



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:18 AM UTC

PDB ID : 2YVK / pdb_00002yvk
Title : Crystal structure of 5-methylthioribose 1-phosphate isomerase product complex from *Bacillus subtilis*
Authors : Tamura, H.; Inoue, T.; Kai, Y.; Matsumura, H.
Deposited on : 2007-04-13
Resolution : 2.40 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

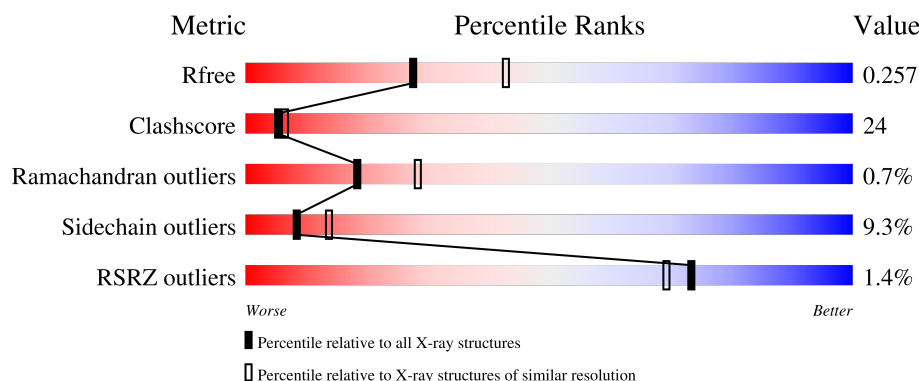
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	374	0.2% 51% 35% 7% 7%
1	B	374	0.2% 51% 37% 5% 7%
1	C	374	0.2% 57% 31% 5% 7%
1	D	374	2% 50% 37% 5% 7%

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	MRU	A	501	-	X	-	-
2	MRU	D	504	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11098 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 Methylthioribose-1-phosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2697	1704	459	524	10			
1	B	349	Total	C	N	O	S	0	0	0
			2697	1704	459	524	10			
1	C	349	Total	C	N	O	S	0	0	0
			2697	1704	459	524	10			
1	D	349	Total	C	N	O	S	0	0	0
			2697	1704	459	524	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O31662
A	-19	GLY	-	expression tag	UNP O31662
A	-18	SER	-	expression tag	UNP O31662
A	-17	SER	-	expression tag	UNP O31662
A	-16	HIS	-	expression tag	UNP O31662
A	-15	HIS	-	expression tag	UNP O31662
A	-14	HIS	-	expression tag	UNP O31662
A	-13	HIS	-	expression tag	UNP O31662
A	-12	HIS	-	expression tag	UNP O31662
A	-11	HIS	-	expression tag	UNP O31662
A	-10	SER	-	expression tag	UNP O31662
A	-9	SER	-	expression tag	UNP O31662
A	-8	GLY	-	expression tag	UNP O31662
A	-7	LEU	-	expression tag	UNP O31662
A	-6	VAL	-	expression tag	UNP O31662
A	-5	PRO	-	expression tag	UNP O31662
A	-4	ARG	-	expression tag	UNP O31662
A	-3	GLY	-	expression tag	UNP O31662
A	-2	SER	-	expression tag	UNP O31662
A	-1	HIS	-	expression tag	UNP O31662
A	0	MET	-	expression tag	UNP O31662

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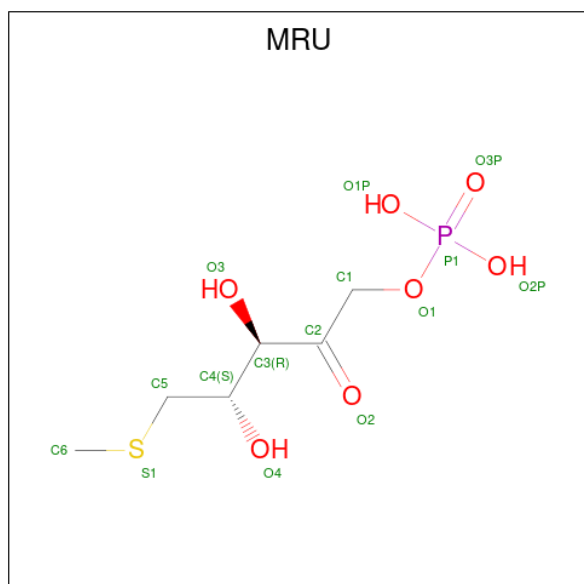
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP O31662
B	-19	GLY	-	expression tag	UNP O31662
B	-18	SER	-	expression tag	UNP O31662
B	-17	SER	-	expression tag	UNP O31662
B	-16	HIS	-	expression tag	UNP O31662
B	-15	HIS	-	expression tag	UNP O31662
B	-14	HIS	-	expression tag	UNP O31662
B	-13	HIS	-	expression tag	UNP O31662
B	-12	HIS	-	expression tag	UNP O31662
B	-11	HIS	-	expression tag	UNP O31662
B	-10	SER	-	expression tag	UNP O31662
B	-9	SER	-	expression tag	UNP O31662
B	-8	GLY	-	expression tag	UNP O31662
B	-7	LEU	-	expression tag	UNP O31662
B	-6	VAL	-	expression tag	UNP O31662
B	-5	PRO	-	expression tag	UNP O31662
B	-4	ARG	-	expression tag	UNP O31662
B	-3	GLY	-	expression tag	UNP O31662
B	-2	SER	-	expression tag	UNP O31662
B	-1	HIS	-	expression tag	UNP O31662
B	0	MET	-	expression tag	UNP O31662
C	-20	MET	-	expression tag	UNP O31662
C	-19	GLY	-	expression tag	UNP O31662
C	-18	SER	-	expression tag	UNP O31662
C	-17	SER	-	expression tag	UNP O31662
C	-16	HIS	-	expression tag	UNP O31662
C	-15	HIS	-	expression tag	UNP O31662
C	-14	HIS	-	expression tag	UNP O31662
C	-13	HIS	-	expression tag	UNP O31662
C	-12	HIS	-	expression tag	UNP O31662
C	-11	HIS	-	expression tag	UNP O31662
C	-10	SER	-	expression tag	UNP O31662
C	-9	SER	-	expression tag	UNP O31662
C	-8	GLY	-	expression tag	UNP O31662
C	-7	LEU	-	expression tag	UNP O31662
C	-6	VAL	-	expression tag	UNP O31662
C	-5	PRO	-	expression tag	UNP O31662
C	-4	ARG	-	expression tag	UNP O31662
C	-3	GLY	-	expression tag	UNP O31662
C	-2	SER	-	expression tag	UNP O31662
C	-1	HIS	-	expression tag	UNP O31662
C	0	MET	-	expression tag	UNP O31662

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP O31662
D	-19	GLY	-	expression tag	UNP O31662
D	-18	SER	-	expression tag	UNP O31662
D	-17	SER	-	expression tag	UNP O31662
D	-16	HIS	-	expression tag	UNP O31662
D	-15	HIS	-	expression tag	UNP O31662
D	-14	HIS	-	expression tag	UNP O31662
D	-13	HIS	-	expression tag	UNP O31662
D	-12	HIS	-	expression tag	UNP O31662
D	-11	HIS	-	expression tag	UNP O31662
D	-10	SER	-	expression tag	UNP O31662
D	-9	SER	-	expression tag	UNP O31662
D	-8	GLY	-	expression tag	UNP O31662
D	-7	LEU	-	expression tag	UNP O31662
D	-6	VAL	-	expression tag	UNP O31662
D	-5	PRO	-	expression tag	UNP O31662
D	-4	ARG	-	expression tag	UNP O31662
D	-3	GLY	-	expression tag	UNP O31662
D	-2	SER	-	expression tag	UNP O31662
D	-1	HIS	-	expression tag	UNP O31662
D	0	MET	-	expression tag	UNP O31662

- Molecule 2 is 5-S-METHYL-1-O-PHOSPHONO-5-THIO-D-RIBULOSE (CCD ID: MRU) (formula: $C_6H_{13}O_7PS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	O	P	S	0	0
			15	6	7	1	1		
2	B	1	Total	C	O	P	S	0	0
			15	6	7	1	1		
2	C	1	Total	C	O	P	S	0	0
			15	6	7	1	1		
2	D	1	Total	C	O	P	S	0	0
			15	6	7	1	1		

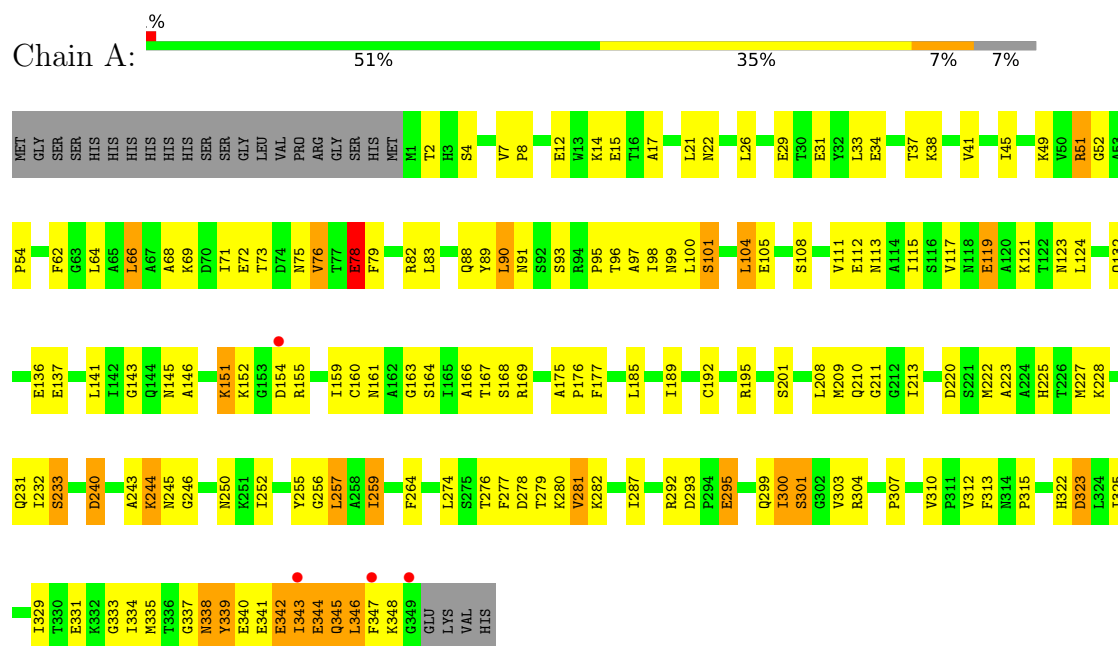
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	56	Total	O	0	0
			56	56		
3	C	68	Total	O	0	0
			68	68		
3	D	65	Total	O	0	0
			65	65		

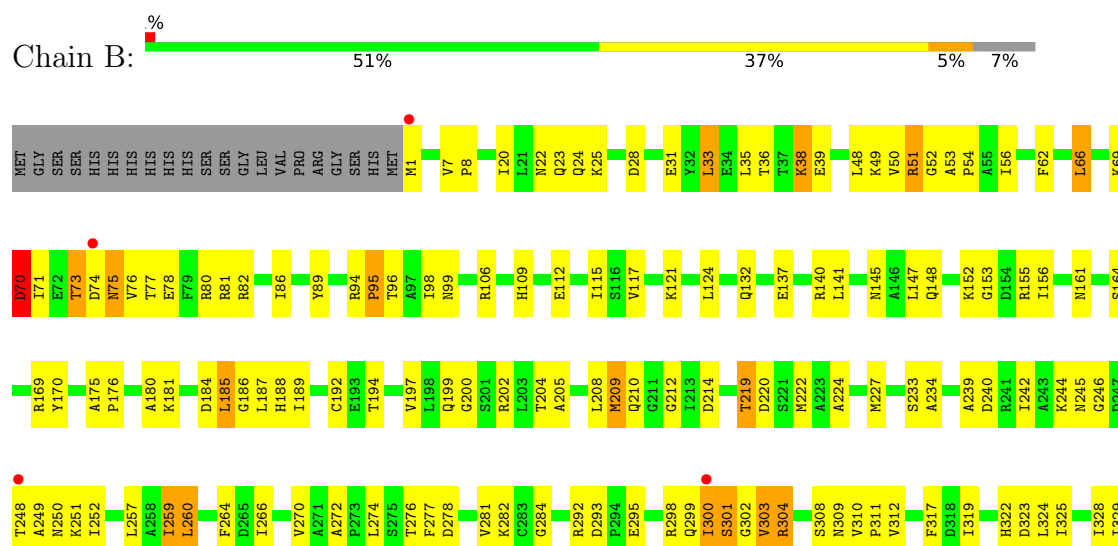
3 Residue-property plots

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: Methylthioribose-1-phosphate isomerase

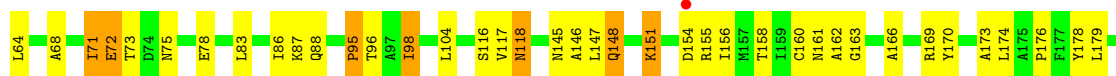
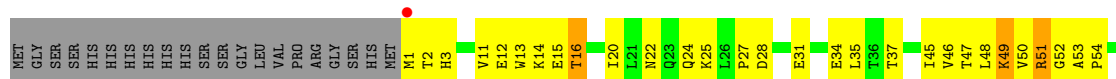


• Molecule 1: Methylthioribose-1-phosphate isomerase

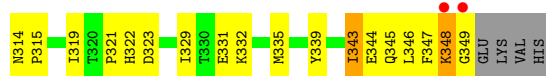
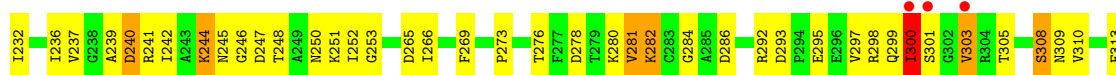
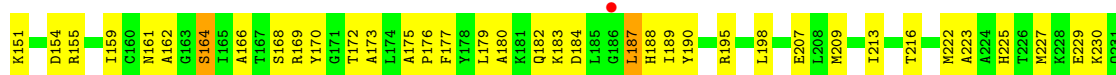
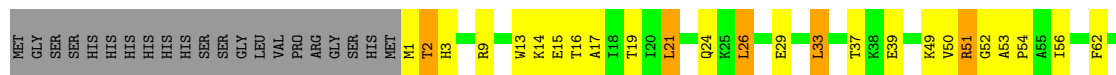




• Molecule 1: Methylthioribose-1-phosphate isomerase



• Molecule 1: Methylthioribose-1-phosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.99Å 84.44Å 95.30Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	63.16 – 2.40 63.16 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (63.16-2.40) 99.2 (63.16-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.40Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.257 0.212 , 0.257	Depositor DCC
R_{free} test set	4968 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11098	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.30% 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: MRU

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	0.49	0/2742	1.02	11/3721 (0.3%)
1	B	0.44	0/2742	0.99	11/3721 (0.3%)
1	C	0.45	0/2742	1.01	13/3721 (0.3%)
1	D	0.50	1/2742 (0.0%)	1.01	13/3721 (0.3%)
All	All	0.47	1/10968 (0.0%)	1.01	48/14884 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	303	VAL	CA-CB	7.67	1.63	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	LYS	N-CA-C	-10.07	100.26	112.54
1	A	96	THR	N-CA-C	9.94	121.70	111.07
1	D	96	THR	N-CA-C	9.36	121.09	111.07
1	C	2	THR	N-CA-C	-8.83	102.42	113.02
1	B	304	ARG	N-CA-C	8.79	123.16	110.24
1	C	96	THR	N-CA-C	8.50	120.47	111.03
1	B	303	VAL	N-CA-C	7.49	119.74	108.80
1	B	308	SER	N-CA-C	6.81	119.28	111.11
1	A	49	LYS	N-CA-C	-6.60	104.71	112.89
1	A	246	GLY	N-CA-C	-6.47	106.22	114.37
1	A	339	TYR	N-CA-C	6.43	117.95	111.07
1	B	49	LYS	N-CA-C	-6.43	104.36	111.82
1	A	338	ASN	N-CA-C	-6.40	102.56	111.39
1	A	287	ILE	N-CA-C	6.30	114.83	107.77
1	D	343	ILE	N-CA-C	-6.29	104.15	111.00
1	A	164	SER	N-CA-C	6.28	118.92	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	THR	N-CA-C	6.16	121.47	111.37
1	B	164	SER	N-CA-C	6.12	118.75	111.71
1	C	334	ILE	N-CA-C	6.06	116.65	108.17
1	C	11	VAL	N-CA-C	6.05	115.81	108.06
1	C	308	SER	N-CA-C	-5.93	102.29	110.35
1	A	78	GLU	N-CA-C	-5.85	105.04	111.82
1	A	334	ILE	N-CA-C	5.84	116.34	108.17
1	D	49	LYS	N-CA-C	-5.79	105.47	112.54
1	D	50	VAL	N-CA-C	-5.66	100.03	108.46
1	B	219	THR	N-CA-C	-5.63	103.27	110.53
1	C	28	ASP	N-CA-C	5.62	117.09	111.07
1	C	246	GLY	N-CA-C	-5.57	106.84	114.64
1	C	300	ILE	N-CA-C	5.52	115.80	107.80
1	D	164	SER	N-CA-C	5.46	117.99	111.71
1	C	249	ALA	N-CA-C	-5.46	99.84	108.73
1	D	314	ASN	N-CA-C	5.40	118.45	108.94
1	D	308	SER	N-CA-C	-5.37	102.93	110.50
1	D	95	PRO	N-CA-C	5.36	123.50	112.47
1	A	344	GLU	N-CA-C	-5.33	105.38	111.14
1	D	282	LYS	N-CA-C	5.32	118.93	112.23
1	D	147	LEU	N-CA-C	5.29	117.13	111.36
1	D	300	ILE	CB-CA-C	-5.21	102.74	111.29
1	D	187	LEU	N-CA-C	5.16	118.04	110.30
1	B	77	THR	N-CA-C	-5.14	105.76	111.36
1	B	209	MET	N-CA-C	-5.12	105.78	111.36
1	C	338	ASN	N-CA-C	-5.10	106.36	112.58
1	B	249	ALA	N-CA-C	-5.07	101.05	109.46
1	A	163	GLY	N-CA-C	5.05	118.80	110.77
1	C	86	ILE	N-CA-C	-5.04	105.50	111.00
1	C	272	ALA	N-CA-C	5.04	114.61	108.11
1	D	119	GLU	N-CA-C	-5.01	105.53	111.69
1	B	39	GLU	N-CA-C	-5.00	105.91	111.36

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	2697	0	2717	144	0
1	B	2697	0	2717	141	0
1	C	2697	0	2717	121	0
1	D	2697	0	2717	134	0
2	A	15	0	10	1	0
2	B	15	0	11	5	0
2	C	15	0	11	3	0
2	D	15	0	11	7	0
3	A	61	0	0	5	0
3	B	56	0	0	3	0
3	C	68	0	0	5	0
3	D	65	0	0	7	0
All	All	11098	0	10911	524	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 24.

All (524) 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:227:MET:HA	1:C:232:ILE:HG12	1.37	1.06
1:A:335:MET:HE1	1:A:343:ILE:HG22	1.37	1.04
1:B:345:GLN:HA	1:B:348:LYS:HE2	1.47	0.96
1:A:51:ARG:HH22	1:A:161:ASN:HD22	1.12	0.95
1:D:244:LYS:HE2	1:D:344:GLU:HG3	1.46	0.94
1:C:151:LYS:NZ	1:C:154:ASP:HB3	1.85	0.91
1:B:303:VAL:HG12	1:B:304:ARG:H	1.37	0.89
1:C:227:MET:HA	1:C:232:ILE:CG1	2.06	0.86
1:C:151:LYS:HZ2	1:C:154:ASP:HB3	1.41	0.85
1:B:227:MET:HE1	1:B:260:LEU:HB3	1.59	0.85
1:B:339:TYR:O	1:B:343:ILE:HG12	1.77	0.85
1:B:22:ASN:HB2	1:B:33:LEU:HD21	1.58	0.84
1:B:54:PRO:HD2	2:B:502:MRU:H63	1.58	0.83
1:A:259:ILE:HD12	1:B:260:LEU:HD12	1.59	0.83
1:D:335:MET:HE3	1:D:346:LEU:HD22	1.61	0.83
1:A:151:LYS:HA	1:A:151:LYS:HE2	1.59	0.82
1:A:115:ILE:HG22	1:A:119:GLU:OE1	1.78	0.82
1:A:51:ARG:NH2	1:A:161:ASN:HD22	1.77	0.82
1:B:240:ASP:OD1	2:B:502:MRU:O4	1.98	0.81
1:B:299:GLN:HG2	1:B:300:ILE:N	1.94	0.81
1:D:323:ASP:HB2	3:D:550:HOH:O	1.79	0.81
1:C:20:ILE:HD12	1:C:50:VAL:HG23	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:HB2	1:A:33:LEU:CD2	2.12	0.79
1:B:322:HIS:HA	1:B:325:ILE:HD12	1.65	0.79
1:C:341:GLU:O	1:C:344:GLU:HB3	1.82	0.78
1:C:68:ALA:O	1:C:71:ILE:HG22	1.83	0.78
1:B:145:ASN:HA	1:B:148:GLN:HE21	1.49	0.77
1:B:251:LYS:HE2	2:B:502:MRU:H11	1.66	0.77
1:B:205:ALA:O	1:B:209:MET:HG3	1.85	0.77
1:A:338:ASN:HD21	1:A:341:GLU:CD	1.93	0.77
1:D:345:GLN:NE2	1:D:348:LYS:HE3	2.00	0.77
1:C:98:ILE:HD12	1:C:278:ASP:HB2	1.69	0.75
1:B:303:VAL:HG12	1:B:304:ARG:N	2.00	0.74
1:A:151:LYS:HD3	1:A:152:LYS:H	1.51	0.74
1:A:348:LYS:O	1:A:348:LYS:HG3	1.88	0.74
1:D:242:ILE:HG12	1:D:248:THR:HG22	1.69	0.73
1:A:293:ASP:OD2	1:A:295:GLU:HB2	1.87	0.73
1:C:22:ASN:OD1	1:C:24:GLN:HG2	1.89	0.73
1:A:341:GLU:O	1:A:345:GLN:HG2	1.88	0.73
1:C:348:LYS:HB2	1:C:348:LYS:NZ	2.03	0.72
1:B:189:ILE:CD1	1:B:208:LEU:HD13	2.19	0.72
1:B:51:ARG:HH12	1:B:161:ASN:HD22	1.35	0.72
1:C:308:SER:O	1:C:309:ASN:HB2	1.88	0.72
1:A:227:MET:HA	1:A:232:ILE:HG12	1.72	0.71
1:D:345:GLN:HA	1:D:348:LYS:HE2	1.72	0.71
1:A:280:LYS:HD2	1:A:281:VAL:HG12	1.73	0.71
1:B:51:ARG:NH1	1:B:161:ASN:HD22	1.89	0.71
1:B:109:HIS:HA	1:B:112:GLU:HG3	1.72	0.71
1:D:227:MET:HA	1:D:232:ILE:HG12	1.73	0.70
1:A:299:GLN:HG3	3:A:526:HOH:O	1.90	0.70
1:B:300:ILE:C	1:B:300:ILE:HD13	2.16	0.70
1:D:90:LEU:O	1:D:93:SER:HB2	1.91	0.70
1:A:22:ASN:HB2	1:A:33:LEU:HD23	1.73	0.70
1:C:293:ASP:OD2	1:C:295:GLU:HB2	1.91	0.70
1:C:53:ALA:HB3	1:C:54:PRO:HD3	1.73	0.70
1:D:227:MET:HA	1:D:232:ILE:CG1	2.22	0.69
1:C:158:THR:HG22	1:C:189:ILE:HD11	1.74	0.69
1:B:54:PRO:CD	2:B:502:MRU:H63	2.22	0.69
1:C:245:ASN:HB2	1:C:282:LYS:O	1.92	0.69
1:A:64:LEU:HD21	1:A:83:LEU:HD21	1.74	0.69
1:A:252:ILE:HG12	1:B:222:MET:HG2	1.75	0.68
1:A:209:MET:HE1	1:B:309:ASN:OD1	1.93	0.68
1:C:192:CYS:HB3	1:C:220:ASP:OD1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ALA:HA	1:B:185:LEU:HD21	1.76	0.68
1:B:189:ILE:HD11	1:B:208:LEU:HD13	1.76	0.68
1:B:155:ARG:HG3	1:B:155:ARG:HH11	1.57	0.68
1:B:147:LEU:HD11	1:B:185:LEU:HD11	1.76	0.67
1:B:22:ASN:OD1	1:B:24:GLN:HG2	1.93	0.67
1:C:75:ASN:HB3	1:C:78:GLU:HB3	1.76	0.67
1:A:168:SER:C	1:A:169:ARG:HG3	2.18	0.67
1:A:151:LYS:HZ3	1:A:185:LEU:HD11	1.59	0.67
1:A:339:TYR:O	1:A:343:ILE:HG23	1.93	0.67
1:C:200:GLY:HA2	1:C:204:THR:HB	1.75	0.67
1:D:244:LYS:HG3	1:D:244:LYS:O	1.93	0.67
1:D:137:GLU:OE1	1:D:140:ARG:HD2	1.95	0.66
1:D:146:ALA:HB3	1:D:176:PRO:HG3	1.76	0.66
1:B:156:ILE:HB	1:B:189:ILE:HG22	1.77	0.66
1:D:51:ARG:HH22	1:D:161:ASN:HD22	1.41	0.66
1:C:51:ARG:NH2	1:C:161:ASN:HD22	1.93	0.66
1:C:154:ASP:HB2	1:C:233:SER:CB	2.25	0.66
1:A:259:ILE:HD13	1:A:259:ILE:C	2.21	0.65
1:C:174:LEU:HD13	1:C:208:LEU:HD11	1.78	0.65
1:A:323:ASP:OD2	1:A:323:ASP:N	2.26	0.65
1:B:36:THR:O	1:B:66:LEU:HD11	1.96	0.65
1:D:278:ASP:OD2	1:D:280:LYS:HE2	1.97	0.65
1:A:98:ILE:HD12	1:A:278:ASP:CG	2.21	0.65
1:C:195:ARG:HH22	1:C:300:ILE:HD11	1.61	0.65
1:D:278:ASP:OD1	1:D:280:LYS:HG2	1.97	0.65
1:B:22:ASN:HB2	1:B:33:LEU:CD2	2.25	0.65
1:C:154:ASP:HB2	1:C:233:SER:OG	1.97	0.65
1:D:53:ALA:HB3	1:D:54:PRO:HD3	1.78	0.64
1:D:308:SER:O	1:D:309:ASN:HB2	1.97	0.64
1:A:299:GLN:HB3	1:A:304:ARG:HA	1.80	0.64
1:B:53:ALA:HB3	1:B:54:PRO:HD3	1.79	0.64
1:C:338:ASN:ND2	1:C:341:GLU:HB3	2.12	0.64
1:D:223:ALA:O	1:D:227:MET:HG3	1.97	0.64
1:B:303:VAL:CG1	1:B:304:ARG:H	2.10	0.64
1:A:52:GLY:HA3	1:A:166:ALA:HB1	1.79	0.64
1:A:225:HIS:HE1	3:A:559:HOH:O	1.80	0.64
1:B:278:ASP:OD1	1:B:281:VAL:HG23	1.97	0.64
1:A:227:MET:HA	1:A:232:ILE:CG1	2.28	0.64
1:C:338:ASN:HD21	1:C:341:GLU:HB3	1.62	0.64
1:B:300:ILE:O	1:B:302:GLY:N	2.31	0.64
1:C:98:ILE:HD12	1:C:278:ASP:CB	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:MET:HG2	1:D:252:ILE:HG12	1.80	0.63
1:A:54:PRO:CG	1:A:167:THR:HG22	2.28	0.63
1:A:335:MET:HG2	1:A:342:GLU:HG2	1.81	0.63
1:C:348:LYS:HB2	1:C:348:LYS:HZ2	1.63	0.63
1:B:300:ILE:HD13	1:B:300:ILE:O	1.99	0.63
1:D:84:GLU:O	1:D:88:GLN:HG3	1.99	0.62
1:B:224:ALA:HA	1:B:227:MET:HE3	1.80	0.62
1:D:281:VAL:HG22	1:D:286:ASP:HB2	1.80	0.62
1:A:146:ALA:HB2	1:A:329:ILE:HD13	1.80	0.62
1:A:151:LYS:CD	1:A:152:LYS:H	2.10	0.62
1:C:195:ARG:HH12	1:C:300:ILE:HG13	1.65	0.62
1:D:51:ARG:HB2	2:D:504:MRU:O3P	2.00	0.62
1:D:300:ILE:HG22	1:D:301:SER:N	2.15	0.62
1:B:303:VAL:HB	3:B:554:HOH:O	2.00	0.62
1:B:251:LYS:CE	2:B:502:MRU:H11	2.30	0.61
1:A:274:LEU:HD13	1:A:331:GLU:CD	2.25	0.61
1:A:2:THR:HA	1:A:211:GLY:HA2	1.81	0.61
1:C:195:ARG:NH1	1:C:300:ILE:HG13	2.15	0.61
1:B:192:CYS:HB3	1:B:220:ASP:OD1	2.01	0.61
1:A:168:SER:O	1:A:169:ARG:HG3	2.01	0.61
1:B:242:ILE:HG12	1:B:248:THR:HG22	1.83	0.61
1:D:151:LYS:HG2	1:D:154:ASP:OD2	2.01	0.60
1:C:147:LEU:HD21	1:C:183:LYS:HD3	1.81	0.60
1:B:33:LEU:N	1:B:33:LEU:HD22	2.17	0.60
1:B:109:HIS:CE1	1:B:112:GLU:OE1	2.54	0.60
1:D:151:LYS:HG2	1:D:154:ASP:CG	2.27	0.60
1:A:51:ARG:HH22	1:A:161:ASN:ND2	1.93	0.60
1:A:101:SER:O	1:A:105:GLU:HB2	2.01	0.60
1:D:246:GLY:O	1:D:248:THR:HG23	2.02	0.60
1:B:62:PHE:HZ	1:B:132:GLN:NE2	2.00	0.60
1:B:340:GLU:O	1:B:344:GLU:HG3	2.02	0.60
1:D:298:ARG:NH1	1:D:310:VAL:O	2.34	0.60
1:B:200:GLY:O	1:B:204:THR:HB	2.02	0.60
1:C:51:ARG:HH22	1:C:161:ASN:HD22	1.50	0.60
1:A:54:PRO:HG3	1:A:167:THR:HG22	1.84	0.59
1:A:345:GLN:HA	1:A:348:LYS:NZ	2.17	0.59
1:B:219:THR:OG1	1:B:222:MET:HG3	2.03	0.59
1:D:117:VAL:HG12	1:D:121:LYS:HE3	1.84	0.59
1:D:347:PHE:O	1:D:349:GLY:N	2.35	0.59
1:D:180:ALA:HB1	1:D:187:LEU:HD22	1.83	0.59
1:B:335:MET:SD	1:B:342:GLU:HB3	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:O	1:A:93:SER:HB2	2.01	0.59
1:A:71:ILE:HG23	1:A:82:ARG:HD3	1.85	0.59
1:C:338:ASN:ND2	1:C:341:GLU:OE1	2.36	0.58
1:B:227:MET:HE1	1:B:260:LEU:CB	2.32	0.58
1:A:8:PRO:HG3	1:A:169:ARG:HD2	1.86	0.58
1:C:87:LYS:HG2	1:C:104:LEU:HB3	1.86	0.58
1:B:137:GLU:OE2	1:B:141:LEU:HD21	2.03	0.57
1:A:141:LEU:HD22	1:A:331:GLU:HB2	1.84	0.57
1:B:137:GLU:O	1:B:141:LEU:HD23	2.04	0.57
1:B:329:ILE:N	1:B:329:ILE:HD12	2.19	0.57
1:D:2:THR:O	1:D:2:THR:CG2	2.52	0.57
1:B:234:ALA:HA	1:B:266:ILE:CG2	2.35	0.57
1:B:76:VAL:O	1:B:80:ARG:HG3	2.04	0.57
1:C:204:THR:O	1:C:208:LEU:HD13	2.04	0.57
1:A:137:GLU:O	1:A:141:LEU:HD13	2.03	0.57
1:C:243:ALA:C	1:C:245:ASN:N	2.61	0.57
1:A:255:TYR:O	1:A:259:ILE:HG22	2.05	0.57
1:A:22:ASN:HB2	1:A:33:LEU:HD21	1.84	0.57
1:D:115:ILE:C	1:D:115:ILE:HD12	2.30	0.57
1:B:224:ALA:HA	1:B:227:MET:CE	2.34	0.57
1:C:243:ALA:C	1:C:245:ASN:H	2.10	0.57
1:C:337:GLY:O	1:C:338:ASN:HB3	2.04	0.57
1:A:141:LEU:HD23	1:A:331:GLU:O	2.04	0.56
1:C:20:ILE:HD12	1:C:50:VAL:CG2	2.33	0.56
1:A:151:LYS:CE	1:A:152:LYS:H	2.19	0.56
1:C:270:VAL:O	1:C:329:ILE:HD12	2.06	0.56
1:D:132:GLN:HG3	1:D:168:SER:OG	2.05	0.56
1:B:245:ASN:HA	1:B:340:GLU:HG2	1.88	0.56
1:C:160:CYS:SG	2:C:503:MRU:H12	2.46	0.56
1:D:78:GLU:OE1	1:D:82:ARG:NH2	2.39	0.56
1:C:87:LYS:CG	1:C:104:LEU:HB3	2.36	0.56
1:B:259:ILE:HG13	1:B:324:LEU:CD1	2.37	0.55
1:B:299:GLN:CG	1:B:300:ILE:N	2.66	0.55
1:C:276:THR:O	1:C:276:THR:HG22	2.06	0.55
1:C:218:ILE:HG22	1:D:313:PHE:HB3	1.88	0.55
1:D:54:PRO:HD2	2:D:504:MRU:H63	1.88	0.55
1:B:299:GLN:HG2	1:B:300:ILE:H	1.68	0.55
1:D:166:ALA:HB1	2:D:504:MRU:H61	1.88	0.55
1:A:155:ARG:NH2	1:A:231:GLN:O	2.34	0.55
1:B:341:GLU:CD	1:C:25:LYS:HE3	2.32	0.55
1:C:178:TYR:CD1	1:C:213:ILE:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:NH1	1:C:300:ILE:CG1	2.70	0.55
1:B:270:VAL:O	1:B:328:ILE:HA	2.07	0.54
1:D:244:LYS:CE	1:D:344:GLU:HG3	2.31	0.54
1:B:71:ILE:HG22	1:B:71:ILE:O	2.07	0.54
1:D:173:ALA:O	1:D:176:PRO:HD2	2.08	0.54
1:A:177:PHE:CD2	1:A:189:ILE:HG12	2.42	0.54
1:A:195:ARG:HB2	3:A:554:HOH:O	2.06	0.54
1:D:189:ILE:N	1:D:189:ILE:HD12	2.23	0.54
1:B:23:GLN:O	1:B:202:ARG:NH2	2.41	0.54
1:A:143:GLY:HA2	1:A:176:PRO:HD3	1.88	0.54
1:B:155:ARG:HA	1:B:188:HIS:O	2.07	0.54
1:D:52:GLY:O	1:D:56:ILE:HG13	2.08	0.54
1:B:189:ILE:HD12	1:B:208:LEU:HD13	1.89	0.54
1:A:21:LEU:HD21	1:A:26:LEU:HD11	1.89	0.54
1:A:340:GLU:O	1:A:344:GLU:HB2	2.07	0.54
1:B:345:GLN:O	1:B:348:LYS:HG2	2.08	0.54
1:C:213:ILE:HG23	3:C:526:HOH:O	2.08	0.53
1:A:151:LYS:HD3	1:A:152:LYS:N	2.19	0.53
1:C:201:SER:OG	1:D:305:THR:O	2.25	0.53
1:C:162:ALA:HB3	1:C:173:ALA:HB3	1.89	0.53
1:D:180:ALA:CB	1:D:187:LEU:HD22	2.38	0.53
1:A:90:LEU:HB3	1:A:104:LEU:HD21	1.90	0.53
1:A:98:ILE:HD12	1:A:278:ASP:CB	2.38	0.53
1:C:13:TRP:CZ2	1:C:15:GLU:HA	2.44	0.53
1:D:2:THR:O	1:D:2:THR:HG22	2.07	0.53
1:C:251:LYS:HD3	1:C:252:ILE:H	1.74	0.53
1:A:99:ASN:HD22	1:A:99:ASN:H	1.56	0.53
1:B:169:ARG:O	1:B:170:TYR:HB2	2.09	0.53
1:C:156:ILE:O	1:C:189:ILE:HD12	2.09	0.53
1:B:70:ASP:OD2	1:B:70:ASP:N	2.35	0.53
1:D:281:VAL:HG22	1:D:286:ASP:CB	2.38	0.52
1:A:98:ILE:HD12	1:A:278:ASP:HB2	1.91	0.52
1:D:244:LYS:O	1:D:343:ILE:HD12	2.10	0.52
1:A:83:LEU:O	1:A:83:LEU:HD23	2.10	0.52
1:B:52:GLY:O	1:B:56:ILE:HG13	2.09	0.52
1:C:244:LYS:HB2	1:C:279:THR:HA	1.92	0.52
1:A:151:LYS:NZ	1:A:185:LEU:HD11	2.23	0.52
1:A:225:HIS:HD2	3:B:535:HOH:O	1.92	0.52
1:C:151:LYS:HZ2	1:C:154:ASP:CB	2.19	0.52
1:A:68:ALA:O	1:A:121:LYS:HE2	2.10	0.52
1:B:20:ILE:HD13	1:B:35:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:HG3	1:B:155:ARG:NH1	2.24	0.52
1:B:38:LYS:HD3	1:B:89:TYR:CE2	2.45	0.52
1:C:251:LYS:HD3	1:C:252:ILE:N	2.25	0.52
1:A:304:ARG:NH1	1:B:28:ASP:OD2	2.40	0.52
1:C:221:SER:O	1:D:253:GLY:HA2	2.10	0.52
1:D:80:ARG:NH2	1:D:114:ALA:O	2.42	0.51
1:B:155:ARG:HG2	1:B:188:HIS:HB3	1.92	0.51
1:B:240:ASP:OD2	1:B:317:PHE:CE1	2.64	0.51
1:D:1:MET:HG3	1:D:2:THR:N	2.26	0.51
1:A:279:THR:HG22	1:A:343:ILE:HD11	1.92	0.51
1:A:54:PRO:HG2	1:A:167:THR:HG22	1.92	0.51
1:A:97:ALA:HB2	1:A:240:ASP:OD2	2.10	0.51
1:C:163:GLY:HA3	1:C:174:LEU:HD12	1.91	0.51
1:D:94:ARG:HB3	3:D:518:HOH:O	2.11	0.51
1:A:189:ILE:HD13	1:A:213:ILE:CG2	2.41	0.51
1:B:7:VAL:HG13	1:B:8:PRO:HD2	1.93	0.51
1:B:338:ASN:OD1	1:B:341:GLU:HB3	2.10	0.51
1:B:343:ILE:O	1:B:346:LEU:HB3	2.11	0.51
1:D:297:VAL:O	1:D:297:VAL:HG12	2.09	0.51
1:A:256:GLY:HA2	1:A:259:ILE:CG2	2.41	0.51
1:C:248:THR:OG1	1:C:320:THR:HB	2.10	0.51
1:A:303:VAL:HG11	1:B:301:SER:HB2	1.93	0.50
1:B:66:LEU:C	1:B:66:LEU:HD13	2.36	0.50
1:D:117:VAL:CG1	1:D:121:LYS:HE3	2.40	0.50
1:D:166:ALA:CB	2:D:504:MRU:H61	2.41	0.50
1:A:38:LYS:HG3	1:A:89:TYR:CE2	2.45	0.50
1:A:91:ASN:C	1:A:93:SER:H	2.18	0.50
1:C:193:GLU:HB2	1:C:201:SER:HB2	1.93	0.50
1:D:225:HIS:CE1	1:D:229:GLU:HG3	2.46	0.50
1:A:277:PHE:HB2	1:A:347:PHE:HZ	1.75	0.50
1:B:180:ALA:HB1	1:B:185:LEU:HG	1.92	0.50
1:C:145:ASN:O	1:C:148:GLN:HG2	2.11	0.50
1:B:189:ILE:HG12	1:B:214:ASP:O	2.11	0.50
1:D:26:LEU:HD12	1:D:29:GLU:O	2.11	0.50
1:B:82:ARG:HG3	1:B:82:ARG:HH11	1.76	0.50
1:C:71:ILE:HD13	1:C:72:GLU:N	2.27	0.50
1:D:159:ILE:HG22	1:D:237:VAL:CG1	2.42	0.50
1:A:335:MET:HE3	1:A:342:GLU:CG	2.42	0.50
1:C:20:ILE:HD13	1:C:35:LEU:HD11	1.93	0.50
1:D:345:GLN:CD	1:D:348:LYS:HE3	2.37	0.50
1:D:345:GLN:HA	1:D:348:LYS:CE	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:PHE:CZ	1:A:315:PRO:HG3	2.47	0.49
1:A:335:MET:HE3	1:A:342:GLU:HG2	1.93	0.49
1:D:115:ILE:HD12	1:D:116:SER:HB3	1.92	0.49
1:D:177:PHE:CD1	1:D:177:PHE:N	2.80	0.49
1:A:41:VAL:O	1:A:45:ILE:HG13	2.12	0.49
1:B:76:VAL:HG21	1:B:115:ILE:O	2.12	0.49
1:C:226:THR:HG22	1:C:232:ILE:HD11	1.94	0.49
1:A:292:ARG:HD3	3:A:553:HOH:O	2.12	0.49
1:B:197:VAL:HB	1:B:199:GLN:OE1	2.11	0.49
1:C:98:ILE:HG12	1:C:98:ILE:O	2.13	0.49
1:D:98:ILE:HD13	1:D:98:ILE:O	2.13	0.49
1:D:159:ILE:HG22	1:D:237:VAL:HG12	1.94	0.49
1:C:51:ARG:NH2	1:C:166:ALA:HB2	2.28	0.49
1:C:195:ARG:HH12	1:C:300:ILE:CG1	2.26	0.49
1:A:322:HIS:HA	1:A:325:ILE:HD12	1.95	0.49
1:D:282:LYS:HD3	1:D:282:LYS:N	2.28	0.49
1:A:7:VAL:HG13	1:A:8:PRO:HD2	1.95	0.49
1:D:295:GLU:HA	1:D:295:GLU:OE1	2.12	0.49
1:A:245:ASN:HB2	1:A:282:LYS:O	2.13	0.48
1:C:147:LEU:CD2	1:C:183:LYS:HD3	2.42	0.48
1:C:244:LYS:HB3	1:C:281:VAL:O	2.13	0.48
1:A:151:LYS:HE2	1:A:151:LYS:CA	2.39	0.48
1:D:146:ALA:CB	1:D:329:ILE:HD13	2.42	0.48
1:D:177:PHE:CD2	1:D:189:ILE:HG12	2.48	0.48
1:D:188:HIS:HE1	1:D:216:THR:OG1	1.95	0.48
1:D:252:ILE:HD13	1:D:315:PRO:HG2	1.95	0.48
1:A:223:ALA:O	1:A:227:MET:HG3	2.13	0.48
1:C:71:ILE:HD13	1:C:71:ILE:C	2.38	0.48
1:C:117:VAL:HG13	1:C:118:ASN:N	2.28	0.48
1:A:21:LEU:HD12	1:A:31:GLU:O	2.13	0.48
1:C:225:HIS:HD2	3:D:560:HOH:O	1.95	0.48
1:C:248:THR:HG21	1:C:270:VAL:HG21	1.95	0.48
1:D:276:THR:HG22	1:D:276:THR:O	2.13	0.48
1:D:164:SER:HB3	1:D:207:GLU:OE1	2.14	0.48
1:D:321:PRO:HB2	3:D:550:HOH:O	2.12	0.48
1:D:335:MET:CE	1:D:346:LEU:HD22	2.40	0.48
1:C:117:VAL:CG1	1:C:118:ASN:N	2.77	0.48
1:C:151:LYS:C	1:C:185:LEU:HD21	2.38	0.48
1:D:146:ALA:HB2	1:D:329:ILE:HD13	1.95	0.48
1:D:169:ARG:O	1:D:170:TYR:HB2	2.13	0.48
1:C:1:MET:C	1:C:3:HIS:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLN:C	1:C:300:ILE:HD12	2.39	0.48
1:D:284:GLY:HA3	1:D:319:ILE:HG21	1.96	0.48
1:A:345:GLN:HA	1:A:348:LYS:HZ2	1.79	0.48
1:C:207:GLU:HG3	1:C:208:LEU:HD12	1.95	0.48
1:B:75:ASN:HB3	1:B:78:GLU:HB3	1.95	0.47
1:B:278:ASP:CG	1:B:281:VAL:HG23	2.38	0.47
1:D:66:LEU:C	1:D:66:LEU:HD23	2.38	0.47
1:A:14:LYS:HB2	1:A:17:ALA:O	2.13	0.47
1:A:222:MET:HG2	1:B:252:ILE:HG12	1.96	0.47
1:C:75:ASN:HB3	1:C:78:GLU:CB	2.42	0.47
1:C:318:ASP:O	1:C:319:ILE:HD12	2.15	0.47
1:A:83:LEU:HD11	1:A:124:LEU:HD11	1.97	0.47
1:A:136:GLU:OE1	1:A:169:ARG:HD2	2.15	0.47
1:B:175:ALA:N	1:B:176:PRO:HD2	2.29	0.47
1:B:246:GLY:O	1:B:248:THR:HG23	2.14	0.47
1:B:299:GLN:CG	1:B:300:ILE:H	2.26	0.47
1:D:19:THR:HA	1:D:33:LEU:O	2.14	0.47
1:D:273:PRO:HA	1:D:331:GLU:OE1	2.14	0.47
1:A:75:ASN:HB3	1:A:78:GLU:HB2	1.96	0.47
1:A:228:LYS:HB2	1:A:264:PHE:CE1	2.49	0.47
1:A:312:VAL:HG12	1:A:313:PHE:N	2.29	0.47
1:B:276:THR:HG22	1:B:276:THR:O	2.13	0.47
1:D:240:ASP:OD2	2:D:504:MRU:O4	2.15	0.47
1:D:62:PHE:HE1	1:D:129:ILE:HG13	1.79	0.47
1:D:137:GLU:OE1	1:D:137:GLU:HA	2.14	0.47
1:A:209:MET:C	1:A:211:GLY:H	2.23	0.47
1:B:274:LEU:HD13	1:B:331:GLU:CD	2.39	0.47
1:C:169:ARG:O	1:C:170:TYR:HB2	2.15	0.47
1:A:343:ILE:HD12	1:A:347:PHE:CE2	2.50	0.47
1:C:281:VAL:HG13	1:C:286:ASP:HB2	1.96	0.47
1:C:200:GLY:O	1:C:204:THR:HB	2.14	0.47
1:D:69:LYS:HA	1:D:121:LYS:HD3	1.97	0.47
1:B:277:PHE:CE1	1:B:343:ILE:HD12	2.50	0.47
1:D:310:VAL:O	1:D:310:VAL:HG13	2.14	0.47
1:C:51:ARG:HH22	1:C:161:ASN:ND2	2.14	0.46
1:D:1:MET:HG3	1:D:3:HIS:H	1.80	0.46
1:D:136:GLU:O	1:D:140:ARG:HG3	2.15	0.46
1:A:154:ASP:HB2	1:A:233:SER:OG	2.16	0.46
1:B:284:GLY:C	1:B:319:ILE:HD13	2.40	0.46
1:D:1:MET:CG	1:D:2:THR:N	2.77	0.46
1:D:241:ARG:NH1	1:D:278:ASP:OD2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:GLN:HE22	1:D:348:LYS:HE3	1.75	0.46
1:A:72:GLU:O	1:A:73:THR:HB	2.15	0.46
1:B:71:ILE:HG22	1:B:73:THR:HG22	1.97	0.46
1:B:197:VAL:HG12	1:B:197:VAL:O	2.15	0.46
1:A:208:LEU:HD22	1:A:213:ILE:HG13	1.98	0.46
1:A:292:ARG:O	1:A:293:ASP:C	2.58	0.46
1:C:282:LYS:HB2	1:C:282:LYS:HE3	1.66	0.46
1:A:228:LYS:HB2	1:A:264:PHE:CZ	2.51	0.46
1:A:337:GLY:O	1:A:338:ASN:C	2.59	0.46
1:C:338:ASN:O	1:C:342:GLU:HG2	2.16	0.46
1:B:117:VAL:O	1:B:121:LYS:HG2	2.16	0.46
1:C:14:LYS:O	1:C:16:THR:N	2.38	0.46
1:C:47:THR:HG21	1:C:49:LYS:HE3	1.98	0.46
1:A:280:LYS:O	1:A:280:LYS:HG2	2.14	0.46
1:C:73:THR:O	1:C:117:VAL:HG21	2.16	0.46
1:C:262:ASN:HB2	3:C:534:HOH:O	2.16	0.46
1:B:272:ALA:O	1:B:330:THR:HG22	2.15	0.45
1:A:37:THR:HG22	1:A:38:LYS:N	2.32	0.45
1:B:300:ILE:O	1:B:301:SER:C	2.59	0.45
1:D:14:LYS:HG2	1:D:17:ALA:O	2.16	0.45
1:B:140:ARG:HD3	1:B:170:TYR:CE2	2.52	0.45
1:A:280:LYS:HB3	1:A:280:LYS:HE3	1.74	0.45
1:A:299:GLN:CB	1:A:304:ARG:HA	2.44	0.45
1:D:292:ARG:HB3	3:D:542:HOH:O	2.16	0.45
1:B:344:GLU:C	1:B:346:LEU:N	2.74	0.45
1:B:82:ARG:HG3	1:B:82:ARG:NH1	2.32	0.45
1:C:71:ILE:O	1:C:71:ILE:HG23	2.17	0.45
1:D:188:HIS:HB2	3:D:538:HOH:O	2.16	0.45
1:A:137:GLU:OE2	1:A:141:LEU:CD1	2.65	0.45
1:A:300:ILE:HG12	1:A:301:SER:OG	2.17	0.45
1:D:339:TYR:O	1:D:343:ILE:HG13	2.17	0.45
1:A:244:LYS:O	1:A:340:GLU:HA	2.17	0.44
1:D:293:ASP:OD1	1:D:293:ASP:C	2.59	0.44
1:D:24:GLN:NE2	3:D:522:HOH:O	2.49	0.44
1:D:100:LEU:O	1:D:104:LEU:HG	2.17	0.44
1:A:15:GLU:O	1:A:69:LYS:NZ	2.50	0.44
1:B:300:ILE:C	1:B:300:ILE:CD1	2.80	0.44
1:D:13:TRP:O	1:D:14:LYS:HD3	2.18	0.44
1:D:151:LYS:CG	1:D:154:ASP:OD2	2.64	0.44
1:D:322:HIS:HB2	1:D:339:TYR:HD2	1.82	0.44
1:A:117:VAL:O	1:A:121:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ALA:CB	1:A:329:ILE:HD13	2.46	0.44
1:C:47:THR:O	1:C:47:THR:HG22	2.17	0.44
1:C:52:GLY:HA3	1:C:166:ALA:HB1	1.98	0.44
1:A:12:GLU:OE2	1:A:14:LYS:NZ	2.51	0.44
1:A:250:ASN:OD1	2:A:501:MRU:H3	2.17	0.44
1:B:94:ARG:HB3	3:B:519:HOH:O	2.16	0.44
1:B:322:HIS:HA	1:B:325:ILE:CD1	2.43	0.44
1:D:162:ALA:HA	2:D:504:MRU:S1	2.57	0.44
1:A:145:ASN:ND2	1:A:333:GLY:HA2	2.33	0.44
1:C:64:LEU:HD11	1:C:83:LEU:HD22	1.98	0.44
1:C:147:LEU:HD22	1:C:179:LEU:HG	1.98	0.44
1:D:345:GLN:CA	1:D:348:LYS:HE2	2.46	0.44
1:A:100:LEU:HD12	1:A:104:LEU:HD22	2.00	0.44
1:A:343:ILE:O	1:A:346:LEU:HB3	2.17	0.44
1:D:232:ILE:HB	1:D:266:ILE:HD13	1.99	0.44
1:C:193:GLU:CB	1:C:201:SER:HB2	2.48	0.44
1:D:251:LYS:HB2	2:D:504:MRU:O2	2.17	0.44
1:A:341:GLU:O	1:A:345:GLN:CG	2.64	0.43
1:B:50:VAL:O	1:B:50:VAL:HG13	2.17	0.43
1:B:153:GLY:HA2	1:B:186:GLY:O	2.18	0.43
1:A:189:ILE:N	1:A:189:ILE:HD12	2.33	0.43
1:C:207:GLU:HB2	3:C:557:HOH:O	2.17	0.43
1:A:243:ALA:C	1:A:245:ASN:N	2.74	0.43
1:A:335:MET:CE	1:A:342:GLU:HG2	2.48	0.43
1:B:33:LEU:CD2	1:B:33:LEU:N	2.80	0.43
1:B:259:ILE:HG13	1:B:324:LEU:HD11	2.00	0.43
1:C:245:ASN:HB2	1:C:283:CYS:HA	2.00	0.43
1:C:252:ILE:HG12	1:D:222:MET:HG2	2.00	0.43
1:D:162:ALA:HB3	1:D:173:ALA:HB3	2.00	0.43
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.86	0.43
1:C:185:LEU:C	1:C:185:LEU:HD23	2.43	0.43
1:D:189:ILE:HD13	1:D:213:ILE:CG2	2.48	0.43
1:A:300:ILE:HG12	1:A:301:SER:N	2.34	0.43
1:A:189:ILE:HD13	1:A:213:ILE:HG22	2.01	0.43
1:C:47:THR:O	1:C:48:LEU:HB2	2.18	0.43
1:C:51:ARG:HH22	1:C:166:ALA:HB2	1.84	0.43
1:D:225:HIS:NE2	1:D:229:GLU:HG3	2.33	0.43
1:A:76:VAL:O	1:A:79:PHE:HB3	2.19	0.43
1:B:94:ARG:HA	1:B:95:PRO:HD3	1.73	0.43
1:D:37:THR:HB	1:D:39:GLU:OE1	2.18	0.43
1:D:308:SER:O	1:D:309:ASN:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ALA:HB1	1:A:34:GLU:HG2	2.01	0.43
1:B:22:ASN:CB	1:B:33:LEU:HD21	2.40	0.43
1:C:47:THR:O	1:C:47:THR:CG2	2.67	0.43
1:D:97:ALA:HB2	1:D:240:ASP:OD1	2.19	0.43
1:A:210:GLN:O	1:A:210:GLN:HG2	2.19	0.43
1:B:1:MET:HG2	1:B:210:GLN:HG2	2.00	0.43
1:B:310:VAL:HA	1:B:311:PRO:HD3	1.91	0.43
1:D:175:ALA:N	1:D:176:PRO:CD	2.82	0.43
1:A:276:THR:O	1:A:276:THR:HG22	2.19	0.42
1:C:162:ALA:HA	2:C:503:MRU:S1	2.58	0.42
1:B:25:LYS:NZ	1:B:31:GLU:OE1	2.50	0.42
1:B:181:LYS:HE3	1:B:212:GLY:O	2.18	0.42
1:B:227:MET:HE3	1:B:264:PHE:CE2	2.55	0.42
1:A:304:ARG:HH12	1:B:28:ASP:HA	1.84	0.42
1:B:338:ASN:OD1	1:B:341:GLU:CB	2.66	0.42
1:C:1:MET:O	1:C:1:MET:SD	2.77	0.42
1:C:14:LYS:C	1:C:16:THR:H	2.23	0.42
1:C:300:ILE:O	1:C:301:SER:HB2	2.19	0.42
1:B:239:ALA:HA	1:B:250:ASN:OD1	2.19	0.42
1:D:87:LYS:HG3	1:D:104:LEU:HB3	2.01	0.42
1:A:151:LYS:HA	1:A:151:LYS:CE	2.41	0.42
1:C:241:ARG:HD2	1:C:287:ILE:HG12	2.01	0.42
1:C:251:LYS:HB2	2:C:503:MRU:O2	2.20	0.42
1:C:341:GLU:HG3	1:C:344:GLU:OE1	2.20	0.42
1:A:113:ASN:HB2	3:A:510:HOH:O	2.18	0.42
1:A:277:PHE:HB2	1:A:347:PHE:CZ	2.53	0.42
1:B:35:LEU:N	1:B:35:LEU:CD1	2.82	0.42
1:D:125:VAL:O	1:D:129:ILE:HD12	2.19	0.42
1:B:98:ILE:HG23	1:B:99:ASN:N	2.35	0.42
1:B:284:GLY:O	1:B:319:ILE:HD13	2.19	0.42
1:C:160:CYS:HA	1:C:194:THR:HG21	2.02	0.42
1:C:293:ASP:HA	1:C:294:PRO:HD3	1.86	0.42
1:D:147:LEU:HD22	1:D:179:LEU:CD2	2.49	0.42
1:D:295:GLU:OE1	1:D:298:ARG:NE	2.46	0.42
1:A:8:PRO:HG3	1:A:169:ARG:CD	2.49	0.42
1:B:300:ILE:HG12	1:B:301:SER:N	2.33	0.42
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.90	0.41
1:B:38:LYS:HD3	1:B:89:TYR:HE2	1.85	0.41
1:D:147:LEU:HD22	1:D:179:LEU:HG	2.02	0.41
1:D:172:THR:OG1	1:D:173:ALA:N	2.52	0.41
1:B:341:GLU:CG	1:C:25:LYS:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ALA:HA	1:D:250:ASN:OD1	2.20	0.41
1:A:307:PRO:O	1:A:310:VAL:HG12	2.20	0.41
1:B:69:LYS:C	1:B:71:ILE:H	2.29	0.41
1:B:147:LEU:HD13	1:B:180:ALA:HB2	2.02	0.41
1:B:234:ALA:HA	1:B:266:ILE:HG22	2.02	0.41
1:B:244:LYS:O	1:B:244:LYS:HG2	2.19	0.41
1:B:341:GLU:HG3	1:C:25:LYS:HE3	2.02	0.41
1:A:312:VAL:CG1	1:A:313:PHE:N	2.83	0.41
1:D:155:ARG:HD3	1:D:230:LYS:O	2.21	0.41
1:D:172:THR:O	1:D:176:PRO:HD3	2.21	0.41
1:D:227:MET:HA	1:D:232:ILE:HG13	2.02	0.41
1:A:62:PHE:O	1:A:66:LEU:HB2	2.21	0.41
1:A:244:LYS:NZ	1:A:244:LYS:CB	2.84	0.41
1:B:292:ARG:O	1:B:293:ASP:C	2.63	0.41
1:B:147:LEU:CD1	1:B:180:ALA:HB2	2.49	0.41
1:B:71:ILE:HD11	1:B:86:ILE:HD12	2.03	0.41
1:B:78:GLU:CD	1:B:81:ARG:HH11	2.29	0.41
1:C:300:ILE:N	1:C:303:VAL:O	2.49	0.41
1:D:247:ASP:OD1	1:D:321:PRO:HA	2.19	0.41
1:D:297:VAL:O	1:D:297:VAL:CG1	2.69	0.41
1:A:175:ALA:N	1:A:176:PRO:HD2	2.35	0.41
1:B:145:ASN:HA	1:B:148:GLN:NE2	2.27	0.41
1:C:348:LYS:NZ	1:C:348:LYS:CB	2.81	0.41
1:A:192:CYS:HB3	1:A:220:ASP:OD1	2.21	0.41
1:A:304:ARG:HH11	1:B:28:ASP:CG	2.28	0.41
1:B:300:ILE:C	1:B:302:GLY:N	2.79	0.41
1:D:79:PHE:CE2	1:D:120:ALA:HB1	2.55	0.41
1:D:107:LEU:HD23	1:D:124:LEU:HD22	2.03	0.41
1:A:151:LYS:HZ3	1:A:185:LEU:CD1	2.31	0.41
1:B:152:LYS:HE2	1:B:152:LYS:HB3	1.91	0.41
1:B:295:GLU:OE2	1:B:298:ARG:HD2	2.21	0.41
1:C:146:ALA:HB3	1:C:176:PRO:HG3	2.03	0.41
1:D:322:HIS:HB2	1:D:339:TYR:CD2	2.55	0.41
1:A:108:SER:O	1:A:111:VAL:HG22	2.21	0.40
1:C:45:ILE:HG23	3:C:513:HOH:O	2.20	0.40
1:D:1:MET:CG	1:D:2:THR:H	2.34	0.40
1:D:236:ILE:HA	1:D:269:PHE:O	2.21	0.40
1:A:159:ILE:HG12	1:A:160:CYS:N	2.36	0.40
1:D:190:TYR:OH	1:D:230:LYS:HD2	2.21	0.40
1:A:243:ALA:C	1:A:245:ASN:H	2.28	0.40
1:B:7:VAL:CG1	1:B:8:PRO:HD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:MET:HE1	1:B:260:LEU:CG	2.52	0.40
1:C:283:CYS:SG	1:C:285:ALA:HB3	2.62	0.40
1:D:146:ALA:HB3	1:D:176:PRO:CG	2.48	0.40
1:D:332:LYS:HD3	1:D:332:LYS:HA	1.87	0.40
1:C:95:PRO:HG2	1:C:290:GLU:HB2	2.02	0.40
1:C:98:ILE:HD12	1:C:278:ASP:CG	2.46	0.40
1:D:9:ARG:O	1:D:21:LEU:HB2	2.21	0.40
1:D:195:ARG:CD	1:D:198:LEU:HD21	2.52	0.40
3:C:544:HOH:O	1:D:225:HIS:HD2	2.04	0.40
1:D:13:TRP:CZ3	1:D:66:LEU:HB2	2.56	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	347/374 (93%)	325 (94%)	21 (6%)	1 (0%)	36	50
1	B	347/374 (93%)	314 (90%)	29 (8%)	4 (1%)	10	16
1	C	347/374 (93%)	332 (96%)	14 (4%)	1 (0%)	36	50
1	D	347/374 (93%)	329 (95%)	14 (4%)	4 (1%)	10	16
All	All	1388/1496 (93%)	1300 (94%)	78 (6%)	10 (1%)	18	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	SER
1	D	93	SER
1	B	337	GLY
1	D	73	THR
1	D	348	LYS

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Mol	Chain	Res	Type
1	B	70	ASP
1	B	95	PRO
1	A	95	PRO
1	C	95	PRO
1	D	95	PRO

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	291/313 (93%)	261 (90%)	30 (10%)	7	11
1	B	291/313 (93%)	267 (92%)	24 (8%)	10	18
1	C	291/313 (93%)	266 (91%)	25 (9%)	10	16
1	D	291/313 (93%)	262 (90%)	29 (10%)	7	11
All	All	1164/1252 (93%)	1056 (91%)	108 (9%)	8	14

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	29	GLU
1	A	51	ARG
1	A	66	LEU
1	A	76	VAL
1	A	78	GLU
1	A	88	GLN
1	A	90	LEU
1	A	101	SER
1	A	104	LEU
1	A	112	GLU
1	A	119	GLU
1	A	123	ASN
1	A	132	GLN
1	A	151	LYS
1	A	201	SER

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Mol	Chain	Res	Type
1	A	233	SER
1	A	240	ASP
1	A	244	LYS
1	A	257	LEU
1	A	259	ILE
1	A	281	VAL
1	A	295	GLU
1	A	300	ILE
1	A	301	SER
1	A	323	ASP
1	A	342	GLU
1	A	343	ILE
1	A	345	GLN
1	A	346	LEU
1	B	33	LEU
1	B	38	LYS
1	B	48	LEU
1	B	51	ARG
1	B	66	LEU
1	B	70	ASP
1	B	73	THR
1	B	74	ASP
1	B	75	ASN
1	B	106	ARG
1	B	124	LEU
1	B	184	ASP
1	B	185	LEU
1	B	187	LEU
1	B	194	THR
1	B	233	SER
1	B	257	LEU
1	B	259	ILE
1	B	260	LEU
1	B	282	LYS
1	B	300	ILE
1	B	312	VAL
1	B	323	ASP
1	B	342	GLU
1	C	12	GLU
1	C	16	THR
1	C	27	PRO
1	C	31	GLU

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Mol	Chain	Res	Type
1	C	34	GLU
1	C	37	THR
1	C	46	VAL
1	C	51	ARG
1	C	71	ILE
1	C	72	GLU
1	C	88	GLN
1	C	98	ILE
1	C	116	SER
1	C	118	ASN
1	C	148	GLN
1	C	151	LYS
1	C	155	ARG
1	C	189	ILE
1	C	244	LYS
1	C	251	LYS
1	C	260	LEU
1	C	279	THR
1	C	282	LYS
1	C	345	GLN
1	C	348	LYS
1	D	2	THR
1	D	15	GLU
1	D	16	THR
1	D	21	LEU
1	D	26	LEU
1	D	33	LEU
1	D	51	ARG
1	D	74	ASP
1	D	78	GLU
1	D	81	ARG
1	D	90	LEU
1	D	93	SER
1	D	95	PRO
1	D	98	ILE
1	D	137	GLU
1	D	144	GLN
1	D	148	GLN
1	D	182	GLN
1	D	183	LYS
1	D	184	ASP
1	D	209	MET

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Mol	Chain	Res	Type
1	D	240	ASP
1	D	244	LYS
1	D	245	ASN
1	D	265	ASP
1	D	281	VAL
1	D	299	GLN
1	D	300	ILE
1	D	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	88	GLN
1	A	99	ASN
1	A	132	GLN
1	A	144	GLN
1	A	161	ASN
1	A	182	GLN
1	A	225	HIS
1	A	338	ASN
1	A	345	GLN
1	B	91	ASN
1	B	132	GLN
1	B	148	GLN
1	B	161	ASN
1	B	231	GLN
1	C	99	ASN
1	C	161	ASN
1	C	225	HIS
1	C	338	ASN
1	D	24	GLN
1	D	88	GLN
1	D	109	HIS
1	D	132	GLN
1	D	161	ASN
1	D	188	HIS
1	D	225	HIS
1	D	309	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	MRU	A	501	-	13,14,14	4.52	11 (84%)	10,19,19	2.66	3 (30%)
2	MRU	D	504	-	13,14,14	0.71	0	10,19,19	1.00	0
2	MRU	B	502	-	13,14,14	1.69	5 (38%)	10,19,19	1.99	3 (30%)
2	MRU	C	503	-	13,14,14	0.71	0	10,19,19	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MRU	A	501	-	-	13/17/17/17	-
2	MRU	D	504	-	-	7/17/17/17	-
2	MRU	B	502	-	-	8/17/17/17	-
2	MRU	C	503	-	-	15/17/17/17	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MRU	O2-C2	-9.38	1.06	1.21
2	A	501	MRU	P1-O1P	-6.95	1.29	1.54
2	A	501	MRU	P1-O3P	-6.43	1.30	1.50
2	A	501	MRU	P1-O2P	-5.52	1.34	1.54
2	A	501	MRU	C5-S1	-3.58	1.72	1.81
2	A	501	MRU	O3-C3	-3.52	1.35	1.42
2	A	501	MRU	P1-O1	-3.48	1.49	1.60
2	B	502	MRU	C1-C2	2.56	1.55	1.51
2	B	502	MRU	P1-O2P	-2.45	1.45	1.54
2	A	501	MRU	C6-S1	-2.28	1.64	1.78
2	B	502	MRU	P1-O1P	-2.26	1.46	1.54
2	B	502	MRU	P1-O3P	-2.25	1.43	1.50
2	A	501	MRU	O4-C4	-2.13	1.38	1.43
2	A	501	MRU	C1-C2	2.12	1.54	1.51
2	A	501	MRU	O1-C1	-2.06	1.41	1.43
2	B	502	MRU	C5-S1	-2.06	1.76	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MRU	O4-C4-C3	6.85	119.63	109.67
2	B	502	MRU	O2P-P1-O1	-5.04	93.54	106.67
2	A	501	MRU	C6-S1-C5	3.26	119.22	101.71
2	A	501	MRU	O1P-P1-O3P	2.52	120.66	110.83
2	B	502	MRU	O2-C2-C1	2.25	124.93	120.44
2	B	502	MRU	O1P-P1-O1	2.06	112.05	106.67

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MRU	C1-O1-P1-O1P
2	A	501	MRU	C1-O1-P1-O2P
2	A	501	MRU	O1-C1-C2-O2
2	A	501	MRU	O1-C1-C2-C3
2	A	501	MRU	C1-C2-C3-O3
2	A	501	MRU	O2-C2-C3-O3
2	A	501	MRU	C2-C3-C4-O4
2	A	501	MRU	C2-C3-C4-C5
2	A	501	MRU	O3-C3-C4-O4
2	A	501	MRU	O3-C3-C4-C5

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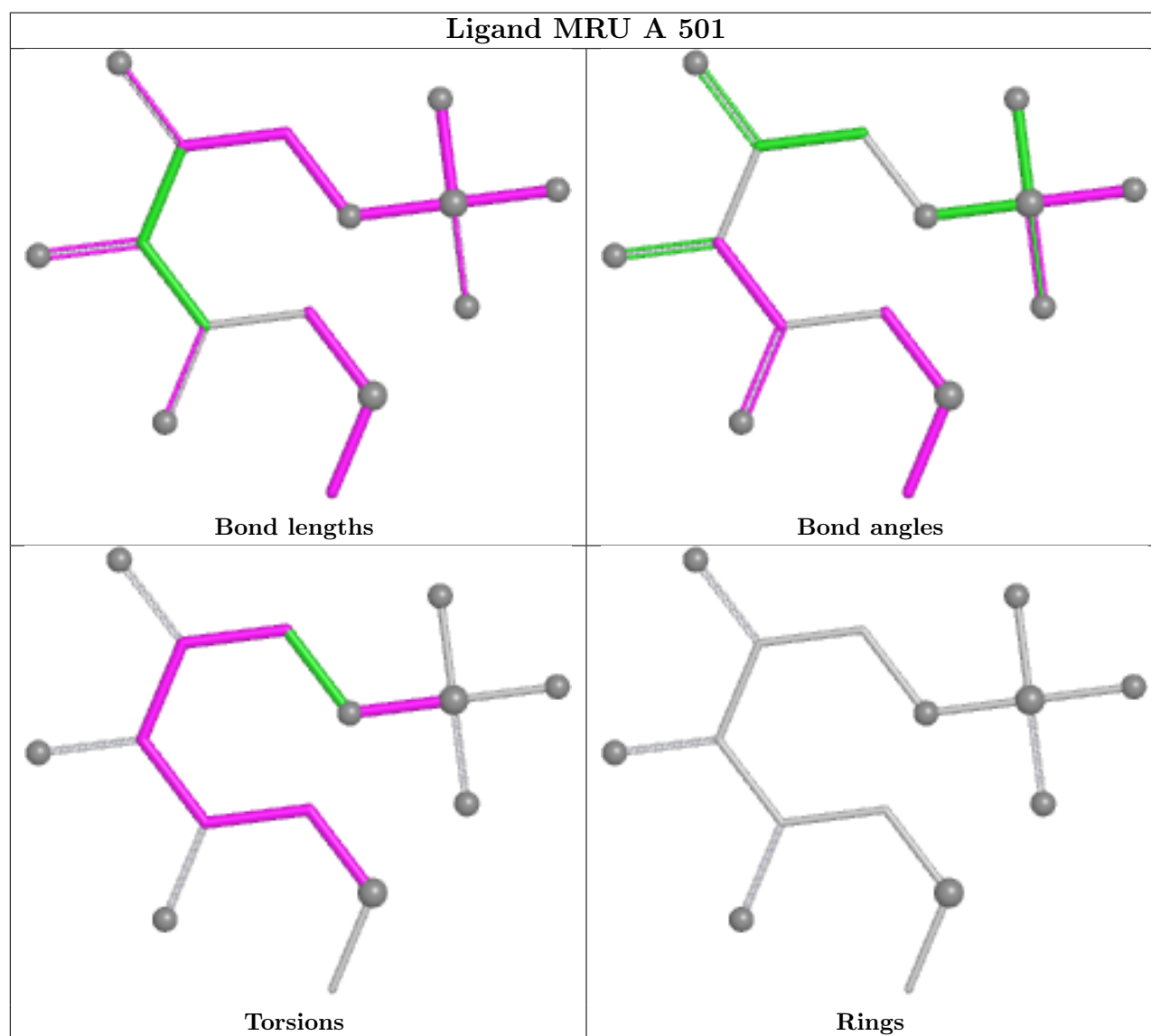
Mol	Chain	Res	Type	Atoms
2	A	501	MRU	C3-C4-C5-S1
2	B	502	MRU	C1-O1-P1-O1P
2	B	502	MRU	C1-O1-P1-O2P
2	B	502	MRU	C3-C4-C5-S1
2	B	502	MRU	O4-C4-C5-S1
2	C	503	MRU	C1-O1-P1-O3P
2	C	503	MRU	C1-O1-P1-O2P
2	C	503	MRU	O1-C1-C2-O2
2	C	503	MRU	O1-C1-C2-C3
2	C	503	MRU	C1-C2-C3-C4
2	C	503	MRU	O2-C2-C3-O3
2	C	503	MRU	O2-C2-C3-C4
2	C	503	MRU	C2-C3-C4-O4
2	C	503	MRU	C2-C3-C4-C5
2	C	503	MRU	O3-C3-C4-O4
2	C	503	MRU	C3-C4-C5-S1
2	C	503	MRU	O4-C4-C5-S1
2	D	504	MRU	O1-C1-C2-O2
2	D	504	MRU	O1-C1-C2-C3
2	D	504	MRU	O3-C3-C4-O4
2	D	504	MRU	O3-C3-C4-C5
2	D	504	MRU	C3-C4-C5-S1
2	D	504	MRU	O4-C4-C5-S1
2	A	501	MRU	C1-O1-P1-O3P
2	B	502	MRU	C1-O1-P1-O3P
2	C	503	MRU	O3-C3-C4-C5
2	B	502	MRU	O2-C2-C3-O3
2	D	504	MRU	C4-C5-S1-C6
2	B	502	MRU	C4-C5-S1-C6
2	C	503	MRU	C1-O1-P1-O1P
2	B	502	MRU	C1-C2-C3-O3
2	A	501	MRU	C4-C5-S1-C6
2	C	503	MRU	C4-C5-S1-C6

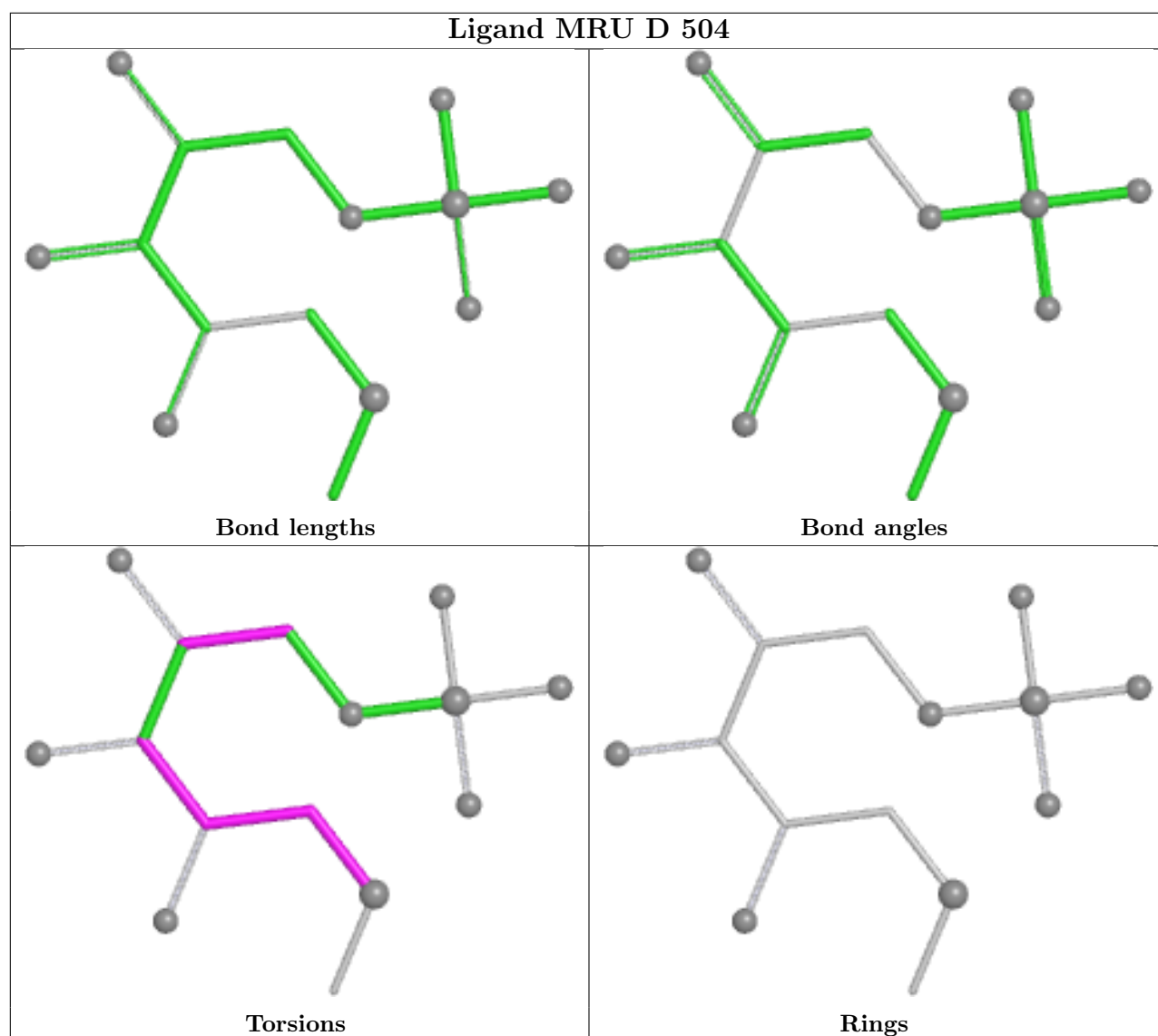
There are no ring outliers.

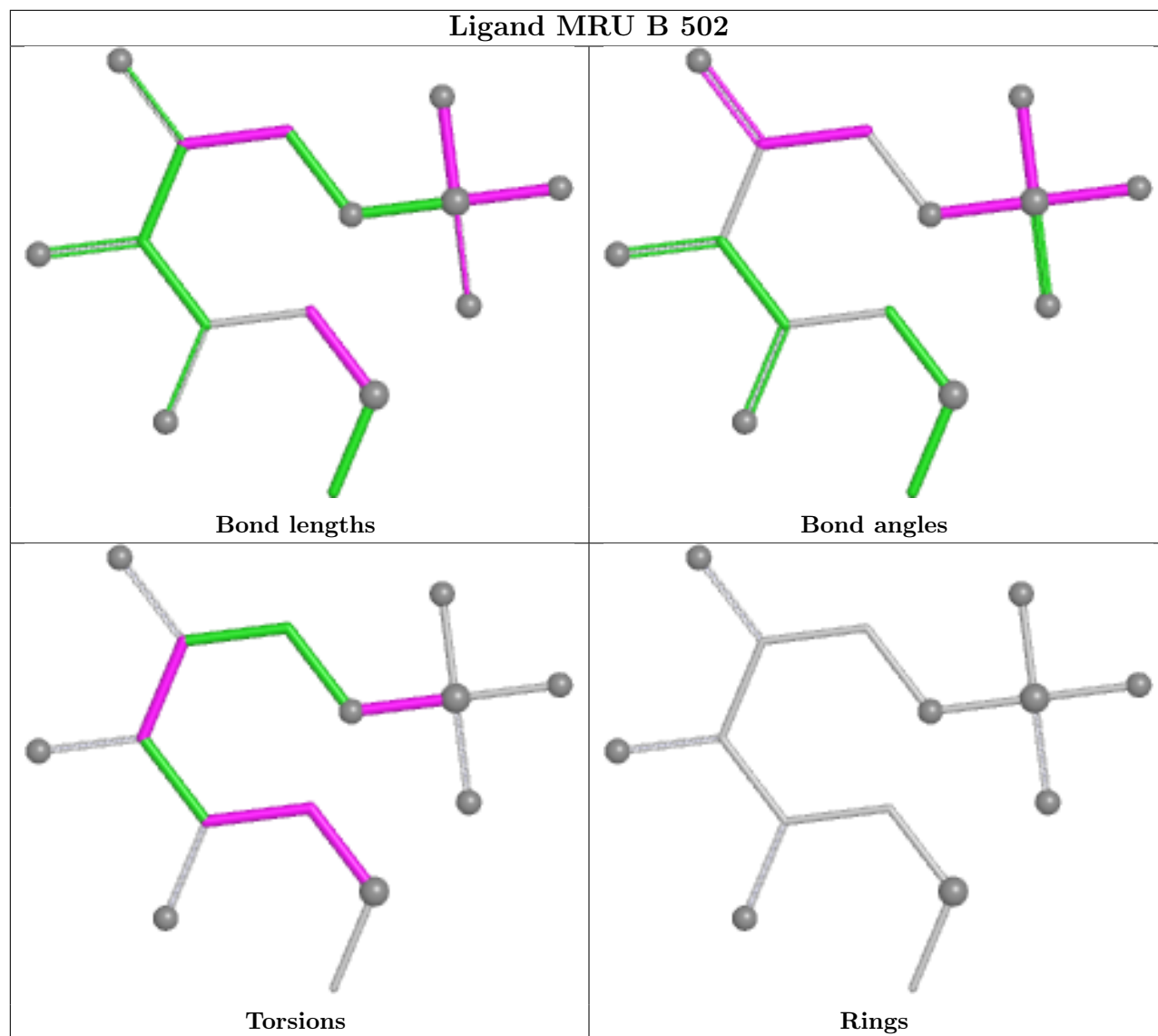
4 monomers are involved in 16 short contacts:

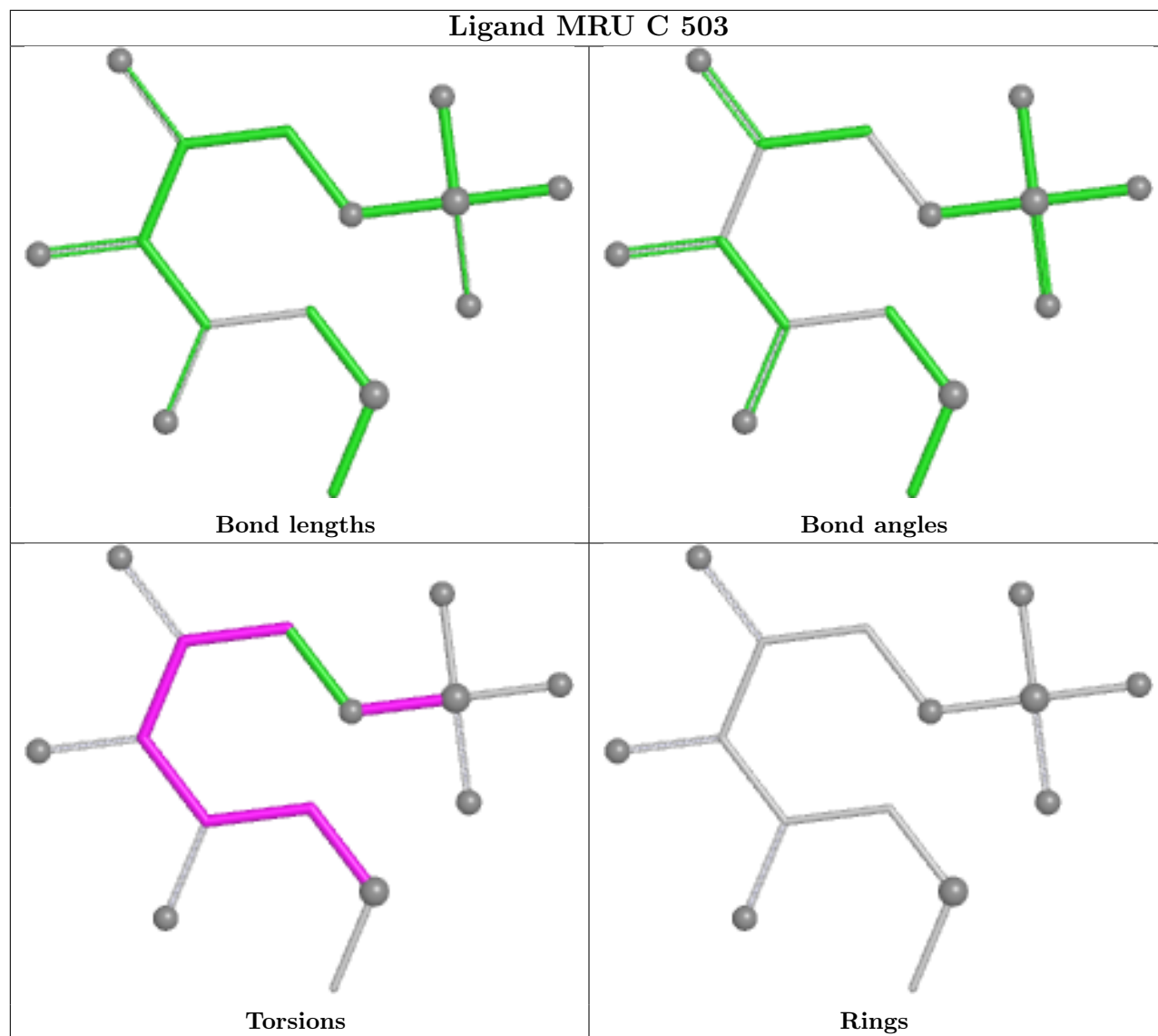
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MRU	1	0
2	D	504	MRU	7	0
2	B	502	MRU	5	0
2	C	503	MRU	3	0

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.









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	349/374 (93%)	0.08	4 (1%) 78 74	12, 25, 42, 64	0
1	B	349/374 (93%)	0.11	5 (1%) 73 69	16, 26, 45, 59	0
1	C	349/374 (93%)	0.10	5 (1%) 73 69	10, 25, 45, 61	0
1	D	349/374 (93%)	0.09	6 (1%) 69 65	14, 25, 41, 60	0
All	All	1396/1496 (93%)	0.09	20 (1%) 73 69	10, 25, 43, 64	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	GLY	3.8
1	A	349	GLY	3.6
1	B	349	GLY	3.4
1	B	300	ILE	3.2
1	D	301	SER	3.1
1	B	74	ASP	2.7
1	B	1	MET	2.5
1	C	1	MET	2.5
1	D	300	ILE	2.4
1	C	154	ASP	2.3
1	D	348	LYS	2.3
1	B	248	THR	2.3
1	A	343	ILE	2.2
1	D	303	VAL	2.2
1	D	186	GLY	2.2
1	C	300	ILE	2.2
1	A	154	ASP	2.2
1	A	347	PHE	2.1
1	C	349	GLY	2.1
1	C	248	THR	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](#)

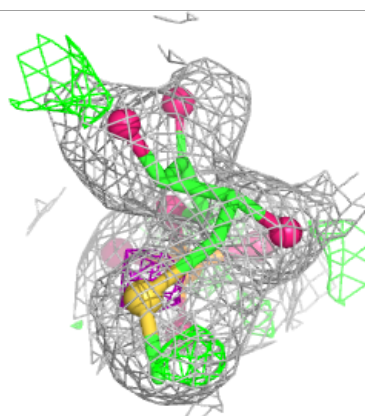
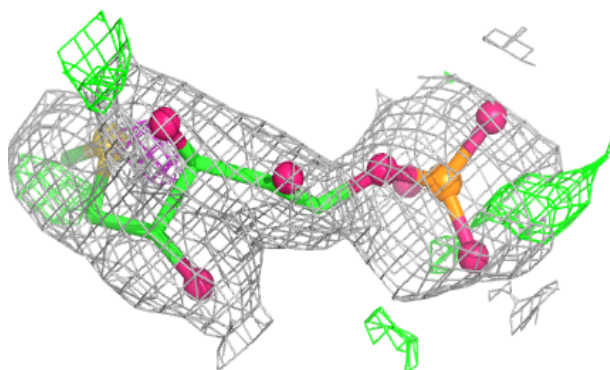
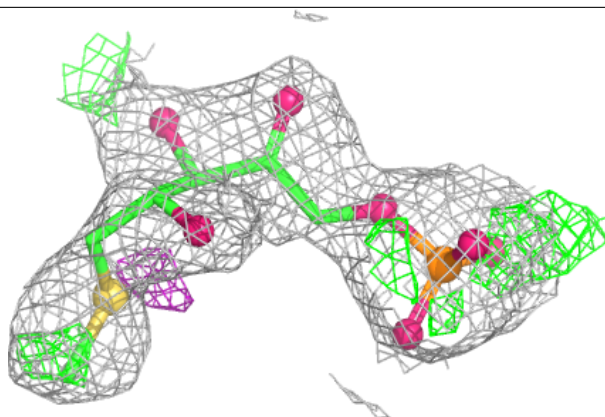
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MRU	D	504	15/15	0.83	0.19	40,49,54,54	0
2	MRU	C	503	15/15	0.87	0.17	49,55,57,58	0
2	MRU	B	502	15/15	0.88	0.18	61,66,68,69	0
2	MRU	A	501	15/15	0.93	0.11	42,49,53,54	0

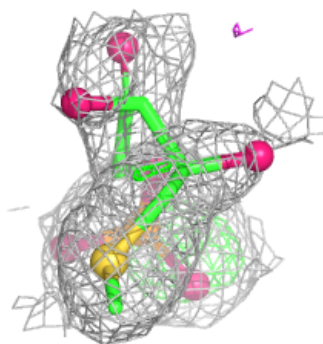
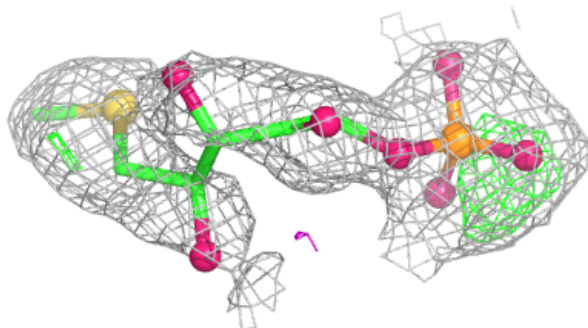
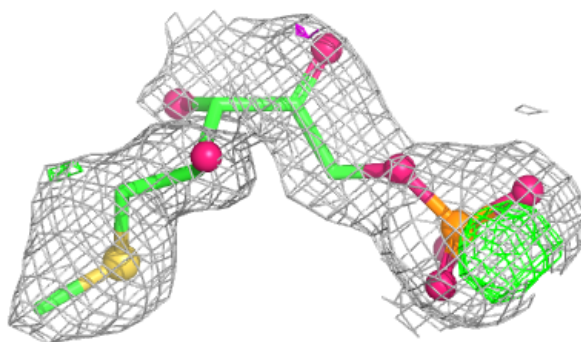
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MRU D 504:

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

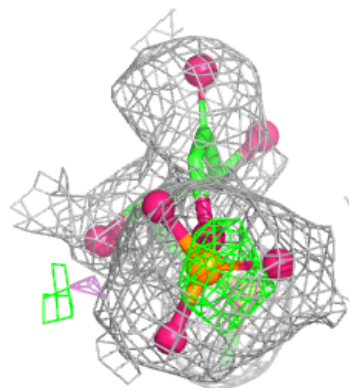
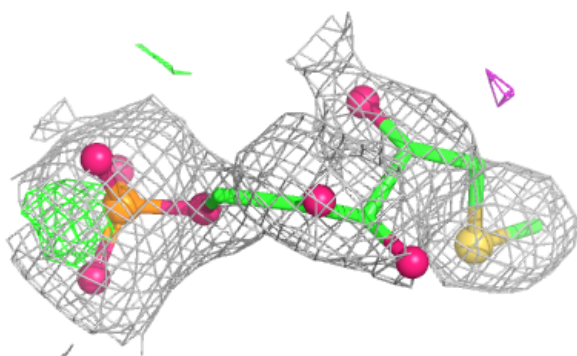
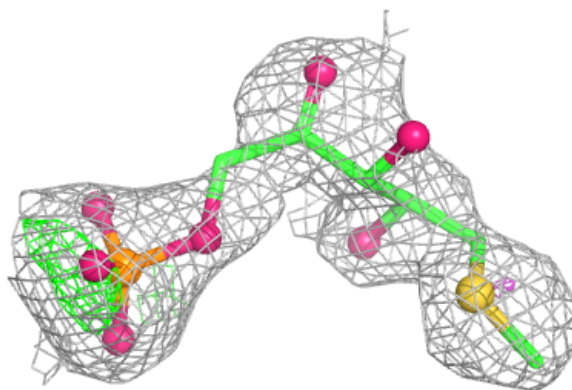
**Electron density around MRU C 503:**

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

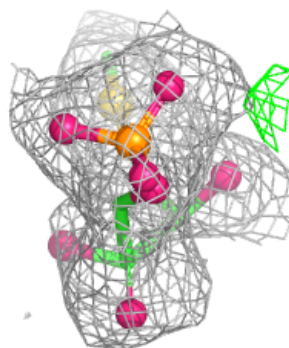
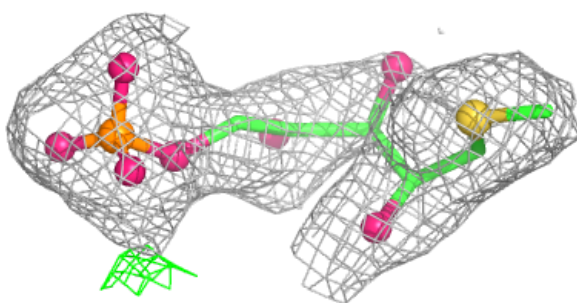
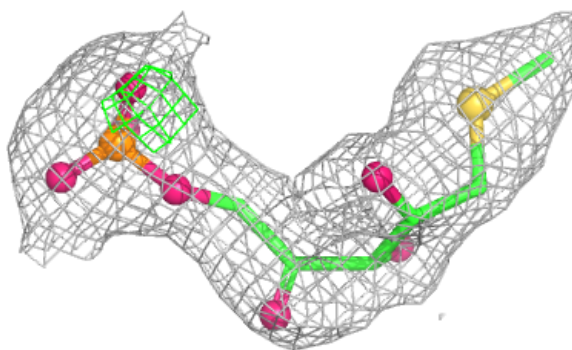


Electron density around MRU B 502:

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

**Electron density around MRU A 501:**

$2mF_o-DF_c$ (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.