	2.51	0.41
1:D:8:LYS:O	1:D:12:LEU:CD2	2.69	0.41
1:D:24:TYR:OH	1:D:246:MET:HB3	2.21	0.41
1:D:180:LEU:HD13	1:D:225:VAL:HA	2.03	0.41
1:A:65:GLY:C	1:A:90:ASN:HB3	2.46	0.41
1:D:81:ILE:CG2	1:D:135:VAL:HG22	2.51	0.41
1:D:251:GLY:C	1:D:252:LEU:HD22	2.45	0.41
1:A:116:ASP:CA	3:A:401:HOH:O	2.68	0.40
1:A:193:LEU:HG	1:A:195:ILE:CD1	2.51	0.40
1:B:218:ARG:HH22	1:D:218:ARG:CB	2.34	0.40
1:B:260:LEU:HA	3:B:412:HOH:O	2.20	0.40
1:A:116:ASP:OD1	1:A:120:ASN:ND2	2.49	0.40
1:B:46:PHE:O	1:B:50:CYS:HB2	2.21	0.40
1:C:8:LYS:HD2	1:C:86:TYR:CE1	2.53	0.40
1:A:193:LEU:HG	1:A:195:ILE:HD12	2.03	0.40
1:A:222:GLU:O	1:A:226:LYS:HG3	2.21	0.40
1:D:84:THR:HG21	1:D:149:LEU:CD2	2.51	0.40
1:B:69:TYR:C	1:B:71:LEU:H	2.29	0.40
1:B:72:LEU:N	1:B:72:LEU:HD12	2.37	0.40
1:B:205:MET:HB2	1:B:246:MET:HA	2.03	0.40
1:C:80:GLU:HG3	1:C:136:LYS:CD	2.50	0.40
1:B:143:VAL:HG13	2:B:301:P0V:C4	2.52	0.40
1:D:8:LYS:HA	1:D:11:TYR:HD2	1.87	0.40
1:D:39:LYS:O	1:D:43:LYS:HG3	2.22	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	268/283 (95%)	257 (96%)	10 (4%)	1 (0%)	30	49
1	B	268/283 (95%)	257 (96%)	9 (3%)	2 (1%)	18	36
1	C	255/283 (90%)	246 (96%)	9 (4%)	0	100	100
1	D	256/283 (90%)	246 (96%)	9 (4%)	1 (0%)	30	49
All	All	1047/1132 (92%)	1006 (96%)	37 (4%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	PRO
1	D	54	VAL
1	A	66	PRO
1	B	54	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	228/245 (93%)	217 (95%)	11 (5%)	23	45
1	B	229/245 (94%)	215 (94%)	14 (6%)	17	35
1	C	219/245 (89%)	202 (92%)	17 (8%)	11	25
1	D	218/245 (89%)	207 (95%)	11 (5%)	22	44
All	All	894/980 (91%)	841 (94%)	53 (6%)	18	36

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	85	ASP
1	A	98	LEU
1	A	143	VAL
1	A	185	SER
1	A	197	ASP
1	A	227	GLU

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Mol	Chain	Res	Type
1	A	236	GLU
1	A	237	VAL
1	A	244	SER
1	A	245	THR
1	B	-4	VAL
1	B	0	SER
1	B	9	ASP
1	B	10	THR
1	B	18	ARG
1	B	76	GLU
1	B	98	LEU
1	B	111	VAL
1	B	122	VAL
1	B	143	VAL
1	B	200	LYS
1	B	225	VAL
1	B	227	GLU
1	B	254	SER
1	C	6	THR
1	C	10	THR
1	C	26	LYS
1	C	95	GLU
1	C	98	LEU
1	C	110	VAL
1	C	122	VAL
1	C	132	ARG
1	C	138	VAL
1	C	154	LEU
1	C	188	LYS
1	C	221	VAL
1	C	233	GLU
1	C	237	VAL
1	C	239	SER
1	C	245	THR
1	C	260	LEU
1	D	12	LEU
1	D	26	LYS
1	D	54	VAL
1	D	87	SER
1	D	127	LYS
1	D	129	GLU
1	D	138	VAL

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Mol	Chain	Res	Type
1	D	202	SER
1	D	225	VAL
1	D	237	VAL
1	D	245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	40	HIS
1	A	44	ASN
1	C	31	HIS
1	C	36	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](#)

4 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	P0V	D	301	-	40,41,41	3.13	19 (47%)	53,58,58	3.90	26 (49%)
2	P0V	C	301	-	40,41,41	2.94	13 (32%)	53,58,58	3.41	16 (30%)
2	P0V	B	301	-	40,41,41	3.05	16 (40%)	53,58,58	3.54	25 (47%)
2	P0V	A	301	-	40,41,41	3.03	16 (40%)	53,58,58	3.71	22 (41%)

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	P0V	D	301	-	-	19/26/43/43	0/4/4/4
2	P0V	C	301	-	-	16/26/43/43	0/4/4/4
2	P0V	B	301	-	-	16/26/43/43	0/4/4/4
2	P0V	A	301	-	-	16/26/43/43	0/4/4/4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	P0V	C33-N34	8.39	1.48	1.33
2	B	301	P0V	C8-N9	-8.38	1.23	1.37
2	A	301	P0V	C8-N9	-8.19	1.23	1.37
2	C	301	P0V	C8-N9	-8.15	1.23	1.37
2	D	301	P0V	C8-N9	-8.12	1.23	1.37
2	D	301	P0V	C2-N9	-7.76	1.21	1.37
2	A	301	P0V	C33-N34	7.65	1.47	1.33
2	B	301	P0V	C2-N9	-7.59	1.21	1.37
2	D	301	P0V	C33-N34	7.56	1.46	1.33
2	B	301	P0V	C33-N34	7.45	1.46	1.33
2	D	301	P0V	O11-C10	7.33	1.58	1.42
2	A	301	P0V	C2-N9	-7.15	1.22	1.37
2	A	301	P0V	O11-C10	6.91	1.58	1.42
2	C	301	P0V	C2-N9	-6.77	1.23	1.37
2	C	301	P0V	O11-C10	6.12	1.56	1.42
2	B	301	P0V	O11-C10	6.07	1.56	1.42
2	D	301	P0V	C24-C25	4.53	1.57	1.47
2	D	301	P0V	C27-C26	4.43	1.55	1.44
2	A	301	P0V	C6-N17	4.43	1.45	1.34
2	B	301	P0V	C6-N17	4.39	1.45	1.34
2	B	301	P0V	C27-C26	4.28	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	P0V	C27-C26	4.26	1.54	1.44
2	D	301	P0V	C6-N17	4.23	1.45	1.34
2	C	301	P0V	C6-N17	4.21	1.45	1.34
2	B	301	P0V	C24-C25	4.16	1.56	1.47
2	A	301	P0V	C24-C25	4.06	1.56	1.47
2	D	301	P0V	O11-C12	3.86	1.53	1.45
2	B	301	P0V	C24-N16	3.86	1.51	1.46
2	A	301	P0V	C24-N16	3.81	1.51	1.46
2	C	301	P0V	C27-C26	3.78	1.53	1.44
2	C	301	P0V	C24-N16	3.77	1.51	1.46
2	C	301	P0V	C24-C25	3.72	1.55	1.47
2	A	301	P0V	O11-C12	3.33	1.52	1.45
2	D	301	P0V	C14-C10	-3.03	1.44	1.53
2	B	301	P0V	C1-N7	2.99	1.44	1.39
2	D	301	P0V	C1-N7	2.96	1.44	1.39
2	D	301	P0V	C24-N16	2.95	1.50	1.46
2	C	301	P0V	C1-N7	2.91	1.44	1.39
2	B	301	P0V	O11-C12	2.86	1.51	1.45
2	C	301	P0V	O11-C12	2.80	1.51	1.45
2	A	301	P0V	C1-N7	2.68	1.44	1.39
2	C	301	P0V	O35-C33	-2.66	1.19	1.24
2	B	301	P0V	C18-N16	2.57	1.53	1.47
2	B	301	P0V	C29-C33	2.53	1.54	1.50
2	C	301	P0V	C29-C33	2.50	1.54	1.50
2	D	301	P0V	C28-C29	2.41	1.43	1.39
2	D	301	P0V	O38-C36	2.39	1.29	1.22
2	B	301	P0V	O38-C36	2.38	1.29	1.22
2	A	301	P0V	C14-C10	-2.37	1.46	1.53
2	A	301	P0V	C29-C33	2.36	1.54	1.50
2	A	301	P0V	O35-C33	-2.36	1.19	1.24
2	D	301	P0V	C29-C33	2.29	1.54	1.50
2	A	301	P0V	C13-C14	-2.28	1.47	1.53
2	D	301	P0V	C18-N16	2.28	1.52	1.47
2	D	301	P0V	C15-N16	2.24	1.51	1.47
2	B	301	P0V	C15-N16	2.23	1.51	1.47
2	B	301	P0V	C14-C10	-2.23	1.46	1.53
2	D	301	P0V	O35-C33	-2.16	1.20	1.24
2	B	301	P0V	C13-C14	-2.15	1.47	1.53
2	C	301	P0V	C14-C10	-2.14	1.46	1.53
2	A	301	P0V	O38-C36	2.10	1.28	1.22
2	D	301	P0V	C13-C14	-2.07	1.47	1.53
2	D	301	P0V	C10-N9	-2.07	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	P0V	C1-C2	2.03	1.42	1.39

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	P0V	C2-N9-C8	16.82	123.40	105.74
2	D	301	P0V	C2-N9-C8	16.40	122.96	105.74
2	C	301	P0V	C2-N9-C8	16.31	122.87	105.74
2	A	301	P0V	C2-N9-C8	15.88	122.41	105.74
2	A	301	P0V	C19-C20-N21	8.56	132.42	110.12
2	A	301	P0V	N3-C2-N9	7.47	139.88	127.17
2	C	301	P0V	N3-C2-N9	7.26	139.52	127.17
2	D	301	P0V	N3-C2-N9	6.55	138.31	127.17
2	D	301	P0V	O37-C36-O38	-6.48	109.38	124.08
2	C	301	P0V	N9-C8-N7	-6.40	104.85	113.94
2	A	301	P0V	C10-N9-C8	-6.35	113.01	127.09
2	B	301	P0V	N3-C2-N9	6.32	137.91	127.17
2	B	301	P0V	N9-C8-N7	-6.24	105.08	113.94
2	B	301	P0V	O37-C36-O38	-6.07	110.31	124.08
2	D	301	P0V	N9-C8-N7	-6.03	105.38	113.94
2	D	301	P0V	O11-C12-C15	-5.77	99.44	108.88
2	A	301	P0V	C1-C2-N3	-5.74	118.81	126.72
2	C	301	P0V	C1-C2-N3	-5.73	118.83	126.72
2	A	301	P0V	O37-C36-O38	-5.67	111.21	124.08
2	C	301	P0V	C10-N9-C8	-5.64	114.58	127.09
2	D	301	P0V	C19-C20-N21	5.63	124.80	110.12
2	A	301	P0V	N9-C8-N7	-5.57	106.03	113.94
2	B	301	P0V	C2-C1-N7	-5.57	104.22	110.58
2	C	301	P0V	C2-C1-N7	-5.53	104.26	110.58
2	D	301	P0V	C2-C1-N7	-5.42	104.38	110.58
2	D	301	P0V	C32-C27-C26	-5.42	111.19	120.78
2	A	301	P0V	C14-C10-N9	5.26	126.37	113.30
2	D	301	P0V	C14-C10-N9	5.26	126.36	113.30
2	A	301	P0V	C2-C1-N7	-5.07	104.79	110.58
2	D	301	P0V	C28-C27-C26	5.04	129.31	120.22
2	D	301	P0V	C10-N9-C8	-5.01	115.98	127.09
2	D	301	P0V	C1-C2-N3	-4.98	119.86	126.72
2	D	301	P0V	N5-C4-N3	-4.97	121.06	128.58
2	C	301	P0V	N5-C4-N3	-4.92	121.13	128.58
2	C	301	P0V	O37-C36-O38	-4.90	112.96	124.08
2	B	301	P0V	N5-C4-N3	-4.87	121.21	128.58
2	B	301	P0V	C10-N9-C8	-4.84	116.36	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	P0V	N5-C4-N3	-4.51	121.75	128.58
2	B	301	P0V	C1-C2-N3	-4.45	120.59	126.72
2	D	301	P0V	O11-C10-C14	-4.45	97.10	106.62
2	A	301	P0V	C13-C14-C10	4.22	109.44	101.46
2	A	301	P0V	C1-C2-N9	-4.13	101.31	105.81
2	B	301	P0V	C1-C2-N9	-3.96	101.50	105.81
2	B	301	P0V	C29-C33-N34	3.93	122.58	117.74
2	D	301	P0V	C19-C20-C36	-3.87	100.20	110.45
2	C	301	P0V	C1-C2-N9	-3.82	101.65	105.81
2	A	301	P0V	C19-C20-C36	-3.79	100.39	110.45
2	C	301	P0V	C4-N3-C2	3.74	120.96	111.83
2	D	301	P0V	C1-C2-N9	-3.65	101.83	105.81
2	B	301	P0V	C14-C13-C12	3.59	109.55	102.61
2	D	301	P0V	C4-N3-C2	3.52	120.42	111.83
2	B	301	P0V	C24-N16-C15	-3.50	104.72	112.91
2	A	301	P0V	C4-N3-C2	3.35	120.01	111.83
2	D	301	P0V	C19-C18-N16	-3.17	105.35	113.69
2	B	301	P0V	C4-N3-C2	3.17	119.56	111.83
2	A	301	P0V	C14-C13-C12	3.11	108.62	102.61
2	A	301	P0V	C19-C18-N16	-3.09	105.56	113.69
2	D	301	P0V	C14-C13-C12	3.05	108.50	102.61
2	D	301	P0V	C25-C24-N16	3.05	120.44	114.08
2	D	301	P0V	C13-C14-C10	3.04	107.21	101.46
2	B	301	P0V	C6-C1-N7	3.01	137.90	132.09
2	C	301	P0V	C12-O11-C10	-2.99	102.87	109.47
2	D	301	P0V	C6-C1-N7	2.98	137.84	132.09
2	B	301	P0V	C2-N9-C10	-2.77	120.16	126.63
2	B	301	P0V	C12-O11-C10	-2.73	103.44	109.47
2	C	301	P0V	C6-C1-N7	2.65	137.20	132.09
2	B	301	P0V	C14-C10-N9	2.65	119.88	113.30
2	A	301	P0V	O11-C12-C15	-2.52	104.75	108.88
2	B	301	P0V	C19-C18-N16	-2.50	107.11	113.69
2	B	301	P0V	O23-C14-C10	-2.47	101.61	110.10
2	B	301	P0V	C18-N16-C15	2.44	117.59	111.89
2	D	301	P0V	C2-N9-C10	-2.44	120.93	126.63
2	B	301	P0V	C19-C20-C36	-2.35	104.23	110.45
2	C	301	P0V	C14-C13-C12	2.34	107.14	102.61
2	D	301	P0V	O22-C13-C12	-2.33	104.39	111.08
2	A	301	P0V	O11-C10-C14	-2.29	101.72	106.62
2	D	301	P0V	C30-C29-C33	-2.26	114.89	121.06
2	A	301	P0V	O35-C33-C29	2.24	122.34	119.60
2	B	301	P0V	O35-C33-N34	-2.23	119.39	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	P0V	C24-N16-C18	-2.20	107.58	112.94
2	C	301	P0V	C14-C10-N9	2.18	118.72	113.30
2	B	301	P0V	O11-C10-N9	2.13	112.19	108.09
2	B	301	P0V	C4-N5-C6	2.13	122.22	118.73
2	A	301	P0V	N17-C6-N5	2.09	123.04	118.38
2	D	301	P0V	C24-N16-C15	-2.05	108.12	112.91
2	A	301	P0V	O23-C14-C10	-2.04	103.08	110.10
2	C	301	P0V	C25-C24-N16	-2.02	109.85	114.08
2	A	301	P0V	C12-O11-C10	-2.01	105.02	109.47
2	B	301	P0V	O22-C13-C14	-2.01	105.36	111.82

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	P0V	C13-C12-C15-N16
2	A	301	P0V	O11-C12-C15-N16
2	A	301	P0V	N21-C20-C36-O38
2	A	301	P0V	C25-C24-N16-C15
2	B	301	P0V	C18-C19-C20-N21
2	B	301	P0V	C13-C12-C15-N16
2	B	301	P0V	O11-C12-C15-N16
2	B	301	P0V	N21-C20-C36-O38
2	B	301	P0V	N16-C24-C25-C26
2	B	301	P0V	C25-C24-N16-C15
2	B	301	P0V	C25-C24-N16-C18
2	C	301	P0V	C13-C12-C15-N16
2	C	301	P0V	O11-C12-C15-N16
2	C	301	P0V	N21-C20-C36-O38
2	C	301	P0V	N16-C24-C25-C26
2	C	301	P0V	C25-C24-N16-C15
2	C	301	P0V	C25-C24-N16-C18
2	D	301	P0V	C18-C19-C20-N21
2	D	301	P0V	C13-C12-C15-N16
2	D	301	P0V	O11-C12-C15-N16
2	D	301	P0V	C25-C24-N16-C15
2	B	301	P0V	C28-C29-C33-O35
2	B	301	P0V	C30-C29-C33-N34
2	B	301	P0V	C30-C29-C33-O35
2	B	301	P0V	C28-C29-C33-N34
2	D	301	P0V	C30-C29-C33-N34
2	D	301	P0V	C30-C29-C33-O35

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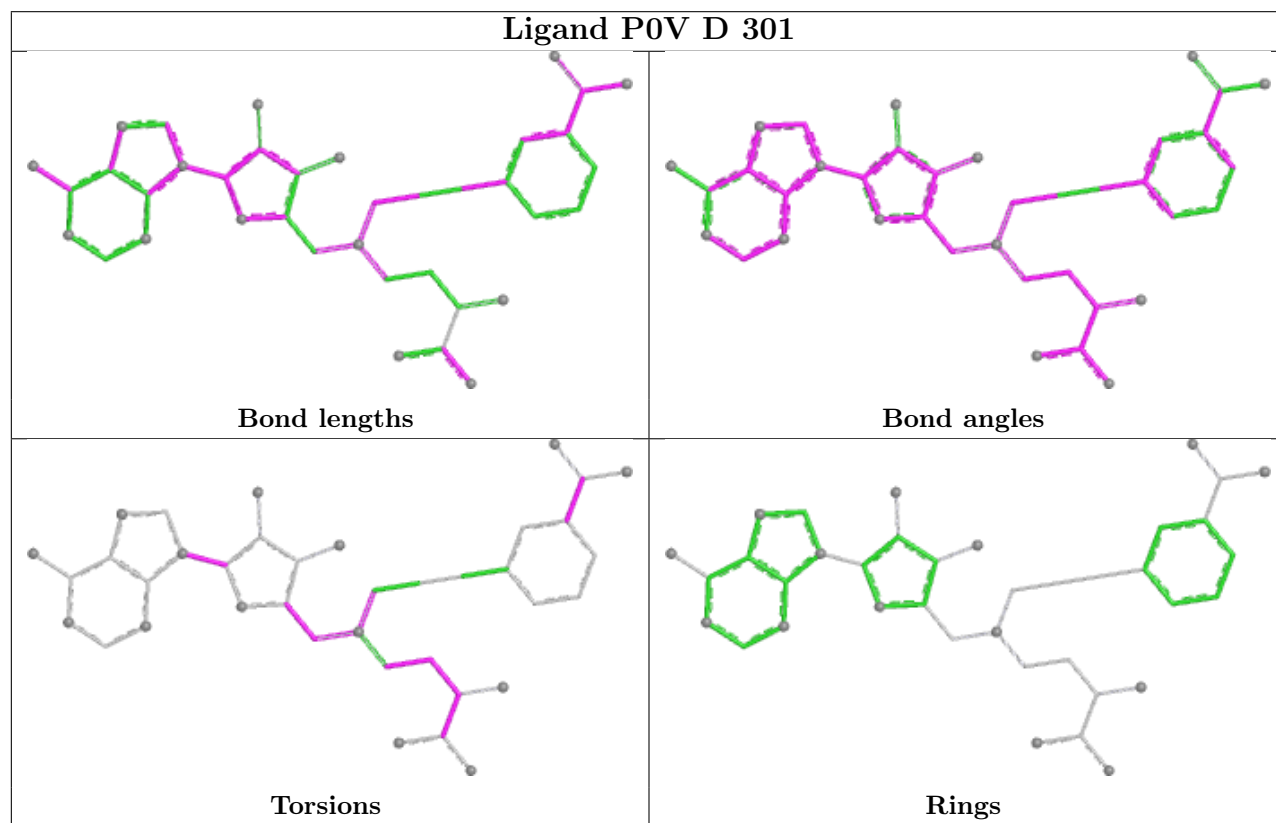
Mol	Chain	Res	Type	Atoms
2	D	301	P0V	C28-C29-C33-N34
2	D	301	P0V	C28-C29-C33-O35
2	A	301	P0V	C30-C29-C33-O35
2	A	301	P0V	C30-C29-C33-N34
2	D	301	P0V	N21-C20-C36-O37
2	A	301	P0V	C28-C29-C33-O35
2	A	301	P0V	N21-C20-C36-O37
2	B	301	P0V	N21-C20-C36-O37
2	C	301	P0V	N21-C20-C36-O37
2	A	301	P0V	C28-C29-C33-N34
2	A	301	P0V	C12-C15-N16-C18
2	B	301	P0V	C12-C15-N16-C18
2	C	301	P0V	C12-C15-N16-C18
2	D	301	P0V	C12-C15-N16-C18
2	C	301	P0V	C28-C29-C33-N34
2	C	301	P0V	C30-C29-C33-N34
2	B	301	P0V	C18-C19-C20-C36
2	A	301	P0V	C25-C24-N16-C18
2	D	301	P0V	C25-C24-N16-C18
2	C	301	P0V	C28-C29-C33-O35
2	B	301	P0V	C19-C20-C36-O38
2	C	301	P0V	C14-C10-N9-C2
2	C	301	P0V	C14-C10-N9-C8
2	D	301	P0V	C14-C10-N9-C8
2	B	301	P0V	C19-C20-C36-O37
2	C	301	P0V	O11-C10-N9-C8
2	A	301	P0V	N16-C24-C25-C26
2	D	301	P0V	C18-C19-C20-C36
2	A	301	P0V	O11-C10-N9-C8
2	D	301	P0V	O11-C10-N9-C8
2	A	301	P0V	C18-C19-C20-N21
2	C	301	P0V	C19-C20-C36-O37
2	C	301	P0V	C19-C20-C36-O38
2	D	301	P0V	C14-C10-N9-C2
2	D	301	P0V	C19-C20-C36-O37
2	D	301	P0V	C19-C20-C36-O38
2	A	301	P0V	N16-C18-C19-C20
2	D	301	P0V	N16-C18-C19-C20
2	A	301	P0V	C19-C20-C36-O37
2	D	301	P0V	N21-C20-C36-O38

There are no ring outliers.

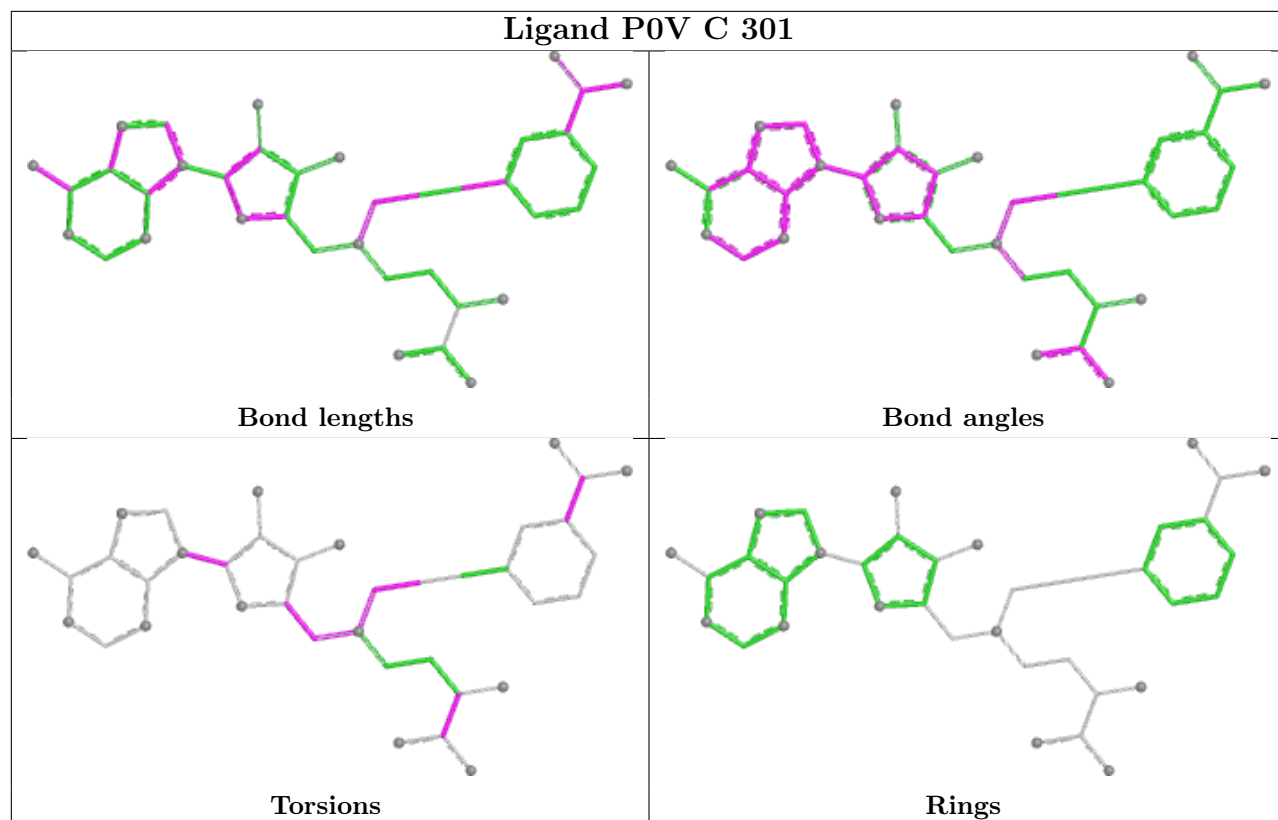
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	P0V	6	0
2	C	301	P0V	1	0
2	B	301	P0V	6	0
2	A	301	P0V	3	0

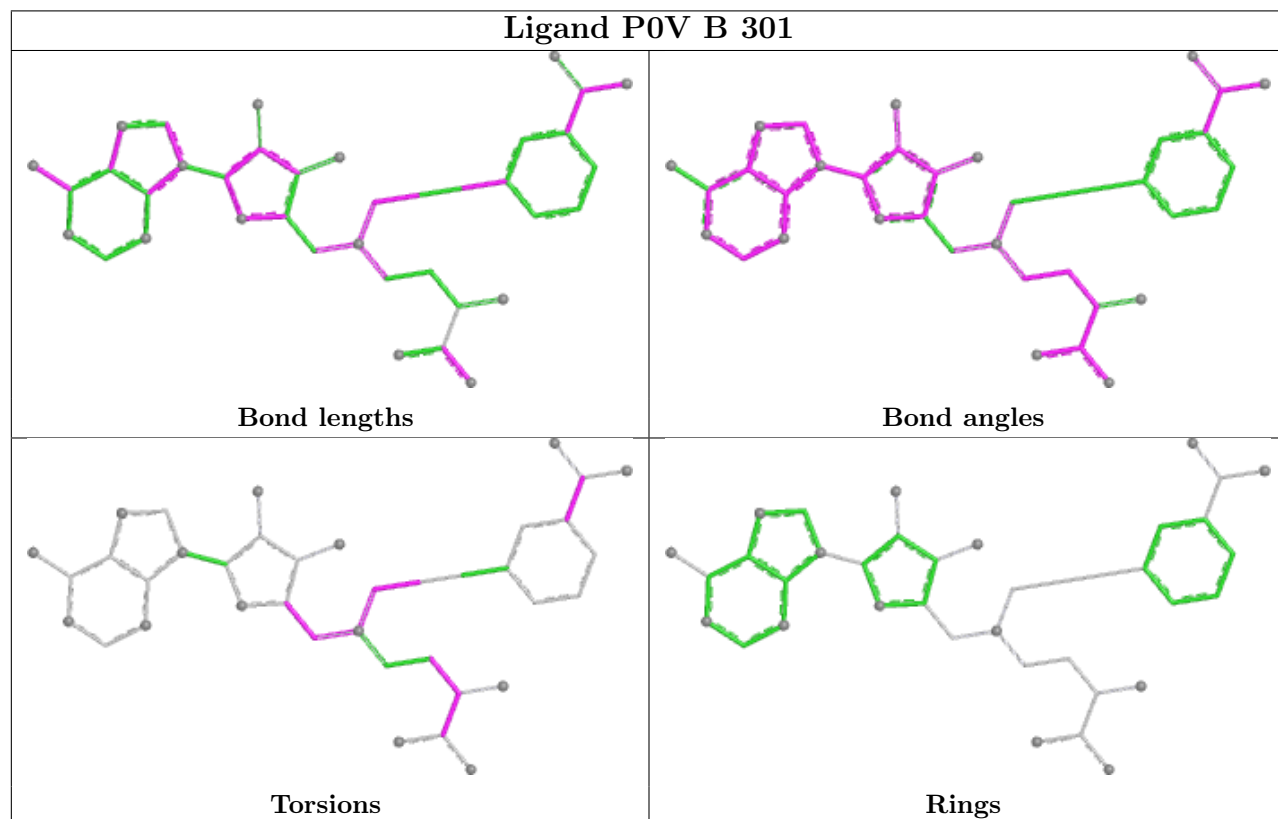
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

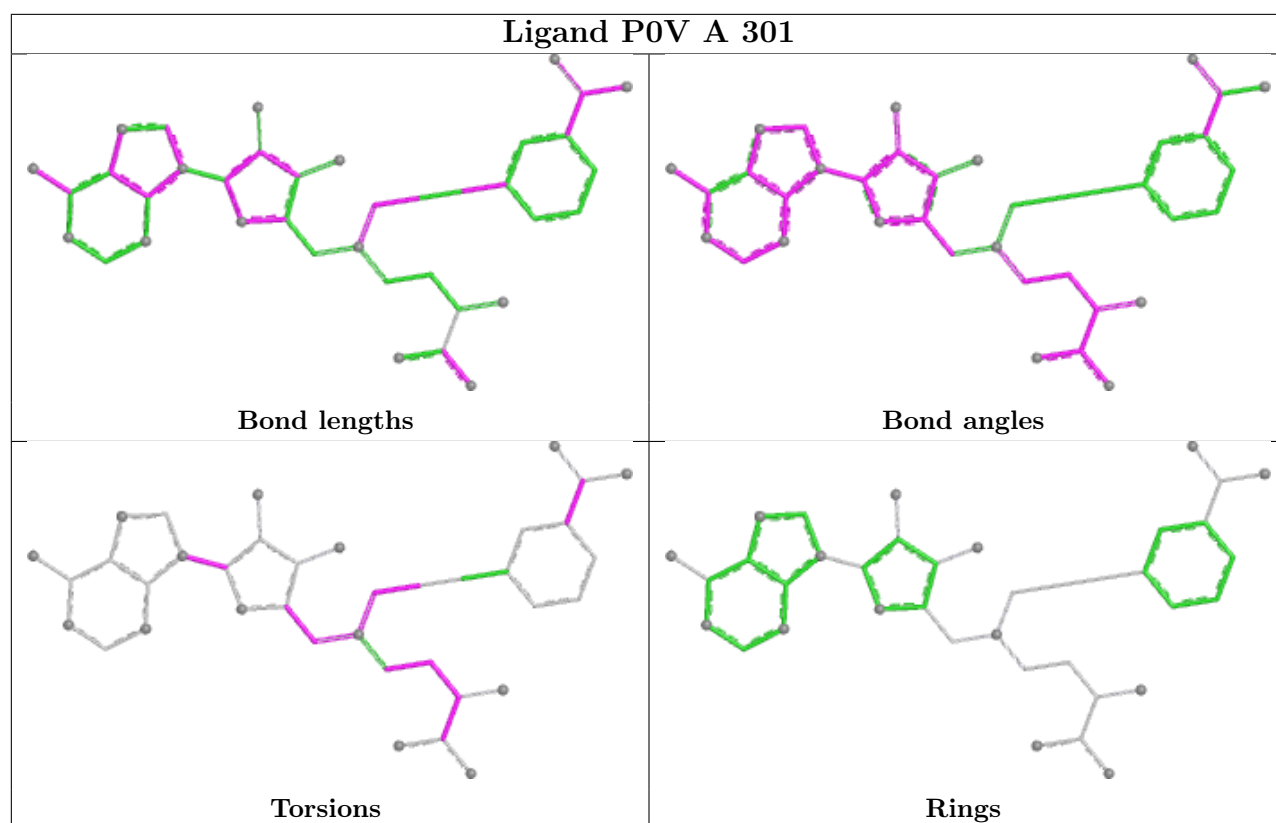


Ligand P0V C 301



Ligand P0V B 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	270/283 (95%)	1.20	39 (14%) 6 5	29, 40, 52, 63	0
1	B	270/283 (95%)	1.24	44 (16%) 4 3	30, 40, 51, 72	0
1	C	257/283 (90%)	1.27	41 (15%) 5 4	38, 48, 64, 80	0
1	D	258/283 (91%)	1.29	42 (16%) 4 3	33, 47, 62, 77	0
All	All	1055/1132 (93%)	1.25	166 (15%) 5 4	29, 43, 60, 80	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	5.9
1	A	138	VAL	5.0
1	B	206	ILE	4.5
1	D	245	THR	4.3
1	A	191	GLY	4.1
1	C	37	ILE	4.0
1	A	183	LEU	3.8
1	A	213	SER	3.6
1	A	53	GLY	3.6
1	D	114	VAL	3.5
1	B	27	PHE	3.5
1	B	-8	SER	3.5
1	A	4	GLY	3.3
1	A	98	LEU	3.3
1	C	14	HIS	3.3
1	A	-8	SER	3.2
1	B	29	SER	3.2
1	A	22	GLU	3.2
1	A	-7	SER	3.2
1	C	237	VAL	3.1
1	A	225	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	232	ILE	3.1
1	C	122	VAL	3.1
1	D	89	GLN	3.0
1	D	17	PRO	3.0
1	B	98	LEU	3.0
1	A	209	GLN	3.0
1	D	216	LEU	3.0
1	B	55	LYS	3.0
1	B	63	GLY	2.9
1	B	-9	HIS	2.9
1	D	156	PRO	2.9
1	B	97	TRP	2.9
1	A	116	ASP	2.9
1	C	32	SER	2.9
1	D	93	GLU	2.9
1	B	122	VAL	2.9
1	C	30	ARG	2.9
1	A	91	LEU	2.9
1	A	238	ILE	2.8
1	C	109	PRO	2.8
1	A	101	ALA	2.8
1	C	38	LEU	2.8
1	A	25	TYR	2.8
1	B	251	GLY	2.8
1	A	29	SER	2.8
1	A	32	SER	2.8
1	D	237	VAL	2.8
1	B	260	LEU	2.8
1	B	208	GLU	2.8
1	B	147	GLN	2.8
1	D	243	SER	2.7
1	B	160	VAL	2.7
1	B	28	GLY	2.7
1	B	228	ALA	2.7
1	D	107	TRP	2.7
1	B	184	GLY	2.6
1	A	-4	VAL	2.6
1	D	157	ALA	2.6
1	B	104	ALA	2.6
1	B	242	TYR	2.6
1	A	54	VAL	2.6
1	A	147	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	82	VAL	2.6
1	C	64	SER	2.6
1	D	18	ARG	2.5
1	D	128	GLU	2.5
1	B	189	PRO	2.5
1	A	234	TRP	2.5
1	B	60	ILE	2.5
1	B	-4	VAL	2.5
1	B	138	VAL	2.5
1	D	122	VAL	2.5
1	D	176	TYR	2.5
1	B	131	LEU	2.5
1	D	39	LYS	2.5
1	A	13	SER	2.5
1	C	29	SER	2.5
1	D	244	SER	2.5
1	C	159	CYS	2.4
1	D	222	GLU	2.4
1	B	143	VAL	2.4
1	B	185	SER	2.4
1	D	212	SER	2.4
1	D	97	TRP	2.4
1	A	247	ALA	2.4
1	B	169	ALA	2.4
1	C	242	TYR	2.4
1	C	192	PHE	2.4
1	D	189	PRO	2.4
1	D	32	SER	2.4
1	C	251	GLY	2.4
1	D	135	VAL	2.4
1	A	104	ALA	2.4
1	A	148	PRO	2.3
1	C	258	ARG	2.3
1	D	258	ARG	2.3
1	B	194	VAL	2.3
1	D	190	GLY	2.3
1	A	59	LEU	2.3
1	C	52	ASP	2.3
1	C	27	PHE	2.3
1	C	179	ALA	2.3
1	C	202	SER	2.3
1	D	171	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	69	TYR	2.3
1	A	184	GLY	2.2
1	B	40	HIS	2.2
1	C	4	GLY	2.2
1	A	187	LEU	2.2
1	A	109	PRO	2.2
1	C	102	PRO	2.2
1	B	90	ASN	2.2
1	D	50	CYS	2.2
1	D	36	GLN	2.2
1	D	213	SER	2.2
1	C	57	ASP	2.2
1	D	118	GLU	2.2
1	C	113	TYR	2.2
1	D	159	CYS	2.2
1	A	72	LEU	2.2
1	C	161	LEU	2.2
1	D	85	ASP	2.2
1	A	127	LYS	2.2
1	B	74	ALA	2.2
1	C	73	SER	2.2
1	D	202	SER	2.2
1	D	88	ASP	2.2
1	B	220	ALA	2.1
1	D	37	ILE	2.1
1	B	116	ASP	2.1
1	B	101	ALA	2.1
1	B	190	GLY	2.1
1	C	41	LEU	2.1
1	C	42	LEU	2.1
1	C	80	GLU	2.1
1	D	165	CYS	2.1
1	A	235	PHE	2.1
1	B	111	VAL	2.1
1	C	137	GLN	2.1
1	A	252	LEU	2.1
1	C	58	LEU	2.1
1	D	124	GLY	2.1
1	D	206	ILE	2.1
1	B	11	TYR	2.1
1	A	40	HIS	2.1
1	A	74	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	224	ALA	2.1
1	A	214	LEU	2.1
1	C	53	GLY	2.1
1	D	251	GLY	2.1
1	C	112	THR	2.1
1	B	235	PHE	2.0
1	A	134	ALA	2.0
1	B	164	LEU	2.0
1	B	199	LEU	2.0
1	C	234	TRP	2.0
1	C	62	ILE	2.0
1	D	136	LYS	2.0
1	B	204	TYR	2.0
1	C	11	TYR	2.0
1	C	17	PRO	2.0
1	B	183	LEU	2.0
1	C	81	ILE	2.0
1	D	62	ILE	2.0
1	D	204	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

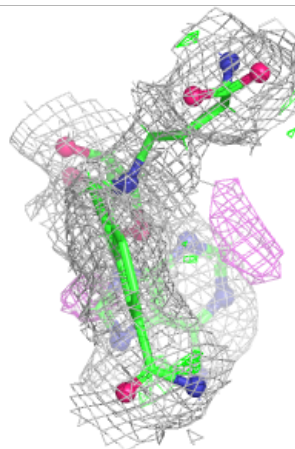
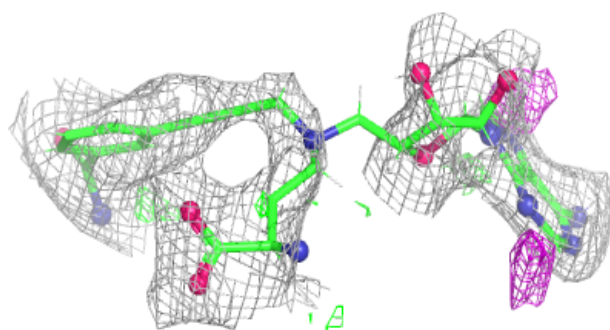
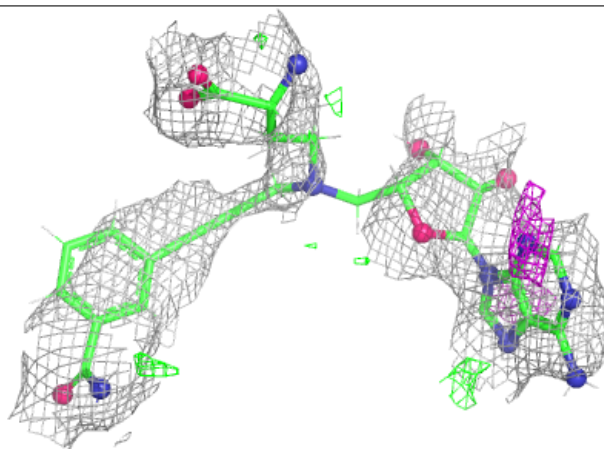
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P0V	D	301	38/38	0.81	0.15	35,47,58,62	0
2	P0V	A	301	38/38	0.84	0.13	31,37,45,48	0
2	P0V	B	301	38/38	0.86	0.13	29,38,47,50	0
2	P0V	C	301	38/38	0.87	0.13	38,49,59,65	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.

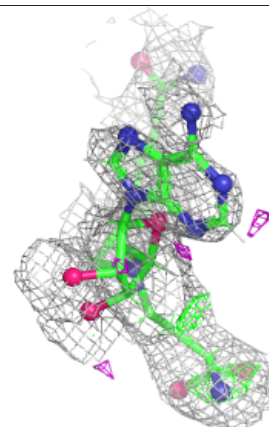
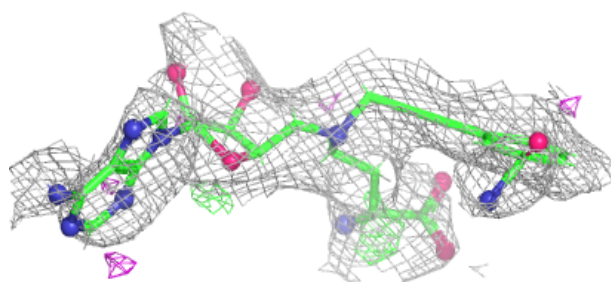
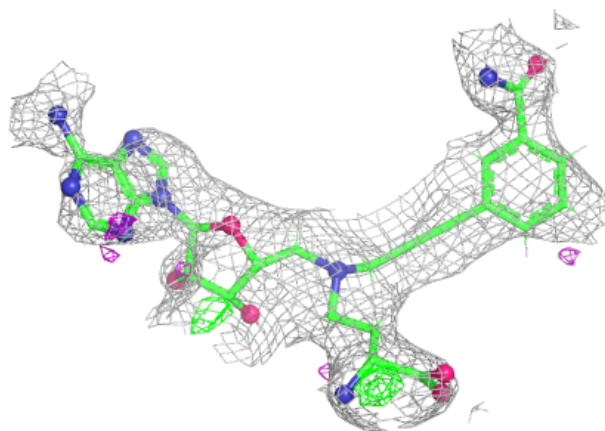
Electron density around P0V D 301:

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



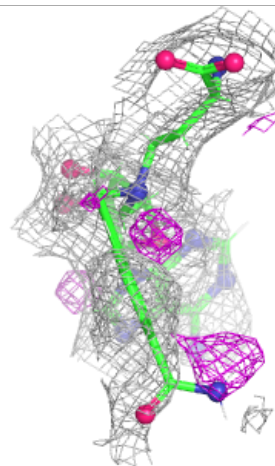
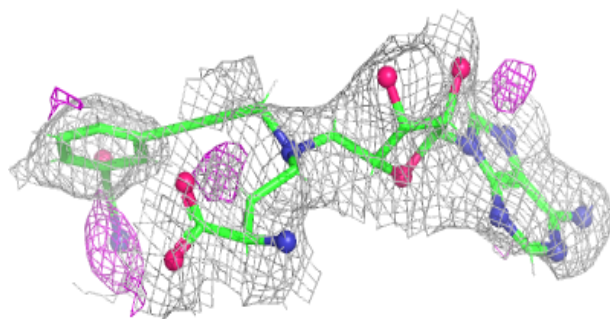
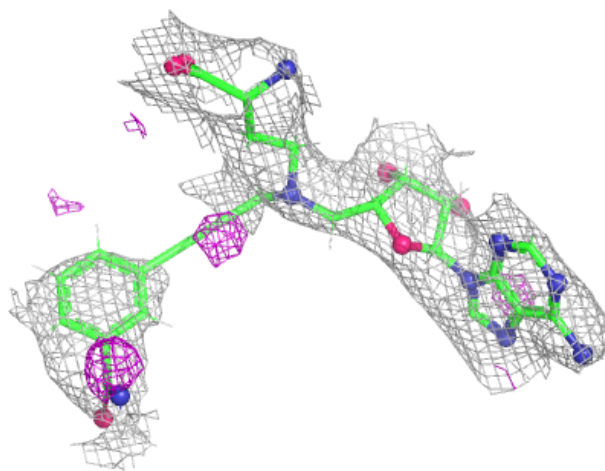
Electron density around P0V A 301:

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



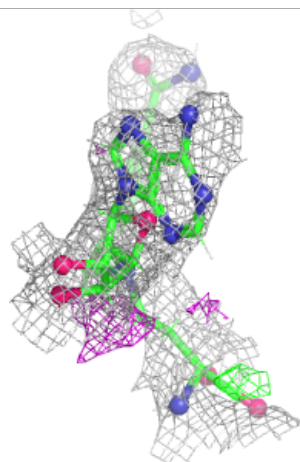
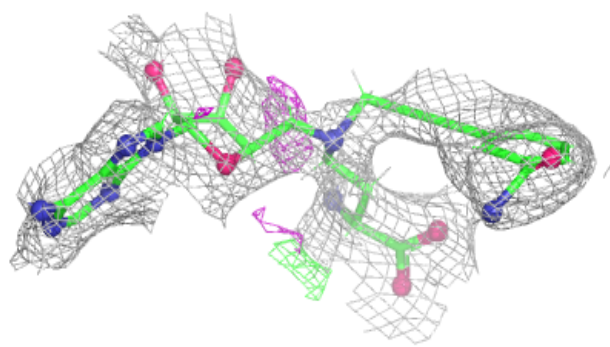
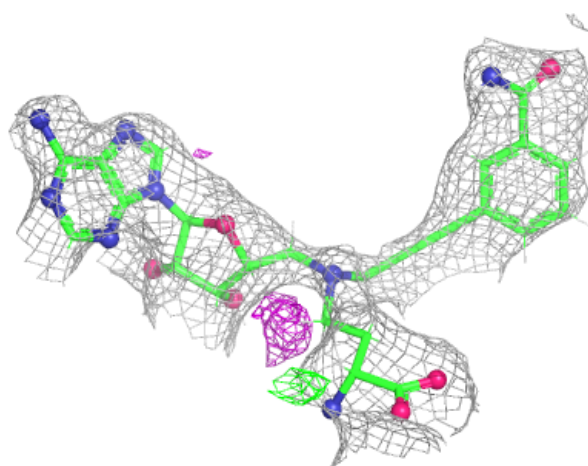
Electron density around P0V B 301:

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



Electron density around P0V C 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.