



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 AM UTC

PDB ID : 3ZRC / pdb_00003zrc
Title : pVHL54-213-EloB-EloC complex (4R)-4-HYDROXY-1-[(3-METHYLISOXAZOL-5-YL)ACETYL]-N-[4-(1,3-OXAZOL-5-YL)BENZYL]-L-PROLINAMIDE bound
Authors : Van Molle, I.; Buckley, D.L.; Crews, C.M.; Ciulli, A.
Deposited on : 2011-06-15
Resolution : 2.90 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

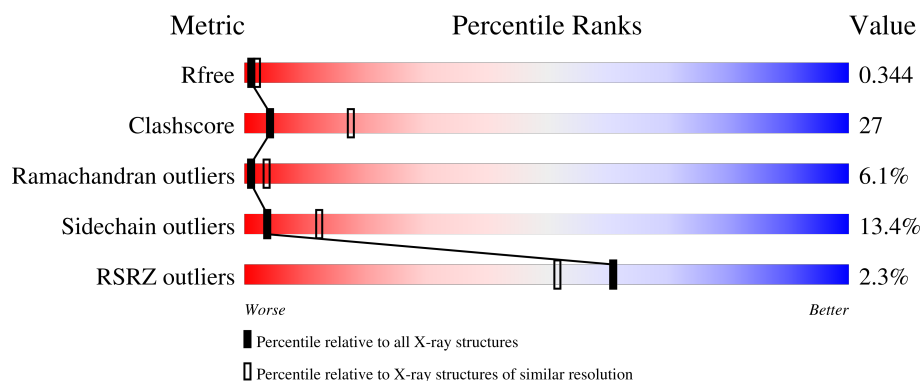
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	118	4% 38% 40% 6% 16%
1	D	118	2% 35% 38% 9% 17%
1	G	118	6% 36% 42% 9% 9%
1	J	118	0% 42% 33% 11% 13%

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Mol	Chain	Length	Quality of chain
2	B	97	41%39%8%11%
2	E	97	% 45%39%. . 10%
2	H	97	31%39%16%. 11%
2	K	97	4% 32%46%10%. 10%
3	C	163	5% 48%29%9%. 13%
3	F	163	% 41%35%9%. 13%
3	I	163	% 39%37%12%. 11%
3	L	163	% 39%37%12%12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10340 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 TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			733	465	122	142	4			
1	D	98	Total	C	N	O	S	0	0	0
			716	454	119	139	4			
1	G	107	Total	C	N	O	S	0	0	0
			819	518	138	158	5			
1	J	103	Total	C	N	O	S	0	0	0
			801	506	136	154	5			

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			663	429	104	124	6			
2	E	87	Total	C	N	O	S	0	0	0
			683	442	110	125	6			
2	H	86	Total	C	N	O	S	0	0	0
			679	440	109	124	6			
2	K	87	Total	C	N	O	S	0	0	0
			687	444	110	127	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15369
E	16	MET	-	expression tag	UNP Q15369
H	16	MET	-	expression tag	UNP Q15369
K	16	MET	-	expression tag	UNP Q15369

- Molecule 3 is a protein called VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR.

There are 12 discrepancies between the modelled and reference sequences:

- Molecule 4 is (4R)-4-HYDROXY-1-[(3-METHYLISOXAZOL-5-YL)ACETYL]-N-[4-(1,3-OXAZOL-5-YL)BENZYL]-L-PROLINAMIDE (CCD ID: L8B) (formula: C₂₁H₂₂N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			30	21	4	5		
4	F	1	Total	C	N	O	0	0
			30	21	4	5		
4	I	1	Total	C	N	O	0	0
			30	21	4	5		
4	L	1	Total	C	N	O	0	0
			30	21	4	5		

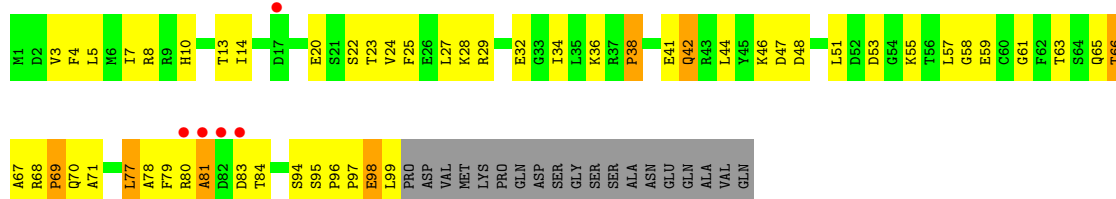
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		
5	G	1	Total	O	0	0
			1	1		
5	H	2	Total	O	0	0
			2	2		
5	I	1	Total	O	0	0
			1	1		
5	L	1	Total	O	0	0
			1	1		

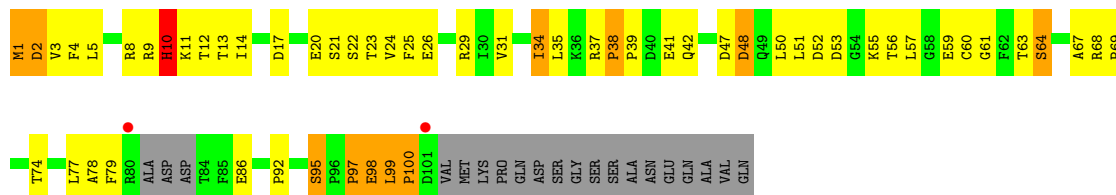
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

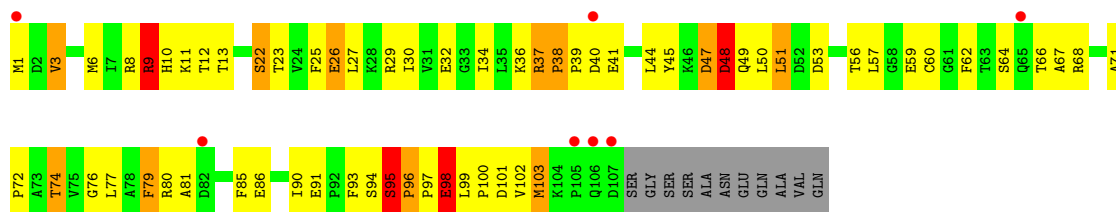
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



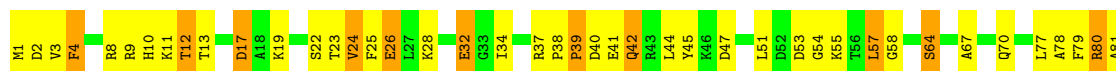
• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2



• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

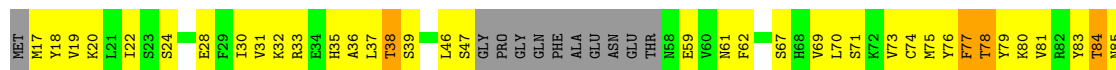


• Molecule 1: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 2

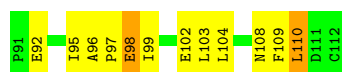
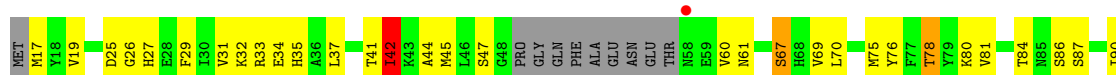




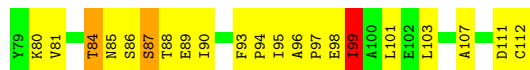
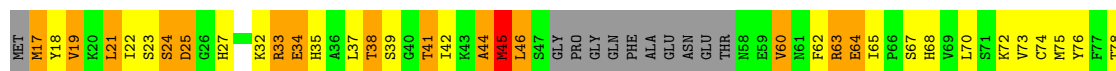
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



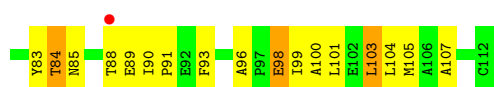
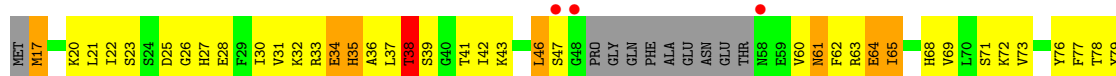
• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1



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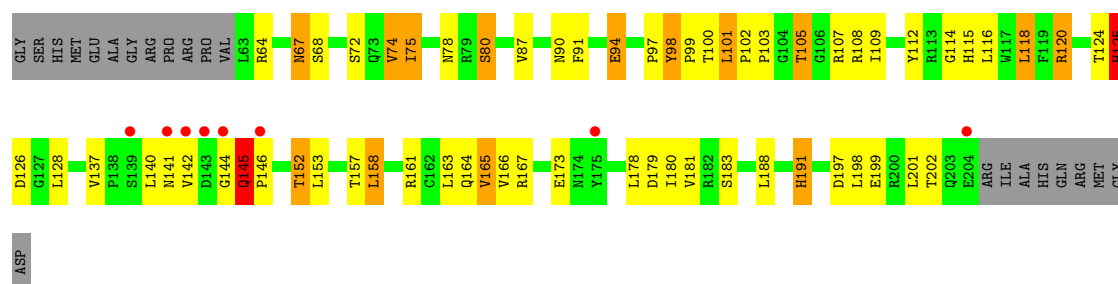


• Molecule 2: TRANSCRIPTION ELONGATION FACTOR B POLYPEPTIDE 1

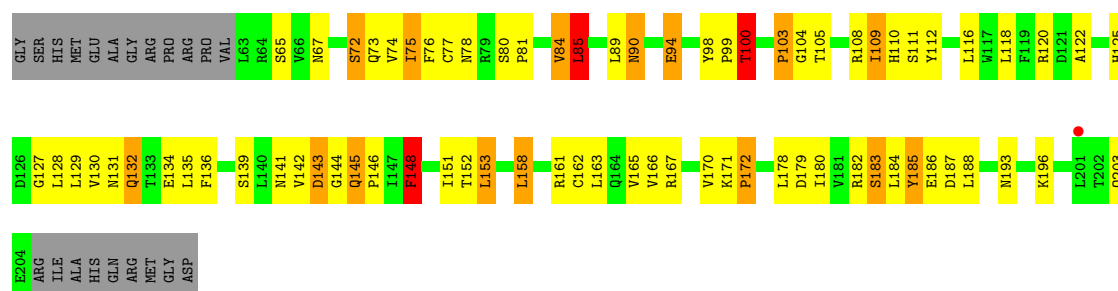


• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR

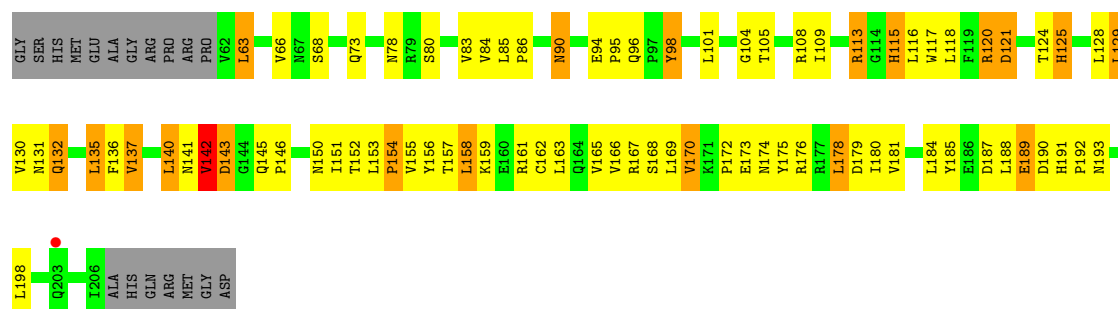




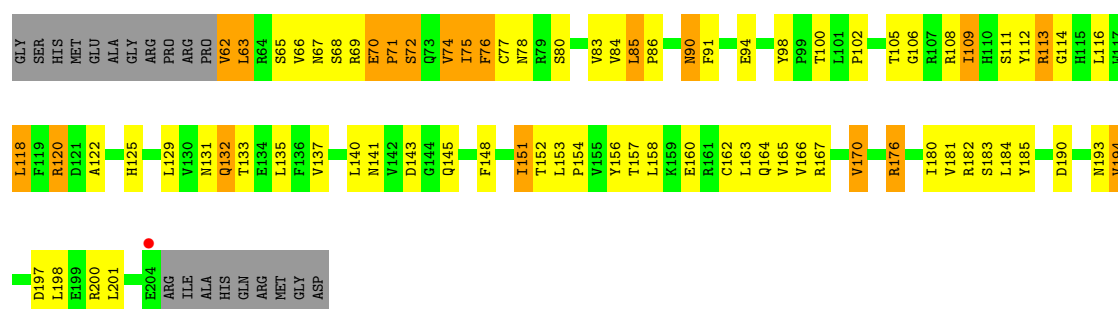
• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



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• Molecule 3: VON HIPPEL-LINDAU DISEASE TUMOR SUPPRESSOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.74Å 93.74Å 363.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.92 – 2.90 41.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (41.92-2.90) 92.0 (41.92-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.350 0.239 , 0.344	Depositor DCC
R_{free} test set	1742 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10340	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 25.80 % 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 2.9627e-03. 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: L8B

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	0.98	0/747	1.27	6/1014 (0.6%)
1	D	0.82	0/730	1.28	11/993 (1.1%)
1	G	0.81	1/836 (0.1%)	1.24	7/1134 (0.6%)
1	J	0.94	0/817	1.35	8/1105 (0.7%)
2	B	0.95	0/677	1.25	3/917 (0.3%)
2	E	0.90	0/697	1.12	2/940 (0.2%)
2	H	0.84	0/693	1.12	3/935 (0.3%)
2	K	1.01	0/701	1.22	5/945 (0.5%)
3	C	0.99	1/1071 (0.1%)	1.38	15/1474 (1.0%)
3	F	0.97	0/1143	1.33	15/1566 (1.0%)
3	I	0.91	0/1166	1.34	16/1599 (1.0%)
3	L	0.97	1/1167 (0.1%)	1.33	9/1597 (0.6%)
All	All	0.93	3/10445 (0.0%)	1.29	100/14219 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	H	0	2
3	I	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	79	PHE	CA-C	5.57	1.60	1.52
3	L	170	VAL	CA-CB	5.34	1.61	1.54
3	C	165	VAL	CA-CB	5.26	1.60	1.54

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	95	SER	CA-C-N	10.67	131.37	120.38
1	G	95	SER	C-N-CA	10.67	131.37	120.38
3	F	153	LEU	CA-C-N	-10.54	109.70	120.98
3	F	153	LEU	C-N-CA	-10.54	109.70	120.98
1	J	83	ASP	N-CA-C	-10.42	88.61	110.80
3	L	185	TYR	N-CA-C	-8.44	102.02	111.14
3	L	70	GLU	CA-C-N	8.29	130.20	119.84
3	L	70	GLU	C-N-CA	8.29	130.20	119.84
3	I	137	VAL	N-CA-C	7.79	115.86	108.15
3	F	100	THR	N-CA-C	7.73	122.41	110.20
1	G	37	ARG	CA-C-N	7.53	128.13	120.38
1	G	37	ARG	C-N-CA	7.53	128.13	120.38
3	C	153	LEU	CA-C-N	-7.44	113.02	120.98
3	C	153	LEU	C-N-CA	-7.44	113.02	120.98
3	I	180	ILE	N-CA-C	7.31	118.87	108.42
1	D	95	SER	CA-C-N	7.10	124.77	119.66
1	D	95	SER	C-N-CA	7.10	124.77	119.66
3	C	101	LEU	CB-CA-C	-7.04	102.35	110.17
3	F	85	LEU	CA-C-N	-7.03	112.19	120.13
3	F	85	LEU	C-N-CA	-7.03	112.19	120.13
1	A	66	THR	N-CA-C	-6.82	102.22	112.04
3	I	113	ARG	N-CA-C	6.47	119.15	110.35
3	C	94	GLU	N-CA-C	6.36	117.39	109.57
3	F	148	PHE	N-CA-C	6.35	119.08	108.73
3	I	170	VAL	N-CA-C	6.33	117.70	108.58
1	A	38	PRO	O-C-N	6.33	124.22	121.31
3	F	185	TYR	N-CA-C	-6.32	103.52	111.11
3	I	129	LEU	CA-C-N	-6.29	115.01	122.93
3	I	129	LEU	C-N-CA	-6.29	115.01	122.93
1	A	96	PRO	CA-C-N	6.23	127.64	120.98
1	A	96	PRO	C-N-CA	6.23	127.64	120.98
3	I	98	TYR	CA-C-N	-6.19	113.29	119.92
3	I	98	TYR	C-N-CA	-6.19	113.29	119.92
1	J	64	SER	N-CA-C	6.15	117.98	111.28
3	C	68	SER	N-CA-C	-6.10	102.32	110.55
3	C	120	ARG	N-CA-C	6.03	118.02	108.79
3	I	96	GLN	CA-C-N	5.99	126.01	119.90
3	I	96	GLN	C-N-CA	5.99	126.01	119.90
1	A	79	PHE	N-CA-C	5.98	118.97	109.65
3	I	68	SER	N-CA-C	-5.92	101.89	110.24
1	J	24	VAL	N-CA-CB	5.90	117.06	110.51
1	G	103	MET	N-CA-C	-5.83	107.97	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	105	THR	N-CA-C	5.79	119.52	110.32
1	D	22	SER	N-CA-C	-5.76	100.75	109.85
3	I	115	HIS	N-CA-C	5.76	117.49	110.41
3	I	154	PRO	CA-C-N	-5.74	116.25	121.65
3	I	154	PRO	C-N-CA	-5.74	116.25	121.65
3	F	72	SER	N-CA-C	5.71	117.55	107.61
1	D	98	GLU	CA-C-N	5.70	131.96	121.70
1	D	98	GLU	C-N-CA	5.70	131.96	121.70
2	B	90	ILE	CA-C-N	5.66	126.12	120.52
2	B	90	ILE	C-N-CA	5.66	126.12	120.52
1	D	23	THR	N-CA-C	5.65	119.31	110.32
3	C	191	HIS	CA-C-N	-5.64	114.16	120.14
3	C	191	HIS	C-N-CA	-5.64	114.16	120.14
3	C	125	HIS	N-CA-C	5.63	122.80	110.80
3	F	94	GLU	N-CA-C	5.52	116.61	109.65
2	E	42	ILE	N-CA-CB	5.47	117.98	110.54
3	C	173	GLU	N-CA-C	-5.44	105.04	110.97
3	F	103	PRO	N-CA-C	5.42	121.07	113.53
2	H	32	LYS	N-CA-C	5.42	117.72	110.35
2	K	26	GLY	N-CA-C	5.40	121.27	114.25
1	J	8	ARG	N-CA-C	5.37	117.83	108.76
1	G	8	ARG	N-CA-C	5.36	117.83	109.52
3	C	98	TYR	CA-C-N	-5.35	114.47	120.14
3	C	98	TYR	C-N-CA	-5.35	114.47	120.14
3	C	152	THR	N-CA-C	5.31	117.89	109.50
3	L	74	VAL	CA-C-N	-5.29	116.28	123.10
3	L	74	VAL	C-N-CA	-5.29	116.28	123.10
2	K	96	ALA	CA-C-N	5.28	126.44	119.84
2	K	96	ALA	C-N-CA	5.28	126.44	119.84
2	B	30	ILE	CB-CA-C	5.27	117.33	110.96
1	J	4	PHE	N-CA-C	5.26	116.98	108.41
3	F	84	VAL	CB-CA-C	-5.22	104.44	110.91
3	L	76	PHE	CA-C-N	-5.19	116.10	122.84
3	L	76	PHE	C-N-CA	-5.19	116.10	122.84
1	J	24	VAL	N-CA-C	-5.18	104.92	110.36
1	G	51	LEU	N-CA-C	5.17	116.81	108.34
3	F	80	SER	CA-C-N	5.13	124.85	119.82
3	F	80	SER	C-N-CA	5.13	124.85	119.82
2	H	96	ALA	CA-C-N	5.13	126.26	119.84
2	H	96	ALA	C-N-CA	5.13	126.26	119.84
2	E	86	SER	N-CA-C	5.13	116.39	107.93
3	I	125	HIS	N-CA-C	5.10	121.65	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	PRO	N-CA-C	5.09	118.60	110.40
1	D	38	PRO	CA-C-N	5.08	124.58	119.19
1	D	38	PRO	C-N-CA	5.08	124.58	119.19
1	D	61	GLY	N-CA-C	5.08	120.78	114.37
3	F	81	PRO	N-CA-C	5.08	120.54	113.98
1	D	37	ARG	CA-C-N	5.08	125.61	120.38
1	D	37	ARG	C-N-CA	5.08	125.61	120.38
3	F	109	ILE	N-CA-C	5.06	115.56	108.17
3	C	145	GLN	CA-C-N	-5.05	114.79	120.14
3	C	145	GLN	C-N-CA	-5.05	114.79	120.14
3	L	170	VAL	N-CA-C	5.04	115.17	108.11
2	K	38	THR	N-CA-C	-5.02	105.80	111.28
1	J	83	ASP	CA-C-N	-5.02	115.74	122.42
1	J	83	ASP	C-N-CA	-5.02	115.74	122.42
2	K	61	ASN	N-CA-C	5.02	118.34	107.49
3	L	193	ASN	N-CA-C	5.00	116.20	107.49

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	111	ASP	Peptide
2	H	87	SER	Peptide
3	I	104	GLY	Peptide
1	J	82	ASP	Peptide

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	733	0	701	32	0
1	D	716	0	667	38	0
1	G	819	0	791	59	1
1	J	801	0	789	45	0
2	B	663	0	637	40	0
2	E	683	0	680	36	0
2	H	679	0	677	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	687	0	684	41	1
3	C	1043	0	950	55	0
3	F	1113	0	1066	57	0
3	I	1136	0	1096	76	0
3	L	1137	0	1107	57	0
4	C	30	0	21	4	0
4	F	30	0	22	2	0
4	I	30	0	22	1	0
4	L	30	0	22	1	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	1	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
All	All	10340	0	9932	551	1

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 27.

All (551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:42:ILE:HG22	2:H:46:LEU:HD23	1.32	1.11
2:K:62:PHE:HB3	2:K:65:ILE:HD13	1.19	1.11
1:J:41:GLU:HG2	1:J:81:ALA:HB2	1.16	1.10
2:H:34:GLU:CD	2:H:34:GLU:H	1.67	1.02
3:L:68:SER:O	3:L:69:ARG:HB2	1.60	1.01
3:C:78:ASN:ND2	3:C:103:PRO:HA	1.78	0.99
1:J:41:GLU:CG	1:J:81:ALA:HB2	1.96	0.96
3:L:108:ARG:O	3:L:109:ILE:HD13	1.68	0.94
3:F:108:ARG:O	3:F:109:ILE:HD13	1.67	0.94
3:F:104:GLY:HA3	2:H:63:ARG:HD2	1.50	0.94
3:I:141:ASN:O	3:I:142:VAL:HG13	1.69	0.92
3:C:102:PRO:O	3:C:105:THR:HB	1.70	0.92
2:E:17:MET:HE3	2:E:32:LYS:HE2	1.54	0.90
3:I:98:TYR:OH	4:I:1207:L8B:O	1.92	0.88
1:J:32:GLU:HG3	1:J:38:PRO:HA	1.58	0.86
1:J:41:GLU:HG2	1:J:81:ALA:CB	2.02	0.86
2:B:105:MET:SD	3:C:180:ILE:HG22	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:ARG:O	2:E:37:LEU:HG	1.76	0.86
3:I:84:VAL:HG22	3:I:128:LEU:CD1	2.07	0.85
3:I:167:ARG:NH1	3:I:192:PRO:HD3	1.92	0.84
3:I:84:VAL:HG22	3:I:128:LEU:HD13	1.59	0.84
1:D:56:THR:OG1	1:D:59:GLU:HB2	1.77	0.83
1:J:9:ARG:NH1	1:J:10:HIS:ND1	2.26	0.83
1:D:79:PHE:H	1:D:86:GLU:HG2	1.44	0.82
2:B:17:MET:HG3	2:B:18:TYR:CD1	2.14	0.82
2:H:42:ILE:CG2	2:H:46:LEU:HD23	2.12	0.80
1:A:24:VAL:HB	1:A:53:ASP:HA	1.65	0.79
3:C:108:ARG:O	3:C:109:ILE:HD13	1.82	0.78
2:K:34:GLU:H	2:K:34:GLU:CD	1.87	0.78
3:F:89:LEU:HD12	3:F:116:LEU:HD23	1.63	0.78
2:B:95:ILE:HB	3:C:165:VAL:HG21	1.65	0.78
3:C:74:VAL:CG1	3:C:75:ILE:N	2.46	0.78
2:K:34:GLU:O	2:K:35:HIS:C	2.27	0.78
2:K:17:MET:SD	2:K:17:MET:O	2.42	0.77
1:D:77:LEU:HD12	1:D:78:ALA:H	1.48	0.77
2:K:65:ILE:N	2:K:65:ILE:HD12	1.99	0.77
3:F:131:ASN:C	3:F:132:GLN:HG2	2.08	0.77
3:I:142:VAL:O	3:I:142:VAL:HG23	1.83	0.77
3:F:84:VAL:HG21	3:F:151:ILE:HG21	1.64	0.77
1:G:22:SER:O	1:G:56:THR:HA	1.84	0.76
2:H:42:ILE:HG22	2:H:46:LEU:CD2	2.15	0.76
1:D:99:LEU:H	1:D:100:PRO:HD3	1.50	0.76
3:L:69:ARG:HG3	3:L:69:ARG:HH11	1.50	0.75
2:B:22:ILE:HG12	2:B:28:GLU:HG2	1.68	0.74
3:C:120:ARG:HD3	3:C:125:HIS:O	1.88	0.74
3:I:172:PRO:HA	3:I:175:TYR:CE1	2.23	0.73
3:L:85:LEU:HD23	3:L:100:THR:HG22	1.71	0.72
1:D:98:GLU:HA	1:D:99:LEU:CB	2.20	0.72
3:F:166:VAL:O	3:F:170:VAL:HG12	1.89	0.72
2:E:80:LYS:O	2:E:84:THR:HG22	1.89	0.72
1:A:25:PHE:HB2	1:A:53:ASP:HB3	1.72	0.72
3:C:120:ARG:HB2	3:C:126:ASP:O	1.90	0.71
1:G:3:VAL:HG22	1:G:67:ALA:HB3	1.72	0.71
2:E:96:ALA:HB1	2:E:98:GLU:OE1	1.90	0.71
3:C:120:ARG:HA	3:C:128:LEU:HD12	1.73	0.70
2:K:23:SER:OG	2:K:25:ASP:OD1	2.09	0.70
3:L:76:PHE:O	3:L:106:GLY:HA2	1.91	0.70
3:F:193:ASN:HB3	3:F:196:LYS:HB2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:PRO:O	1:G:98:GLU:HB2	1.89	0.70
2:H:33:ARG:O	2:H:37:LEU:HG	1.90	0.70
3:F:104:GLY:CA	2:H:63:ARG:HD2	2.21	0.70
3:I:141:ASN:HD21	3:I:146:PRO:HA	1.57	0.70
3:C:178:LEU:O	3:C:180:ILE:HG13	1.91	0.70
2:H:18:TYR:O	2:H:19:VAL:HG12	1.92	0.69
3:C:64:ARG:HD2	3:C:91:PHE:O	1.91	0.69
1:G:23:THR:N	1:G:26:GLU:OE2	2.23	0.69
1:J:44:LEU:O	1:J:51:LEU:HB2	1.92	0.69
3:L:90:ASN:HB2	3:L:94:GLU:O	1.92	0.69
3:I:175:TYR:O	3:I:185:TYR:HE1	1.75	0.69
3:C:102:PRO:HD2	3:C:105:THR:HG21	1.75	0.69
1:G:9:ARG:HD3	1:G:77:LEU:HD23	1.75	0.69
2:B:36:ALA:O	2:B:38:THR:N	2.25	0.69
2:E:95:ILE:HB	3:F:165:VAL:HG21	1.75	0.69
1:J:94:SER:HB3	2:K:25:ASP:OD2	1.94	0.68
3:L:154:PRO:HG2	3:L:156:TYR:CE1	2.28	0.68
1:G:11:LYS:HA	2:H:27:HIS:CD2	2.27	0.68
1:D:21:SER:HA	1:D:56:THR:HB	1.76	0.68
3:F:73:GLN:OE1	3:F:110:HIS:CD2	2.47	0.67
3:L:116:LEU:HG	3:L:137:VAL:HG22	1.76	0.67
3:C:180:ILE:HD12	3:C:180:ILE:O	1.94	0.67
3:C:102:PRO:O	3:C:105:THR:CB	2.42	0.67
3:L:62:VAL:O	3:L:63:LEU:HB2	1.95	0.67
3:F:90:ASN:HD22	3:F:94:GLU:HB2	1.59	0.66
2:H:35:HIS:O	2:H:38:THR:HB	1.95	0.66
2:K:34:GLU:O	2:K:37:LEU:N	2.28	0.66
2:H:62:PHE:CD2	2:H:65:ILE:HD12	2.30	0.66
2:B:36:ALA:C	2:B:38:THR:H	2.03	0.66
3:L:194:VAL:O	3:L:198:LEU:HB2	1.95	0.66
3:L:116:LEU:HG	3:L:137:VAL:CG2	2.26	0.65
1:D:1:MET:HG2	1:D:64:SER:OG	1.97	0.65
1:D:55:LYS:HD2	1:D:59:GLU:OE1	1.96	0.65
2:H:23:SER:OG	2:H:25:ASP:OD1	2.14	0.64
3:I:141:ASN:C	3:I:142:VAL:HG13	2.21	0.64
3:C:67:ASN:HA	3:C:91:PHE:CE1	2.33	0.64
3:F:158:LEU:O	3:F:158:LEU:HD12	1.97	0.63
3:I:131:ASN:O	3:I:132:GLN:HB2	1.97	0.63
3:F:163:LEU:O	3:F:167:ARG:HG3	1.98	0.63
2:H:64:GLU:HB2	5:H:2002:HOH:O	1.99	0.63
3:I:142:VAL:O	3:I:142:VAL:CG2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:162:CYS:O	3:L:166:VAL:HG23	1.99	0.63
3:C:199:GLU:O	3:C:202:THR:HG22	1.99	0.63
2:H:34:GLU:CD	2:H:34:GLU:N	2.47	0.63
3:I:132:GLN:OE1	3:I:132:GLN:HA	1.98	0.63
1:G:34:ILE:HG12	2:H:18:TYR:CE2	2.34	0.63
2:H:80:LYS:O	2:H:84:THR:HB	1.99	0.63
3:L:163:LEU:O	3:L:167:ARG:HG3	1.98	0.63
3:C:74:VAL:HG12	3:C:75:ILE:N	2.14	0.62
2:K:35:HIS:O	2:K:38:THR:HB	1.99	0.62
3:C:67:ASN:HA	3:C:91:PHE:HE1	1.64	0.62
1:J:1:MET:SD	1:J:64:SER:OG	2.52	0.62
2:K:35:HIS:HD2	2:K:78:THR:HG22	1.63	0.62
3:F:167:ARG:HH21	3:F:188:LEU:HA	1.64	0.62
3:I:131:ASN:OD1	3:I:150:ASN:HB2	2.00	0.62
1:G:66:THR:O	1:G:66:THR:HG22	1.99	0.62
3:I:84:VAL:HG21	3:I:151:ILE:HG21	1.81	0.62
3:L:102:PRO:HD2	3:L:105:THR:OG1	2.00	0.61
1:G:25:PHE:HD2	1:G:53:ASP:HB3	1.64	0.61
1:J:4:PHE:H	1:J:67:ALA:HB1	1.65	0.61
2:B:87:SER:O	2:B:89:GLU:N	2.34	0.61
1:D:14:ILE:HD13	1:D:34:ILE:HD12	1.80	0.61
1:J:37:ARG:NH1	1:J:41:GLU:OE1	2.32	0.61
3:L:67:ASN:OD1	3:L:67:ASN:O	2.18	0.61
1:A:77:LEU:HD12	1:A:78:ALA:N	2.15	0.61
3:F:120:ARG:HD3	3:F:127:GLY:HA2	1.81	0.61
1:G:79:PHE:HB3	1:G:80:ARG:HA	1.80	0.61
1:D:8:ARG:HG2	1:D:13:THR:HG23	1.83	0.61
1:G:57:LEU:O	1:G:62:PHE:HB2	2.01	0.61
1:A:8:ARG:HG2	1:A:13:THR:HG23	1.83	0.61
2:E:42:ILE:HA	2:E:45:MET:HB2	1.84	0.60
1:D:50:LEU:HG	1:D:51:LEU:H	1.65	0.60
3:F:120:ARG:HD2	3:F:125:HIS:O	2.01	0.60
3:I:173:GLU:N	3:I:173:GLU:CD	2.59	0.60
3:C:98:TYR:HB3	3:C:99:PRO:CD	2.31	0.60
3:L:85:LEU:HD23	3:L:100:THR:CG2	2.31	0.60
2:H:101:LEU:HD22	3:I:178:LEU:HD21	1.84	0.60
3:C:145:GLN:CB	3:C:146:PRO:HD3	2.31	0.60
3:F:111:SER:C	3:F:112:TYR:CD1	2.80	0.60
1:A:24:VAL:HG23	1:A:55:LYS:O	2.02	0.59
2:B:76:TYR:OH	3:C:157:THR:HA	2.02	0.59
2:E:108:ASN:ND2	3:F:184:LEU:HD21	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:118:LEU:HD12	3:L:118:LEU:C	2.26	0.59
2:H:35:HIS:HD2	2:H:78:THR:HG22	1.67	0.59
1:G:94:SER:HB3	2:H:25:ASP:OD2	2.02	0.59
2:B:17:MET:HG3	2:B:18:TYR:HD1	1.68	0.59
2:B:71:SER:O	2:B:75:MET:HG3	2.02	0.59
2:K:65:ILE:HD12	2:K:65:ILE:H	1.67	0.59
3:C:87:VAL:HB	3:C:118:LEU:HD12	1.85	0.59
1:G:25:PHE:HE1	1:G:29:ARG:HH21	1.51	0.59
2:H:87:SER:HB3	3:I:132:GLN:NE2	2.18	0.59
3:C:80:SER:O	3:C:103:PRO:HB3	2.03	0.59
2:E:17:MET:HE3	2:E:32:LYS:CE	2.31	0.59
3:I:167:ARG:HH12	3:I:192:PRO:HD3	1.66	0.59
3:C:98:TYR:OH	4:C:1205:L8B:HB1C	2.03	0.59
2:E:25:ASP:OD2	2:E:67:SER:OG	2.21	0.59
1:G:100:PRO:C	1:G:102:VAL:H	2.10	0.59
3:L:109:ILE:HD11	4:L:1205:L8B:CAJ	2.33	0.59
1:D:9:ARG:O	1:D:10:HIS:C	2.45	0.58
3:F:108:ARG:C	3:F:109:ILE:HD13	2.27	0.58
1:G:11:LYS:H	1:G:91:GLU:HB2	1.68	0.58
1:A:32:GLU:O	1:A:36:LYS:HA	2.03	0.58
3:C:74:VAL:HG13	3:C:75:ILE:H	1.68	0.58
1:J:25:PHE:CE1	1:J:39:PRO:HB3	2.38	0.58
2:H:103:LEU:O	2:H:107:ALA:N	2.34	0.58
1:D:69:PRO:HB3	2:E:78:THR:HG22	1.86	0.58
1:J:37:ARG:HH21	1:J:79:PHE:HB3	1.68	0.58
1:G:41:GLU:O	1:G:85:PHE:HE1	1.87	0.58
3:I:175:TYR:O	3:I:185:TYR:CE1	2.56	0.58
3:I:121:ASP:OD2	3:I:124:THR:OG1	2.16	0.57
1:A:68:ARG:O	1:A:69:PRO:C	2.45	0.57
2:H:18:TYR:O	2:H:19:VAL:CG1	2.52	0.57
1:A:70:GLN:HG2	2:B:79:TYR:CD2	2.38	0.57
3:I:163:LEU:CD2	3:I:188:LEU:HD23	2.34	0.57
2:B:17:MET:HG3	2:B:18:TYR:CE1	2.39	0.57
2:K:34:GLU:CD	2:K:34:GLU:N	2.61	0.57
3:C:74:VAL:HG13	3:C:75:ILE:N	2.20	0.57
1:G:41:GLU:O	1:G:85:PHE:CE1	2.57	0.57
3:F:72:SER:HA	3:F:141:ASN:HD21	1.70	0.57
3:F:130:VAL:HG11	3:F:136:PHE:HB2	1.87	0.57
2:K:20:LYS:HE2	2:K:28:GLU:HB3	1.87	0.57
3:I:141:ASN:O	3:I:142:VAL:CG1	2.48	0.56
3:C:124:THR:O	3:C:126:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HG3	1:D:2:ASP:N	2.19	0.56
1:D:98:GLU:CA	1:D:99:LEU:CB	2.84	0.56
2:E:99:ILE:CG2	2:E:99:ILE:O	2.54	0.56
1:G:79:PHE:O	1:G:86:GLU:HG2	2.05	0.56
1:J:37:ARG:NH2	1:J:79:PHE:HB3	2.19	0.56
3:F:65:SER:OG	3:F:89:LEU:O	2.21	0.56
2:K:65:ILE:N	2:K:65:ILE:CD1	2.68	0.56
2:B:39:SER:OG	2:B:110:LEU:HB3	2.06	0.56
3:F:143:ASP:C	3:F:145:GLN:H	2.14	0.56
3:C:112:TYR:HB2	3:C:115:HIS:CD2	2.41	0.55
3:L:69:ARG:HH11	3:L:69:ARG:CG	2.19	0.55
3:C:109:ILE:HG23	4:C:1205:L8B:HAH	1.87	0.55
3:I:113:ARG:CD	3:I:140:LEU:HD12	2.37	0.55
3:I:173:GLU:CD	3:I:173:GLU:H	2.14	0.55
3:L:135:LEU:HD21	3:L:201:LEU:HD11	1.89	0.55
2:B:31:VAL:HG12	2:B:32:LYS:N	2.22	0.55
1:A:29:ARG:NH1	1:A:32:GLU:OE1	2.39	0.54
1:D:77:LEU:HD12	1:D:78:ALA:N	2.19	0.54
3:L:62:VAL:O	3:L:63:LEU:CB	2.55	0.54
2:E:99:ILE:HG22	2:E:103:LEU:HB2	1.88	0.54
3:I:189:GLU:O	3:I:191:HIS:N	2.39	0.54
3:L:72:SER:HA	3:L:141:ASN:HD21	1.72	0.54
1:A:70:GLN:HG2	2:B:79:TYR:HD2	1.71	0.54
2:K:107:ALA:HB2	3:L:158:LEU:HG	1.89	0.54
3:I:142:VAL:O	3:I:143:ASP:C	2.51	0.54
1:J:19:LYS:O	1:J:22:SER:HB3	2.07	0.54
2:B:79:TYR:CD1	2:B:79:TYR:C	2.86	0.54
1:D:47:ASP:O	1:D:48:ASP:CB	2.55	0.54
2:H:46:LEU:HG	2:H:46:LEU:O	2.08	0.54
3:I:152:THR:HG22	3:I:153:LEU:N	2.23	0.54
3:L:120:ARG:HD3	3:L:125:HIS:O	2.08	0.54
1:A:44:LEU:O	1:A:51:LEU:HB2	2.08	0.53
2:E:109:PHE:HD1	2:E:110:LEU:HD23	1.73	0.53
3:F:85:LEU:HA	3:F:100:THR:HG22	1.89	0.53
2:K:83:TYR:CE2	2:K:91:PRO:HD2	2.43	0.53
3:L:70:GLU:OE1	3:L:113:ARG:HD3	2.08	0.53
2:E:60:VAL:HG12	2:E:61:ASN:H	1.74	0.53
2:H:95:ILE:HB	3:I:165:VAL:HG21	1.89	0.53
3:F:179:ASP:O	3:F:180:ILE:HG23	2.09	0.53
2:K:107:ALA:CB	3:L:158:LEU:HG	2.38	0.53
1:G:25:PHE:CD2	1:G:53:ASP:HB3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:LEU:HD22	1:G:60:CYS:SG	2.48	0.53
2:B:84:THR:O	2:B:85:ASN:HB2	2.09	0.53
3:F:85:LEU:HD23	3:F:100:THR:HG23	1.91	0.53
3:I:174:ASN:C	3:I:176:ARG:N	2.65	0.53
2:K:83:TYR:O	2:K:84:THR:C	2.50	0.53
2:E:87:SER:HB3	3:F:132:GLN:HE22	1.74	0.52
2:H:37:LEU:C	2:H:39:SER:N	2.66	0.52
3:I:141:ASN:O	3:I:142:VAL:HG22	2.09	0.52
2:K:35:HIS:CD2	2:K:78:THR:HG22	2.43	0.52
1:A:28:LYS:NZ	1:A:53:ASP:OD1	2.34	0.52
1:J:77:LEU:HD12	1:J:78:ALA:H	1.75	0.52
2:K:46:LEU:O	2:K:47:SER:CB	2.56	0.52
1:A:29:ARG:O	1:A:32:GLU:N	2.43	0.52
2:H:97:PRO:C	2:H:99:ILE:H	2.17	0.52
3:C:120:ARG:CB	3:C:126:ASP:O	2.57	0.52
3:F:167:ARG:NH2	3:F:187:ASP:O	2.43	0.52
1:G:9:ARG:O	1:G:12:THR:HB	2.09	0.52
3:I:141:ASN:ND2	3:I:145:GLN:O	2.40	0.52
3:I:173:GLU:O	3:I:174:ASN:ND2	2.42	0.52
1:D:25:PHE:HB2	1:D:53:ASP:HB3	1.91	0.52
3:F:131:ASN:O	3:F:132:GLN:HG2	2.10	0.52
3:I:73:GLN:OE1	3:I:108:ARG:HD2	2.09	0.52
3:I:78:ASN:OD1	3:I:78:ASN:C	2.52	0.51
1:J:81:ALA:O	1:J:83:ASP:HB3	2.10	0.51
2:E:29:PHE:CD2	2:E:70:LEU:HD23	2.45	0.51
3:C:72:SER:HA	3:C:141:ASN:CB	2.40	0.51
3:L:75:ILE:HD11	3:L:148:PHE:CE2	2.46	0.51
1:A:77:LEU:HD12	1:A:78:ALA:H	1.76	0.51
2:B:76:TYR:O	2:B:80:LYS:N	2.42	0.51
3:I:90:ASN:HB2	3:I:94:GLU:N	2.25	0.51
3:C:108:ARG:C	3:C:109:ILE:HD13	2.35	0.51
1:G:47:ASP:O	1:G:49:GLN:N	2.42	0.51
2:E:99:ILE:CG2	2:E:103:LEU:HB2	2.41	0.51
1:G:38:PRO:HG2	1:G:41:GLU:OE1	2.10	0.51
1:A:25:PHE:O	1:A:28:LYS:HB2	2.11	0.51
3:F:129:LEU:HD22	3:F:132:GLN:O	2.10	0.51
3:I:166:VAL:O	3:I:170:VAL:HG22	2.10	0.51
2:K:98:GLU:CD	2:K:98:GLU:H	2.19	0.51
2:K:83:TYR:HB3	2:K:90:ILE:HG12	1.93	0.50
1:A:4:PHE:O	1:A:67:ALA:HB1	2.12	0.50
3:F:90:ASN:HB3	3:F:94:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:200:ARG:O	3:L:201:LEU:C	2.54	0.50
3:I:158:LEU:HD12	3:I:162:CYS:SG	2.52	0.50
2:K:76:TYR:CD1	2:K:76:TYR:C	2.90	0.50
3:L:131:ASN:C	3:L:133:THR:H	2.19	0.50
1:A:68:ARG:O	1:A:71:ALA:N	2.44	0.50
3:L:129:LEU:O	3:L:151:ILE:HA	2.12	0.50
2:E:87:SER:HB3	3:F:132:GLN:NE2	2.27	0.50
1:J:28:LYS:HB3	1:J:42:GLN:NE2	2.27	0.50
1:G:100:PRO:O	1:G:103:MET:HB2	2.11	0.50
3:I:184:LEU:HA	3:I:187:ASP:HB2	1.94	0.50
3:L:75:ILE:HD11	3:L:77:CYS:HB2	1.93	0.50
2:B:35:HIS:O	2:B:77:PHE:CD2	2.64	0.50
3:F:180:ILE:HG13	3:F:185:TYR:CE1	2.47	0.50
4:F:1205:L8B:OAB	4:F:1205:L8B:C	2.60	0.50
3:I:117:TRP:HB2	3:I:136:PHE:HB3	1.93	0.50
3:I:163:LEU:HD23	3:I:188:LEU:HD23	1.94	0.50
1:A:8:ARG:CG	1:A:13:THR:HG23	2.41	0.50
1:D:99:LEU:N	1:D:100:PRO:HD3	2.21	0.50
1:G:96:PRO:O	1:G:97:PRO:C	2.54	0.50
3:C:112:TYR:HB2	3:C:115:HIS:NE2	2.27	0.49
3:F:142:VAL:C	3:F:144:GLY:H	2.19	0.49
3:L:135:LEU:HD11	3:L:201:LEU:HD13	1.94	0.49
1:G:9:ARG:HD3	1:G:77:LEU:CD2	2.42	0.49
2:H:80:LYS:HA	3:I:155:VAL:HG11	1.94	0.49
3:F:78:ASN:ND2	3:F:103:PRO:HA	2.27	0.49
4:F:1205:L8B:OAB	4:F:1205:L8B:O	2.29	0.49
3:I:185:TYR:O	3:I:188:LEU:N	2.45	0.49
1:A:70:GLN:CG	2:B:79:TYR:HD2	2.25	0.49
2:B:36:ALA:C	2:B:38:THR:N	2.65	0.49
2:B:73:VAL:HG13	2:B:77:PHE:CE1	2.47	0.49
3:I:115:HIS:O	3:I:137:VAL:HG13	2.11	0.49
1:D:50:LEU:HG	1:D:51:LEU:N	2.25	0.49
3:C:188:LEU:C	3:C:188:LEU:HD23	2.37	0.49
2:B:77:PHE:O	2:B:81:VAL:HG23	2.12	0.49
3:C:141:ASN:O	3:C:145:GLN:O	2.29	0.49
2:E:42:ILE:HG22	2:E:60:VAL:HG21	1.95	0.49
2:H:33:ARG:C	2:H:37:LEU:HG	2.37	0.49
1:A:41:GLU:HG2	1:A:81:ALA:HB2	1.95	0.49
3:I:120:ARG:HD3	3:I:125:HIS:O	2.12	0.49
3:L:157:THR:O	3:L:158:LEU:C	2.55	0.49
3:F:130:VAL:HG13	3:F:130:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:ALA:N	1:G:72:PRO:CD	2.76	0.49
1:G:1:MET:HB3	1:G:64:SER:OG	2.12	0.48
2:B:83:TYR:HB3	2:B:90:ILE:HG12	1.94	0.48
3:L:197:ASP:O	3:L:200:ARG:HB2	2.12	0.48
1:G:9:ARG:HG2	1:G:10:HIS:HB2	1.94	0.48
1:J:38:PRO:O	1:J:39:PRO:C	2.57	0.48
3:C:120:ARG:HA	3:C:128:LEU:CD1	2.41	0.48
1:G:38:PRO:HB2	1:G:40:ASP:OD1	2.13	0.48
2:H:112:CYS:OXT	3:I:157:THR:HB	2.13	0.48
3:I:165:VAL:O	3:I:168:SER:OG	2.27	0.48
3:L:118:LEU:HD12	3:L:118:LEU:O	2.14	0.48
1:G:32:GLU:C	1:G:34:ILE:H	2.21	0.48
3:I:163:LEU:HD22	3:I:188:LEU:HD23	1.95	0.48
3:F:131:ASN:C	3:F:132:GLN:CG	2.84	0.48
1:G:37:ARG:HA	1:G:38:PRO:HD2	1.63	0.48
3:I:109:ILE:C	3:I:109:ILE:HD12	2.39	0.48
1:J:19:LYS:HB2	1:J:22:SER:HB2	1.94	0.48
2:K:103:LEU:HD13	3:L:158:LEU:HD11	1.96	0.48
1:D:55:LYS:HA	1:D:59:GLU:OE1	2.14	0.48
3:F:100:THR:HG21	3:F:122:ALA:HB2	1.96	0.48
1:A:68:ARG:O	1:A:70:GLN:N	2.46	0.48
2:H:44:ALA:O	2:H:45:MET:C	2.56	0.48
1:J:12:THR:CG2	1:J:13:THR:N	2.77	0.48
3:L:143:ASP:CB	3:L:145:GLN:HB2	2.44	0.48
3:C:101:LEU:N	3:C:101:LEU:HD12	2.29	0.48
1:J:81:ALA:O	1:J:82:ASP:C	2.56	0.48
2:B:98:GLU:H	2:B:98:GLU:CD	2.22	0.47
3:I:154:PRO:HG2	3:I:156:TYR:CE1	2.49	0.47
1:A:23:THR:O	1:A:24:VAL:C	2.56	0.47
1:D:4:PHE:O	1:D:67:ALA:HB1	2.14	0.47
1:D:20:GLU:OE2	1:D:63:THR:HG22	2.15	0.47
2:H:17:MET:O	2:H:17:MET:SD	2.72	0.47
2:B:20:LYS:HB3	2:B:59:GLU:HG2	1.96	0.47
3:F:76:PHE:CE2	3:F:109:ILE:HG13	2.50	0.47
3:F:85:LEU:CA	3:F:100:THR:HG22	2.44	0.47
1:G:37:ARG:NH2	1:G:80:ARG:HA	2.29	0.47
2:H:74:CYS:O	2:H:75:MET:C	2.56	0.47
2:H:112:CYS:SG	3:I:158:LEU:HD23	2.55	0.47
1:G:32:GLU:OE1	1:G:39:PRO:HD3	2.14	0.47
2:H:72:LYS:O	2:H:73:VAL:C	2.57	0.47
1:J:34:ILE:HG21	2:K:30:ILE:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:C	1:A:61:GLY:H	2.22	0.47
3:L:69:ARG:HG3	3:L:69:ARG:NH1	2.23	0.47
2:E:99:ILE:O	2:E:99:ILE:HG22	2.13	0.47
2:K:61:ASN:O	2:K:63:ARG:HD2	2.15	0.47
3:L:181:VAL:HG12	3:L:183:SER:H	1.80	0.47
1:G:6:MET:HE2	1:G:74:THR:OG1	2.13	0.47
1:G:44:LEU:CD2	1:G:76:GLY:O	2.63	0.47
2:H:37:LEU:C	2:H:39:SER:H	2.22	0.47
3:L:160:GLU:O	3:L:164:GLN:HG3	2.14	0.47
3:I:90:ASN:HB2	3:I:94:GLU:O	2.15	0.47
1:J:79:PHE:HB2	1:J:86:GLU:OE2	2.15	0.47
1:A:63:THR:C	1:A:65:GLN:H	2.23	0.47
3:I:118:LEU:HD11	3:I:135:LEU:HD22	1.97	0.47
2:K:79:TYR:CE2	2:K:93:PHE:HB2	2.50	0.47
1:G:95:SER:HA	1:G:96:PRO:HD2	1.54	0.46
3:I:161:ARG:O	3:I:165:VAL:HG23	2.15	0.46
3:I:174:ASN:C	3:I:176:ARG:H	2.23	0.46
2:H:22:ILE:HA	2:H:27:HIS:O	2.16	0.46
2:H:76:TYR:HA	2:H:93:PHE:HE2	1.80	0.46
1:J:70:GLN:CD	1:J:70:GLN:H	2.22	0.46
1:G:56:THR:N	1:G:59:GLU:OE1	2.35	0.46
2:H:37:LEU:HD23	2:H:46:LEU:HD21	1.98	0.46
2:B:88:THR:O	2:B:89:GLU:C	2.58	0.46
2:E:67:SER:C	2:E:69:VAL:H	2.22	0.46
1:G:47:ASP:C	1:G:49:GLN:H	2.24	0.46
1:J:94:SER:O	2:K:68:HIS:HB3	2.15	0.46
3:C:80:SER:O	3:C:103:PRO:CB	2.63	0.46
3:I:198:LEU:HD23	3:I:198:LEU:HA	1.73	0.46
1:J:79:PHE:O	1:J:80:ARG:CB	2.64	0.46
1:J:37:ARG:HA	1:J:38:PRO:HD3	1.80	0.46
3:I:84:VAL:CG2	3:I:128:LEU:HD13	2.39	0.46
1:J:26:GLU:H	1:J:26:GLU:HG2	1.53	0.46
2:K:62:PHE:CB	2:K:65:ILE:HD13	2.14	0.46
1:D:68:ARG:O	1:D:69:PRO:C	2.58	0.46
3:F:182:ARG:HA	3:F:185:TYR:CD2	2.51	0.46
1:G:93:PHE:CD1	2:H:67:SER:HB2	2.51	0.46
2:H:97:PRO:HB3	3:I:169:LEU:HD11	1.97	0.46
3:C:120:ARG:CA	3:C:128:LEU:HD12	2.45	0.45
3:C:158:LEU:O	3:C:158:LEU:HD12	2.15	0.45
1:D:10:HIS:O	1:D:12:THR:N	2.41	0.45
3:I:130:VAL:HG11	3:I:136:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:GLU:OE1	3:I:95:PRO:HD2	2.16	0.45
1:A:57:LEU:O	1:A:58:GLY:C	2.60	0.45
2:B:73:VAL:CG1	2:B:77:PHE:CE1	2.99	0.45
3:I:141:ASN:ND2	3:I:146:PRO:HA	2.27	0.45
2:K:65:ILE:H	2:K:65:ILE:CD1	2.26	0.45
2:B:74:CYS:O	2:B:78:THR:HG23	2.17	0.45
1:J:1:MET:HG2	1:J:2:ASP:H	1.80	0.45
1:J:38:PRO:HD2	1:J:41:GLU:HG3	1.98	0.45
1:G:34:ILE:HG12	2:H:18:TYR:CD2	2.52	0.45
1:G:47:ASP:C	1:G:48:ASP:OD1	2.60	0.45
2:H:97:PRO:O	2:H:99:ILE:N	2.43	0.45
2:K:34:GLU:HG2	2:K:35:HIS:H	1.81	0.45
3:L:83:VAL:HG12	3:L:122:ALA:HB3	1.98	0.45
3:C:198:LEU:O	3:C:202:THR:HB	2.16	0.45
1:D:52:ASP:HB2	1:D:55:LYS:HG2	1.98	0.45
3:C:114:GLY:HA2	3:C:137:VAL:CG1	2.47	0.45
3:L:180:ILE:CG2	3:L:184:LEU:HB2	2.47	0.45
1:A:47:ASP:O	1:A:48:ASP:HB2	2.17	0.45
2:B:31:VAL:HG12	2:B:32:LYS:H	1.82	0.45
3:C:90:ASN:HB2	3:C:94:GLU:O	2.16	0.45
1:G:66:THR:O	1:G:66:THR:CG2	2.65	0.45
2:K:72:LYS:O	2:K:73:VAL:C	2.60	0.45
2:B:19:VAL:HG13	2:B:33:ARG:HG3	1.99	0.45
1:J:28:LYS:HA	1:J:42:GLN:HE22	1.81	0.45
3:L:69:ARG:CG	3:L:69:ARG:NH1	2.76	0.45
1:D:57:LEU:HA	1:D:57:LEU:HD23	1.71	0.44
3:F:131:ASN:O	3:F:132:GLN:CG	2.65	0.44
2:H:88:THR:HG22	2:H:89:GLU:H	1.82	0.44
1:J:23:THR:OG1	1:J:26:GLU:HG2	2.17	0.44
2:B:46:LEU:O	2:B:47:SER:C	2.58	0.44
1:D:51:LEU:HD22	1:D:60:CYS:SG	2.57	0.44
2:E:44:ALA:O	2:E:45:MET:C	2.60	0.44
3:I:162:CYS:O	3:I:166:VAL:HG23	2.17	0.44
1:A:14:ILE:HD13	1:A:34:ILE:HG21	2.00	0.44
2:E:34:GLU:H	2:E:34:GLU:CD	2.22	0.44
2:H:76:TYR:HA	2:H:93:PHE:CE2	2.52	0.44
2:K:36:ALA:HA	2:K:77:PHE:CE2	2.53	0.44
3:L:65:SER:O	3:L:91:PHE:HD1	2.01	0.44
3:L:78:ASN:OD1	3:L:78:ASN:C	2.60	0.44
2:B:20:LYS:HD3	2:B:28:GLU:HG2	2.00	0.44
1:G:98:GLU:CD	1:G:99:LEU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HG2	1:A:47:ASP:HB2	1.99	0.44
3:I:175:TYR:HD1	3:I:175:TYR:H	1.65	0.44
2:B:67:SER:C	2:B:69:VAL:H	2.25	0.44
2:E:29:PHE:HD2	2:E:70:LEU:HD23	1.83	0.44
2:H:18:TYR:C	2:H:19:VAL:CG1	2.91	0.44
2:K:99:ILE:O	2:K:100:ALA:C	2.59	0.44
3:L:113:ARG:NE	3:L:140:LEU:HB2	2.32	0.44
3:F:145:GLN:HB2	3:F:146:PRO:HD3	1.99	0.44
3:F:162:CYS:O	3:F:163:LEU:C	2.60	0.44
1:J:17:ASP:OD1	1:J:17:ASP:C	2.61	0.44
3:C:67:ASN:CA	3:C:91:PHE:CE1	3.01	0.43
1:D:42:GLN:HB2	1:D:77:LEU:HD11	2.00	0.43
1:G:3:VAL:HG22	1:G:67:ALA:CB	2.47	0.43
3:I:120:ARG:NH1	3:I:125:HIS:O	2.51	0.43
2:K:17:MET:SD	2:K:17:MET:C	2.99	0.43
3:F:74:VAL:HG12	3:F:75:ILE:N	2.33	0.43
1:G:27:LEU:HD22	1:G:57:LEU:HD21	2.00	0.43
2:H:90:ILE:HD13	3:I:155:VAL:HG23	2.00	0.43
1:D:24:VAL:HB	1:D:53:ASP:HA	2.00	0.43
1:G:32:GLU:O	1:G:36:LYS:N	2.50	0.43
3:I:113:ARG:HD3	3:I:140:LEU:HD12	1.99	0.43
2:H:21:LEU:HA	2:H:60:VAL:O	2.19	0.43
2:K:37:LEU:HD22	2:K:43:LYS:HG3	2.00	0.43
1:J:57:LEU:O	1:J:58:GLY:C	2.61	0.43
3:L:111:SER:C	3:L:112:TYR:CD1	2.96	0.43
2:E:35:HIS:CE1	2:E:81:VAL:HG11	2.54	0.43
3:F:118:LEU:HD21	3:F:120:ARG:CZ	2.49	0.43
3:I:152:THR:HG22	3:I:153:LEU:O	2.17	0.43
3:L:118:LEU:C	3:L:118:LEU:CD1	2.91	0.43
3:F:73:GLN:N	3:F:73:GLN:CD	2.76	0.43
3:I:63:LEU:HD12	3:I:63:LEU:HA	1.90	0.43
1:J:1:MET:HG2	1:J:2:ASP:N	2.33	0.43
1:J:28:LYS:HG2	1:J:44:LEU:CD1	2.48	0.43
3:C:105:THR:HG23	2:K:64:GLU:OE1	2.19	0.43
3:C:100:THR:O	3:C:107:ARG:NH2	2.51	0.42
2:E:17:MET:CE	2:E:32:LYS:HE2	2.35	0.42
2:E:102:GLU:O	2:E:103:LEU:C	2.61	0.42
1:J:10:HIS:O	1:J:11:LYS:HB2	2.19	0.42
1:J:23:THR:O	1:J:24:VAL:C	2.60	0.42
1:D:5:LEU:HD11	1:D:57:LEU:CD1	2.49	0.42
3:L:143:ASP:C	3:L:145:GLN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:143:ASP:C	3:L:145:GLN:N	2.76	0.42
1:D:31:VAL:O	1:D:35:LEU:HB2	2.20	0.42
2:E:26:GLY:O	2:E:27:HIS:C	2.61	0.42
1:G:98:GLU:OE1	1:G:99:LEU:N	2.25	0.42
3:I:129:LEU:HD13	3:I:132:GLN:O	2.19	0.42
3:L:75:ILE:C	3:L:75:ILE:HD12	2.44	0.42
1:G:97:PRO:O	1:G:98:GLU:CB	2.62	0.42
3:L:66:VAL:HG12	3:L:67:ASN:N	2.33	0.42
3:L:176:ARG:HA	3:L:176:ARG:HD3	1.70	0.42
1:A:38:PRO:HD2	1:A:41:GLU:OE1	2.19	0.42
2:B:19:VAL:CG1	2:B:33:ARG:HG2	2.50	0.42
3:C:198:LEU:HA	3:C:198:LEU:HD23	1.61	0.42
2:B:24:SER:HB3	2:B:62:PHE:O	2.20	0.42
3:C:144:GLY:O	3:C:145:GLN:CB	2.68	0.42
1:D:1:MET:CG	1:D:2:ASP:N	2.82	0.42
2:K:21:LEU:C	2:K:22:ILE:HG13	2.44	0.42
3:C:107:ARG:HD2	4:C:1205:L8B:NAP	2.34	0.42
1:G:44:LEU:HD23	1:G:76:GLY:O	2.19	0.42
3:F:76:PHE:CD2	3:F:109:ILE:HG13	2.54	0.42
1:G:11:LYS:HA	2:H:27:HIS:NE2	2.35	0.42
2:H:34:GLU:O	2:H:35:HIS:C	2.62	0.42
1:A:98:GLU:O	1:A:99:LEU:CB	2.68	0.42
2:E:31:VAL:CG1	2:E:32:LYS:N	2.83	0.42
2:H:41:THR:HG22	2:H:42:ILE:N	2.35	0.42
1:J:11:LYS:HA	2:K:27:HIS:CD2	2.55	0.42
3:L:84:VAL:HG12	3:L:85:LEU:N	2.34	0.41
3:L:86:PRO:HG2	3:L:98:TYR:HB2	2.02	0.41
1:A:42:GLN:HB2	1:A:77:LEU:HD11	2.02	0.41
1:G:9:ARG:O	1:G:12:THR:CB	2.68	0.41
3:I:85:LEU:HA	3:I:86:PRO:HD3	1.94	0.41
3:I:172:PRO:HA	3:I:175:TYR:CD1	2.55	0.41
1:J:38:PRO:HB2	1:J:40:ASP:OD1	2.20	0.41
1:J:45:TYR:CG	1:J:88:LEU:HD22	2.55	0.41
3:L:68:SER:O	3:L:69:ARG:CB	2.41	0.41
2:B:99:ILE:O	2:B:99:ILE:HG22	2.20	0.41
2:E:90:ILE:HG22	3:F:153:LEU:HB2	2.02	0.41
3:I:113:ARG:HD2	3:I:140:LEU:HD12	2.01	0.41
3:I:157:THR:C	3:I:159:LYS:N	2.76	0.41
1:J:24:VAL:O	1:J:25:PHE:C	2.62	0.41
2:K:69:VAL:HG13	2:K:103:LEU:HD23	2.02	0.41
3:C:197:ASP:O	3:C:201:LEU:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:HIS:HB3	2:E:29:PHE:CE2	2.55	0.41
1:G:57:LEU:HD23	1:G:62:PHE:HD2	1.84	0.41
2:H:18:TYR:HB3	2:H:19:VAL:H	1.77	0.41
2:E:109:PHE:CD1	2:E:109:PHE:C	2.98	0.41
3:C:166:VAL:O	3:C:167:ARG:C	2.62	0.41
1:D:38:PRO:HA	1:D:39:PRO:HD3	1.85	0.41
2:E:76:TYR:CE2	3:F:158:LEU:HB2	2.55	0.41
3:F:84:VAL:HG22	3:F:128:LEU:HD13	2.03	0.41
1:J:101:ASP:HB3	1:J:102:VAL:H	1.71	0.41
2:E:92:GLU:HG3	3:F:161:ARG:NH2	2.36	0.41
3:F:118:LEU:C	3:F:118:LEU:HD23	2.45	0.41
1:G:97:PRO:HD3	2:H:68:HIS:CE1	2.55	0.41
2:H:94:PRO:O	2:H:95:ILE:HG13	2.20	0.41
1:J:79:PHE:N	1:J:86:GLU:OE2	2.49	0.41
2:B:95:ILE:HD12	3:C:161:ARG:HG3	2.02	0.41
3:F:90:ASN:ND2	3:F:94:GLU:HB2	2.31	0.41
3:I:90:ASN:CB	3:I:94:GLU:H	2.33	0.41
3:L:67:ASN:OD1	3:L:67:ASN:C	2.63	0.41
3:C:116:LEU:HD23	3:C:137:VAL:HG22	2.02	0.41
3:F:148:PHE:CZ	2:H:45:MET:HG3	2.56	0.41
1:G:26:GLU:O	1:G:30:ILE:HG13	2.21	0.41
1:J:95:SER:HA	1:J:96:PRO:HD2	1.89	0.41
1:A:7:ILE:HD11	1:A:27:LEU:HD11	2.04	0.40
1:D:39:PRO:HA	1:D:42:GLN:HE21	1.86	0.40
2:H:68:HIS:CD2	2:H:68:HIS:C	3.00	0.40
3:I:113:ARG:HE	3:I:113:ARG:HB3	1.31	0.40
2:B:80:LYS:O	2:B:84:THR:OG1	2.38	0.40
1:D:92:PRO:O	2:E:27:HIS:HE1	2.04	0.40
1:D:97:PRO:HB2	1:D:98:GLU:H	1.69	0.40
3:F:171:LYS:HA	3:F:172:PRO:HD2	1.90	0.40
1:G:29:ARG:NH2	1:G:39:PRO:HG2	2.35	0.40
3:C:99:PRO:HD2	4:C:1205:L8B:NAP	2.36	0.40
3:C:163:LEU:O	3:C:164:GLN:C	2.65	0.40
1:D:26:GLU:O	1:D:29:ARG:HB2	2.20	0.40
1:G:10:HIS:O	1:G:11:LYS:HB2	2.22	0.40
1:G:79:PHE:H	1:G:86:GLU:HG2	1.86	0.40
3:I:165:VAL:O	3:I:169:LEU:HG	2.22	0.40
2:B:35:HIS:HA	2:B:81:VAL:HG21	2.03	0.40
2:E:42:ILE:HD11	2:E:110:LEU:HD11	2.03	0.40
3:F:98:TYR:HB3	3:F:99:PRO:CD	2.52	0.40
1:G:93:PHE:HD1	2:H:67:SER:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:41:THR:O	2:K:42:ILE:C	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ASP:OD2	2:K:33:ARG:NH1[1_655]	2.18	0.02

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	97/118 (82%)	79 (81%)	9 (9%)	9 (9%)	0	1
1	D	94/118 (80%)	80 (85%)	7 (7%)	7 (7%)	1	2
1	G	105/118 (89%)	76 (72%)	22 (21%)	7 (7%)	1	3
1	J	101/118 (86%)	82 (81%)	12 (12%)	7 (7%)	1	2
2	B	82/97 (84%)	70 (85%)	9 (11%)	3 (4%)	2	11
2	E	83/97 (86%)	64 (77%)	15 (18%)	4 (5%)	2	7
2	H	82/97 (84%)	65 (79%)	10 (12%)	7 (8%)	0	1
2	K	83/97 (86%)	64 (77%)	15 (18%)	4 (5%)	2	7
3	C	140/163 (86%)	110 (79%)	20 (14%)	10 (7%)	1	2
3	F	140/163 (86%)	115 (82%)	18 (13%)	7 (5%)	1	6
3	I	143/163 (88%)	113 (79%)	24 (17%)	6 (4%)	2	9
3	L	141/163 (86%)	108 (77%)	25 (18%)	8 (6%)	1	4
All	All	1291/1512 (85%)	1026 (80%)	186 (14%)	79 (6%)	1	4

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	A	83	ASP
1	A	84	THR
1	A	98	GLU
2	B	37	LEU
2	B	88	THR
2	B	89	GLU
3	C	67	ASN
3	C	105	THR
3	C	125	HIS
3	C	145	GLN
3	C	191	HIS
1	D	99	LEU
3	F	145	GLN
1	G	48	ASP
1	G	98	GLU
2	H	44	ALA
2	H	45	MET
3	I	142	VAL
3	I	143	ASP
3	I	190	ASP
1	J	55	LYS
1	J	80	ARG
1	J	83	ASP
1	J	101	ASP
3	L	71	PRO
3	L	90	ASN
1	A	22	SER
3	C	140	LEU
3	C	179	ASP
1	D	10	HIS
1	D	48	ASP
3	F	67	ASN
1	G	81	ALA
2	H	85	ASN
1	J	102	VAL
2	K	89	GLU
3	L	63	LEU
3	L	113	ARG
3	L	190	ASP
1	A	10	HIS
1	A	80	ARG
1	D	11	LYS

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Mol	Chain	Res	Type
1	D	97	PRO
3	F	139	SER
3	F	143	ASP
3	F	183	SER
3	F	203	GLN
1	G	9	ARG
1	G	47	ASP
1	G	96	PRO
2	H	24	SER
2	H	25	ASP
2	H	98	GLU
3	I	179	ASP
1	J	82	ASP
2	K	35	HIS
1	A	94	SER
1	G	38	PRO
3	I	132	GLN
2	K	98	GLU
3	L	132	GLN
3	C	142	VAL
1	D	64	SER
2	E	41	THR
2	E	47	SER
2	E	98	GLU
3	F	172	PRO
3	L	182	ARG
1	D	100	PRO
2	H	99	ILE
3	L	114	GLY
3	C	181	VAL
2	E	97	PRO
2	K	60	VAL
1	A	69	PRO
3	C	97	PRO
3	I	83	VAL
1	J	54	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	75/103 (73%)	68 (91%)	7 (9%)	8	27
1	D	72/103 (70%)	63 (88%)	9 (12%)	4	15
1	G	87/103 (84%)	74 (85%)	13 (15%)	3	10
1	J	87/103 (84%)	75 (86%)	12 (14%)	3	12
2	B	71/86 (83%)	64 (90%)	7 (10%)	7	24
2	E	75/86 (87%)	68 (91%)	7 (9%)	8	27
2	H	75/86 (87%)	57 (76%)	18 (24%)	1	2
2	K	76/86 (88%)	59 (78%)	17 (22%)	1	3
3	C	103/149 (69%)	96 (93%)	7 (7%)	14	42
3	F	121/149 (81%)	106 (88%)	15 (12%)	4	15
3	I	124/149 (83%)	108 (87%)	16 (13%)	4	13
3	L	125/149 (84%)	107 (86%)	18 (14%)	3	11
All	All	1091/1352 (81%)	945 (87%)	146 (13%)	4	12

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	5	LEU
1	A	20	GLU
1	A	42	GLN
1	A	66	THR
1	A	77	LEU
1	A	95	SER
2	B	38	THR
2	B	61	ASN
2	B	70	LEU
2	B	77	PHE
2	B	78	THR
2	B	84	THR
2	B	98	GLU
3	C	74	VAL
3	C	75	ILE
3	C	80	SER
3	C	118	LEU
3	C	152	THR

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Mol	Chain	Res	Type
3	C	158	LEU
3	C	183	SER
1	D	1	MET
1	D	2	ASP
1	D	3	VAL
1	D	10	HIS
1	D	17	ASP
1	D	34	ILE
1	D	41	GLU
1	D	74	THR
1	D	95	SER
2	E	19	VAL
2	E	42	ILE
2	E	67	SER
2	E	75	MET
2	E	78	THR
2	E	104	LEU
2	E	110	LEU
3	F	75	ILE
3	F	77	CYS
3	F	85	LEU
3	F	90	ASN
3	F	100	THR
3	F	105	THR
3	F	132	GLN
3	F	134	GLU
3	F	135	LEU
3	F	148	PHE
3	F	152	THR
3	F	158	LEU
3	F	178	LEU
3	F	183	SER
3	F	186	GLU
1	G	3	VAL
1	G	9	ARG
1	G	13	THR
1	G	22	SER
1	G	26	GLU
1	G	45	TYR
1	G	48	ASP
1	G	50	LEU
1	G	68	ARG

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Mol	Chain	Res	Type
1	G	74	THR
1	G	90	ILE
1	G	95	SER
1	G	98	GLU
2	H	17	MET
2	H	19	VAL
2	H	21	LEU
2	H	24	SER
2	H	33	ARG
2	H	34	GLU
2	H	38	THR
2	H	41	THR
2	H	45	MET
2	H	46	LEU
2	H	60	VAL
2	H	63	ARG
2	H	64	GLU
2	H	70	LEU
2	H	81	VAL
2	H	84	THR
2	H	86	SER
2	H	99	ILE
3	I	63	LEU
3	I	66	VAL
3	I	80	SER
3	I	90	ASN
3	I	101	LEU
3	I	116	LEU
3	I	120	ARG
3	I	121	ASP
3	I	135	LEU
3	I	140	LEU
3	I	142	VAL
3	I	158	LEU
3	I	178	LEU
3	I	181	VAL
3	I	189	GLU
3	I	193	ASN
1	J	3	VAL
1	J	12	THR
1	J	17	ASP
1	J	26	GLU

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Mol	Chain	Res	Type
1	J	32	GLU
1	J	39	PRO
1	J	42	GLN
1	J	47	ASP
1	J	53	ASP
1	J	57	LEU
1	J	84	THR
1	J	90	ILE
2	K	17	MET
2	K	31	VAL
2	K	32	LYS
2	K	34	GLU
2	K	38	THR
2	K	39	SER
2	K	46	LEU
2	K	64	GLU
2	K	65	ILE
2	K	71	SER
2	K	84	THR
2	K	85	ASN
2	K	88	THR
2	K	101	LEU
2	K	103	LEU
2	K	104	LEU
2	K	105	MET
3	L	62	VAL
3	L	71	PRO
3	L	72	SER
3	L	74	VAL
3	L	75	ILE
3	L	80	SER
3	L	85	LEU
3	L	109	ILE
3	L	118	LEU
3	L	120	ARG
3	L	132	GLN
3	L	151	ILE
3	L	152	THR
3	L	153	LEU
3	L	165	VAL
3	L	170	VAL
3	L	176	ARG

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Mol	Chain	Res	Type
3	L	194	VAL

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

Mol	Chain	Res	Type
1	A	49	GLN
2	B	27	HIS
3	C	96	GLN
2	E	35	HIS
2	E	61	ASN
3	F	90	ASN
3	F	110	HIS
3	F	115	HIS
3	F	132	GLN
3	F	141	ASN
3	F	174	ASN
1	G	49	GLN
2	H	27	HIS
2	H	35	HIS
2	H	108	ASN
3	I	96	GLN
3	I	174	ASN
3	I	193	ASN
3	I	195	GLN
1	J	42	GLN
1	J	49	GLN
2	K	27	HIS
3	L	132	GLN
3	L	141	ASN
3	L	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
4	L8B	C	1205	-	33,33,33	2.70	18 (54%)	40,46,46	2.18	16 (40%)
4	L8B	L	1205	-	33,33,33	1.58	4 (12%)	40,46,46	2.49	15 (37%)
4	L8B	F	1205	-	33,33,33	2.13	13 (39%)	40,46,46	1.69	9 (22%)
4	L8B	I	1207	-	33,33,33	2.29	17 (51%)	40,46,46	2.45	16 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L8B	C	1205	-	-	5/21/33/33	0/4/4/4
4	L8B	L	1205	-	-	7/21/33/33	0/4/4/4
4	L8B	F	1205	-	-	0/21/33/33	0/4/4/4
4	L8B	I	1207	-	-	5/21/33/33	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1205	L8B	CAY-CBA	-5.96	1.34	1.48
4	C	1205	L8B	CAK-CAW	-5.81	1.30	1.40
4	C	1205	L8B	OAT-NAQ	-5.46	1.32	1.42
4	F	1205	L8B	CAK-CAW	-4.90	1.31	1.40
4	I	1207	L8B	CAY-CBA	-4.89	1.36	1.48
4	C	1205	L8B	CAY-CBA	-4.74	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1205	L8B	CAJ-NAP	-4.36	1.30	1.37
4	I	1207	L8B	CAK-CAW	-4.29	1.32	1.40
4	F	1205	L8B	CAY-CBA	-4.19	1.38	1.48
4	I	1207	L8B	CAJ-NAP	-4.15	1.30	1.37
4	I	1207	L8B	OAS-CBA	-3.93	1.30	1.37
4	C	1205	L8B	CAJ-CBA	-3.90	1.29	1.34
4	C	1205	L8B	CB-CG	-3.88	1.45	1.52
4	C	1205	L8B	OAS-CBA	-3.72	1.31	1.37
4	F	1205	L8B	CAJ-CBA	-3.58	1.29	1.34
4	C	1205	L8B	OAS-CAI	-3.54	1.30	1.35
4	F	1205	L8B	OAT-NAQ	-3.54	1.35	1.42
4	F	1205	L8B	CAJ-NAP	-3.53	1.31	1.37
4	I	1207	L8B	CB-CG	-3.47	1.46	1.52
4	L	1205	L8B	CAK-CAW	-3.37	1.34	1.40
4	I	1207	L8B	CAJ-CBA	-3.33	1.30	1.34
4	I	1207	L8B	OAT-NAQ	-3.02	1.36	1.42
4	C	1205	L8B	CB-CA	-3.01	1.48	1.53
4	I	1207	L8B	CD2-N	-2.88	1.43	1.47
4	F	1205	L8B	OAS-CBA	-2.84	1.32	1.37
4	C	1205	L8B	CD2-CG	-2.78	1.48	1.52
4	C	1205	L8B	CAK-CAZ	-2.69	1.30	1.34
4	I	1207	L8B	CAK-CAZ	-2.60	1.30	1.34
4	C	1205	L8B	CAH-CAY	-2.57	1.35	1.39
4	F	1205	L8B	CD2-N	-2.52	1.43	1.47
4	F	1205	L8B	CB-CA	-2.48	1.49	1.53
4	F	1205	L8B	OAS-CAI	-2.45	1.32	1.35
4	C	1205	L8B	OAT-CAZ	-2.44	1.31	1.35
4	C	1205	L8B	CD2-N	-2.42	1.43	1.47
4	F	1205	L8B	OAT-CAZ	-2.41	1.31	1.35
4	F	1205	L8B	CD2-CG	-2.40	1.49	1.52
4	I	1207	L8B	OAT-CAZ	-2.40	1.31	1.35
4	C	1205	L8B	OD1-CG	-2.32	1.36	1.43
4	C	1205	L8B	CAL-CAX	-2.29	1.46	1.51
4	I	1207	L8B	CB-CA	-2.23	1.49	1.53
4	L	1205	L8B	CAJ-NAP	-2.21	1.33	1.37
4	I	1207	L8B	OAS-CAI	-2.17	1.32	1.35
4	I	1207	L8B	CAG-CAY	-2.15	1.36	1.39
4	I	1207	L8B	CAH-CAY	-2.12	1.36	1.39
4	F	1205	L8B	CAK-CAZ	-2.04	1.31	1.34
4	L	1205	L8B	CAM-CAZ	2.04	1.52	1.49
4	I	1207	L8B	CD2-CG	-2.03	1.49	1.52
4	C	1205	L8B	CAG-CAY	-2.03	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1207	L8B	OD1-CG	-2.03	1.37	1.43
4	I	1207	L8B	CAF-CAX	-2.02	1.35	1.38
4	C	1205	L8B	CAF-CAX	-2.02	1.35	1.38
4	F	1205	L8B	CAU-N	-2.01	1.29	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1207	L8B	CAY-CBA-CAJ	-7.31	126.41	135.21
4	L	1205	L8B	CAG-CAY-CBA	-6.41	110.59	120.77
4	L	1205	L8B	CAH-CAY-CBA	6.36	130.87	120.77
4	I	1207	L8B	CAA-CAW-NAQ	5.76	124.68	119.97
4	L	1205	L8B	CAA-CAW-NAQ	5.33	124.33	119.97
4	I	1207	L8B	CD2-N-CAU	-5.02	119.73	129.13
4	C	1205	L8B	CG-CB-CA	-4.65	98.32	103.75
4	F	1205	L8B	OAS-CAI-NAP	-4.34	104.94	114.64
4	C	1205	L8B	CAA-CAW-NAQ	4.28	123.47	119.97
4	C	1205	L8B	CAY-CBA-CAJ	-4.23	130.12	135.21
4	C	1205	L8B	CAX-CAL-NAR	-4.19	104.24	113.07
4	L	1205	L8B	CG-CD2-N	4.15	107.00	103.00
4	L	1205	L8B	CAZ-OAT-NAQ	-4.05	105.25	108.30
4	F	1205	L8B	CAY-CBA-CAJ	-4.02	130.38	135.21
4	C	1205	L8B	OAS-CAI-NAP	-4.01	105.69	114.64
4	I	1207	L8B	CB-CA-C	-3.95	103.79	111.36
4	C	1205	L8B	CD2-N-CA	-3.89	106.67	111.83
4	L	1205	L8B	CB-CA-C	-3.83	104.02	111.36
4	L	1205	L8B	CAU-CAM-CAZ	-3.64	101.47	112.13
4	C	1205	L8B	CB-CG-CD2	-3.41	99.38	103.18
4	F	1205	L8B	CD2-N-CAU	-3.29	122.96	129.13
4	I	1207	L8B	OAS-CAI-NAP	-3.28	107.32	114.64
4	F	1205	L8B	CAM-CAU-N	3.13	122.95	117.83
4	I	1207	L8B	CAL-NAR-C	3.11	126.56	122.29
4	C	1205	L8B	CAJ-NAP-CAI	3.07	110.95	104.05
4	L	1205	L8B	OAS-CAI-NAP	-3.02	107.90	114.64
4	F	1205	L8B	CAJ-NAP-CAI	2.91	110.60	104.05
4	I	1207	L8B	OAT-CAZ-CAK	-2.85	107.08	109.73
4	I	1207	L8B	CAH-CAY-CBA	-2.78	116.34	120.77
4	I	1207	L8B	CAA-CAW-CAK	-2.72	124.54	128.62
4	L	1205	L8B	CD2-N-CAU	-2.70	124.07	129.13
4	I	1207	L8B	CA-N-CAU	2.68	128.76	120.83
4	L	1205	L8B	CAA-CAW-CAK	-2.67	124.62	128.62
4	F	1205	L8B	CB-CA-N	-2.64	100.03	103.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1207	L8B	CAE-CAG-CAY	-2.61	118.01	120.80
4	I	1207	L8B	CA-C-NAR	-2.60	110.38	115.99
4	L	1205	L8B	CAM-CAU-N	2.58	122.05	117.83
4	C	1205	L8B	CAM-CAU-N	2.58	122.05	117.83
4	C	1205	L8B	CB-CA-C	-2.56	106.45	111.36
4	C	1205	L8B	CA-N-CAU	2.50	128.23	120.83
4	L	1205	L8B	CG-CB-CA	2.49	106.66	103.75
4	L	1205	L8B	CB-CA-N	2.40	106.02	103.17
4	C	1205	L8B	CAA-CAW-CAK	-2.36	125.08	128.62
4	I	1207	L8B	CAG-CAY-CBA	2.25	124.35	120.77
4	L	1205	L8B	CAJ-NAP-CAI	2.23	109.06	104.05
4	C	1205	L8B	OAB-CAU-CAM	-2.21	116.19	121.28
4	L	1205	L8B	CAL-NAR-C	2.17	125.27	122.29
4	C	1205	L8B	CD2-N-CAU	-2.15	125.09	129.13
4	I	1207	L8B	CAL-CAX-CAF	-2.12	116.61	120.94
4	I	1207	L8B	OAS-CBA-CAY	2.10	125.17	118.34
4	C	1205	L8B	CAU-CAM-CAZ	-2.09	106.00	112.13
4	F	1205	L8B	CAA-CAW-NAQ	2.09	121.68	119.97
4	I	1207	L8B	CAJ-NAP-CAI	2.08	108.73	104.05
4	C	1205	L8B	OAT-CAZ-CAK	-2.03	107.84	109.73
4	F	1205	L8B	CAG-CAY-CBA	-2.03	117.55	120.77
4	F	1205	L8B	CAU-CAM-CAZ	-2.00	106.26	112.13

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1205	L8B	CAH-CAY-CBA-CAJ
4	L	1205	L8B	CAG-CAY-CBA-CAJ
4	L	1205	L8B	CAH-CAY-CBA-OAS
4	L	1205	L8B	CAG-CAY-CBA-OAS
4	I	1207	L8B	CAG-CAY-CBA-OAS
4	I	1207	L8B	CAH-CAY-CBA-OAS
4	I	1207	L8B	CAG-CAY-CBA-CAJ
4	I	1207	L8B	CAH-CAY-CBA-CAJ
4	C	1205	L8B	CAG-CAY-CBA-OAS
4	C	1205	L8B	CAH-CAY-CBA-OAS
4	L	1205	L8B	CAU-CAM-CAZ-CAK
4	C	1205	L8B	CAZ-CAM-CAU-OAB
4	L	1205	L8B	CAU-CAM-CAZ-OAT
4	C	1205	L8B	CAG-CAY-CBA-CAJ
4	C	1205	L8B	CAH-CAY-CBA-CAJ

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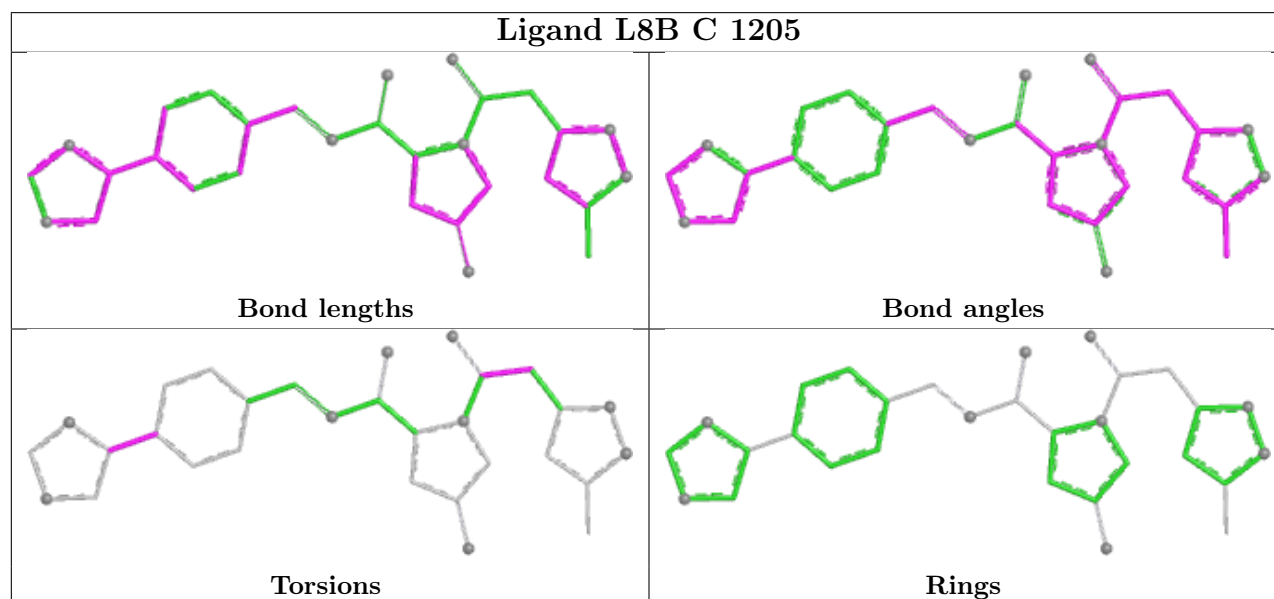
Mol	Chain	Res	Type	Atoms
4	I	1207	L8B	CAZ-CAM-CAU-OAB
4	L	1205	L8B	CAZ-CAM-CAU-OAB

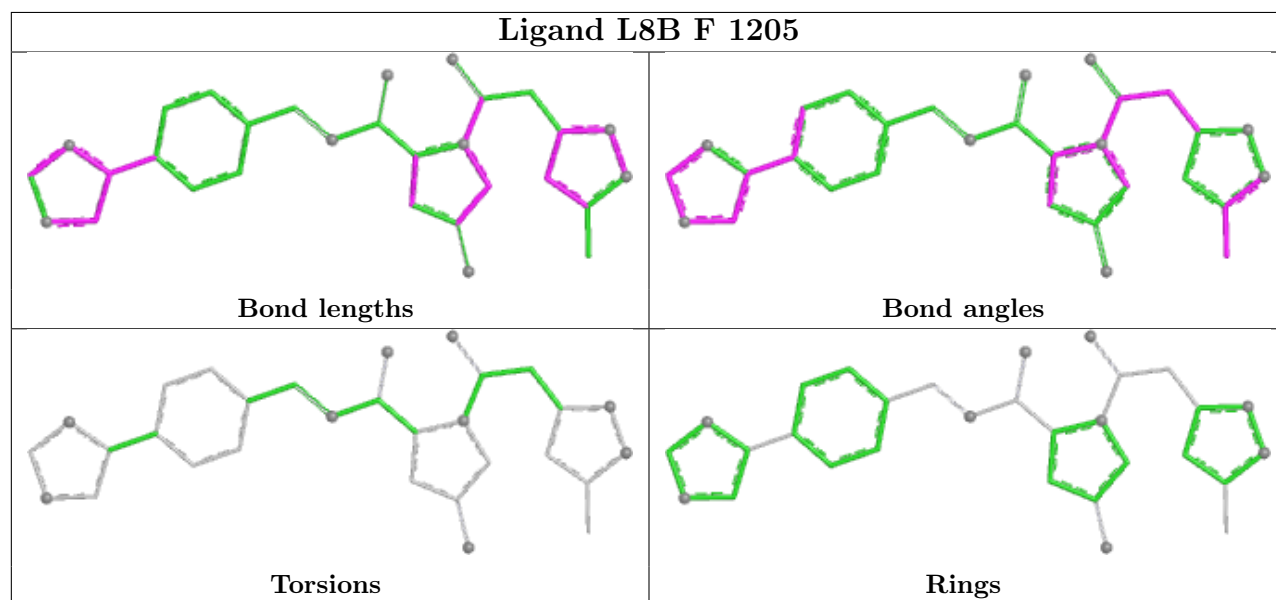
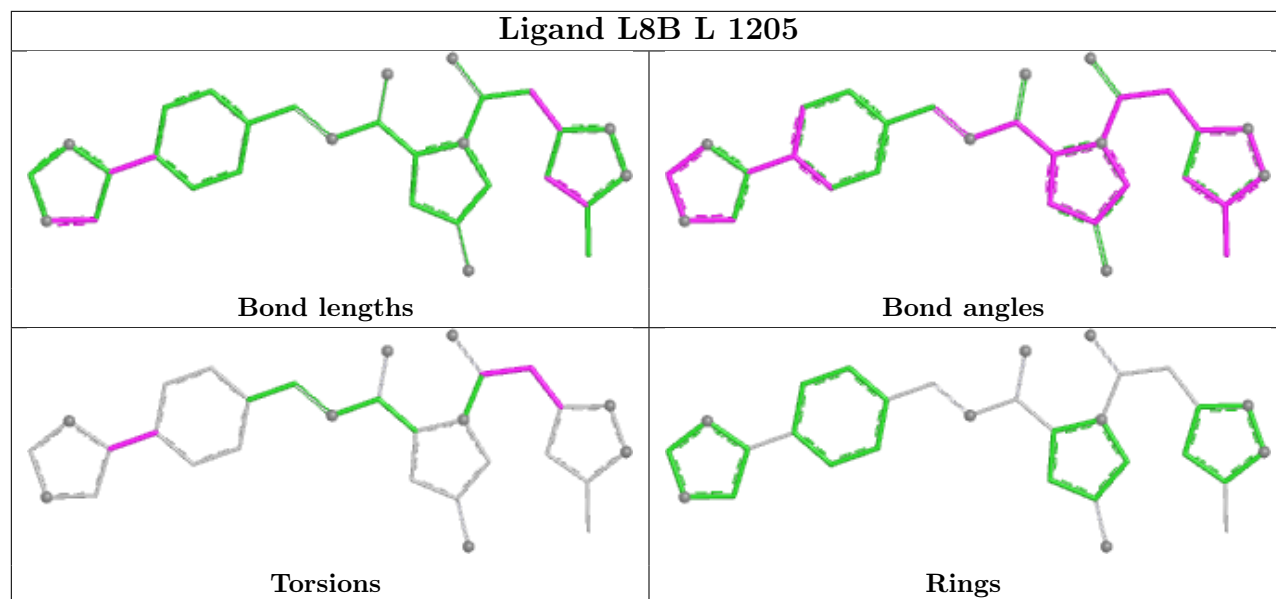
There are no ring outliers.

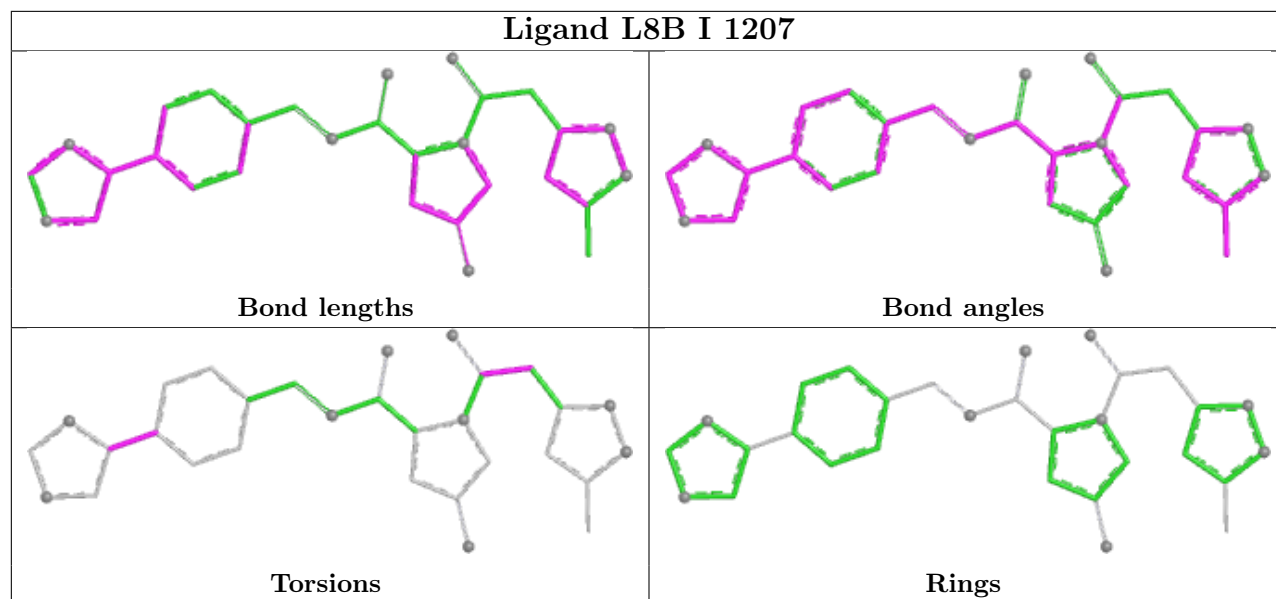
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1205	L8B	4	0
4	L	1205	L8B	1	0
4	F	1205	L8B	2	0
4	I	1207	L8B	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	99/118 (83%)	0.10	5 (5%) 33 26	16, 37, 53, 57	0
1	D	98/118 (83%)	0.46	2 (2%) 65 56	32, 50, 70, 74	0
1	G	107/118 (90%)	0.44	7 (6%) 25 20	31, 51, 68, 82	0
1	J	103/118 (87%)	0.12	1 (0%) 79 73	19, 38, 55, 75	0
2	B	86/97 (88%)	-0.16	0 100 100	18, 34, 46, 53	0
2	E	87/97 (89%)	0.03	1 (1%) 78 71	25, 40, 49, 57	0
2	H	86/97 (88%)	0.09	0 100 100	30, 44, 55, 57	0
2	K	87/97 (89%)	0.12	4 (4%) 37 29	20, 35, 53, 58	0
3	C	142/163 (87%)	0.17	8 (5%) 30 23	16, 34, 54, 61	0
3	F	142/163 (87%)	-0.01	1 (0%) 84 79	16, 35, 57, 65	0
3	I	145/163 (88%)	0.01	1 (0%) 84 79	18, 36, 60, 64	0
3	L	143/163 (87%)	0.01	1 (0%) 84 79	9, 32, 53, 56	0
All	All	1325/1512 (87%)	0.11	31 (2%) 61 52	9, 38, 60, 82	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	82	ASP	4.3
1	A	80	ARG	4.1
1	G	105	PRO	4.1
1	J	82	ASP	3.8
2	K	58	ASN	3.8
3	C	141	ASN	3.7
1	D	80	ARG	3.6
3	L	204	GLU	3.5
1	G	106	GLN	3.4
2	K	88	THR	3.2
3	C	175	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	82	ASP	3.1
3	C	144	GLY	2.8
3	C	142	VAL	2.7
2	K	48	GLY	2.5
3	C	204	GLU	2.5
3	F	201	LEU	2.4
1	G	1	MET	2.4
1	A	83	ASP	2.4
1	A	81	ALA	2.3
3	C	143	ASP	2.3
1	G	107	ASP	2.3
1	D	101	ASP	2.2
3	C	139	SER	2.2
1	G	40	ASP	2.2
1	G	65	GLN	2.1
3	I	203	GLN	2.1
2	E	58	ASN	2.1
1	A	17	ASP	2.1
2	K	47	SER	2.0
3	C	146	PRO	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.

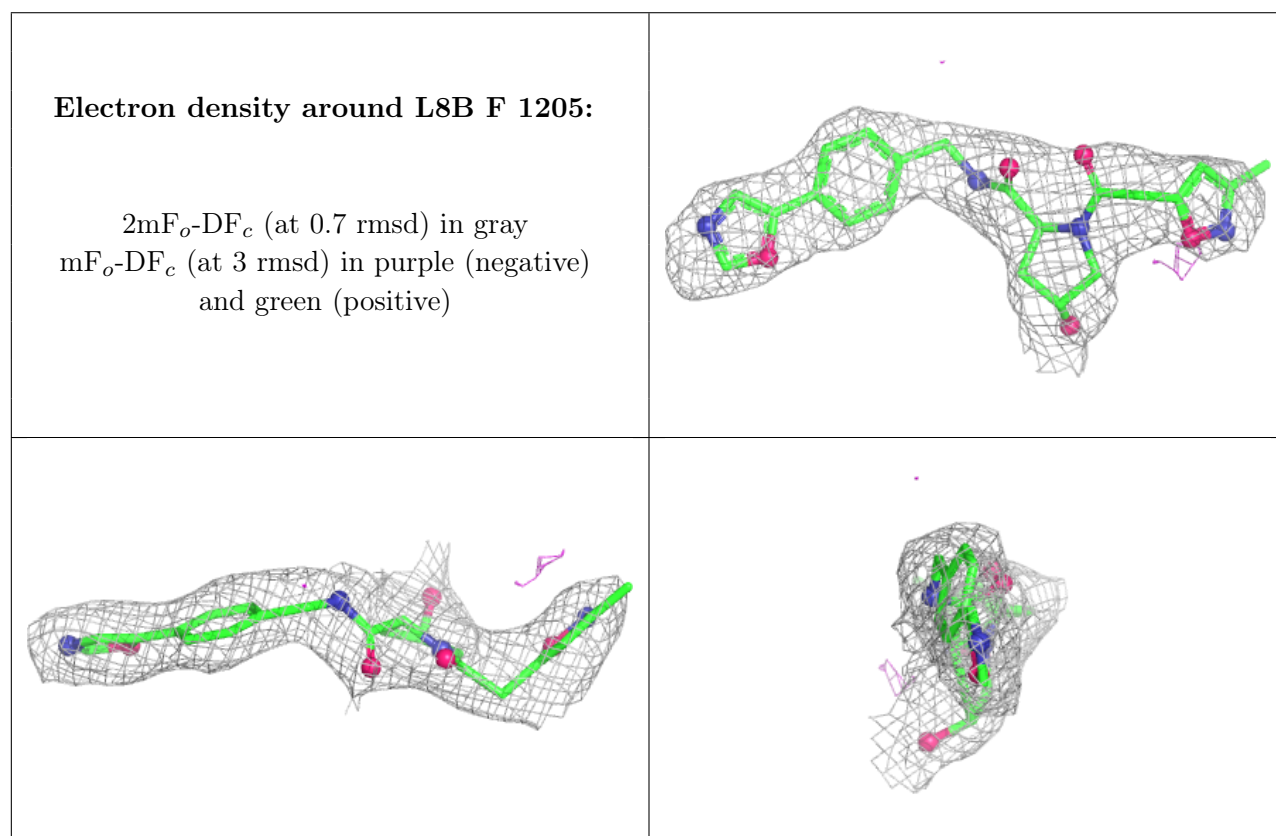
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	L8B	F	1205	30/30	0.88	0.12	39,43,52,53	0
4	L8B	I	1207	30/30	0.88	0.12	37,41,52,53	0
4	L8B	C	1205	30/30	0.90	0.11	41,42,44,45	0

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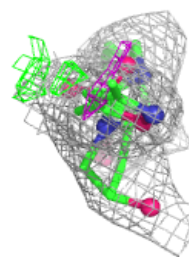
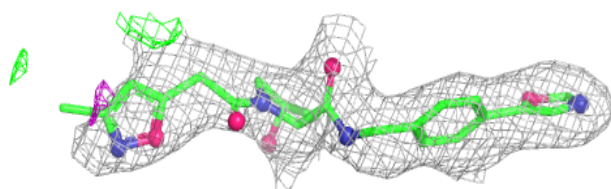
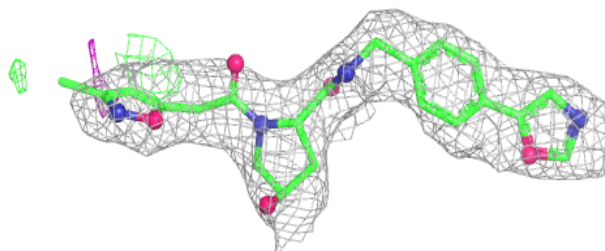
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	L8B	L	1205	30/30	0.93	0.10	22,28,38,38	0

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.

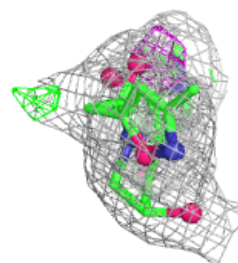
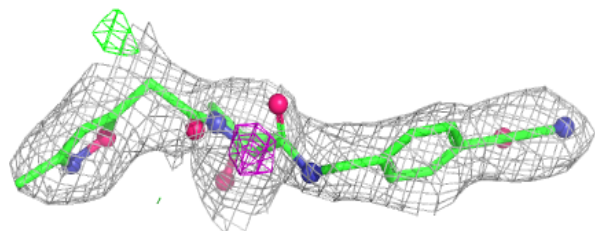
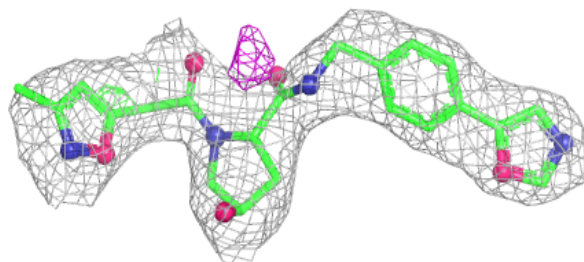


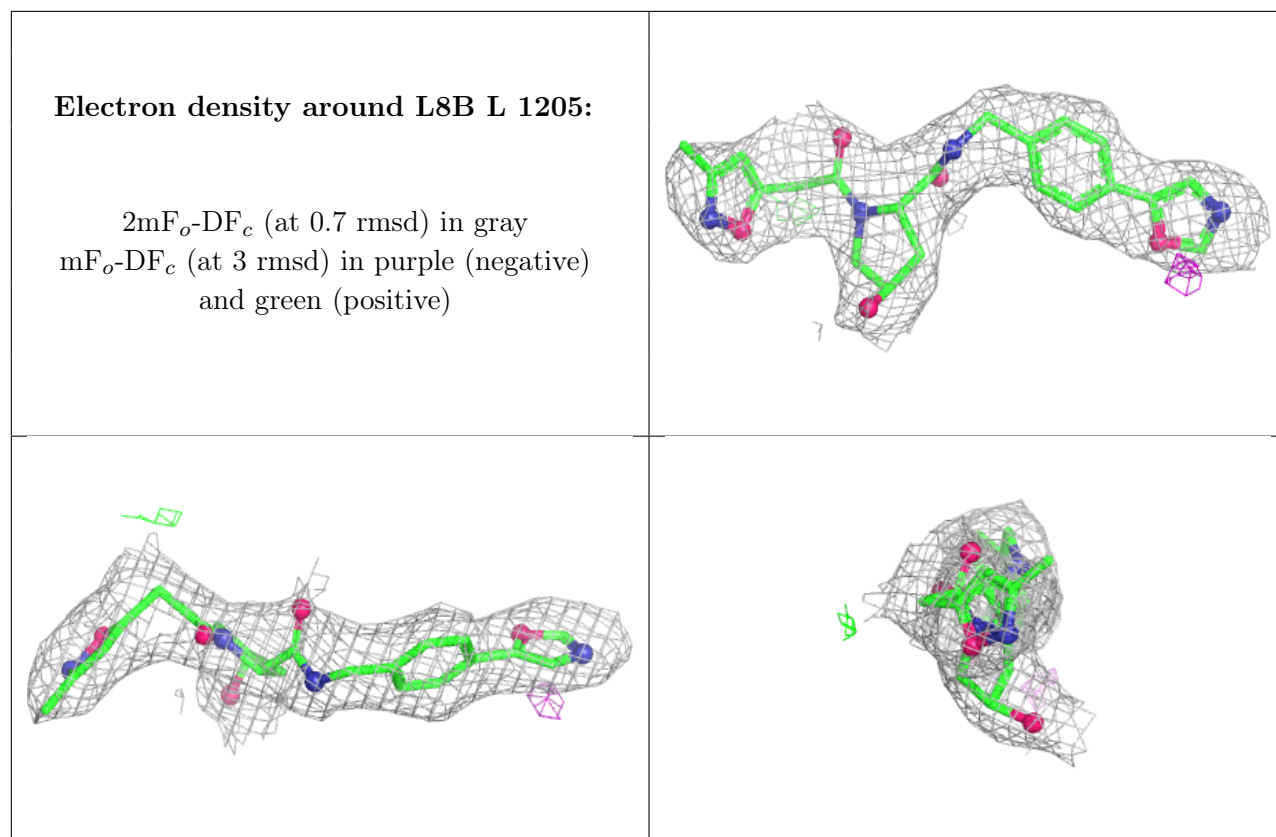
Electron density around L8B I 1207:

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

**Electron density around L8B C 1205:**

$2mF_o-DF_c$ (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.