



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:38 AM UTC

PDB ID : 4YJ5 / pdb_00004yj5
Title : Crystal structure of PKM2 mutant
Authors : Liu, J.-S.; Wu, C.-W.; Wang, W.-C.
Deposited on : 2015-03-03
Resolution : 2.41 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

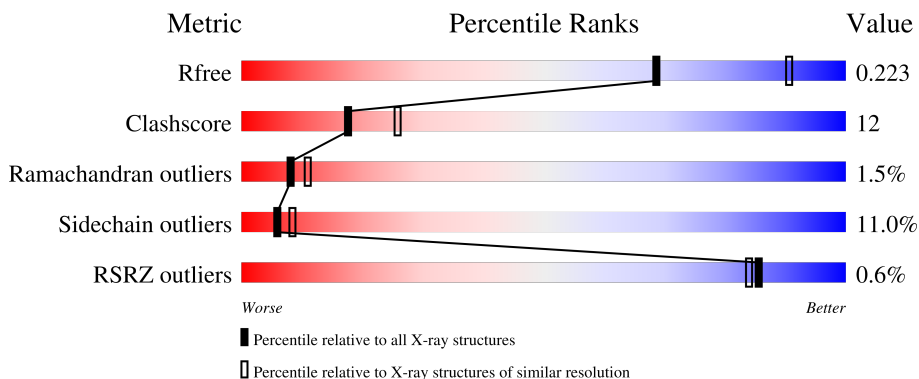
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	518	% 78% 16% 5% .
1	B	518	68% 26% 5% .
1	C	518	% 72% 24% .
1	D	518	% 72% 21% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16419 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.

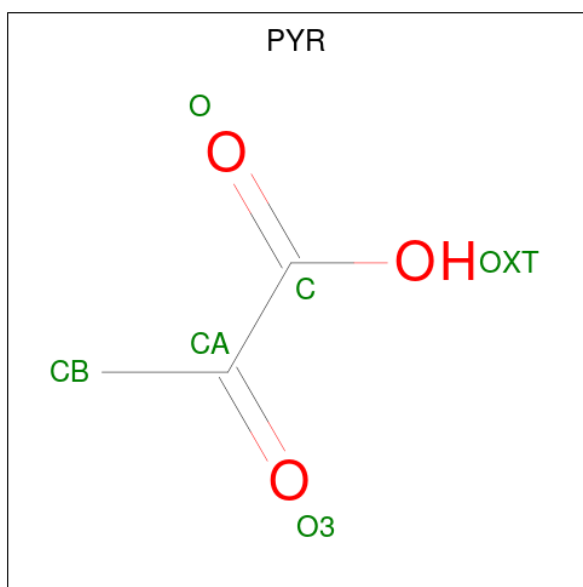
- Molecule 1 is a protein called Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3967	2495	702	745	25			
1	B	518	Total	C	N	O	S	0	0	0
			3967	2495	702	745	25			
1	C	518	Total	C	N	O	S	0	0	0
			3967	2495	702	745	25			
1	D	518	Total	C	N	O	S	0	0	0
			3967	2495	702	745	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	TYR	HIS	engineered mutation	UNP P14618
B	391	TYR	HIS	engineered mutation	UNP P14618
C	391	TYR	HIS	engineered mutation	UNP P14618
D	391	TYR	HIS	engineered mutation	UNP P14618

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).

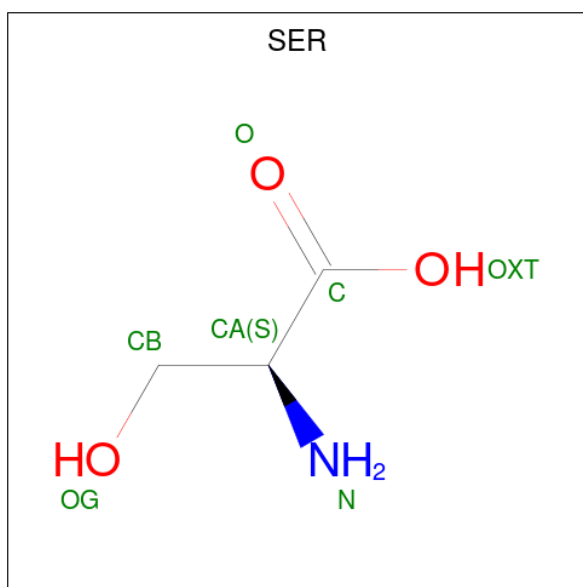


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

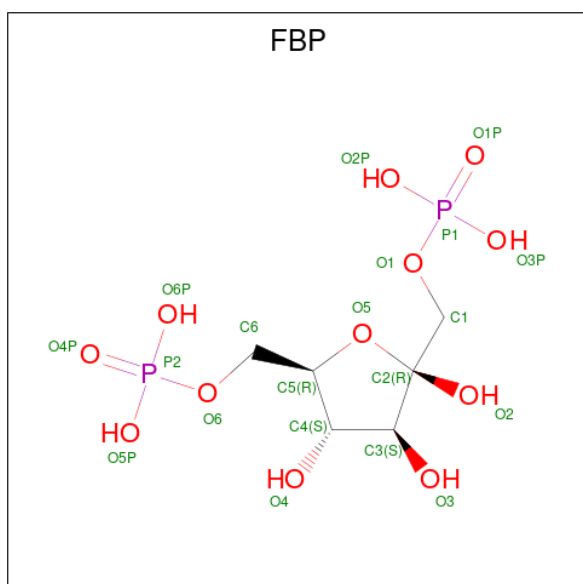
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	3	1	3		
4	B	1	Total	C	N	O	0	0
			7	3	1	3		
4	C	1	Total	C	N	O	0	0
			7	3	1	3		
4	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 5 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



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

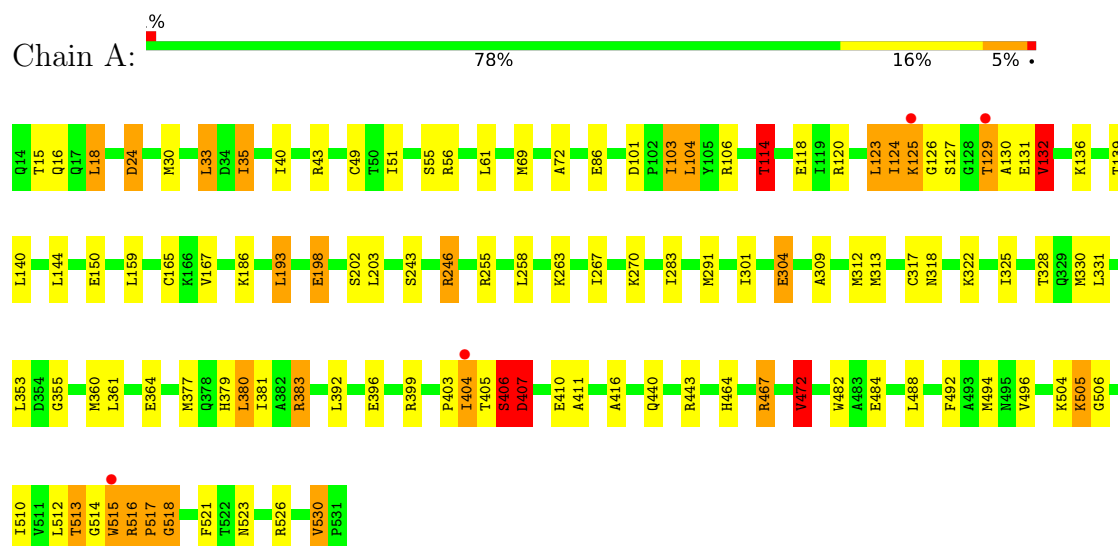
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	96	Total	O	0	0
			96	96		
6	C	95	Total	O	0	0
			95	95		
6	D	111	Total	O	0	0
			111	111		

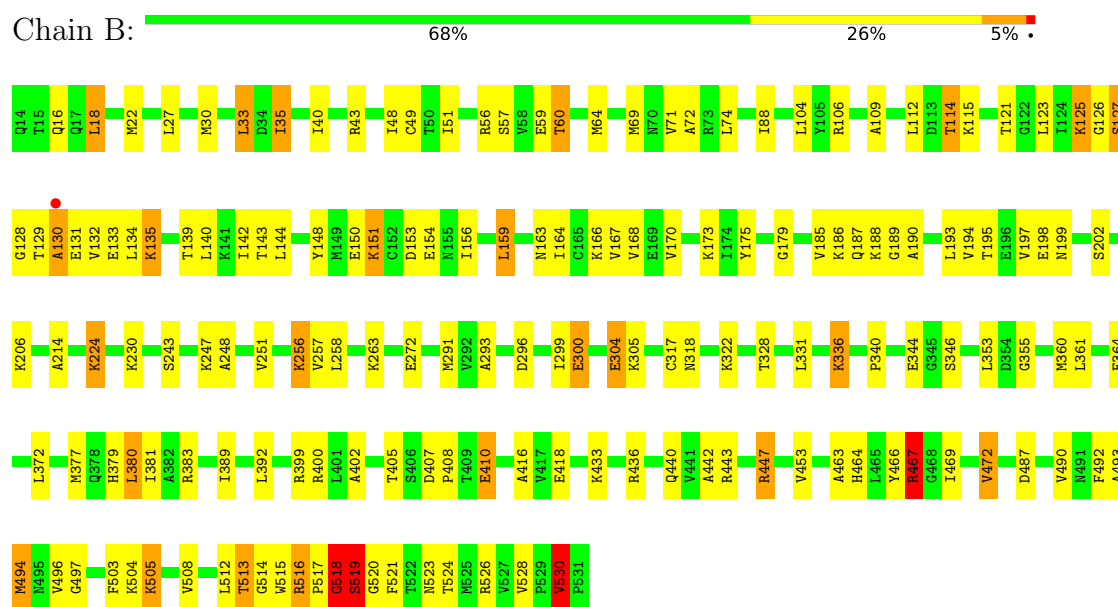
3 Residue-property plots

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.

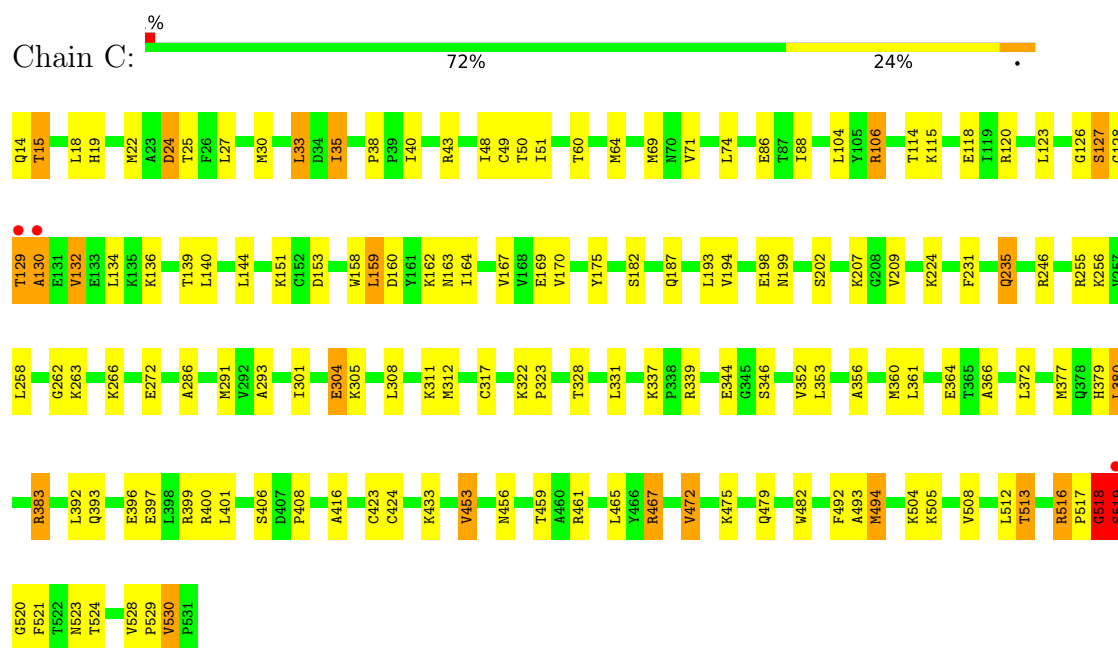
• Molecule 1: Pyruvate kinase PKM



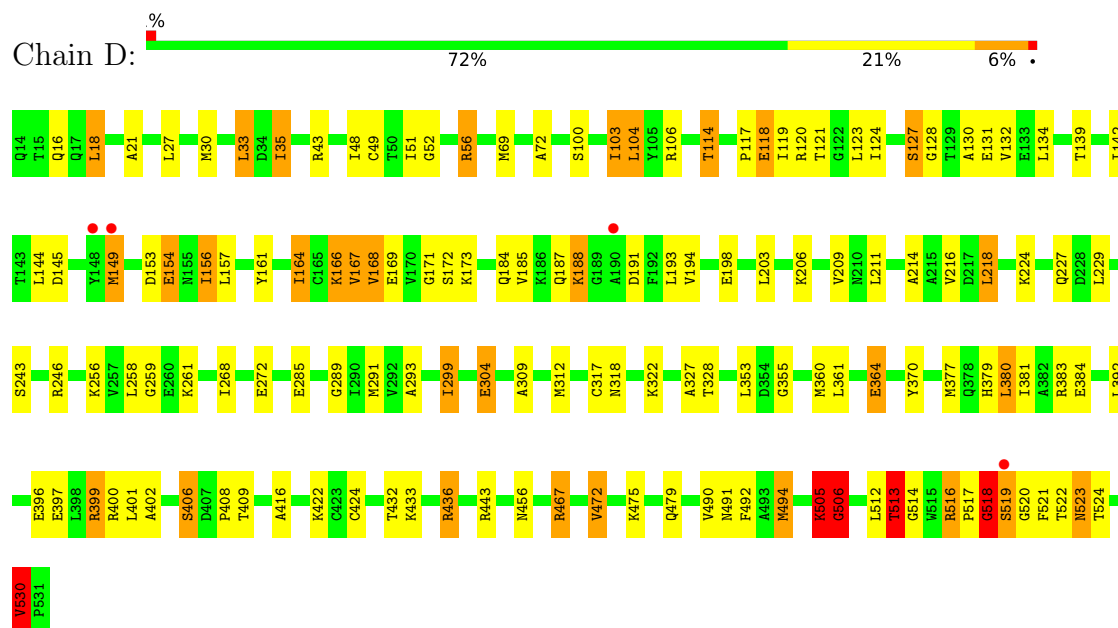
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.22Å 140.89Å 108.72Å 90.00° 93.97° 90.00°	Depositor
Resolution (Å)	20.00 – 2.41 20.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.41) 98.6 (20.00-2.41)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.144 , 0.217 0.158 , 0.223	Depositor DCC
R_{free} test set	4222 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16419	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: FBP, MG, PYR

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	1.03	0/4031	1.22	10/5444 (0.2%)
1	B	1.01	2/4031 (0.0%)	1.18	10/5444 (0.2%)
1	C	1.00	2/4031 (0.0%)	1.17	8/5444 (0.1%)
1	D	0.96	2/4031 (0.0%)	1.18	16/5444 (0.3%)
All	All	1.00	6/16124 (0.0%)	1.19	44/21776 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	GLY	N-CA	5.81	1.53	1.45
1	B	520	GLY	CA-C	5.75	1.59	1.51
1	D	520	GLY	CA-C	5.74	1.59	1.51
1	D	106	ARG	C-O	-5.57	1.20	1.25
1	B	520	GLY	N-CA	5.36	1.53	1.45
1	C	520	GLY	CA-C	5.03	1.58	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126	GLY	N-CA-C	-7.65	102.27	112.14
1	D	467	ARG	CG-CD-NE	-7.59	95.31	112.00
1	A	407	ASP	CA-C-N	7.58	128.26	119.47
1	A	407	ASP	C-N-CA	7.58	128.26	119.47
1	D	530	VAL	N-CA-CB	7.38	117.59	109.99
1	C	106	ARG	CA-C-N	-7.38	112.40	119.85
1	C	106	ARG	C-N-CA	-7.38	112.40	119.85
1	A	467	ARG	NE-CZ-NH2	-7.16	112.75	119.20
1	D	383	ARG	CB-CG-CD	-7.00	95.20	111.30
1	A	467	ARG	CG-CD-NE	-6.97	96.66	112.00
1	C	461	ARG	N-CA-C	-6.51	104.98	113.12
1	B	467	ARG	NE-CZ-NH2	-6.41	113.43	119.20
1	C	286	ALA	N-CA-C	6.30	118.96	111.71
1	B	467	ARG	CG-CD-NE	-6.29	98.16	112.00
1	A	472	VAL	CB-CA-C	5.90	118.14	110.12
1	A	35	ILE	CA-CB-CG2	5.78	120.32	110.50
1	C	352	VAL	CB-CA-C	-5.77	104.59	111.97
1	A	515	TRP	CA-CB-CG	5.75	124.52	113.60
1	B	299	ILE	CA-C-N	5.72	127.94	120.28
1	B	299	ILE	C-N-CA	5.72	127.94	120.28
1	D	399	ARG	N-CA-C	5.67	117.46	111.28
1	A	114	THR	N-CA-CB	-5.64	102.05	110.17
1	D	506	GLY	N-CA-C	5.62	119.47	112.73
1	D	168	VAL	N-CA-C	5.59	115.64	108.82
1	B	189	GLY	N-CA-C	5.56	118.53	111.85
1	D	467	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	D	402	ALA	CA-C-N	-5.47	114.70	120.66
1	D	402	ALA	C-N-CA	-5.47	114.70	120.66
1	D	56	ARG	N-CA-C	5.40	118.08	111.82
1	B	410	GLU	N-CA-C	-5.38	105.50	111.36
1	B	442	ALA	CA-C-N	5.34	128.18	120.38
1	B	442	ALA	C-N-CA	5.34	128.18	120.38
1	D	505	LYS	CA-C-N	-5.32	114.08	119.98
1	D	505	LYS	C-N-CA	-5.32	114.08	119.98
1	A	496	VAL	N-CA-C	-5.29	105.37	110.72
1	C	453	VAL	CB-CA-C	-5.24	104.63	110.96
1	D	370	TYR	CA-C-N	-5.19	113.69	119.19
1	D	370	TYR	C-N-CA	-5.19	113.69	119.19
1	D	513	THR	N-CA-CB	-5.19	103.52	111.56
1	D	523	ASN	N-CA-C	-5.18	104.95	113.50
1	B	56	ARG	N-CA-CB	-5.14	102.02	110.40
1	A	56	ARG	N-CA-CB	-5.11	102.47	110.44
1	C	255	ARG	N-CA-C	-5.08	105.83	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	VAL	N-CA-CB	5.03	115.61	110.23

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ILE	Peptide
1	A	406	SER	Peptide
1	B	518	GLY	Peptide
1	C	518	GLY	Peptide
1	D	506	GLY	Peptide
1	D	518	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3967	0	4051	92	0
1	B	3967	0	4051	124	0
1	C	3967	0	4051	105	0
1	D	3967	0	4051	111	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	7	0	4	1	0
4	B	7	0	4	1	0
4	C	7	0	4	0	0
4	D	7	0	4	0	0
5	B	20	0	10	1	0
5	C	20	0	10	0	0
5	D	20	0	10	3	0
6	A	133	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	96	0	0	4	0
6	C	95	0	0	4	0
6	D	111	0	0	5	0
All	All	16419	0	16250	399	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 12.

All (399) 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:49:CYS:HB2	1:D:69:MET:HE3	1.18	1.16
1:A:126:GLY:HA3	1:A:127:SER:HB3	1.18	1.12
1:C:35:ILE:HD11	1:D:309:ALA:HB2	1.25	1.09
1:D:51:ILE:HD11	1:D:69:MET:HE1	1.32	1.09
1:C:35:ILE:CD1	1:D:309:ALA:HB2	1.81	1.09
1:B:49:CYS:HB2	1:B:69:MET:HE3	1.16	1.08
1:B:51:ILE:HD11	1:B:69:MET:HE1	1.25	1.08
1:C:127:SER:N	1:C:128:GLY:HA2	1.67	1.07
1:A:124:ILE:HG22	1:A:125:LYS:HB3	1.38	1.04
1:A:126:GLY:HA3	1:A:127:SER:CB	1.90	1.01
1:C:127:SER:H	1:C:128:GLY:HA2	0.88	1.00
1:D:139:THR:HG23	6:D:749:HOH:O	1.63	0.98
1:A:291:MET:HE2	1:A:360:MET:HE1	1.43	0.97
1:A:103:ILE:HG22	1:A:104:LEU:HD13	1.47	0.97
1:B:43:ARG:HE	1:B:379:HIS:HD2	1.10	0.96
1:C:494:MET:HE1	1:C:530:VAL:HB	1.46	0.95
1:C:356:ALA:O	1:C:467:ARG:NH1	1.99	0.95
1:D:291:MET:SD	1:D:360:MET:HE1	2.09	0.93
1:C:380:LEU:HB3	1:D:304:GLU:HG2	1.51	0.90
1:B:114:THR:HG21	6:B:705:HOH:O	1.70	0.90
1:C:304:GLU:HG2	1:D:380:LEU:HB3	1.54	0.90
1:D:169:GLU:O	1:D:185:VAL:HG21	1.70	0.89
1:B:518:GLY:HA3	1:B:521:PHE:CD2	2.07	0.89
1:C:43:ARG:HE	1:C:379:HIS:HD2	1.19	0.89
1:D:49:CYS:HB2	1:D:69:MET:CE	2.00	0.89
1:B:472:VAL:HG13	1:B:492:PHE:HE2	1.39	0.88
1:A:126:GLY:CA	1:A:127:SER:HB3	2.03	0.88
1:C:127:SER:H	1:C:128:GLY:CA	1.82	0.88
1:D:43:ARG:HE	1:D:379:HIS:HD2	1.17	0.88
1:D:118:GLU:HG2	1:D:120:ARG:HE	1.38	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLU:HG2	1:B:380:LEU:HB3	1.55	0.87
1:A:124:ILE:O	1:A:125:LYS:HG2	1.76	0.86
1:C:246:ARG:HD2	6:C:753:HOH:O	1.77	0.84
1:A:43:ARG:HE	1:A:379:HIS:HD2	1.26	0.84
1:A:380:LEU:HB3	1:B:304:GLU:HG2	1.57	0.84
1:C:291:MET:CE	1:C:360:MET:HE1	2.07	0.83
1:A:410:GLU:HG2	1:D:422:LYS:HE2	1.61	0.83
1:B:291:MET:HE2	1:B:360:MET:HE1	1.61	0.82
1:B:518:GLY:HA3	1:B:521:PHE:CE2	2.13	0.82
1:B:167:VAL:HG12	1:B:214:ALA:HB1	1.62	0.81
1:C:291:MET:HE2	1:C:360:MET:HE1	1.60	0.81
1:B:43:ARG:HE	1:B:379:HIS:CD2	1.98	0.81
1:B:472:VAL:HG13	1:B:492:PHE:CE2	2.15	0.81
1:B:433:LYS:HD3	1:B:519:SER:HA	1.63	0.80
1:D:49:CYS:CB	1:D:69:MET:HE3	2.08	0.78
1:A:136:LYS:HD3	1:A:198:GLU:O	1.84	0.78
1:A:406:SER:HB3	1:A:407:ASP:HB3	1.66	0.77
1:D:291:MET:CE	1:D:360:MET:HE1	2.14	0.77
1:C:361:LEU:HD22	1:C:364:GLU:HG3	1.67	0.77
1:C:43:ARG:HE	1:C:379:HIS:CD2	2.03	0.77
1:C:35:ILE:HD11	1:D:309:ALA:CB	2.11	0.76
1:D:161:TYR:O	1:D:164:ILE:HG22	1.85	0.76
1:B:402:ALA:HB3	6:B:725:HOH:O	1.85	0.76
1:B:74:LEU:HD21	1:B:88:ILE:HG13	1.66	0.76
1:C:304:GLU:HG3	1:D:377:MET:HE1	1.68	0.75
1:B:49:CYS:CB	1:B:69:MET:HE3	2.08	0.75
1:C:518:GLY:HA3	1:C:521:PHE:CD2	2.21	0.75
1:B:49:CYS:HB2	1:B:69:MET:CE	2.09	0.74
1:A:124:ILE:HG22	1:A:125:LYS:CB	2.17	0.74
1:A:49:CYS:HB2	1:A:69:MET:HE3	1.69	0.72
1:C:401:LEU:HD12	1:D:27:LEU:HD23	1.69	0.72
1:D:149:MET:HE3	1:D:206:LYS:NZ	2.05	0.72
1:A:69:MET:CE	1:A:72:ALA:HA	2.20	0.71
1:B:16:GLN:HG2	1:B:40:ILE:HG23	1.72	0.71
1:C:361:LEU:HD22	1:C:364:GLU:CG	2.21	0.71
1:D:16:GLN:HG3	1:D:18:LEU:HD23	1.72	0.70
1:B:187:GLN:HB2	1:B:194:VAL:HB	1.73	0.70
1:C:518:GLY:HA3	1:C:521:PHE:CE2	2.27	0.70
1:B:516:ARG:HB2	1:B:517:PRO:HD2	1.73	0.70
1:C:472:VAL:HG13	1:C:492:PHE:HE2	1.56	0.69
1:C:377:MET:HE1	1:D:304:GLU:HG3	1.72	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:MET:CE	1:B:530:VAL:HB	2.22	0.69
1:B:51:ILE:HD11	1:B:69:MET:CE	2.13	0.69
1:A:131:GLU:O	1:A:203:LEU:O	2.10	0.69
1:B:132:VAL:HG12	1:B:133:GLU:N	2.07	0.69
1:D:188:LYS:HA	1:D:193:LEU:HD23	1.74	0.69
1:A:51:ILE:HD11	1:A:69:MET:HE1	1.75	0.69
1:B:18:LEU:HD23	1:B:22:MET:HE2	1.74	0.69
1:A:406:SER:HA	1:A:407:ASP:CB	2.23	0.69
1:A:464:HIS:HD1	4:A:603:SER:N	1.91	0.69
1:B:472:VAL:CG1	1:B:492:PHE:CE2	2.76	0.69
1:C:182:SER:OG	1:C:199:ASN:HB2	1.93	0.68
1:B:185:VAL:HA	1:B:195:THR:HG22	1.76	0.67
1:A:380:LEU:HB3	1:B:304:GLU:CG	2.24	0.67
1:D:30:MET:HA	1:D:33:LEU:HD22	1.76	0.67
1:B:291:MET:CE	1:B:360:MET:HE1	2.23	0.67
1:B:472:VAL:CG1	1:B:492:PHE:HE2	2.07	0.67
1:D:505:LYS:HA	1:D:530:VAL:HG22	1.77	0.67
1:C:48:ILE:HG21	1:C:360:MET:HE2	1.75	0.67
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.77	0.66
1:B:410:GLU:OE1	1:B:440:GLN:HG2	1.95	0.66
1:A:304:GLU:HG3	1:B:377:MET:HE1	1.76	0.66
1:B:48:ILE:HG21	1:B:360:MET:HE2	1.77	0.66
1:D:118:GLU:HG2	1:D:120:ARG:NE	2.10	0.66
1:B:361:LEU:HD22	1:B:364:GLU:HG3	1.77	0.66
1:D:505:LYS:HB3	6:D:706:HOH:O	1.95	0.66
1:B:361:LEU:HD22	1:B:364:GLU:CG	2.26	0.65
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.77	0.65
1:B:518:GLY:HA3	1:B:521:PHE:HD2	1.61	0.65
1:A:513:THR:HG22	1:A:514:GLY:O	1.96	0.65
1:D:43:ARG:HE	1:D:379:HIS:CD2	2.07	0.65
1:C:433:LYS:HD3	1:C:519:SER:HA	1.78	0.65
1:A:125:LYS:HD3	1:A:130:ALA:H	1.62	0.64
1:A:406:SER:HA	1:A:407:ASP:HB3	1.78	0.64
1:C:291:MET:HE2	1:C:360:MET:CE	2.27	0.64
1:C:291:MET:HE1	1:C:360:MET:HE1	1.80	0.64
1:B:156:ILE:HD12	1:B:156:ILE:O	1.98	0.63
1:A:291:MET:CE	1:A:360:MET:HE1	2.22	0.63
1:A:406:SER:CB	1:A:407:ASP:HB3	2.29	0.63
1:B:114:THR:HG22	1:B:243:SER:HB2	1.80	0.63
1:A:515:TRP:HD1	1:A:523:ASN:HD21	1.45	0.63
1:A:406:SER:CA	1:A:407:ASP:HB3	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:TRP:HD1	1:A:523:ASN:ND2	1.97	0.62
1:D:169:GLU:O	1:D:185:VAL:CG2	2.46	0.62
1:D:149:MET:HE3	1:D:206:LYS:HZ3	1.65	0.62
1:D:103:ILE:HG22	1:D:104:LEU:HD13	1.81	0.62
1:B:464:HIS:HD1	4:B:603:SER:N	1.97	0.62
1:C:472:VAL:HG13	1:C:492:PHE:CE2	2.35	0.61
1:B:517:PRO:O	1:B:518:GLY:O	2.19	0.61
1:C:51:ILE:HD11	1:C:69:MET:HE1	1.82	0.61
1:C:406:SER:O	1:C:408:PRO:HD3	2.01	0.61
1:C:266:LYS:NZ	6:C:787:HOH:O	2.33	0.60
1:A:318:ASN:HD21	1:A:355:GLY:HA3	1.66	0.60
1:B:128:GLY:HA3	6:B:743:HOH:O	2.00	0.60
1:C:118:GLU:OE2	1:C:120:ARG:HD2	2.01	0.60
1:A:43:ARG:HE	1:A:379:HIS:CD2	2.11	0.60
1:D:436:ARG:CZ	1:D:436:ARG:HB2	2.30	0.60
1:A:404:ILE:O	1:A:404:ILE:HG22	1.99	0.60
1:B:256:LYS:N	1:B:256:LYS:HD2	2.17	0.60
1:B:447:ARG:HG2	1:B:447:ARG:HH11	1.67	0.60
1:B:494:MET:HE1	1:B:530:VAL:HB	1.82	0.60
1:A:124:ILE:C	1:A:125:LYS:HG2	2.25	0.60
1:B:256:LYS:HA	1:B:256:LYS:HZ2	1.67	0.60
1:B:513:THR:HG22	1:B:524:THR:HB	1.84	0.59
1:A:516:ARG:C	1:A:518:GLY:H	2.11	0.59
1:B:115:LYS:HD3	1:B:224:LYS:HE3	1.84	0.59
1:C:106:ARG:HD3	6:C:719:HOH:O	2.02	0.59
1:B:272:GLU:HB3	1:B:293:ALA:HB3	1.85	0.59
1:D:121:THR:HB	1:D:157:LEU:HD11	1.85	0.58
1:B:132:VAL:CG1	1:B:154:GLU:HB3	2.33	0.58
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.86	0.58
1:D:48:ILE:HB	1:D:360:MET:HG3	1.84	0.58
1:A:309:ALA:HB2	1:B:35:ILE:HD13	1.85	0.58
1:A:411:ALA:HA	1:D:422:LYS:HG2	1.85	0.58
1:A:325:ILE:HG21	1:A:360:MET:HE3	1.84	0.58
1:B:127:SER:OG	1:B:128:GLY:HA2	2.04	0.57
1:A:506:GLY:HA3	6:A:778:HOH:O	2.04	0.57
1:B:132:VAL:HG12	1:B:133:GLU:H	1.68	0.57
1:C:272:GLU:HB3	1:C:293:ALA:HB3	1.86	0.57
1:A:361:LEU:HD22	1:A:364:GLU:CG	2.35	0.57
1:A:505:LYS:O	1:A:530:VAL:O	2.22	0.57
1:B:256:LYS:HA	1:B:256:LYS:NZ	2.19	0.57
1:B:167:VAL:CG1	1:B:214:ALA:HB1	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ILE:CD1	1:D:309:ALA:CB	2.72	0.57
1:A:24:ASP:HB3	1:D:400:ARG:HH22	1.70	0.56
1:D:505:LYS:HD2	1:D:506:GLY:N	2.20	0.56
1:A:114:THR:HG22	1:A:243:SER:H	1.71	0.56
1:A:515:TRP:CD1	1:A:523:ASN:HD21	2.23	0.56
1:C:129:THR:O	1:C:130:ALA:HB3	2.06	0.56
1:B:518:GLY:CA	1:B:521:PHE:CE2	2.87	0.56
1:D:377:MET:HE3	1:D:381:ILE:HG13	1.88	0.55
1:D:518:GLY:HA3	1:D:521:PHE:HD2	1.70	0.55
1:C:40:ILE:O	1:C:383:ARG:HD3	2.06	0.55
1:C:517:PRO:O	1:C:518:GLY:O	2.23	0.55
1:B:64:MET:HG3	1:B:372:LEU:CD2	2.37	0.55
1:D:505:LYS:CB	6:D:706:HOH:O	2.52	0.55
1:D:361:LEU:HD22	1:D:364:GLU:HG2	1.88	0.55
1:B:132:VAL:HG11	1:B:154:GLU:HB3	1.89	0.55
1:A:106:ARG:HD3	6:A:731:HOH:O	2.06	0.55
1:B:505:LYS:O	1:B:530:VAL:O	2.25	0.55
1:A:30:MET:HA	1:A:33:LEU:HD22	1.87	0.54
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.43	0.54
1:B:125:LYS:HD2	1:B:153:ASP:HB3	1.89	0.54
1:A:131:GLU:O	1:A:132:VAL:HB	2.07	0.54
1:D:472:VAL:HG13	1:D:492:PHE:CE2	2.43	0.54
1:A:69:MET:HE2	1:A:72:ALA:CA	2.38	0.54
1:B:494:MET:HE3	1:B:494:MET:HA	1.90	0.54
1:D:361:LEU:HD22	1:D:364:GLU:CG	2.38	0.54
1:A:406:SER:CA	1:A:407:ASP:CB	2.86	0.53
1:C:513:THR:HG22	1:C:524:THR:HB	1.89	0.53
1:D:166:LYS:HG3	1:D:167:VAL:N	2.24	0.53
1:D:406:SER:O	1:D:408:PRO:HD3	2.09	0.53
1:C:163:ASN:O	1:C:164:ILE:C	2.50	0.53
1:C:361:LEU:HB3	1:C:364:GLU:HG2	1.91	0.53
1:A:69:MET:CE	1:A:72:ALA:CA	2.87	0.53
1:B:514:GLY:HA3	5:B:604:FBP:O3	2.09	0.53
1:A:472:VAL:HG13	1:A:492:PHE:CE2	2.44	0.53
1:C:317:CYS:HB3	1:C:322:LYS:O	2.08	0.52
1:C:377:MET:CE	1:D:304:GLU:HG3	2.39	0.52
1:A:526:ARG:HA	1:D:523:ASN:O	2.10	0.52
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.91	0.52
1:C:308:LEU:HD11	1:D:384:GLU:HG3	1.91	0.52
1:B:112:LEU:HD23	1:B:112:LEU:C	2.35	0.52
1:D:517:PRO:O	1:D:518:GLY:O	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.40	0.51
1:D:69:MET:HE2	1:D:72:ALA:HA	1.92	0.51
1:B:516:ARG:HD2	1:B:521:PHE:CD2	2.46	0.51
1:C:453:VAL:CG2	1:C:493:ALA:HB2	2.40	0.51
1:C:516:ARG:HD2	1:C:518:GLY:H	1.76	0.51
1:C:482:TRP:CD1	1:C:517:PRO:HB3	2.46	0.51
1:C:393:GLN:O	1:C:397:GLU:HG3	2.11	0.50
1:D:142:ILE:HA	1:D:157:LEU:O	2.12	0.50
1:A:124:ILE:O	1:A:125:LYS:CG	2.55	0.50
1:D:166:LYS:HG3	1:D:167:VAL:HG22	1.93	0.50
1:B:517:PRO:O	1:B:518:GLY:C	2.55	0.50
1:C:25:THR:HB	1:D:397:GLU:CD	2.37	0.50
1:B:151:LYS:O	1:B:156:ILE:HD11	2.11	0.50
1:C:305:LYS:HB3	1:D:35:ILE:HG13	1.94	0.50
1:D:513:THR:HG22	1:D:524:THR:HB	1.92	0.50
1:B:518:GLY:CA	1:B:521:PHE:HE2	2.24	0.49
1:B:526:ARG:HA	1:C:523:ASN:O	2.12	0.49
1:C:231:PHE:O	1:C:235:GLN:HB2	2.13	0.49
1:C:456:ASN:OD1	1:C:456:ASN:C	2.54	0.49
1:C:50:THR:HG22	1:C:366:ALA:HB2	1.95	0.49
1:D:171:GLY:N	1:D:185:VAL:HG23	2.27	0.49
1:D:318:ASN:HD21	1:D:355:GLY:HA3	1.76	0.49
1:A:403:PRO:CB	1:A:405:THR:HG23	2.43	0.49
1:A:516:ARG:O	1:A:518:GLY:N	2.45	0.49
1:A:123:LEU:HD22	1:A:150:GLU:HG2	1.94	0.49
1:B:123:LEU:HD22	1:B:150:GLU:HG2	1.95	0.49
1:B:142:ILE:HG21	1:B:159:LEU:HD22	1.95	0.49
1:C:24:ASP:OD1	1:C:24:ASP:N	2.45	0.49
1:C:30:MET:HA	1:C:33:LEU:HD22	1.94	0.49
1:B:317:CYS:HB3	1:B:322:LYS:O	2.12	0.49
1:C:304:GLU:HG3	1:D:377:MET:CE	2.40	0.49
1:B:74:LEU:HD21	1:B:88:ILE:CG1	2.39	0.49
1:D:291:MET:HE2	1:D:360:MET:HE1	1.93	0.49
1:D:154:GLU:CD	1:D:154:GLU:H	2.21	0.49
1:C:158:TRP:CH2	1:C:160:ASP:HB3	2.47	0.49
1:D:123:LEU:HD22	1:D:128:GLY:HA2	1.95	0.49
1:D:327:ALA:HB2	1:D:360:MET:HE3	1.95	0.49
1:B:106:ARG:NE	1:B:106:ARG:HA	2.27	0.48
1:B:418:GLU:OE2	1:C:399:ARG:NH1	2.45	0.48
1:C:516:ARG:C	1:C:518:GLY:H	2.20	0.48
1:B:399:ARG:O	1:B:400:ARG:C	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LYS:HE3	1:D:198:GLU:HG3	1.95	0.48
1:B:43:ARG:NE	1:B:379:HIS:HD2	1.93	0.48
1:D:127:SER:HB2	1:D:130:ALA:HB2	1.94	0.48
1:A:15:THR:O	1:A:16:GLN:CB	2.61	0.48
1:B:291:MET:HE2	1:B:360:MET:CE	2.38	0.48
1:D:117:PRO:HB3	1:D:218:LEU:HB3	1.96	0.48
1:B:164:ILE:O	1:B:168:VAL:HG22	2.14	0.48
1:D:119:ILE:CG2	1:D:209:VAL:HB	2.43	0.48
1:D:173:LYS:NZ	1:D:184:GLN:HE21	2.11	0.48
1:D:272:GLU:HG2	1:D:293:ALA:HB3	1.95	0.48
1:D:514:GLY:HA3	5:D:604:FBP:O3	2.14	0.48
1:B:132:VAL:CG1	1:B:133:GLU:N	2.77	0.47
1:D:52:GLY:O	1:D:56:ARG:HB2	2.13	0.47
1:A:255:ARG:HG2	1:A:267:ILE:CD1	2.45	0.47
1:A:482:TRP:NE1	1:A:517:PRO:HA	2.28	0.47
1:D:153:ASP:CG	1:D:156:ILE:HG22	2.39	0.47
1:A:301:ILE:HD12	1:B:35:ILE:HG12	1.97	0.47
1:A:403:PRO:C	1:A:405:THR:H	2.22	0.47
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.96	0.47
1:C:51:ILE:HD11	1:C:69:MET:CE	2.45	0.47
1:C:115:LYS:HD3	1:C:224:LYS:HE3	1.97	0.47
1:D:153:ASP:OD1	1:D:156:ILE:HG22	2.15	0.47
1:D:171:GLY:H	1:D:185:VAL:HG23	1.78	0.47
1:A:55:SER:O	1:A:61:LEU:HG	2.15	0.47
1:D:149:MET:HE3	1:D:206:LYS:HZ1	1.77	0.47
1:A:403:PRO:HB3	1:A:405:THR:HG23	1.97	0.47
1:D:433:LYS:HE2	5:D:604:FBP:O3P	2.15	0.46
1:C:518:GLY:HA3	1:C:521:PHE:HD2	1.74	0.46
1:B:57:SER:OG	1:B:60:THR:HG23	2.14	0.46
1:C:482:TRP:NE1	1:C:517:PRO:HB3	2.29	0.46
1:A:126:GLY:CA	1:A:127:SER:CB	2.70	0.46
1:C:15:THR:HA	1:C:38:PRO:HD2	1.98	0.46
1:A:309:ALA:HB2	1:B:35:ILE:CD1	2.46	0.46
1:A:399:ARG:HH22	1:D:399:ARG:HH22	1.62	0.46
1:B:163:ASN:HD21	1:B:166:LYS:HD3	1.80	0.46
1:B:490:VAL:O	1:B:494:MET:HG2	2.16	0.46
1:B:133:GLU:HB3	1:B:135:LYS:HE3	1.97	0.46
1:B:494:MET:HE2	1:B:530:VAL:HB	1.98	0.46
1:A:361:LEU:HD22	1:A:364:GLU:HG2	1.96	0.46
1:D:490:VAL:O	1:D:494:MET:HG2	2.16	0.46
1:A:377:MET:HE3	1:A:381:ILE:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:MET:HG3	1:B:372:LEU:HD23	1.98	0.45
1:B:305:LYS:NZ	6:B:788:HOH:O	2.48	0.45
1:B:361:LEU:HD22	1:B:364:GLU:HG2	1.97	0.45
1:C:175:TYR:CE1	1:C:182:SER:HB3	2.51	0.45
1:C:187:GLN:HB3	1:C:194:VAL:HB	1.98	0.45
1:C:167:VAL:HG12	1:C:167:VAL:O	2.16	0.45
1:C:383:ARG:NH1	6:C:762:HOH:O	2.45	0.45
1:D:119:ILE:HG22	1:D:209:VAL:HB	1.98	0.45
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.75	0.45
1:C:169:GLU:O	1:C:170:VAL:C	2.59	0.45
1:C:304:GLU:CD	1:C:304:GLU:H	2.22	0.45
1:C:74:LEU:HD21	1:C:88:ILE:HG13	1.98	0.45
1:C:331:LEU:HD12	1:C:361:LEU:HD21	1.98	0.45
1:C:339:ARG:HD3	6:D:711:HOH:O	2.16	0.45
1:A:69:MET:HE2	1:A:72:ALA:HA	1.95	0.45
1:D:149:MET:CE	1:D:206:LYS:NZ	2.79	0.45
1:A:129:THR:O	1:A:130:ALA:HB3	2.18	0.44
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.69	0.44
1:D:416:ALA:HB2	1:D:512:LEU:HD21	2.00	0.44
1:D:443:ARG:NE	6:D:715:HOH:O	2.51	0.44
1:D:516:ARG:HD2	1:D:518:GLY:H	1.82	0.44
1:C:453:VAL:HG22	1:C:493:ALA:HB2	1.99	0.44
1:D:173:LYS:HA	1:D:173:LYS:HD3	1.73	0.44
1:D:268:ILE:HD12	1:D:289:GLY:HA3	1.98	0.44
1:B:114:THR:CG2	1:B:243:SER:H	2.30	0.44
1:B:163:ASN:ND2	1:B:166:LYS:HD3	2.31	0.44
1:C:15:THR:HG22	1:C:38:PRO:HG2	2.00	0.44
1:A:16:GLN:HG3	1:A:40:ILE:HG23	1.98	0.44
1:A:309:ALA:HB1	1:A:313:MET:HE2	1.98	0.44
1:B:377:MET:HE3	1:B:381:ILE:HG13	2.00	0.44
1:C:129:THR:O	1:C:130:ALA:CB	2.66	0.44
1:D:187:GLN:HB3	1:D:194:VAL:CG1	2.48	0.44
1:C:132:VAL:HG21	1:C:153:ASP:HA	2.00	0.43
1:C:159:LEU:HD11	1:C:209:VAL:HG21	2.00	0.43
1:C:331:LEU:HD23	1:C:344:GLU:HB3	1.99	0.43
1:B:331:LEU:HD23	1:B:344:GLU:HB3	2.00	0.43
1:A:101:ASP:OD2	1:A:104:LEU:HD22	2.17	0.43
1:C:262:GLY:O	1:C:263:LYS:C	2.60	0.43
1:B:389:ILE:HD11	1:B:467:ARG:NH2	2.33	0.43
1:B:516:ARG:HD3	1:B:518:GLY:H	1.84	0.43
1:D:317:CYS:HB3	1:D:322:LYS:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:THR:HA	5:D:604:FBP:H61	2.01	0.43
1:A:361:LEU:HD22	1:A:364:GLU:HG3	2.00	0.43
1:B:71:VAL:HG22	1:B:109:ALA:HB3	2.00	0.43
1:B:148:TYR:HA	1:B:151:LYS:HB2	2.01	0.43
1:B:248:ALA:O	1:B:251:VAL:N	2.51	0.43
1:C:361:LEU:HD22	1:C:364:GLU:HG2	1.99	0.43
1:C:516:ARG:O	1:C:518:GLY:N	2.52	0.43
1:B:48:ILE:HG12	1:B:71:VAL:HB	2.01	0.43
1:B:405:THR:O	1:C:423:CYS:HA	2.19	0.43
1:B:463:ALA:HB1	1:B:469:ILE:HG21	2.00	0.43
1:C:127:SER:N	1:C:128:GLY:CA	2.55	0.43
1:C:305:LYS:O	1:D:35:ILE:HD11	2.19	0.43
1:D:127:SER:HB3	1:D:130:ALA:H	1.84	0.43
1:A:165:CYS:SG	1:A:193:LEU:HD13	2.58	0.42
1:C:19:HIS:O	1:C:22:MET:HG2	2.19	0.42
1:D:114:THR:HG22	1:D:243:SER:H	1.83	0.42
1:A:118:GLU:OE2	1:A:120:ARG:HD2	2.18	0.42
1:B:340:PRO:HG3	1:B:377:MET:HG2	2.01	0.42
1:A:246:ARG:C	1:A:283:ILE:HD11	2.44	0.42
1:B:407:ASP:HA	1:B:408:PRO:HD3	1.83	0.42
1:C:323:PRO:HB3	1:C:465:LEU:O	2.19	0.42
1:D:18:LEU:O	1:D:21:ALA:HB3	2.19	0.42
1:D:409:THR:HG23	1:D:522:THR:HB	1.99	0.42
1:D:494:MET:CE	1:D:530:VAL:HB	2.49	0.42
1:A:114:THR:CG2	1:A:243:SER:H	2.32	0.42
1:B:173:LYS:HE3	1:B:198:GLU:HG3	2.01	0.42
1:C:64:MET:HG3	1:C:372:LEU:HD23	2.01	0.42
1:C:516:ARG:C	1:C:518:GLY:N	2.77	0.42
1:B:494:MET:CE	1:B:494:MET:HA	2.50	0.42
1:C:27:LEU:HD23	1:D:401:LEU:HD12	2.02	0.42
1:C:516:ARG:CD	1:C:518:GLY:H	2.31	0.42
1:C:49:CYS:HB2	1:C:69:MET:HE3	2.01	0.42
1:A:472:VAL:CG1	1:A:492:PHE:CE2	3.03	0.42
1:C:64:MET:HG3	1:C:372:LEU:CD2	2.49	0.42
1:A:186:LYS:HA	1:A:186:LYS:HD3	1.76	0.42
1:C:301:ILE:HD12	1:D:35:ILE:HG12	2.02	0.42
1:D:214:ALA:O	1:D:216:VAL:HG23	2.20	0.42
1:B:121:THR:HA	1:B:159:LEU:HD12	2.02	0.41
1:D:172:SER:H	1:D:185:VAL:CG2	2.33	0.41
1:D:299:ILE:H	1:D:299:ILE:HG12	1.60	0.41
1:B:69:MET:HE2	1:B:72:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASP:O	1:B:300:GLU:HB2	2.20	0.41
1:C:162:LYS:HD3	1:C:162:LYS:HA	1.69	0.41
1:A:106:ARG:HA	1:A:106:ARG:NE	2.35	0.41
1:A:383:ARG:HD2	6:A:750:HOH:O	2.21	0.41
1:B:515:TRP:CH2	1:B:516:ARG:HG2	2.55	0.41
1:D:224:LYS:O	1:D:227:GLN:HB2	2.20	0.41
1:D:475:LYS:HD3	1:D:475:LYS:HA	1.86	0.41
1:A:165:CYS:SG	1:A:193:LEU:CD1	3.08	0.41
1:D:456:ASN:C	1:D:456:ASN:OD1	2.63	0.41
1:A:440:GLN:O	1:A:443:ARG:HG2	2.20	0.41
1:B:121:THR:O	1:B:206:LYS:HA	2.19	0.41
1:D:161:TYR:CE1	1:D:218:LEU:HD13	2.56	0.41
1:A:405:THR:OG1	1:A:406:SER:N	2.54	0.41
1:B:129:THR:O	1:B:130:ALA:HB2	2.20	0.41
1:C:199:ASN:HD22	1:C:199:ASN:HA	1.64	0.41
1:A:51:ILE:HD11	1:A:69:MET:CE	2.47	0.41
1:A:330:MET:O	1:A:331:LEU:HD23	2.20	0.41
1:B:126:GLY:O	1:B:129:THR:HB	2.21	0.41
1:B:143:THR:HG21	1:B:148:TYR:CD2	2.55	0.41
1:B:416:ALA:HB2	1:B:512:LEU:HD21	2.02	0.41
1:C:120:ARG:HA	1:C:207:LYS:O	2.20	0.41
1:D:49:CYS:SG	1:D:69:MET:HG3	2.61	0.41
1:D:166:LYS:HE2	1:D:167:VAL:HA	2.03	0.41
1:B:114:THR:HG22	1:B:243:SER:H	1.86	0.41
1:A:416:ALA:HB2	1:A:512:LEU:HD21	2.03	0.40
1:B:121:THR:HG22	1:B:159:LEU:CD1	2.51	0.40
1:B:336:LYS:HA	1:B:336:LYS:HD2	1.92	0.40
1:C:48:ILE:HG12	1:C:71:VAL:HB	2.03	0.40
1:D:229:LEU:HD23	1:D:229:LEU:HA	1.91	0.40
1:B:30:MET:HA	1:B:33:LEU:HD22	2.04	0.40
1:D:173:LYS:HZ1	1:D:184:GLN:HE21	1.69	0.40
1:A:243:SER:HA	1:A:270:LYS:HB2	2.02	0.40
1:A:505:LYS:HD2	1:A:506:GLY:N	2.36	0.40
1:C:528:VAL:HG12	1:C:529:PRO:O	2.20	0.40
1:A:317:CYS:HB3	1:A:322:LYS:O	2.21	0.40
1:B:318:ASN:HD21	1:B:355:GLY:HA3	1.87	0.40
1:C:356:ALA:C	1:C:467:ARG:HH12	2.12	0.40
1:D:134:LEU:HD21	1:D:203:LEU:HD22	2.04	0.40
1:D:144:LEU:HD12	1:D:191:ASP:HA	2.04	0.40
1:D:304:GLU:CD	1:D:304:GLU:H	2.28	0.40
1:C:311:LYS:O	1:D:30:MET:HE2	2.21	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	516/518 (100%)	485 (94%)	21 (4%)	10 (2%)	6	7
1	B	516/518 (100%)	487 (94%)	20 (4%)	9 (2%)	7	9
1	C	516/518 (100%)	490 (95%)	20 (4%)	6 (1%)	10	15
1	D	516/518 (100%)	486 (94%)	25 (5%)	5 (1%)	12	18
All	All	2064/2072 (100%)	1948 (94%)	86 (4%)	30 (2%)	8	11

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	B	130	ALA
1	B	188	LYS
1	B	518	GLY
1	B	519	SER
1	C	518	GLY
1	C	519	SER
1	D	518	GLY
1	B	125	LYS
1	B	190	ALA
1	C	129	THR
1	C	130	ALA
1	D	145	ASP
1	D	259	GLY
1	D	519	SER
1	A	263	LYS
1	A	517	PRO
1	A	521	PHE
1	B	197	VAL
1	D	328	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	THR
1	B	328	THR
1	B	523	ASN
1	C	15	THR
1	C	328	THR
1	A	132	VAL
1	A	505	LYS
1	A	404	ILE
1	A	407	ASP
1	A	518	GLY

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	426/426 (100%)	387 (91%)	39 (9%)	8	13
1	B	426/426 (100%)	374 (88%)	52 (12%)	5	6
1	C	426/426 (100%)	377 (88%)	49 (12%)	5	7
1	D	426/426 (100%)	378 (89%)	48 (11%)	5	8
All	All	1704/1704 (100%)	1516 (89%)	188 (11%)	6	8

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	24	ASP
1	A	33	LEU
1	A	35	ILE
1	A	86	GLU
1	A	103	ILE
1	A	104	LEU
1	A	114	THR
1	A	123	LEU
1	A	129	THR
1	A	132	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	THR
1	A	140	LEU
1	A	144	LEU
1	A	159	LEU
1	A	167	VAL
1	A	193	LEU
1	A	198	GLU
1	A	202	SER
1	A	246	ARG
1	A	258	LEU
1	A	304	GLU
1	A	312	MET
1	A	353	LEU
1	A	380	LEU
1	A	383	ARG
1	A	392	LEU
1	A	396	GLU
1	A	406	SER
1	A	467	ARG
1	A	472	VAL
1	A	484	GLU
1	A	488	LEU
1	A	494	MET
1	A	504	LYS
1	A	510	ILE
1	A	513	THR
1	A	516	ARG
1	A	530	VAL
1	B	18	LEU
1	B	27	LEU
1	B	33	LEU
1	B	35	ILE
1	B	59	GLU
1	B	60	THR
1	B	104	LEU
1	B	114	THR
1	B	127	SER
1	B	131	GLU
1	B	134	LEU
1	B	135	LYS
1	B	139	THR
1	B	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	144	LEU
1	B	151	LYS
1	B	159	LEU
1	B	170	VAL
1	B	186	LYS
1	B	193	LEU
1	B	199	ASN
1	B	202	SER
1	B	224	LYS
1	B	230	LYS
1	B	247	LYS
1	B	256	LYS
1	B	257	VAL
1	B	258	LEU
1	B	263	LYS
1	B	300	GLU
1	B	304	GLU
1	B	336	LYS
1	B	346	SER
1	B	353	LEU
1	B	380	LEU
1	B	383	ARG
1	B	392	LEU
1	B	436	ARG
1	B	443	ARG
1	B	447	ARG
1	B	467	ARG
1	B	472	VAL
1	B	487	ASP
1	B	494	MET
1	B	504	LYS
1	B	505	LYS
1	B	508	VAL
1	B	513	THR
1	B	516	ARG
1	B	519	SER
1	B	528	VAL
1	B	530	VAL
1	C	14	GLN
1	C	18	LEU
1	C	24	ASP
1	C	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	35	ILE
1	C	60	THR
1	C	86	GLU
1	C	104	LEU
1	C	114	THR
1	C	123	LEU
1	C	127	SER
1	C	132	VAL
1	C	134	LEU
1	C	136	LYS
1	C	139	THR
1	C	140	LEU
1	C	144	LEU
1	C	151	LYS
1	C	159	LEU
1	C	193	LEU
1	C	198	GLU
1	C	202	SER
1	C	235	GLN
1	C	256	LYS
1	C	258	LEU
1	C	304	GLU
1	C	312	MET
1	C	337	LYS
1	C	346	SER
1	C	353	LEU
1	C	380	LEU
1	C	383	ARG
1	C	392	LEU
1	C	396	GLU
1	C	400	ARG
1	C	424	CYS
1	C	459	THR
1	C	467	ARG
1	C	472	VAL
1	C	475	LYS
1	C	479	GLN
1	C	494	MET
1	C	504	LYS
1	C	505	LYS
1	C	508	VAL
1	C	513	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	516	ARG
1	C	519	SER
1	C	530	VAL
1	D	18	LEU
1	D	33	LEU
1	D	35	ILE
1	D	100	SER
1	D	103	ILE
1	D	104	LEU
1	D	114	THR
1	D	118	GLU
1	D	124	ILE
1	D	127	SER
1	D	131	GLU
1	D	132	VAL
1	D	149	MET
1	D	154	GLU
1	D	156	ILE
1	D	164	ILE
1	D	166	LYS
1	D	167	VAL
1	D	168	VAL
1	D	188	LYS
1	D	211	LEU
1	D	218	LEU
1	D	246	ARG
1	D	256	LYS
1	D	258	LEU
1	D	261	LYS
1	D	285	GLU
1	D	299	ILE
1	D	304	GLU
1	D	312	MET
1	D	353	LEU
1	D	364	GLU
1	D	380	LEU
1	D	392	LEU
1	D	396	GLU
1	D	406	SER
1	D	424	CYS
1	D	436	ARG
1	D	467	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	472	VAL
1	D	479	GLN
1	D	491	ASN
1	D	494	MET
1	D	505	LYS
1	D	513	THR
1	D	516	ARG
1	D	519	SER
1	D	530	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	90	ASN
1	A	199	ASN
1	A	210	ASN
1	A	318	ASN
1	A	379	HIS
1	A	440	GLN
1	B	14	GLN
1	B	90	ASN
1	B	184	GLN
1	B	187	GLN
1	B	252	HIS
1	B	318	ASN
1	B	379	HIS
1	B	440	GLN
1	C	14	GLN
1	C	78	HIS
1	C	90	ASN
1	C	184	GLN
1	C	199	ASN
1	C	227	GLN
1	C	252	HIS
1	C	318	ASN
1	C	379	HIS
1	C	393	GLN
1	D	90	ASN
1	D	146	ASN
1	D	184	GLN
1	D	210	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	GLN
1	D	264	ASN
1	D	318	ASN
1	D	379	HIS
1	D	393	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FBP	C	604	-	18,20,20	0.77	1 (5%)	21,32,32	1.34	3 (14%)
5	FBP	D	604	-	18,20,20	0.94	0	21,32,32	1.32	2 (9%)
2	PYR	B	601	-	5,5,5	1.38	0	3,6,6	2.36	2 (66%)
4	SER	A	603	-	4,6,6	1.08	0	2,7,7	1.15	0
4	SER	B	603	-	4,6,6	1.01	0	2,7,7	0.51	0
4	SER	D	603	-	4,6,6	1.09	0	2,7,7	1.99	1 (50%)
5	FBP	B	604	-	18,20,20	0.92	1 (5%)	21,32,32	1.31	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PYR	D	601	-	5,5,5	1.51	1 (20%)	3,6,6	1.86	0
2	PYR	A	601	-	5,5,5	1.32	1 (20%)	3,6,6	1.62	1 (33%)
4	SER	C	603	-	4,6,6	1.01	0	2,7,7	1.21	0
2	PYR	C	601	-	5,5,5	1.09	0	3,6,6	1.65	1 (33%)

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
5	FBP	C	604	-	-	2/13/32/32	0/1/1/1
5	FBP	D	604	-	-	3/13/32/32	0/1/1/1
2	PYR	B	601	-	-	0/4/4/4	-
4	SER	A	603	-	-	0/6/6/6	-
4	SER	B	603	-	-	0/6/6/6	-
4	SER	D	603	-	-	0/6/6/6	-
5	FBP	B	604	-	-	2/13/32/32	0/1/1/1
2	PYR	D	601	-	-	0/4/4/4	-
2	PYR	A	601	-	-	0/4/4/4	-
4	SER	C	603	-	-	0/6/6/6	-
2	PYR	C	601	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	604	FBP	O2-C2	2.67	1.45	1.40
2	D	601	PYR	OXT-C	-2.33	1.24	1.30
2	A	601	PYR	O-C	2.18	1.28	1.22
5	C	604	FBP	O2-C2	2.13	1.44	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	604	FBP	O1-P1-O1P	-3.75	96.31	106.44
5	B	604	FBP	O3P-P1-O2P	3.49	120.90	107.80
2	B	601	PYR	OXT-C-CA	3.00	121.91	113.59
5	D	604	FBP	O5-C5-C6	2.91	116.33	109.50
5	B	604	FBP	O6-P2-O4P	-2.84	98.77	106.44
4	D	603	SER	OXT-C-O	-2.69	117.97	124.08
5	C	604	FBP	O2P-P1-O1P	2.59	120.91	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PYR	O3-CA-CB	2.46	125.28	119.77
2	C	601	PYR	OXT-C-CA	2.32	120.02	113.59
5	D	604	FBP	O3P-P1-O1	-2.31	100.64	106.67
2	A	601	PYR	OXT-C-CA	2.19	119.65	113.59
5	C	604	FBP	O5P-P2-O6	-2.01	101.43	106.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

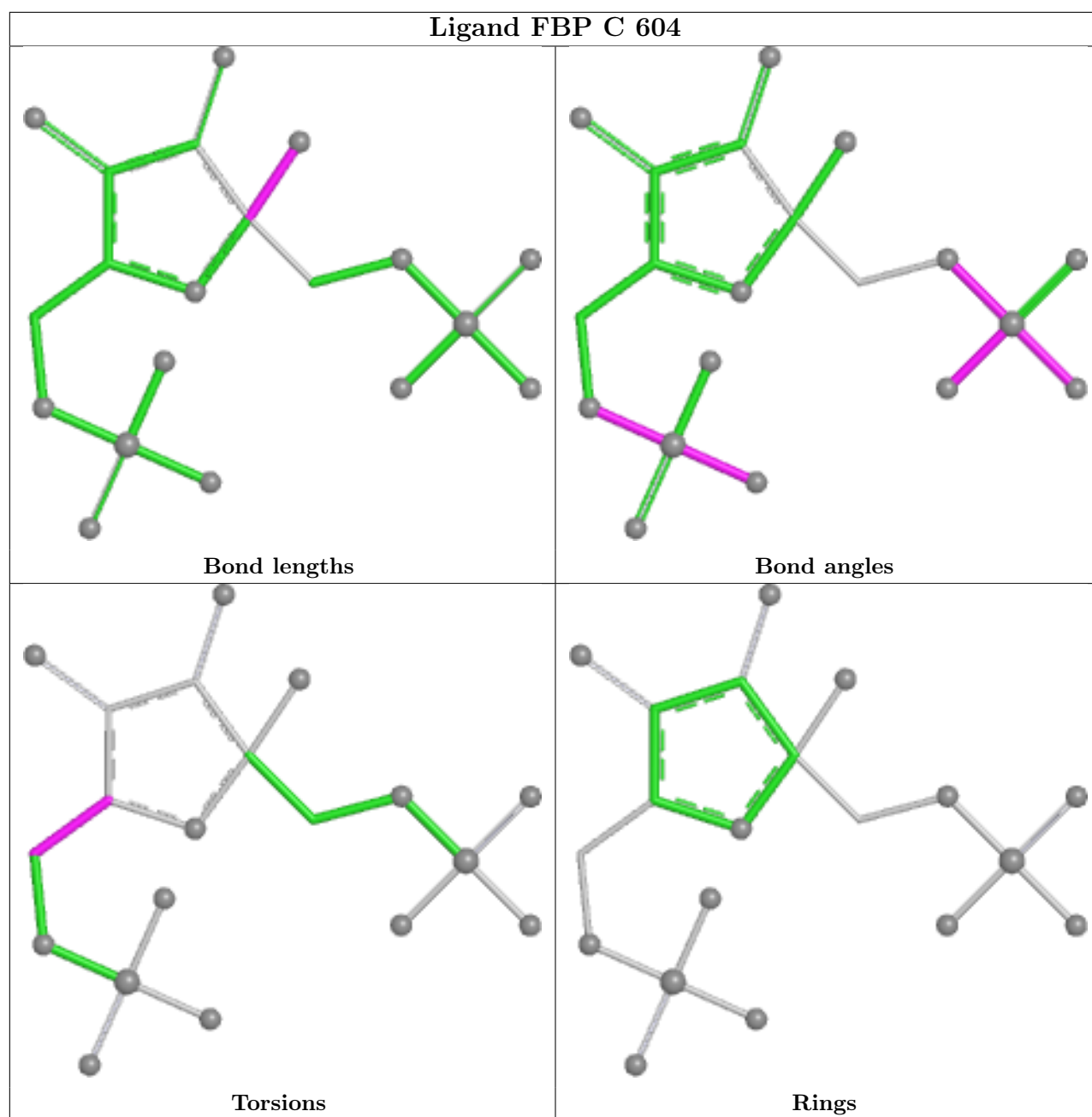
Mol	Chain	Res	Type	Atoms
5	D	604	FBP	O1-C1-C2-O5
5	D	604	FBP	C4-C5-C6-O6
5	B	604	FBP	C4-C5-C6-O6
5	C	604	FBP	C4-C5-C6-O6
5	D	604	FBP	O5-C5-C6-O6
5	B	604	FBP	O5-C5-C6-O6
5	C	604	FBP	O5-C5-C6-O6

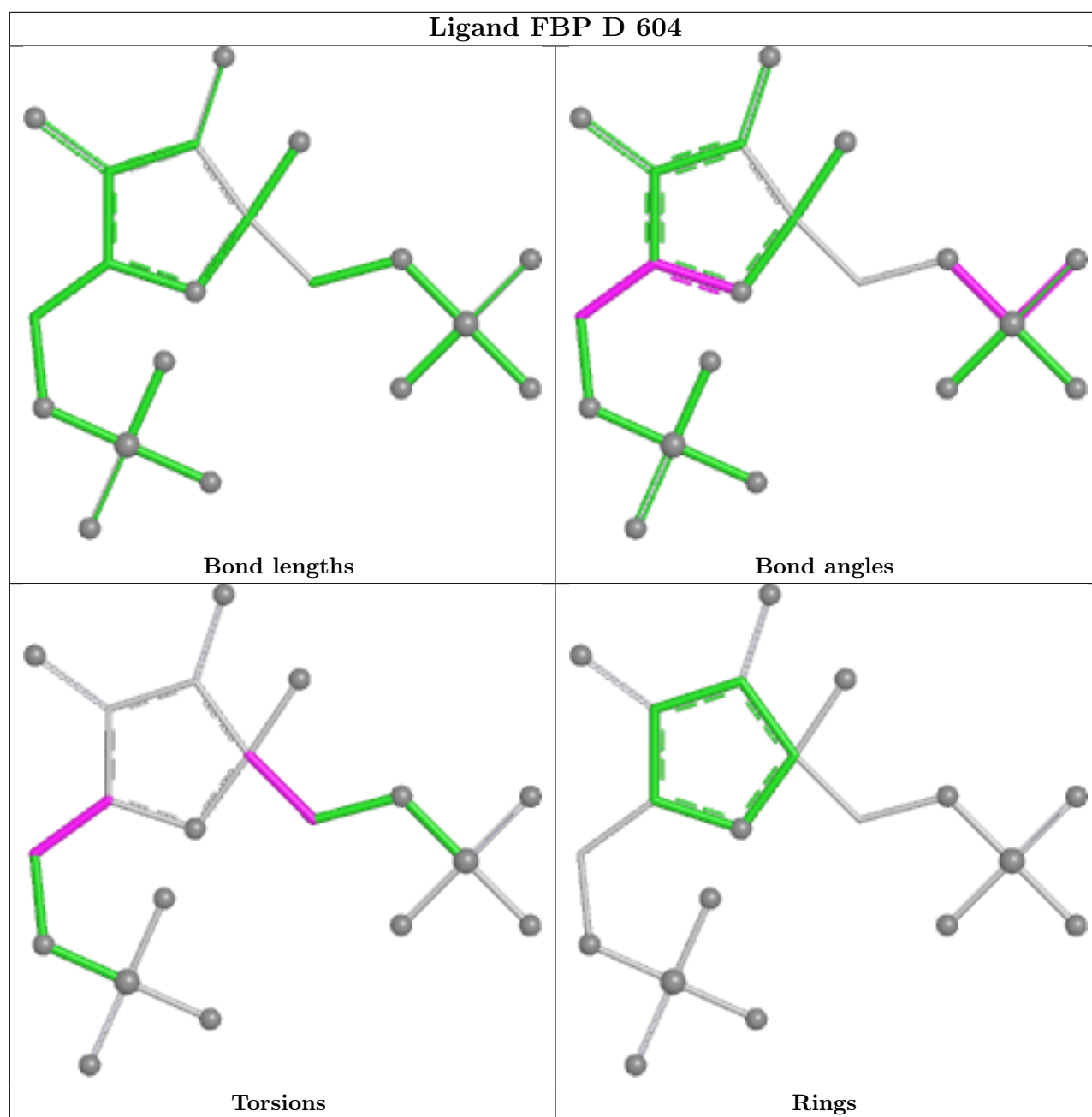
There are no ring outliers.

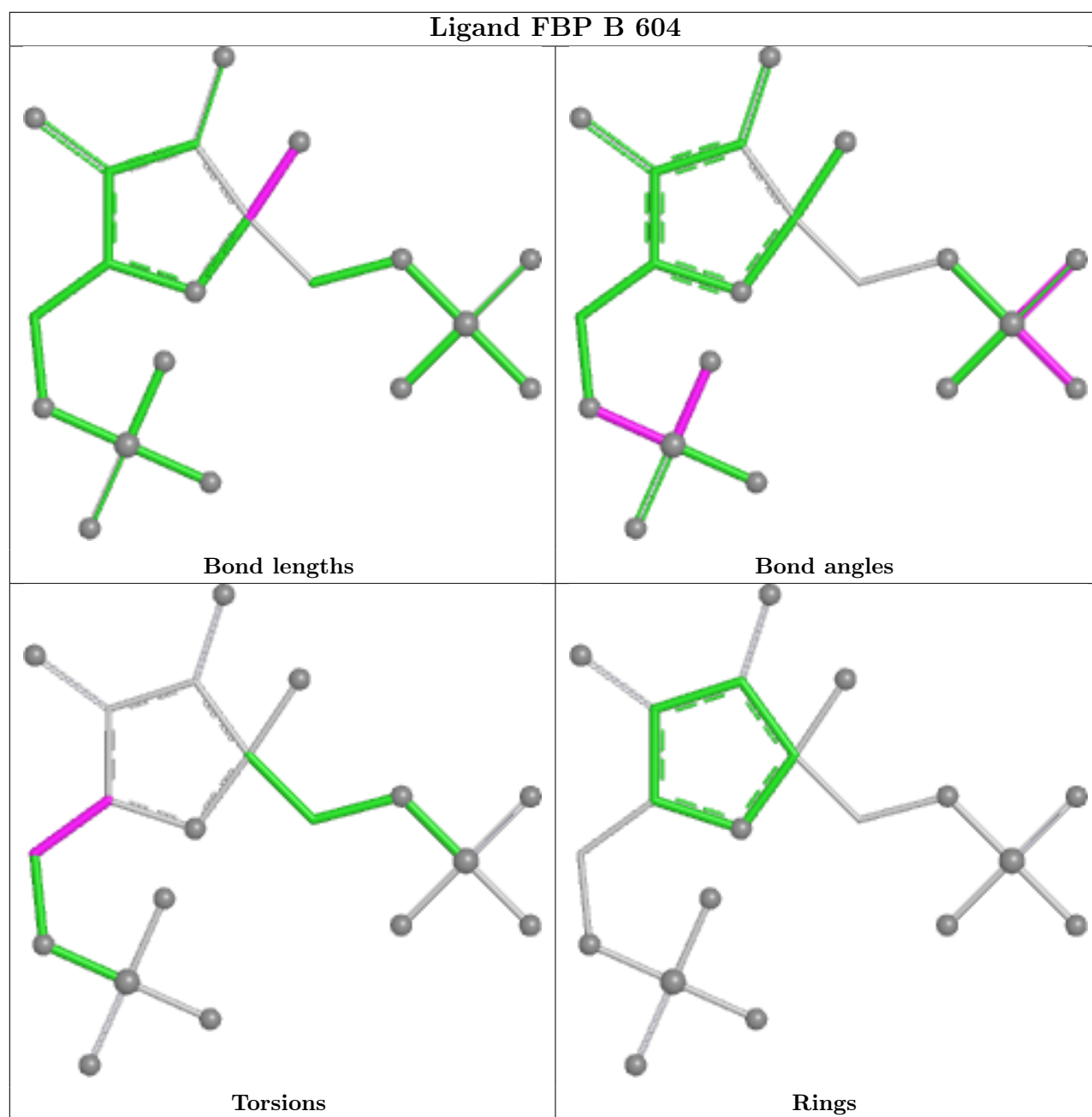
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	604	FBP	3	0
4	A	603	SER	1	0
4	B	603	SER	1	0
5	B	604	FBP	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	518/518 (100%)	-0.76	4 (0%) 82 80	18, 32, 67, 119	0
1	B	518/518 (100%)	-0.70	1 (0%) 91 90	20, 34, 75, 151	0
1	C	518/518 (100%)	-0.64	3 (0%) 85 84	24, 39, 68, 100	0
1	D	518/518 (100%)	-0.59	4 (0%) 82 80	21, 38, 82, 110	0
All	All	2072/2072 (100%)	-0.67	12 (0%) 85 84	18, 36, 75, 151	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	TRP	4.1
1	A	129	THR	3.4
1	B	130	ALA	3.1
1	C	130	ALA	3.0
1	A	404	ILE	2.7
1	D	190	ALA	2.7
1	D	148	TYR	2.7
1	C	129	THR	2.6
1	C	519	SER	2.3
1	D	519	SER	2.1
1	A	125	LYS	2.0
1	D	149	MET	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

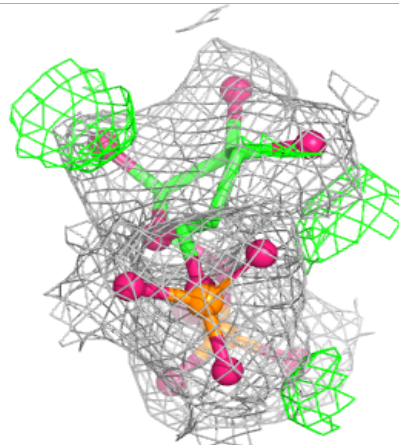
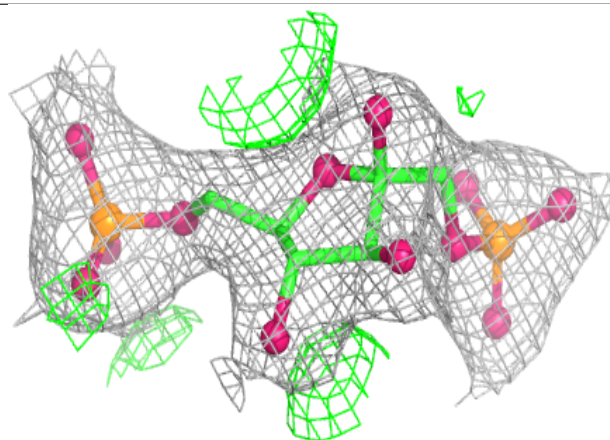
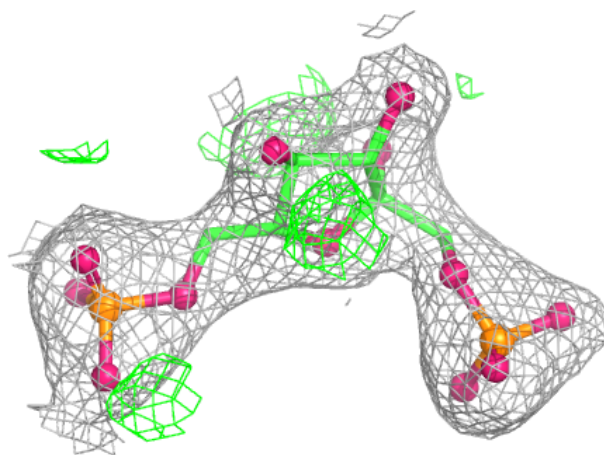
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PYR	B	601	6/6	0.78	0.13	40,45,53,57	0
2	PYR	D	601	6/6	0.82	0.12	46,50,60,60	0
2	PYR	C	601	6/6	0.88	0.10	34,44,51,63	0
2	PYR	A	601	6/6	0.93	0.08	37,42,44,51	0
3	MG	D	602	1/1	0.95	0.04	39,39,39,39	0
4	SER	C	603	7/7	0.95	0.06	36,38,40,42	0
4	SER	D	603	7/7	0.96	0.06	31,33,35,35	0
4	SER	A	603	7/7	0.97	0.06	26,27,30,30	0
5	FBP	B	604	20/20	0.97	0.05	33,40,49,51	0
4	SER	B	603	7/7	0.98	0.05	27,28,30,31	0
3	MG	C	602	1/1	0.98	0.03	20,20,20,20	0
5	FBP	C	604	20/20	0.98	0.04	33,39,43,45	0
5	FBP	D	604	20/20	0.98	0.05	33,41,46,52	0
3	MG	B	602	1/1	0.99	0.04	18,18,18,18	0
3	MG	A	602	1/1	0.99	0.03	15,15,15,15	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.

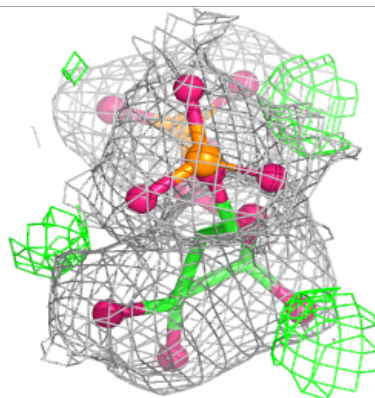
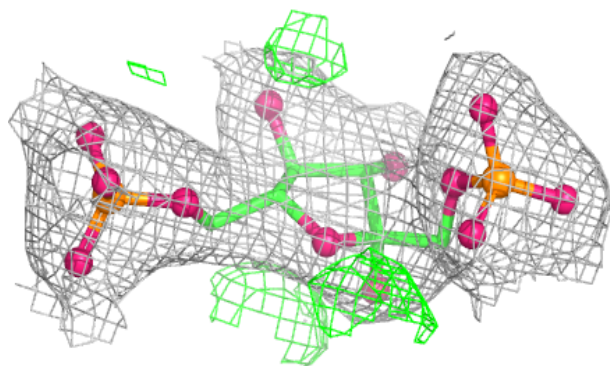
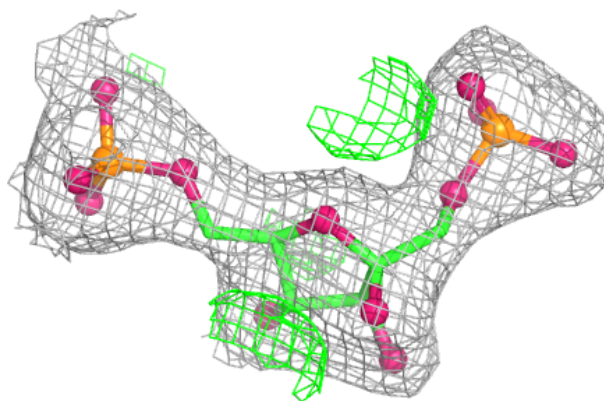
Electron density around FBP B 604:

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

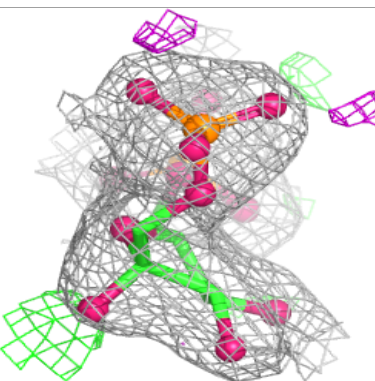
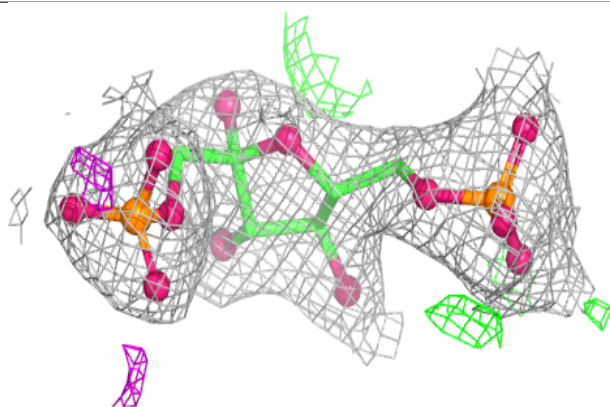
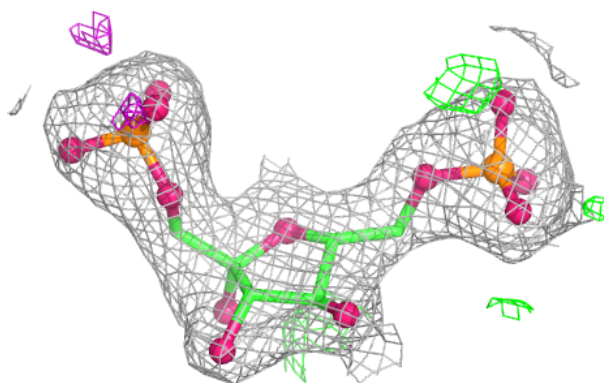


Electron density around FBP C 604:

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

**Electron density around FBP D 604:**

$2mF_o-DF_c$ (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.