



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2025 – 04:11 PM JST

PDB ID : 9IQQ / pdb_00009iqq
Title : Crystal structure of PKM2 in complex with a natural activator
Authors : Chen, T.J.; Wang, W.C.
Deposited on : 2024-07-13
Resolution : 2.70 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

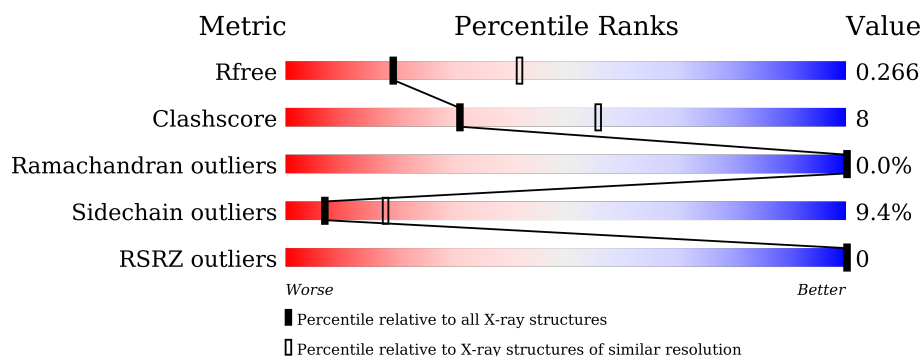
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	551	
1	B	551	
1	C	551	
1	D	551	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15854 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3942	2479	699	739	25			
1	B	503	Total	C	N	O	S	0	0	0
			3865	2429	687	725	24			
1	C	513	Total	C	N	O	S	0	0	0
			3935	2475	698	737	25			
1	D	506	Total	C	N	O	S	0	0	0
			3888	2445	691	727	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
B	-19	MET	-	initiating methionine	UNP P14618

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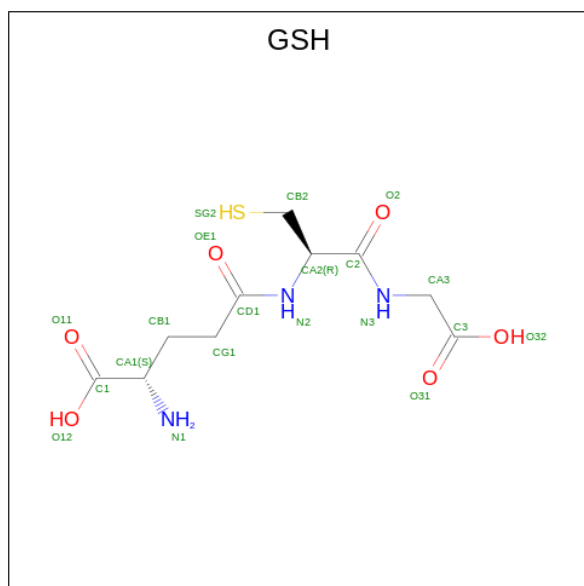
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
C	-19	MET	-	initiating methionine	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
D	-19	MET	-	initiating methionine	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618

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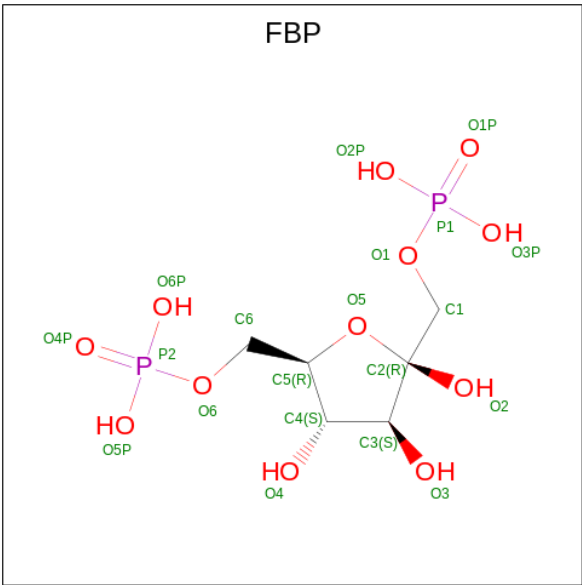
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			20	6	12	2		
3	C	1	Total	C	O	P	0	0
			20	6	12	2		
3	D	1	Total	C	O	P	0	0
			20	6	12	2		

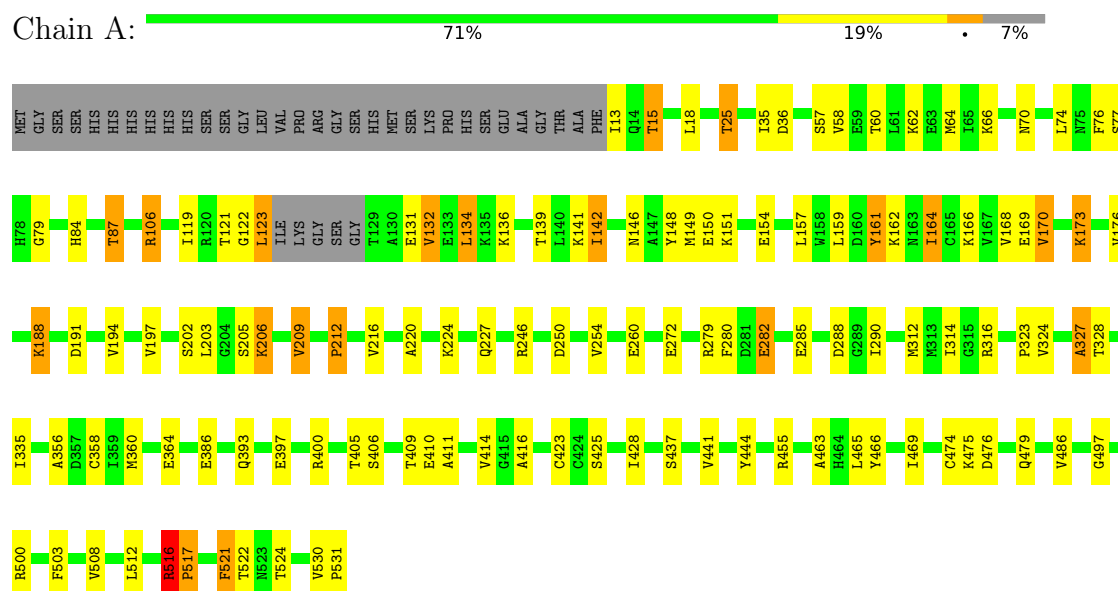
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	40	Total	O	0	0
			40	40		
4	C	34	Total	O	0	0
			34	34		
4	D	29	Total	O	0	0
			29	29		

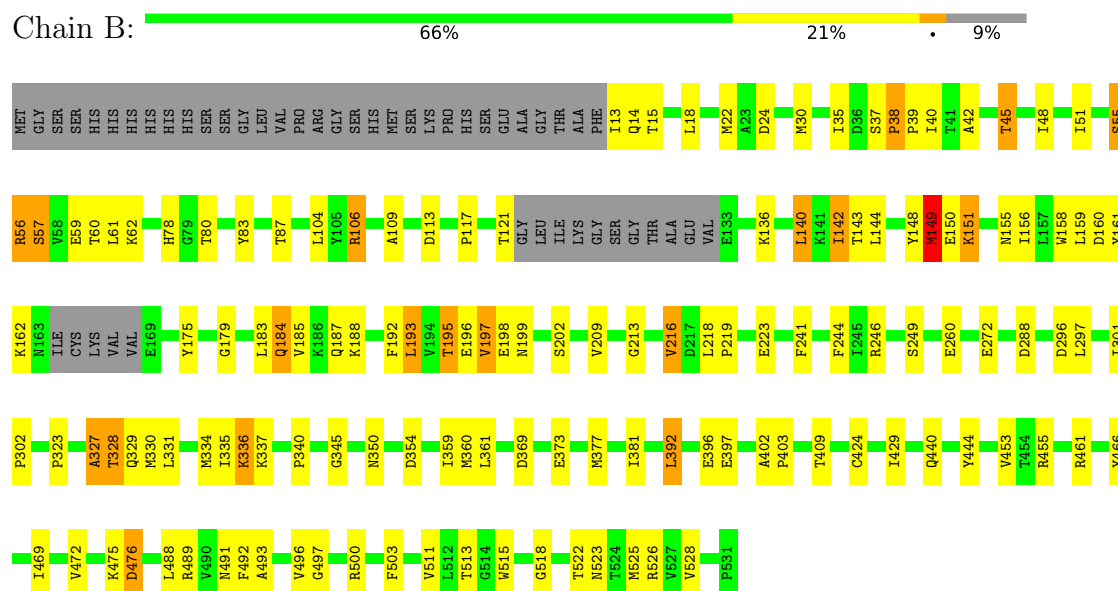
3 Residue-property plots [i](#)

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

• Molecule 1: Pyruvate kinase PKM

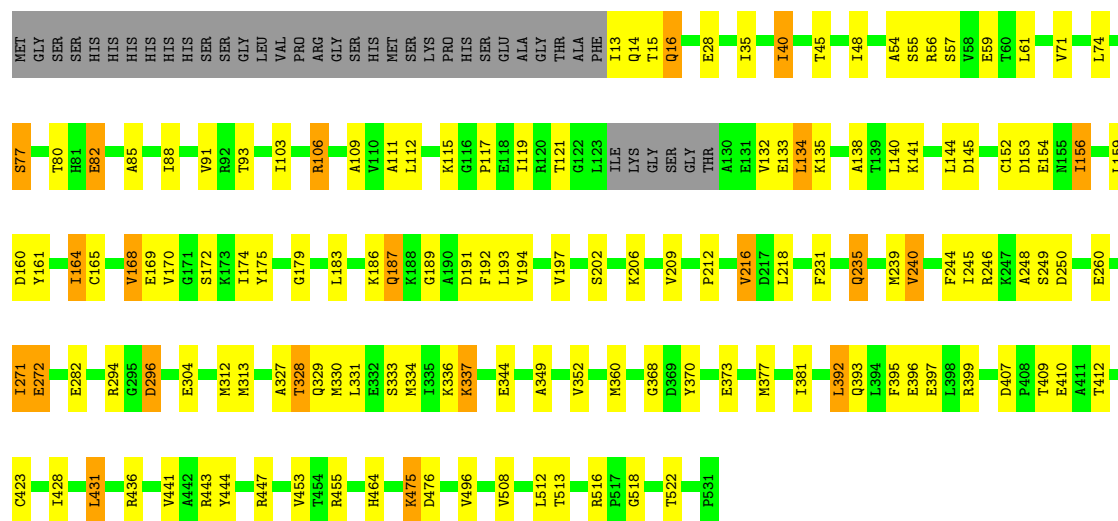


• Molecule 1: Pyruvate kinase PKM



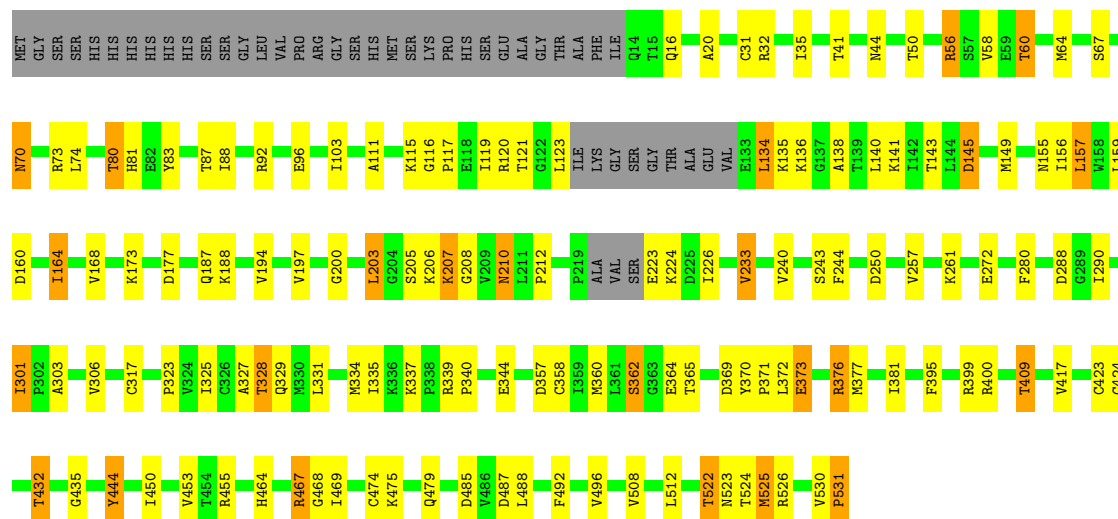
• Molecule 1: Pyruvate kinase PKM

Chain C:  68% 22% 7%



• Molecule 1: Pyruvate kinase PKM

Chain D:  66% 21% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.82Å 130.29Å 104.46Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.1 (30.00-2.70) 72.2 (30.00-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.256 , 0.264 0.257 , 0.266	Depositor DCC
R_{free} test set	2395 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15854	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

5.1 Standard geometry

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

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	0.92	0/4005	1.46	22/5409 (0.4%)
1	B	0.92	0/3927	1.42	22/5301 (0.4%)
1	C	0.91	0/3998	1.39	10/5399 (0.2%)
1	D	0.90	0/3950	1.41	15/5331 (0.3%)
All	All	0.91	0/15880	1.42	69/21440 (0.3%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	ALA	N-CA-C	8.68	123.82	112.72
1	B	327	ALA	N-CA-C	8.18	124.18	114.04
1	A	191	ASP	N-CA-C	-7.43	102.72	112.24
1	A	475	LYS	N-CA-C	-6.98	104.64	113.72
1	A	444	TYR	CB-CA-C	6.85	122.35	110.01
1	C	35	ILE	N-CA-C	-6.79	104.49	112.98
1	A	212	PRO	N-CA-C	6.73	123.09	113.47
1	C	447	ARG	N-CA-C	-6.70	104.12	112.90
1	C	328	THR	N-CA-C	6.68	120.35	109.59
1	A	76	PHE	CB-CA-C	6.67	122.25	110.37
1	B	38	PRO	N-CA-C	6.62	117.66	110.58
1	C	518	GLY	CA-C-O	-6.57	117.95	122.22
1	B	328	THR	N-CA-C	6.47	119.44	108.90
1	A	328	THR	N-CA-C	6.43	120.30	109.76
1	A	164	ILE	N-CA-C	-6.39	104.10	110.62
1	A	70	ASN	N-CA-C	-6.37	106.15	114.04
1	B	350	ASN	CB-CA-C	6.31	121.58	110.85
1	A	161	TYR	CB-CA-C	6.22	118.71	110.06
1	A	220	ALA	N-CA-C	-6.22	104.50	111.28
1	D	371	PRO	N-CA-C	6.19	121.70	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ARG	N-CA-C	-6.18	104.60	111.71
1	C	444	TYR	CB-CA-C	6.11	121.72	110.11
1	D	531	PRO	N-CA-CB	-6.10	96.29	103.00
1	D	328	THR	N-CA-C	6.10	119.46	109.76
1	D	35	ILE	N-CA-C	-6.05	105.13	113.00
1	C	77	SER	N-CA-C	-5.98	105.09	112.38
1	B	455	ARG	N-CA-C	-5.94	105.69	113.17
1	B	296	ASP	CB-CA-C	5.90	122.01	110.67
1	B	162	LYS	N-CA-C	-5.88	106.07	113.72
1	B	476	ASP	CB-CA-C	5.86	116.82	108.68
1	D	432	THR	CA-CB-OG1	-5.81	100.89	109.60
1	B	35	ILE	N-CA-C	-5.79	106.14	112.80
1	B	144	LEU	N-CA-C	-5.74	106.08	112.57
1	D	70	ASN	N-CA-C	-5.74	106.93	114.04
1	C	475	LYS	N-CA-C	-5.72	106.06	113.16
1	D	444	TYR	CB-CA-C	5.71	120.93	110.36
1	B	39	PRO	N-CA-C	5.67	119.58	111.13
1	A	79	GLY	CA-C-O	-5.66	118.54	122.22
1	D	56	ARG	CB-CA-C	-5.65	100.17	110.63
1	B	149	MET	N-CA-C	-5.57	105.21	111.28
1	C	455	ARG	N-CA-C	-5.56	106.85	113.97
1	B	518	GLY	CA-C-O	-5.48	118.19	122.52
1	A	76	PHE	N-CA-C	-5.47	106.46	113.02
1	A	36	ASP	CB-CA-C	5.45	119.94	110.72
1	A	524	THR	CB-CA-C	5.43	120.56	111.22
1	A	327	ALA	N-CA-C	5.34	122.19	110.80
1	B	213	GLY	N-CA-C	5.34	119.61	112.77
1	A	35	ILE	N-CA-C	-5.34	106.66	112.80
1	B	475	LYS	N-CA-C	-5.30	106.12	112.59
1	A	246	ARG	N-CA-C	-5.30	107.47	114.31
1	A	406	SER	N-CA-C	-5.30	106.50	113.17
1	B	444	TYR	CB-CA-C	5.30	119.54	110.01
1	D	188	LYS	CB-CA-C	-5.29	108.81	116.54
1	B	369	ASP	N-CA-C	-5.29	106.88	113.38
1	B	302	PRO	CB-CA-C	5.24	118.25	111.64
1	B	327	ALA	CA-C-N	-5.23	115.62	122.99
1	B	327	ALA	C-N-CA	-5.23	115.62	122.99
1	D	80	THR	N-CA-C	-5.22	102.17	109.69
1	A	386	GLU	N-CA-C	-5.15	105.66	111.28
1	D	455	ARG	N-CA-C	-5.14	106.41	113.30
1	C	160	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	516	ARG	CB-CA-C	5.08	120.18	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	THR	CB-CA-C	5.08	118.13	109.75
1	B	440	GLN	CB-CA-C	5.07	119.20	110.79
1	D	160	ASP	N-CA-C	-5.06	106.88	113.16
1	D	56	ARG	N-CA-C	-5.05	105.90	111.71
1	A	455	ARG	N-CA-C	-5.04	106.06	113.61
1	D	115	LYS	N-CA-C	-5.03	105.87	111.36
1	D	365	THR	CB-CA-C	5.01	118.07	109.15

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	3942	0	4024	56	0
1	B	3865	0	3935	67	0
1	C	3935	0	4017	68	0
1	D	3888	0	3966	76	0
2	B	20	0	15	1	0
3	B	20	0	10	1	0
3	C	20	0	10	0	0
3	D	20	0	10	0	0
4	A	41	0	0	0	0
4	B	40	0	0	0	0
4	C	34	0	0	1	0
4	D	29	0	0	0	0
All	All	15854	0	15987	257	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 8.

All (257) 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:D:117:PRO:HD2	1:D:244:PHE:HB2	1.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG23	1:A:203:LEU:HB3	1.54	0.89
1:C:16:GLN:HG2	1:C:40:ILE:HG22	1.61	0.82
1:B:185:VAL:HA	1:B:195:THR:HG21	1.62	0.80
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.65	0.79
1:A:134:LEU:HB3	1:A:197:VAL:HG11	1.67	0.77
1:C:153:ASP:HB3	1:C:156:ILE:HG13	1.69	0.74
1:D:123:LEU:HB2	1:D:149:MET:O	1.86	0.74
1:D:103:ILE:HG23	1:D:496:VAL:HA	1.73	0.69
1:D:123:LEU:HA	1:D:205:SER:HB3	1.75	0.68
1:A:148:TYR:HA	1:A:151:LYS:HG3	1.75	0.68
1:A:58:VAL:HG12	1:A:62:LYS:HE3	1.75	0.67
1:B:472:VAL:HG21	1:B:496:VAL:HG21	1.76	0.67
1:D:280:PHE:HE1	1:D:290:ILE:HG21	1.60	0.67
1:B:188:LYS:HA	1:B:193:LEU:HB3	1.76	0.67
1:A:122:GLY:HA2	1:A:206:LYS:H	1.59	0.66
1:C:331:LEU:HD23	1:C:344:GLU:HB3	1.78	0.66
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.77	0.65
1:D:136:LYS:HG3	1:D:200:GLY:HA3	1.79	0.65
1:D:134:LEU:HB2	1:D:203:LEU:HB2	1.79	0.64
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.79	0.64
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.79	0.63
1:A:159:LEU:HD21	1:A:209:VAL:HG21	1.79	0.63
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.80	0.63
1:C:103:ILE:HG23	1:C:496:VAL:HA	1.82	0.62
1:D:141:LYS:HG2	1:D:194:VAL:HG22	1.81	0.62
1:D:233:VAL:HG11	1:D:261:LYS:HB3	1.83	0.60
1:A:119:ILE:HG22	1:A:159:LEU:HD22	1.82	0.60
1:A:173:LYS:O	1:A:212:PRO:HD2	2.01	0.60
1:B:288:ASP:O	1:B:323:PRO:HD2	2.03	0.59
1:C:168:VAL:HG13	1:C:172:SER:HB2	1.84	0.59
1:D:73:ARG:HA	1:D:111:ALA:HB3	1.85	0.59
1:D:288:ASP:O	1:D:323:PRO:HD2	2.03	0.58
1:D:120:ARG:HD3	1:D:206:LYS:HG2	1.86	0.58
1:D:20:ALA:HB2	1:D:32:ARG:O	2.04	0.57
1:C:88:ILE:HD13	1:C:235:GLN:HG2	1.86	0.57
1:C:134:LEU:HB3	1:C:197:VAL:HG11	1.85	0.57
1:C:117:PRO:HD2	1:C:244:PHE:HB2	1.86	0.57
1:D:103:ILE:HA	1:D:496:VAL:HG22	1.86	0.57
1:D:370:TYR:HB3	1:D:373:GLU:OE1	2.05	0.57
1:C:272:GLU:HB2	1:C:296:ASP:HB2	1.87	0.56
1:A:170:VAL:HG22	1:A:188:LYS:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:THR:HG23	1:D:522:THR:HB	1.86	0.56
1:B:80:THR:HG23	1:B:83:TYR:H	1.71	0.56
1:A:280:PHE:HE1	1:A:290:ILE:HG21	1.71	0.56
1:A:84:HIS:HA	1:A:87:THR:HG23	1.88	0.56
1:C:170:VAL:HG13	1:C:186:LYS:HA	1.88	0.55
1:B:216:VAL:HG23	1:B:246:ARG:HD3	1.88	0.55
1:B:354:ASP:OD1	2:B:601:GSH:HA32	2.06	0.55
1:C:334:MET:HA	1:C:337:LYS:O	2.07	0.54
1:A:516:ARG:HB3	1:A:517:PRO:CD	2.37	0.54
1:C:431:LEU:HD22	1:C:453:VAL:HB	1.90	0.54
1:C:132:VAL:HG11	1:C:154:GLU:HB2	1.90	0.53
1:D:73:ARG:HH12	1:D:362:SER:HB3	1.73	0.53
1:D:334:MET:HA	1:D:337:LYS:O	2.09	0.53
1:D:119:ILE:O	1:D:208:GLY:HA2	2.09	0.53
1:B:15:THR:HG22	1:B:38:PRO:HD2	1.90	0.53
1:D:60:THR:O	1:D:64:MET:HG2	2.07	0.53
1:D:70:ASN:HB3	1:D:464:HIS:ND1	2.24	0.53
1:C:144:LEU:HB2	1:C:191:ASP:CB	2.39	0.53
1:D:67:SER:HB3	1:D:376:ARG:HD3	1.89	0.53
1:A:132:VAL:O	1:A:202:SER:HA	2.08	0.53
1:A:146:ASN:HA	1:A:149:MET:HB2	1.91	0.53
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.90	0.52
1:C:111:ALA:HB2	1:C:239:MET:HG3	1.91	0.52
1:C:121:THR:O	1:C:206:LYS:HA	2.08	0.52
1:B:331:LEU:HD12	1:B:361:LEU:HD21	1.92	0.52
1:C:396:GLU:HA	1:C:399:ARG:NH1	2.25	0.52
1:C:248:ALA:HB2	1:C:282:GLU:HG2	1.91	0.52
1:A:437:SER:HB3	1:A:522:THR:HG21	1.90	0.52
1:A:161:TYR:O	1:A:164:ILE:HG12	2.10	0.52
1:B:476:ASP:HB3	1:B:488:LEU:HD21	1.91	0.52
1:B:523:ASN:O	1:D:526:ARG:HA	2.10	0.52
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.92	0.52
1:B:429:ILE:O	1:B:511:VAL:HA	2.09	0.51
1:D:159:LEU:HD12	1:D:164:ILE:HD13	1.91	0.51
1:A:84:HIS:HA	1:A:87:THR:CG2	2.41	0.51
1:C:349:ALA:HB2	1:C:381:ILE:HG22	1.91	0.51
1:D:50:THR:HA	1:D:73:ARG:HB3	1.94	0.50
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.93	0.50
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.46	0.50
1:A:25:THR:HG22	1:B:397:GLU:HG2	1.94	0.50
1:B:59:GLU:HA	1:B:62:LYS:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:HG3	1:C:138:ALA:HB2	1.94	0.50
1:A:142:ILE:HG22	1:A:157:LEU:HB3	1.93	0.50
1:B:334:MET:HA	1:B:337:LYS:O	2.12	0.50
1:D:56:ARG:HB3	1:D:87:THR:HG22	1.94	0.49
1:B:55:SER:O	1:B:61:LEU:HG	2.11	0.49
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.94	0.49
1:B:183:LEU:HD23	1:B:197:VAL:HA	1.94	0.49
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.93	0.49
1:D:140:LEU:HD21	1:D:157:LEU:HD23	1.95	0.49
1:B:515:TRP:H	1:B:515:TRP:CD1	2.29	0.49
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.95	0.49
1:A:314:ILE:HD13	1:A:356:ALA:HB2	1.95	0.49
1:D:492:PHE:O	1:D:496:VAL:HG23	2.13	0.49
1:C:80:THR:OG1	1:C:82:GLU:HG3	2.13	0.48
1:C:174:ILE:HB	1:C:183:LEU:HD12	1.96	0.48
1:B:40:ILE:HD12	1:B:42:ALA:HB3	1.95	0.48
1:C:272:GLU:CB	1:C:296:ASP:HB2	2.43	0.48
1:D:143:THR:HG23	1:D:145:ASP:H	1.77	0.48
1:B:113:ASP:HA	1:B:241:PHE:HB2	1.96	0.48
1:D:303:ALA:HA	1:D:306:VAL:HG23	1.95	0.48
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.49	0.48
1:A:60:THR:O	1:A:64:MET:HG2	2.14	0.48
1:D:335:ILE:HG12	1:D:364:GLU:HA	1.95	0.48
1:C:45:THR:HG21	1:C:352:VAL:HG22	1.95	0.48
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.49	0.48
1:C:144:LEU:HB2	1:C:191:ASP:HB3	1.96	0.47
1:B:472:VAL:HG22	1:B:492:PHE:HE2	1.79	0.47
1:C:106:ARG:HH12	1:C:464:HIS:HE1	1.61	0.47
1:A:314:ILE:HG23	1:A:324:VAL:HG11	1.97	0.47
1:A:335:ILE:HG12	1:A:364:GLU:HA	1.95	0.47
1:A:405:THR:O	1:C:423:CYS:HA	2.14	0.47
1:B:409:THR:HG23	1:B:522:THR:HB	1.96	0.47
1:C:112:LEU:HB3	1:C:240:VAL:HG22	1.96	0.47
1:C:187:GLN:HB2	1:C:194:VAL:HB	1.96	0.47
1:C:132:VAL:CG1	1:C:154:GLU:HB2	2.45	0.47
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.96	0.47
1:D:92:ARG:O	1:D:96:GLU:HG2	2.14	0.47
1:D:116:GLY:HA3	1:D:243:SER:HB2	1.97	0.47
1:A:141:LYS:HG2	1:A:194:VAL:HG22	1.96	0.47
1:A:288:ASP:O	1:A:323:PRO:HD2	2.15	0.47
1:C:164:ILE:O	1:C:168:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:HG	1:D:135:LYS:H	1.79	0.46
1:D:210:ASN:HD22	1:D:210:ASN:HA	1.60	0.46
1:B:472:VAL:HG22	1:B:492:PHE:CE2	2.50	0.46
1:C:333:SER:HB2	1:C:337:LYS:HE3	1.96	0.46
1:D:450:ILE:HB	1:D:469:ILE:HA	1.96	0.46
1:B:14:GLN:O	1:B:37:SER:HA	2.16	0.46
1:D:226:ILE:HG23	1:D:257:VAL:HG13	1.97	0.46
1:C:141:LYS:HA	1:C:193:LEU:O	2.15	0.46
1:C:216:VAL:HG13	1:C:218:LEU:H	1.80	0.46
1:D:50:THR:OG1	1:D:362:SER:HA	2.15	0.46
1:A:279:ARG:O	1:A:282:GLU:HG3	2.16	0.46
1:B:121:THR:HA	1:B:158:TRP:O	2.16	0.46
1:C:312:MET:HG2	1:D:31:CYS:O	2.15	0.46
1:C:119:ILE:HG23	1:C:161:TYR:HB2	1.98	0.46
1:A:312:MET:HA	1:B:30:MET:O	2.16	0.46
1:D:423:CYS:O	1:D:424:CYS:C	2.59	0.46
1:C:111:ALA:CB	1:C:239:MET:HG3	2.46	0.46
1:C:409:THR:HG23	1:C:522:THR:HB	1.97	0.46
1:B:175:TYR:O	1:B:209:VAL:HA	2.16	0.45
1:C:165:CYS:SG	1:C:189:GLY:N	2.89	0.45
1:D:177:ASP:HA	1:D:207:LYS:HG3	1.98	0.45
1:C:294:ARG:NH2	1:C:330:MET:HG2	2.31	0.45
1:A:517:PRO:O	1:A:521:PHE:HE1	2.00	0.45
1:D:207:LYS:HA	1:D:207:LYS:HD3	1.66	0.45
1:D:376:ARG:H	1:D:376:ARG:HG2	1.62	0.45
1:B:297:LEU:O	1:B:301:ILE:HG12	2.17	0.45
1:D:44:ASN:HB3	1:D:468:GLY:HA2	1.98	0.45
1:D:120:ARG:HA	1:D:207:LYS:O	2.16	0.45
1:C:370:TYR:HB3	1:C:373:GLU:HB2	1.98	0.45
1:D:325:ILE:HG12	1:D:358:CYS:HB2	1.98	0.45
1:B:48:ILE:HB	1:B:360:MET:HG3	1.97	0.45
1:C:428:ILE:HG21	1:C:441:VAL:HG11	1.99	0.45
1:A:393:GLN:O	1:A:397:GLU:HG3	2.18	0.45
1:B:526:ARG:HA	1:D:523:ASN:O	2.17	0.45
1:C:159:LEU:HD22	1:C:209:VAL:HG21	1.99	0.44
1:D:357:ASP:HA	1:D:467:ARG:HB2	1.99	0.44
1:B:56:ARG:NH2	1:B:83:TYR:O	2.50	0.44
1:A:400:ARG:HG2	1:C:392:LEU:HD21	1.98	0.44
1:C:15:THR:C	1:C:16:GLN:HG3	2.42	0.44
1:C:117:PRO:HG3	1:C:246:ARG:HH21	1.83	0.44
1:C:334:MET:HE2	1:C:334:MET:HB3	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:HD21	1:D:400:ARG:HG2	1.99	0.44
1:D:417:VAL:HG21	1:D:444:TYR:HB2	1.99	0.44
1:B:327:ALA:HB1	1:B:360:MET:HE2	1.99	0.44
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.99	0.44
1:D:334:MET:O	1:D:370:TYR:HB2	2.18	0.44
1:B:453:VAL:HG21	1:B:493:ALA:HB2	2.00	0.43
1:C:77:SER:HA	1:C:115:LYS:HB2	1.99	0.43
1:D:210:ASN:O	1:D:212:PRO:HD3	2.18	0.43
1:B:489:ARG:HH12	3:B:602:FBP:P1	2.41	0.43
1:C:304:GLU:HB2	1:D:381:ILE:HA	2.00	0.43
1:D:530:VAL:HA	1:D:531:PRO:HD3	1.85	0.43
1:A:123:LEU:HD12	1:A:205:SER:CB	2.48	0.43
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.00	0.43
1:C:271:ILE:HG21	1:C:313:MET:SD	2.59	0.43
1:D:80:THR:H	1:D:83:TYR:CB	2.32	0.43
1:B:525:MET:HE3	1:D:525:MET:HE3	2.01	0.43
1:C:85:ALA:HB2	1:C:231:PHE:HZ	1.83	0.43
1:B:104:LEU:O	1:B:500:ARG:NH1	2.52	0.43
1:C:175:TYR:HE1	1:C:212:PRO:HG2	1.82	0.43
1:C:396:GLU:HA	1:C:399:ARG:HH11	1.83	0.43
1:D:395:PHE:CE2	1:D:399:ARG:HD2	2.54	0.43
1:D:432:THR:HG21	1:D:435:GLY:HA2	2.01	0.43
1:B:117:PRO:HD2	1:B:244:PHE:HB2	2.01	0.43
1:B:136:LYS:HG3	1:B:199:ASN:HA	1.99	0.43
1:B:142:ILE:HG23	1:B:192:PHE:HB2	2.01	0.43
1:B:402:ALA:HA	1:B:403:PRO:HD3	1.87	0.43
1:C:144:LEU:HD23	1:C:144:LEU:HA	1.83	0.43
1:C:189:GLY:HA3	1:C:192:PHE:CE1	2.53	0.43
1:A:411:ALA:O	1:A:414:VAL:HG12	2.19	0.43
1:A:164:ILE:O	1:A:168:VAL:HG22	2.19	0.43
1:D:187:GLN:HB2	1:D:194:VAL:HB	2.01	0.42
1:C:168:VAL:HA	4:C:708:HOH:O	2.18	0.42
1:A:121:THR:O	1:A:206:LYS:N	2.52	0.42
1:B:159:LEU:HD22	1:B:209:VAL:HG21	2.00	0.42
1:D:44:ASN:CB	1:D:468:GLY:HA2	2.49	0.42
1:A:224:LYS:O	1:A:227:GLN:HB2	2.19	0.42
1:A:123:LEU:C	1:A:123:LEU:HD13	2.45	0.42
1:B:109:ALA:HB2	1:B:461:ARG:HB3	2.01	0.42
1:C:245:ILE:HG23	1:C:250:ASP:HB2	2.02	0.42
1:D:512:LEU:HA	1:D:524:THR:O	2.19	0.42
1:B:106:ARG:HG2	1:B:500:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HD22	1:B:219:PRO:HD2	2.02	0.42
1:B:140:LEU:HB3	1:B:195:THR:O	2.18	0.42
1:B:193:LEU:H	1:B:193:LEU:HG	1.56	0.42
1:D:280:PHE:HZ	1:D:317:CYS:SG	2.43	0.42
1:B:51:ILE:HD12	1:B:61:LEU:HD21	2.02	0.42
1:C:48:ILE:HB	1:C:360:MET:HG3	2.02	0.42
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.55	0.42
1:D:479:GLN:HB2	1:D:485:ASP:HB2	2.01	0.42
1:A:15:THR:O	1:A:18:LEU:HG	2.20	0.41
1:B:57:SER:HB2	1:B:60:THR:HB	2.02	0.41
1:B:188:LYS:HG2	1:B:193:LEU:HD22	2.02	0.41
1:C:407:ASP:HB3	1:C:410:GLU:HB2	2.01	0.41
1:B:331:LEU:HD22	1:B:340:PRO:HB3	2.01	0.41
1:C:14:GLN:HG2	1:C:15:THR:H	1.85	0.41
1:A:66:LYS:HA	1:A:106:ARG:HH22	1.86	0.41
1:B:148:TYR:HD1	1:B:151:LYS:HD3	1.84	0.41
1:B:330:MET:HE2	1:B:330:MET:HB3	1.96	0.41
1:C:54:ALA:HB2	1:C:368:GLY:H	1.85	0.41
1:D:64:MET:HG2	1:D:64:MET:H	1.72	0.41
1:A:106:ARG:HG3	1:A:500:ARG:HH22	1.85	0.41
1:A:327:ALA:HA	1:A:360:MET:HB3	2.01	0.41
1:A:409:THR:HG23	1:A:522:THR:HB	2.03	0.41
1:B:18:LEU:O	1:B:22:MET:HG3	2.21	0.41
1:B:184:GLN:O	1:B:195:THR:HB	2.20	0.41
1:D:88:ILE:O	1:D:92:ARG:HG3	2.20	0.41
1:D:121:THR:HB	1:D:157:LEU:HD12	2.02	0.41
1:D:223:GLU:HG3	1:D:224:LYS:H	1.84	0.41
1:A:358:CYS:SG	1:A:465:LEU:HA	2.61	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.94	0.41
1:A:416:ALA:HB2	1:A:512:LEU:HD11	2.03	0.41
1:A:423:CYS:SG	1:A:425:SER:HB3	2.61	0.41
1:A:428:ILE:HG21	1:A:441:VAL:HG11	2.02	0.41
1:A:516:ARG:HB3	1:A:517:PRO:HD2	2.02	0.41
1:B:335:ILE:HG22	1:B:336:LYS:HE3	2.03	0.41
1:C:61:LEU:HD13	1:C:91:VAL:HA	2.03	0.41
1:D:432:THR:OG1	1:D:435:GLY:N	2.53	0.41
1:A:250:ASP:O	1:A:254:VAL:HG23	2.21	0.41
1:A:161:TYR:CD2	1:A:164:ILE:HG23	2.56	0.40
1:B:345:GLY:HA2	1:B:381:ILE:HD13	2.03	0.40
1:C:393:GLN:O	1:C:397:GLU:HG3	2.21	0.40
1:C:328:THR:HG22	1:C:329:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:HD23	1:D:372:LEU:HA	1.84	0.40
1:A:530:VAL:HA	1:A:531:PRO:HD3	1.86	0.40
1:B:45:THR:HG22	1:B:359:ILE:HG12	2.02	0.40
1:B:106:ARG:HA	1:B:106:ARG:HD2	1.53	0.40
1:B:149:MET:HG3	1:B:150:GLU:N	2.36	0.40
1:B:159:LEU:CD2	1:B:209:VAL:HG21	2.51	0.40
1:B:158:TRP:CZ2	1:B:160:ASP:HA	2.56	0.40
1:D:138:ALA:H	1:D:197:VAL:HB	1.86	0.40
1:D:301:ILE:HD11	1:D:306:VAL:HA	2.04	0.40
1:D:173:LYS:O	1:D:212:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/551 (93%)	498 (98%)	11 (2%)	1 (0%)	44	68
1	B	497/551 (90%)	481 (97%)	16 (3%)	0	100	100
1	C	509/551 (92%)	500 (98%)	9 (2%)	0	100	100
1	D	500/551 (91%)	485 (97%)	15 (3%)	0	100	100
All	All	2016/2204 (92%)	1964 (97%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	ARG

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	424/453 (94%)	384 (91%)	40 (9%)	7	18
1	B	415/453 (92%)	378 (91%)	37 (9%)	8	20
1	C	423/453 (93%)	378 (89%)	45 (11%)	5	13
1	D	418/453 (92%)	382 (91%)	36 (9%)	8	21
All	All	1680/1812 (93%)	1522 (91%)	158 (9%)	7	18

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	15	THR
1	A	25	THR
1	A	57	SER
1	A	74	LEU
1	A	77	SER
1	A	87	THR
1	A	106	ARG
1	A	123	LEU
1	A	131	GLU
1	A	132	VAL
1	A	134	LEU
1	A	136	LYS
1	A	139	THR
1	A	142	ILE
1	A	150	GLU
1	A	154	GLU
1	A	162	LYS
1	A	166	LYS
1	A	169	GLU
1	A	170	VAL
1	A	173	LYS
1	A	176	VAL
1	A	188	LYS

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Mol	Chain	Res	Type
1	A	206	LYS
1	A	209	VAL
1	A	216	VAL
1	A	260	GLU
1	A	272	GLU
1	A	282	GLU
1	A	285	GLU
1	A	410	GLU
1	A	474	CYS
1	A	476	ASP
1	A	479	GLN
1	A	486	VAL
1	A	508	VAL
1	A	516	ARG
1	A	517	PRO
1	A	521	PHE
1	B	13	ILE
1	B	24	ASP
1	B	55	SER
1	B	56	ARG
1	B	57	SER
1	B	78	HIS
1	B	87	THR
1	B	106	ARG
1	B	140	LEU
1	B	142	ILE
1	B	143	THR
1	B	149	MET
1	B	151	LYS
1	B	155	ASN
1	B	156	ILE
1	B	161	TYR
1	B	184	GLN
1	B	187	GLN
1	B	193	LEU
1	B	195	THR
1	B	196	GLU
1	B	197	VAL
1	B	198	GLU
1	B	202	SER
1	B	216	VAL
1	B	223	GLU

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Mol	Chain	Res	Type
1	B	249	SER
1	B	260	GLU
1	B	272	GLU
1	B	336	LYS
1	B	373	GLU
1	B	392	LEU
1	B	396	GLU
1	B	424	CYS
1	B	491	ASN
1	B	513	THR
1	B	528	VAL
1	C	13	ILE
1	C	16	GLN
1	C	28	GLU
1	C	40	ILE
1	C	55	SER
1	C	56	ARG
1	C	57	SER
1	C	59	GLU
1	C	74	LEU
1	C	82	GLU
1	C	93	THR
1	C	106	ARG
1	C	133	GLU
1	C	134	LEU
1	C	140	LEU
1	C	145	ASP
1	C	152	CYS
1	C	156	ILE
1	C	164	ILE
1	C	168	VAL
1	C	169	GLU
1	C	187	GLN
1	C	202	SER
1	C	216	VAL
1	C	235	GLN
1	C	240	VAL
1	C	249	SER
1	C	260	GLU
1	C	271	ILE
1	C	272	GLU
1	C	296	ASP

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Mol	Chain	Res	Type
1	C	336	LYS
1	C	337	LYS
1	C	377	MET
1	C	392	LEU
1	C	412	THR
1	C	431	LEU
1	C	436	ARG
1	C	443	ARG
1	C	475	LYS
1	C	476	ASP
1	C	508	VAL
1	C	512	LEU
1	C	513	THR
1	C	516	ARG
1	D	16	GLN
1	D	41	THR
1	D	58	VAL
1	D	60	THR
1	D	74	LEU
1	D	81	HIS
1	D	134	LEU
1	D	145	ASP
1	D	155	ASN
1	D	156	ILE
1	D	157	LEU
1	D	164	ILE
1	D	168	VAL
1	D	203	LEU
1	D	207	LYS
1	D	210	ASN
1	D	233	VAL
1	D	240	VAL
1	D	250	ASP
1	D	272	GLU
1	D	301	ILE
1	D	339	ARG
1	D	362	SER
1	D	369	ASP
1	D	373	GLU
1	D	376	ARG
1	D	409	THR
1	D	453	VAL

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Mol	Chain	Res	Type
1	D	467	ARG
1	D	474	CYS
1	D	475	LYS
1	D	487	ASP
1	D	488	LEU
1	D	508	VAL
1	D	522	THR
1	D	525	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	146	ASN
1	A	155	ASN
1	A	235	GLN
1	A	456	ASN
1	A	458	GLN
1	A	479	GLN
1	A	495	ASN
1	B	184	GLN
1	B	187	GLN
1	B	440	GLN
1	C	14	GLN
1	C	155	ASN
1	C	227	GLN
1	C	235	GLN
1	C	440	GLN
1	D	16	GLN
1	D	81	HIS
1	D	146	ASN
1	D	199	ASN
1	D	210	ASN
1	D	440	GLN
1	D	464	HIS

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	$\# Z > 2$
3	FBP	B	602	-	18,20,20	0.86	0	23,32,32	1.17	2 (8%)
3	FBP	D	601	-	18,20,20	0.71	0	23,32,32	0.94	1 (4%)
2	GSH	B	601	-	18,19,19	0.73	0	23,24,24	1.42	4 (17%)
3	FBP	C	601	-	18,20,20	0.83	0	23,32,32	1.02	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBP	B	602	-	-	6/13/32/32	0/1/1/1
3	FBP	D	601	-	-	5/13/32/32	0/1/1/1
2	GSH	B	601	-	-	9/24/24/24	-
3	FBP	C	601	-	-	7/13/32/32	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GSH	CB1-CG1-CD1	3.51	120.88	113.04
2	B	601	GSH	CA2-N2-CD1	3.01	129.38	121.65
2	B	601	GSH	CB2-CA2-N2	2.91	115.44	111.28
2	B	601	GSH	CB1-CA1-C1	2.44	116.11	110.30
3	B	602	FBP	O5P-P2-O6	-2.23	100.80	106.73
3	B	602	FBP	O2P-P1-O1	-2.20	100.87	106.73
3	C	601	FBP	O6P-P2-O5P	2.19	116.02	107.64
3	D	601	FBP	O6P-P2-O5P	2.12	115.75	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GSH	CB2-CA2-N2-CD1
2	B	601	GSH	O2-C2-CA2-CB2
2	B	601	GSH	N3-C2-CA2-CB2
2	B	601	GSH	O31-C3-CA3-N3
2	B	601	GSH	O32-C3-CA3-N3
3	B	602	FBP	O1-C1-C2-O2
3	B	602	FBP	O1-C1-C2-C3
3	B	602	FBP	O1-C1-C2-O5
3	B	602	FBP	C6-O6-P2-O4P
3	C	601	FBP	C1-O1-P1-O2P
3	C	601	FBP	C1-O1-P1-O3P
3	C	601	FBP	O1-C1-C2-O2
3	C	601	FBP	O1-C1-C2-C3
3	C	601	FBP	O1-C1-C2-O5
3	D	601	FBP	C1-O1-P1-O3P
3	D	601	FBP	O1-C1-C2-O2
3	D	601	FBP	O1-C1-C2-C3
3	D	601	FBP	O1-C1-C2-O5
2	B	601	GSH	O12-C1-CA1-N1
2	B	601	GSH	OE1-CD1-N2-CA2
3	D	601	FBP	C6-O6-P2-O4P
2	B	601	GSH	N2-CA2-CB2-SG2
2	B	601	GSH	O11-C1-CA1-N1
3	B	602	FBP	C6-O6-P2-O5P
3	C	601	FBP	C6-O6-P2-O4P
3	B	602	FBP	C4-C5-C6-O6
3	C	601	FBP	C4-C5-C6-O6

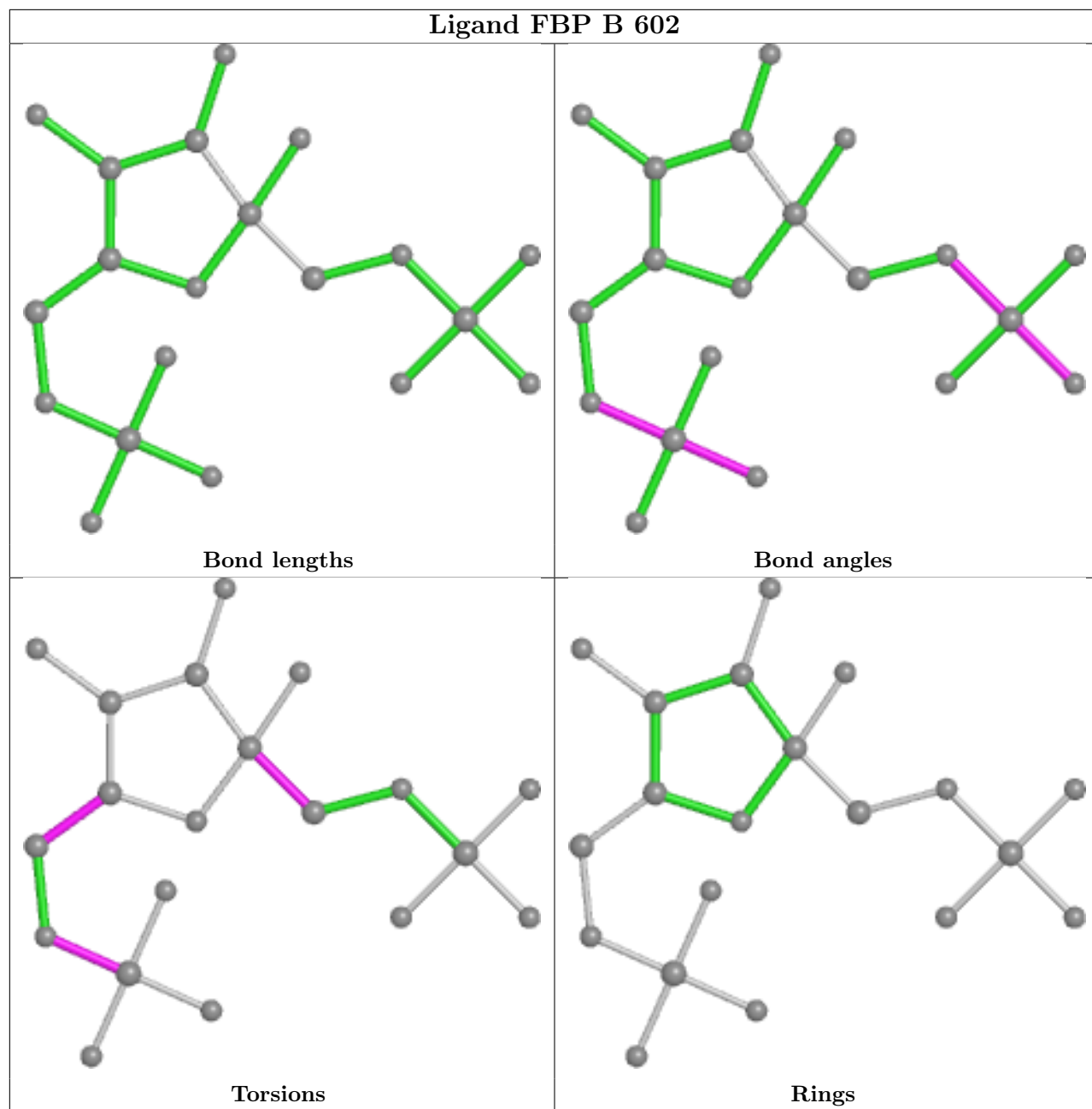
There are no ring outliers.

2 monomers are involved in 2 short contacts:

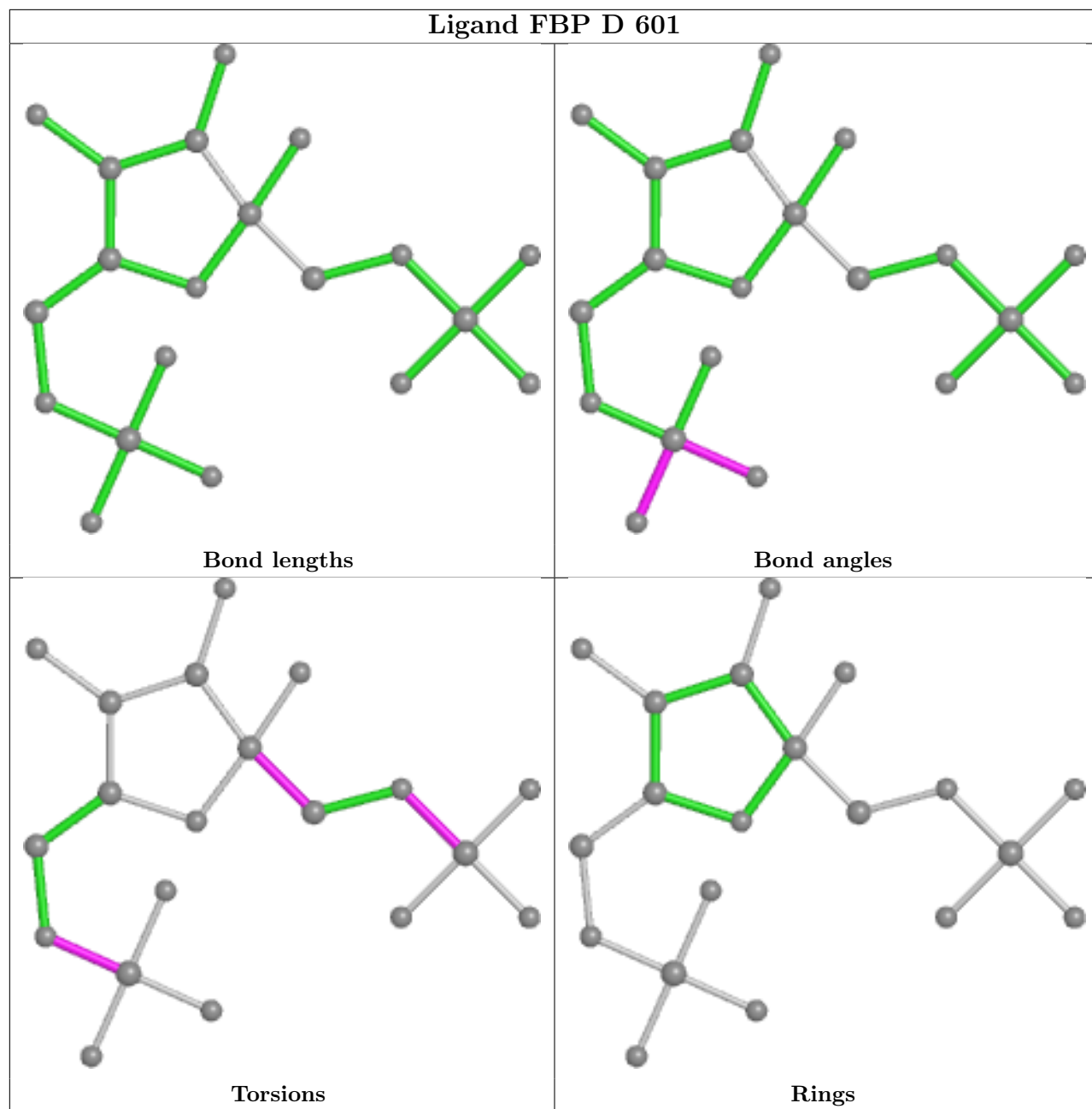
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	FBP	1	0
2	B	601	GSH	1	0

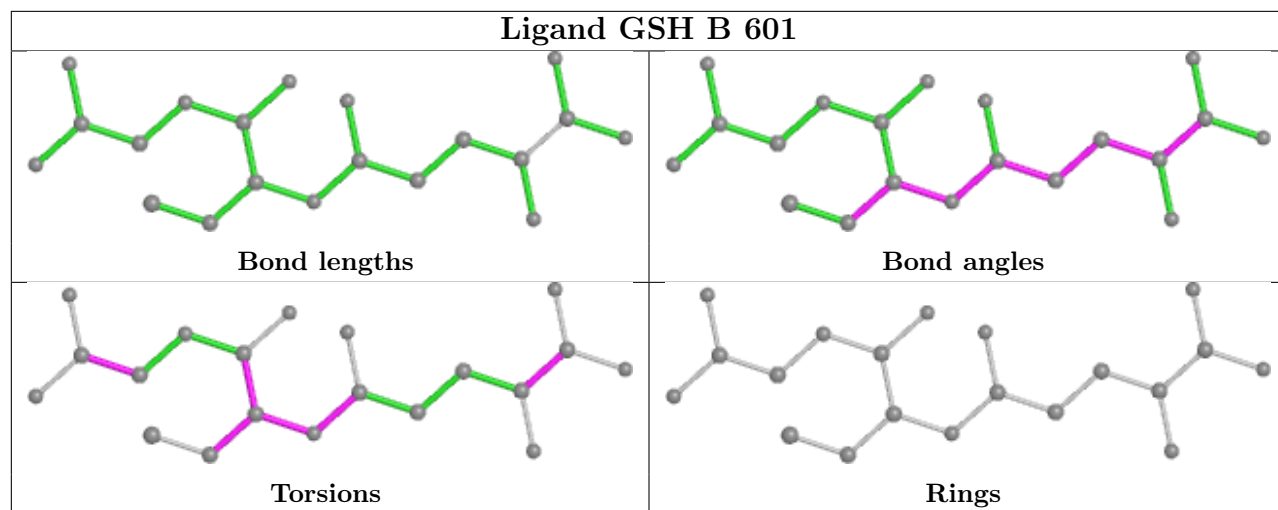
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

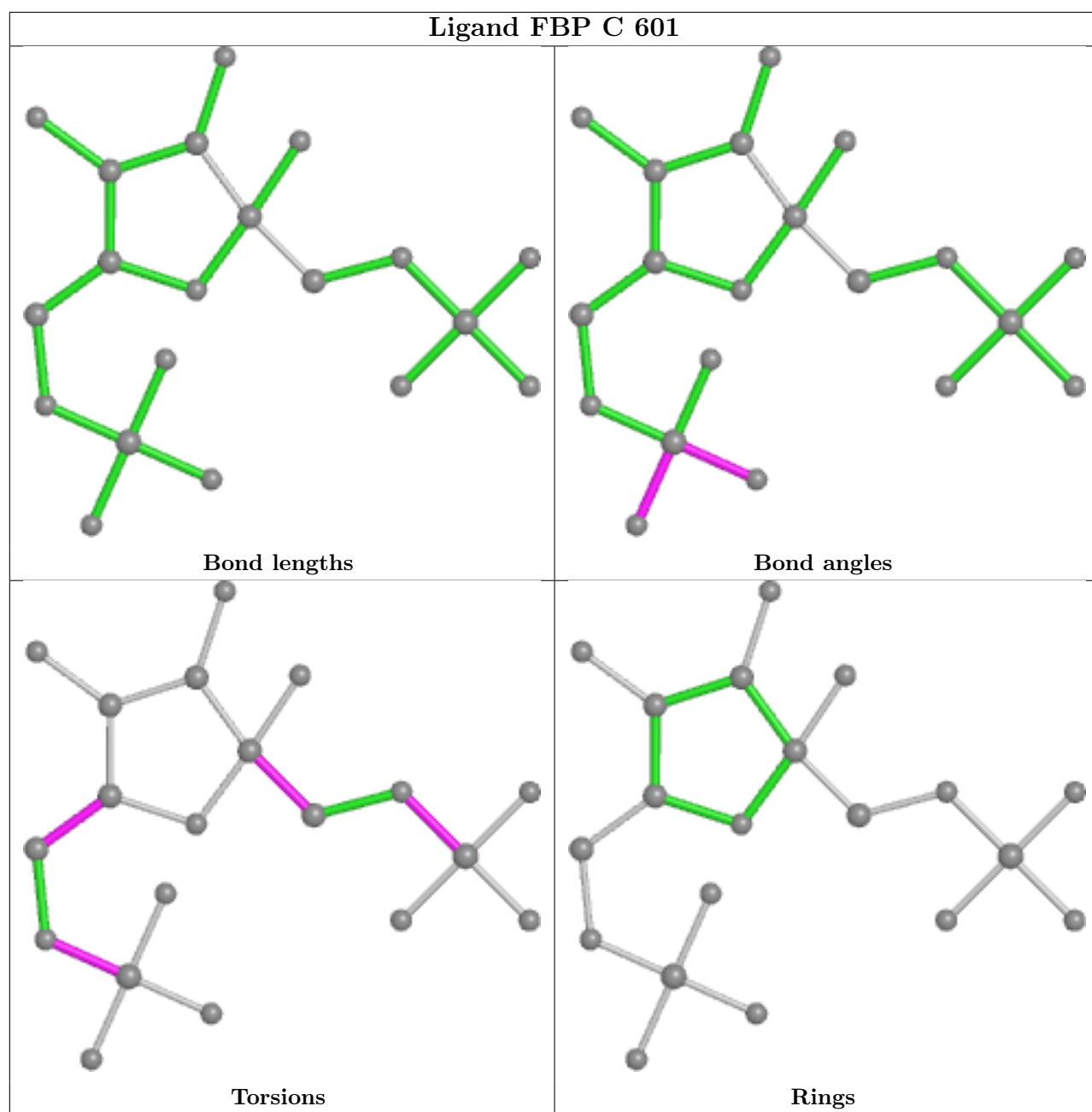
Ligand FBP B 602



Ligand FBP D 601







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	514/551 (93%)	-1.66	0 100 100	13, 33, 79, 107	0
1	B	503/551 (91%)	-1.57	0 100 100	16, 42, 103, 138	0
1	C	513/551 (93%)	-1.58	0 100 100	16, 44, 96, 135	0
1	D	506/551 (91%)	-1.52	0 100 100	20, 50, 86, 125	0
All	All	2036/2204 (92%)	-1.58	0 100 100	13, 42, 92, 138	0

There are no RSRZ outliers to report.

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](#)

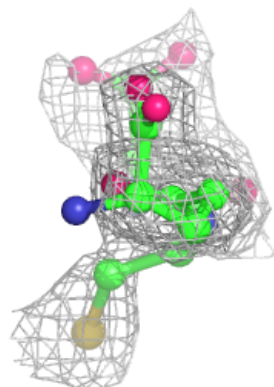
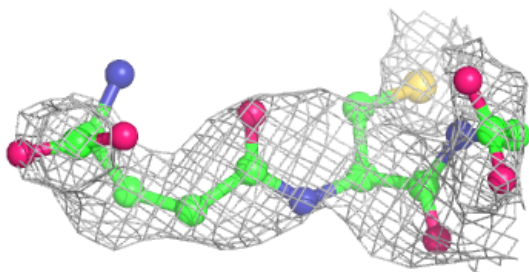
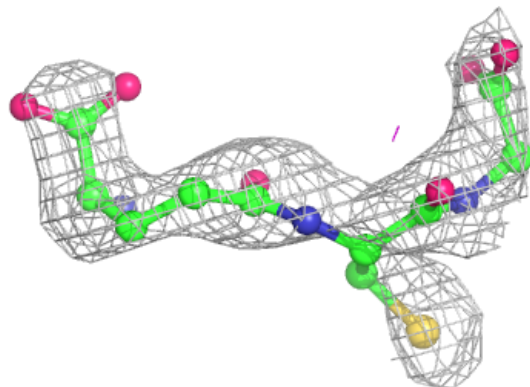
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GSH	B	601	20/20	0.99	0.04	56,62,67,69	0
3	FBP	B	602	20/20	0.99	0.03	32,42,44,49	0
3	FBP	D	601	20/20	0.99	0.03	34,42,53,54	0
3	FBP	C	601	20/20	1.00	0.02	32,35,48,48	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.

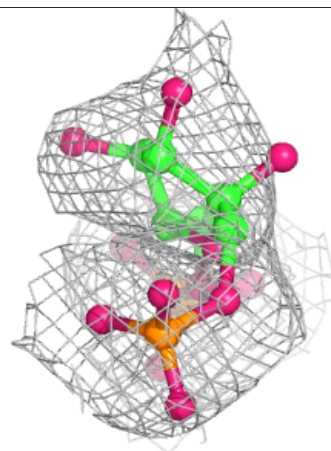
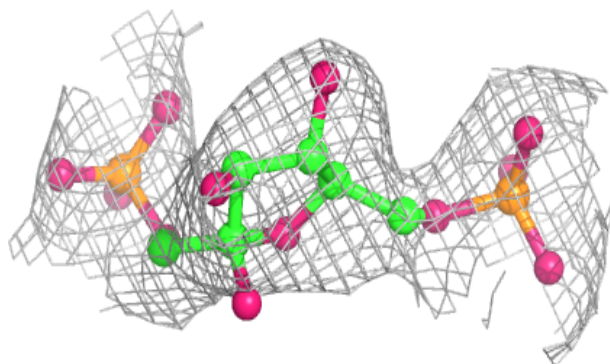
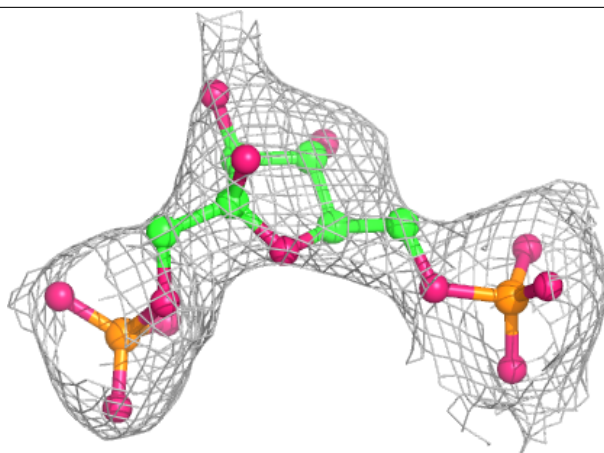
Electron density around GSH B 601:

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

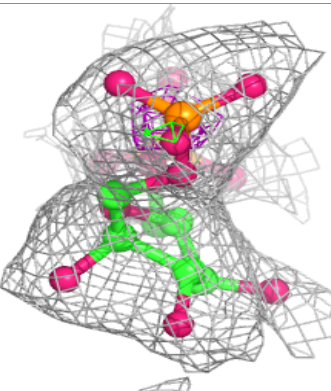
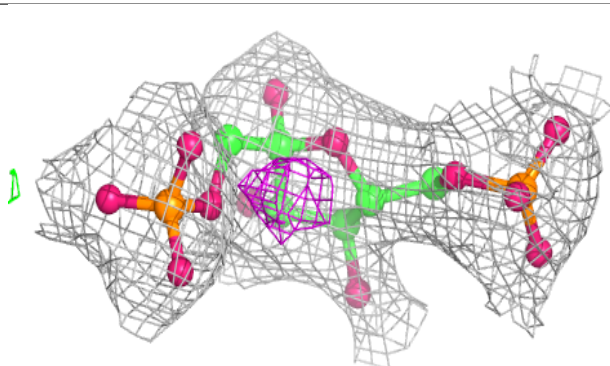
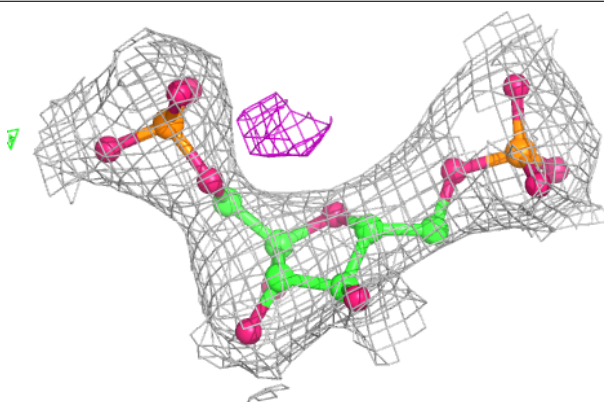


Electron density around FBP B 602:

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

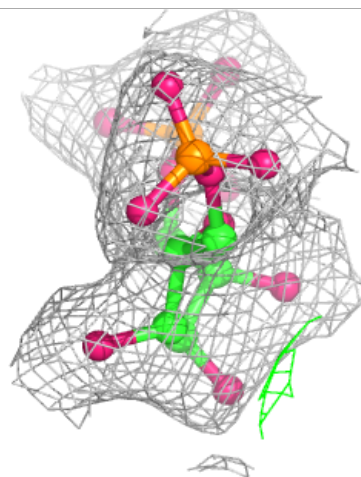
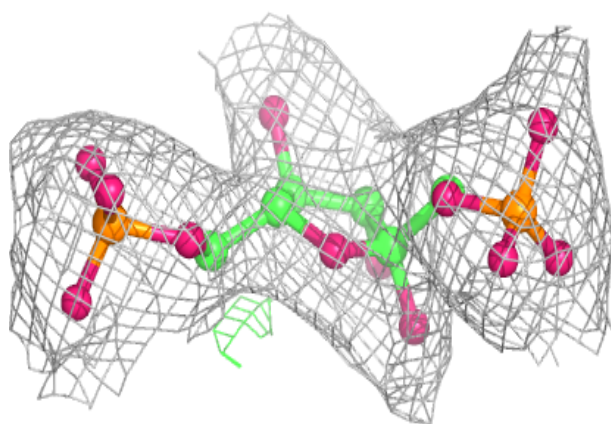
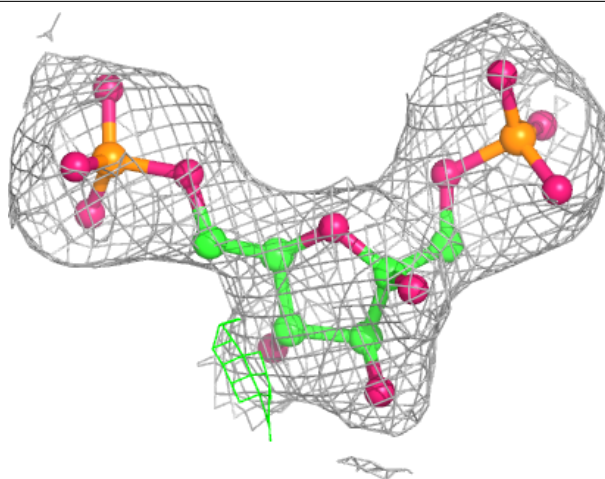
**Electron density around FBP D 601:**

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



Electron density around FBP C 601:

$2mF_o-DF_c$ (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.