



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 05:14 AM UTC

PDB ID : 8IAV / pdb_00008iav
Title : Crystal structure of Streptococcus pneumoniae pyruvate kinase in complex with fructose 1,6-bisphosphate
Authors : Nakashima, R.; Taguchi, A.
Deposited on : 2023-02-09
Resolution : 2.59 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

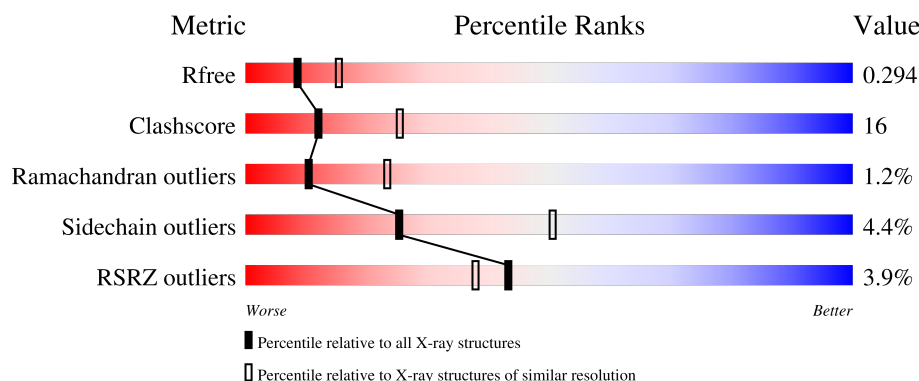
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	521	
1	B	521	
1	C	521	
1	D	521	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13962 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3443	2153	592	681	17			
1	B	445	Total	C	N	O	S	0	0	0
			3396	2117	590	672	17			
1	C	460	Total	C	N	O	S	0	0	0
			3508	2188	609	694	17			
1	D	460	Total	C	N	O	S	0	0	0
			3517	2195	609	696	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	-19	MET	-	initiating methionine	UNP Q8DQ84

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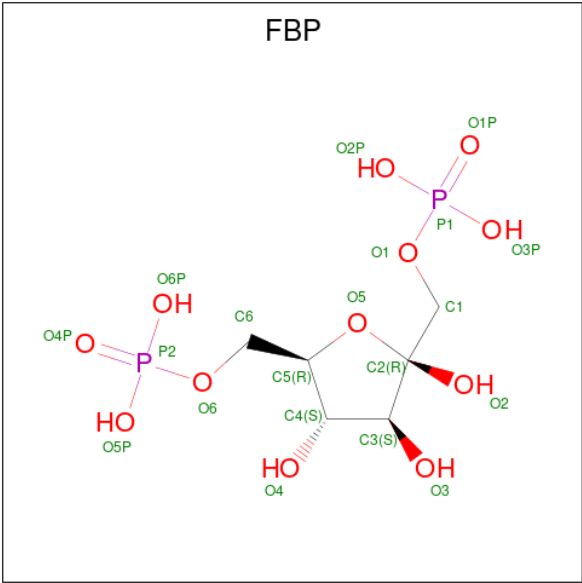
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q8DQ84
B	-17	SER	-	expression tag	UNP Q8DQ84
B	-16	SER	-	expression tag	UNP Q8DQ84
B	-15	HIS	-	expression tag	UNP Q8DQ84
B	-14	HIS	-	expression tag	UNP Q8DQ84
B	-13	HIS	-	expression tag	UNP Q8DQ84
B	-12	HIS	-	expression tag	UNP Q8DQ84
B	-11	HIS	-	expression tag	UNP Q8DQ84
B	-10	HIS	-	expression tag	UNP Q8DQ84
B	-9	SER	-	expression tag	UNP Q8DQ84
B	-8	SER	-	expression tag	UNP Q8DQ84
B	-7	GLY	-	expression tag	UNP Q8DQ84
B	-6	LEU	-	expression tag	UNP Q8DQ84
B	-5	VAL	-	expression tag	UNP Q8DQ84
B	-4	PRO	-	expression tag	UNP Q8DQ84
B	-3	ARG	-	expression tag	UNP Q8DQ84
B	-2	GLY	-	expression tag	UNP Q8DQ84
B	-1	SER	-	expression tag	UNP Q8DQ84
B	0	HIS	-	expression tag	UNP Q8DQ84
C	-19	MET	-	initiating methionine	UNP Q8DQ84
C	-18	GLY	-	expression tag	UNP Q8DQ84
C	-17	SER	-	expression tag	UNP Q8DQ84
C	-16	SER	-	expression tag	UNP Q8DQ84
C	-15	HIS	-	expression tag	UNP Q8DQ84
C	-14	HIS	-	expression tag	UNP Q8DQ84
C	-13	HIS	-	expression tag	UNP Q8DQ84
C	-12	HIS	-	expression tag	UNP Q8DQ84
C	-11	HIS	-	expression tag	UNP Q8DQ84
C	-10	HIS	-	expression tag	UNP Q8DQ84
C	-9	SER	-	expression tag	UNP Q8DQ84
C	-8	SER	-	expression tag	UNP Q8DQ84
C	-7	GLY	-	expression tag	UNP Q8DQ84
C	-6	LEU	-	expression tag	UNP Q8DQ84
C	-5	VAL	-	expression tag	UNP Q8DQ84
C	-4	PRO	-	expression tag	UNP Q8DQ84
C	-3	ARG	-	expression tag	UNP Q8DQ84
C	-2	GLY	-	expression tag	UNP Q8DQ84
C	-1	SER	-	expression tag	UNP Q8DQ84
C	0	HIS	-	expression tag	UNP Q8DQ84
D	-19	MET	-	initiating methionine	UNP Q8DQ84
D	-18	GLY	-	expression tag	UNP Q8DQ84
D	-17	SER	-	expression tag	UNP Q8DQ84

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q8DQ84
D	-15	HIS	-	expression tag	UNP Q8DQ84
D	-14	HIS	-	expression tag	UNP Q8DQ84
D	-13	HIS	-	expression tag	UNP Q8DQ84
D	-12	HIS	-	expression tag	UNP Q8DQ84
D	-11	HIS	-	expression tag	UNP Q8DQ84
D	-10	HIS	-	expression tag	UNP Q8DQ84
D	-9	SER	-	expression tag	UNP Q8DQ84
D	-8	SER	-	expression tag	UNP Q8DQ84
D	-7	GLY	-	expression tag	UNP Q8DQ84
D	-6	LEU	-	expression tag	UNP Q8DQ84
D	-5	VAL	-	expression tag	UNP Q8DQ84
D	-4	PRO	-	expression tag	UNP Q8DQ84
D	-3	ARG	-	expression tag	UNP Q8DQ84
D	-2	GLY	-	expression tag	UNP Q8DQ84
D	-1	SER	-	expression tag	UNP Q8DQ84
D	0	HIS	-	expression tag	UNP Q8DQ84

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂).



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

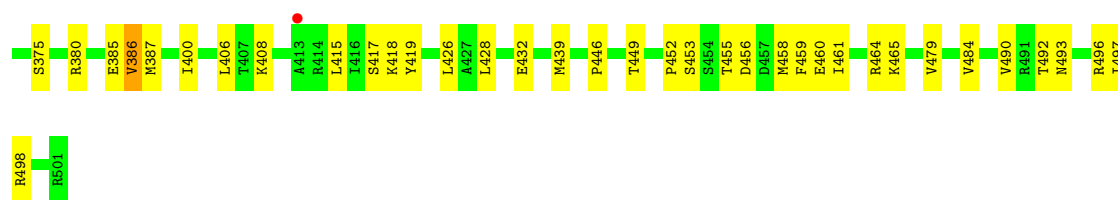
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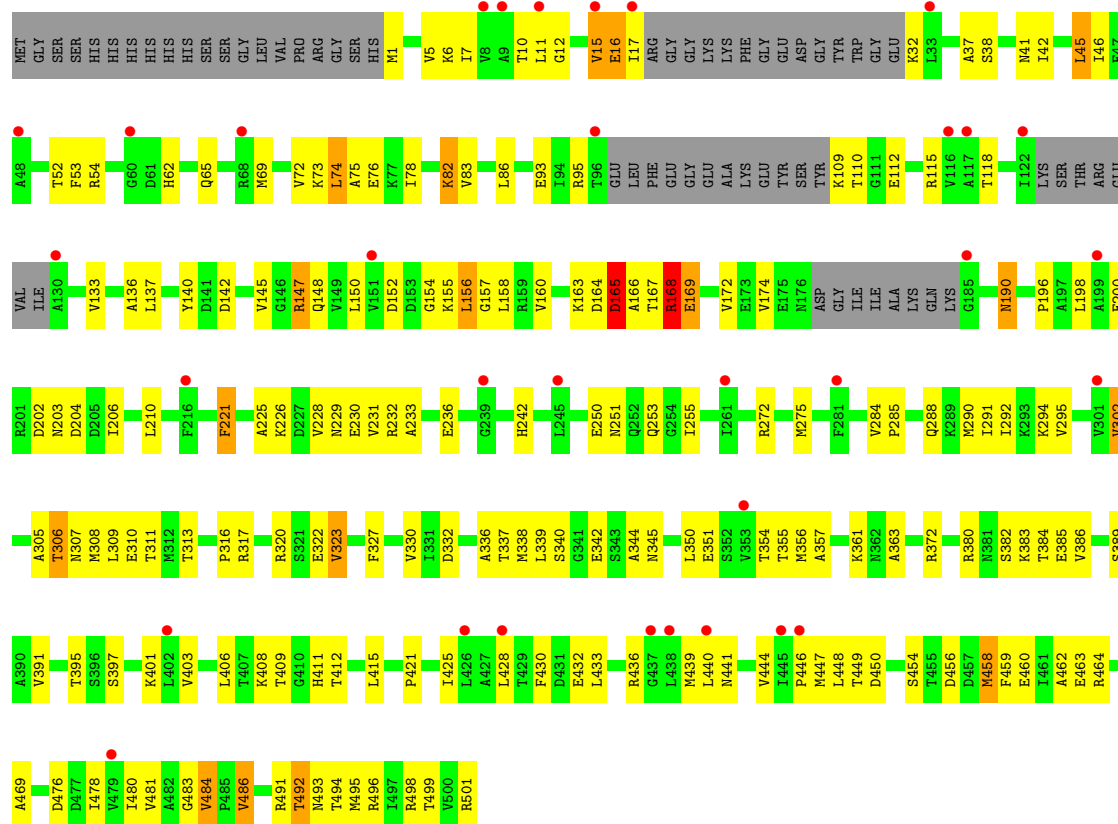
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is water.

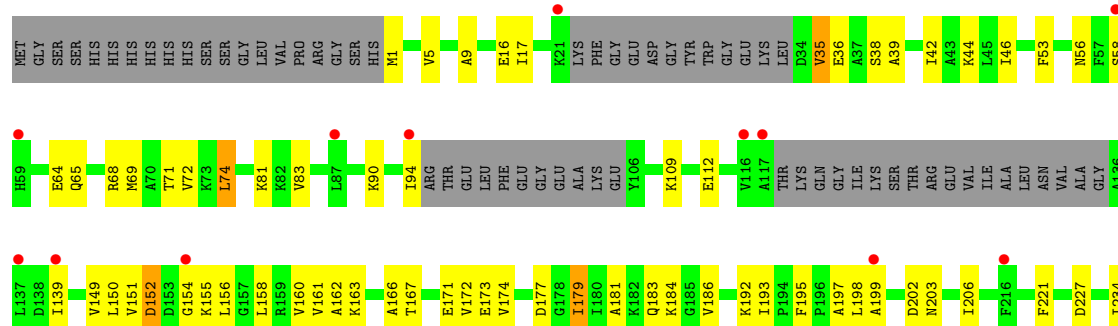
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	5	Total	O	0	0
			5	5		
3	C	3	Total	O	0	0
			3	3		
3	D	7	Total	O	0	0
			7	7		



• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.03Å 86.79Å 129.86Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	47.69 – 2.59 47.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.69-2.59) 99.2 (47.69-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.234 , 0.298 0.233 , 0.294	Depositor DCC
R_{free} test set	3621 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13962	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: 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	0.89	0/3482	1.05	2/4699 (0.0%)
1	B	0.91	0/3429	1.10	1/4618 (0.0%)
1	C	0.88	0/3542	1.02	3/4776 (0.1%)
1	D	0.88	0/3554	1.03	0/4791
All	All	0.89	0/14007	1.05	6/18884 (0.0%)

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	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ILE	CA-C-N	6.03	128.63	120.38
1	A	139	ILE	C-N-CA	6.03	128.63	120.38
1	C	16	GLU	CB-CG-CD	-5.98	102.43	112.60
1	C	15	VAL	CA-C-N	-5.74	114.09	122.65
1	C	15	VAL	C-N-CA	-5.74	114.09	122.65
1	B	459	PHE	CA-CB-CG	-5.09	108.71	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	179	ILE	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	3443	0	3472	97	0
1	B	3396	0	3443	94	0
1	C	3508	0	3566	169	0
1	D	3517	0	3565	106	0
2	A	20	0	10	2	0
2	B	20	0	10	0	0
2	C	20	0	10	3	0
2	D	20	0	10	1	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
3	C	3	0	0	0	0
3	D	7	0	0	0	0
All	All	13962	0	14086	440	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 16.

All (440) 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:115:ARG:HH12	1:C:169:GLU:CD	1.67	1.01
1:C:459:PHE:CE2	1:C:496:ARG:NH2	2.28	1.00
1:D:412:THR:HG23	2:D:601:FBP:O1P	1.70	0.92
1:C:42:ILE:HG21	1:C:72:VAL:HG12	1.51	0.91
1:B:386:VAL:HG11	1:D:398:MET:HG3	1.50	0.91
1:C:460:GLU:OE1	1:C:464:ARG:CZ	2.21	0.89
1:A:160:VAL:HA	1:A:172:VAL:HG12	1.57	0.86
1:C:308:MET:HE1	1:C:337:THR:HB	1.56	0.86
1:C:459:PHE:CD2	1:C:496:ARG:CZ	2.58	0.86
1:D:412:THR:HG21	1:D:492:THR:OG1	1.76	0.85
1:B:21:LYS:HE2	1:B:25:GLU:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:PHE:HE2	1:C:496:ARG:NH2	1.73	0.83
1:A:200:GLU:OE1	1:A:200:GLU:N	2.12	0.82
1:C:454:SER:HA	1:C:486:VAL:HG13	1.62	0.82
1:A:372:ARG:HH21	1:A:372:ARG:HG3	1.46	0.80
1:C:459:PHE:CE2	1:C:496:ARG:CZ	2.65	0.80
1:D:152:ASP:OD1	1:D:184:LYS:HG2	1.81	0.80
1:A:275:MET:HE3	1:A:284:VAL:HG13	1.65	0.77
1:D:42:ILE:HD11	1:D:72:VAL:HA	1.64	0.77
1:C:198:LEU:HD13	1:C:230:GLU:HB3	1.67	0.77
1:C:115:ARG:NH1	1:C:169:GLU:HG3	2.00	0.76
1:C:150:LEU:HB3	1:C:154:GLY:HA2	1.67	0.76
1:D:348:TYR:HB3	1:D:351:GLU:HB2	1.68	0.76
1:A:372:ARG:NH1	1:B:370:TYR:O	2.20	0.75
1:C:115:ARG:NH1	1:C:169:GLU:CD	2.43	0.74
1:B:313:THR:HG22	1:B:342:GLU:HA	1.70	0.74
1:C:408:LYS:HD2	1:C:430:PHE:HD2	1.52	0.73
1:D:181:ALA:HB3	1:D:184:LYS:HD3	1.69	0.72
1:B:317:ARG:HG2	1:B:317:ARG:HH11	1.53	0.72
1:A:484:VAL:HG22	1:A:494:THR:HG21	1.71	0.71
1:B:109:LYS:HZ2	1:B:177:ASP:HB3	1.55	0.71
1:D:162:ALA:HB3	1:D:171:GLU:HB3	1.72	0.71
1:D:308:MET:HE2	1:D:326:VAL:HG12	1.72	0.71
1:A:447:MET:HE1	1:A:469:ALA:HB2	1.73	0.70
1:C:439:MET:HG3	1:C:446:PRO:HG2	1.72	0.70
1:B:385:GLU:HG3	1:B:415:LEU:HD22	1.72	0.70
1:A:275:MET:O	1:A:279:VAL:HG22	1.90	0.70
1:C:76:GLU:HG2	1:C:82:LYS:HA	1.74	0.69
1:C:206:ILE:O	1:C:210:LEU:HG	1.93	0.69
1:C:412:THR:HG21	1:C:492:THR:HG21	1.74	0.68
1:C:7:ILE:HD13	1:C:356:MET:HG2	1.74	0.68
1:C:115:ARG:NH1	1:C:169:GLU:CG	2.57	0.68
1:D:39:ALA:CB	1:D:74:LEU:HD12	2.23	0.68
1:D:94:ILE:HG22	1:D:186:VAL:HB	1.74	0.68
1:D:35:VAL:HG13	1:D:36:GLU:N	2.09	0.67
1:C:167:THR:HB	1:C:169:GLU:OE2	1.95	0.67
1:D:474:SER:HA	1:D:500:VAL:HG23	1.78	0.66
1:D:35:VAL:HG13	1:D:36:GLU:H	1.60	0.66
1:C:5:VAL:HG21	1:C:330:VAL:HG13	1.78	0.66
1:B:57:PHE:HA	1:B:65:GLN:HE22	1.60	0.66
1:B:380:ARG:HB3	1:B:386:VAL:HG12	1.79	0.65
1:C:118:THR:CG2	1:C:168:ARG:O	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ALA:HB3	1:D:74:LEU:HD12	1.78	0.64
1:B:199:ALA:HB3	1:B:202:ASP:OD2	1.97	0.64
1:D:42:ILE:HD13	1:D:72:VAL:HG12	1.78	0.64
1:A:368:ASN:OD1	1:A:422:ASN:ND2	2.31	0.64
1:C:118:THR:HG23	1:C:168:ARG:O	1.98	0.63
1:C:478:ILE:HD12	1:C:480:ILE:HD11	1.78	0.63
1:C:167:THR:O	1:C:168:ARG:HB2	1.97	0.63
1:D:5:VAL:HG21	1:D:330:VAL:HG22	1.80	0.63
1:A:146:GLY:H	1:A:160:VAL:HG13	1.64	0.63
1:C:255:ILE:HD11	1:C:275:MET:HE3	1.80	0.63
1:C:140:TYR:HD2	1:C:168:ARG:O	1.82	0.62
1:C:46:ILE:HD11	1:C:53:PHE:CE2	2.34	0.62
1:A:372:ARG:HG3	1:A:372:ARG:NH2	2.15	0.62
1:C:340:SER:N	1:C:342:GLU:OE2	2.32	0.62
1:C:115:ARG:NH1	1:C:169:GLU:OE1	2.24	0.61
1:B:57:PHE:HA	1:B:65:GLN:NE2	2.15	0.61
1:C:167:THR:HG21	1:C:169:GLU:OE1	2.01	0.61
1:B:65:GLN:O	1:B:69:MET:HG3	2.00	0.61
1:B:142:ASP:OD2	1:B:194:PRO:HD3	2.01	0.61
1:B:497:ILE:HG13	1:D:387:MET:HE1	1.83	0.61
1:C:46:ILE:HD12	1:C:83:VAL:HG11	1.82	0.61
1:C:351:GLU:O	1:C:355:THR:HG23	2.00	0.61
1:C:408:LYS:HD2	1:C:430:PHE:CD2	2.34	0.61
1:B:56:ASN:HA	1:B:88:ASP:HB3	1.83	0.61
1:D:109:LYS:HA	1:D:177:ASP:OD1	2.00	0.61
1:D:499:THR:O	1:D:501:ARG:NH1	2.34	0.61
1:B:10:THR:OG1	1:B:54:ARG:NH1	2.34	0.60
1:C:164:ASP:HB3	1:C:167:THR:HG1	1.67	0.60
1:D:410:GLY:O	1:D:414:ARG:HG3	2.01	0.60
1:A:6:LYS:O	1:A:336:ALA:HA	2.01	0.60
1:C:164:ASP:HB3	1:C:167:THR:OG1	2.01	0.60
1:A:406:LEU:HD22	1:A:458:MET:HB3	1.82	0.60
1:A:386:VAL:HG23	1:C:397:SER:HB2	1.82	0.60
1:A:354:THR:O	1:A:358:THR:HG23	2.01	0.60
1:A:398:MET:CG	1:C:386:VAL:HG11	2.32	0.60
1:D:449:THR:HB	1:D:465:LYS:HE2	1.83	0.60
1:A:206:ILE:HD13	1:A:231:VAL:HG13	1.85	0.59
1:A:439:MET:HG3	1:A:446:PRO:HG2	1.84	0.59
1:A:458:MET:CE	1:A:484:VAL:HG12	2.32	0.59
1:A:460:GLU:OE1	1:A:460:GLU:HA	2.01	0.59
1:B:284:VAL:HG22	1:B:285:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:O	1:A:160:VAL:HG12	2.02	0.59
1:C:458:MET:HE1	1:C:483:GLY:O	2.02	0.59
1:B:16:GLU:OE1	1:B:68:ARG:NH1	2.37	0.58
1:B:426:LEU:HG	1:B:428:LEU:CD2	2.34	0.58
1:A:383:LYS:O	1:A:386:VAL:HG12	2.03	0.58
1:B:275:MET:O	1:B:279:VAL:HG22	2.03	0.58
1:C:411:HIS:CE1	1:C:415:LEU:HD21	2.39	0.58
1:B:317:ARG:HH11	1:B:317:ARG:CG	2.16	0.57
1:B:406:LEU:HD22	1:B:458:MET:HB3	1.86	0.57
1:D:149:VAL:CG1	1:D:158:LEU:HB2	2.34	0.57
1:D:463:GLU:OE2	1:D:498:ARG:NH2	2.38	0.57
1:C:232:ARG:O	1:C:236:GLU:HG2	2.05	0.57
1:C:320:ARG:HD3	1:D:276:GLY:HA3	1.86	0.57
1:C:206:ILE:HD13	1:C:231:VAL:HG13	1.87	0.57
1:B:114:ILE:HG23	1:B:172:VAL:CG2	2.35	0.57
1:C:460:GLU:OE1	1:C:464:ARG:NH1	2.37	0.57
1:A:155:LYS:HG2	1:B:316:PRO:HG2	1.85	0.57
1:C:383:LYS:HA	1:C:386:VAL:HG22	1.87	0.57
1:D:489:ALA:O	1:D:490:VAL:HB	2.03	0.57
1:C:242:HIS:CE1	1:C:433:LEU:HG	2.40	0.57
1:D:109:LYS:NZ	1:D:177:ASP:OD2	2.26	0.57
1:C:140:TYR:CD2	1:C:168:ARG:O	2.57	0.56
1:C:448:LEU:HD12	1:C:449:THR:N	2.20	0.56
1:C:459:PHE:CD2	1:C:496:ARG:NH1	2.73	0.56
1:B:93:GLU:O	1:B:94:ILE:HG13	2.05	0.56
1:A:417:SER:HB2	1:A:442:TRP:O	2.06	0.56
1:B:114:ILE:HG23	1:B:172:VAL:HG23	1.87	0.56
1:B:460:GLU:HG2	1:B:498:ARG:HH12	1.71	0.56
1:A:146:GLY:N	1:A:160:VAL:HG13	2.21	0.56
1:B:68:ARG:O	1:B:71:THR:N	2.38	0.56
1:A:270:ILE:HG22	1:A:272:ARG:HG3	1.88	0.55
1:C:272:ARG:O	1:D:320:ARG:NE	2.39	0.55
1:B:89:THR:O	1:B:220:SER:OG	2.23	0.55
1:C:6:LYS:NZ	1:C:441:ASN:O	2.33	0.55
1:C:15:VAL:O	1:C:41:ASN:ND2	2.39	0.55
1:C:458:MET:HE3	1:C:484:VAL:HG12	1.89	0.55
1:A:149:VAL:HG22	1:A:188:ILE:HG12	1.87	0.55
1:B:380:ARG:CB	1:B:386:VAL:HG12	2.37	0.55
1:A:398:MET:HG3	1:C:386:VAL:HG11	1.90	0.54
1:C:167:THR:HG1	1:C:169:GLU:CD	2.15	0.54
1:D:402:LEU:HB3	1:D:478:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LYS:O	1:C:112:GLU:HG3	2.07	0.54
1:A:496:ARG:HG3	1:C:494:THR:HG22	1.89	0.54
1:C:17:ILE:HG13	1:C:37:ALA:HB1	1.89	0.54
1:C:308:MET:HE3	1:C:356:MET:HE1	1.90	0.54
1:D:150:LEU:HB3	1:D:154:GLY:HA2	1.90	0.54
1:A:225:ALA:HB2	1:A:260:GLU:HG3	1.89	0.54
1:C:118:THR:HG21	1:C:140:TYR:HD2	1.73	0.54
1:C:305:ALA:HB1	1:C:338:MET:HE2	1.90	0.54
1:A:383:LYS:HB2	1:A:491:ARG:HD3	1.90	0.54
1:B:150:LEU:HB3	1:B:154:GLY:HA2	1.90	0.54
1:A:270:ILE:HD11	1:A:291:ILE:HB	1.89	0.53
1:C:226:LYS:HD3	1:C:229:ASN:HD22	1.71	0.53
1:B:452:PRO:HG3	1:B:458:MET:HE3	1.89	0.53
1:B:92:PRO:HB3	1:B:195:PHE:CG	2.44	0.53
1:C:156:LEU:HD12	1:C:157:GLY:H	1.74	0.53
1:C:458:MET:CE	1:C:483:GLY:O	2.57	0.53
1:A:217:ILE:HD12	1:A:243:VAL:HG11	1.91	0.53
1:C:225:ALA:O	1:C:228:VAL:HG22	2.09	0.53
1:D:68:ARG:HA	1:D:71:THR:CG2	2.39	0.53
1:D:351:GLU:O	1:D:355:THR:OG1	2.23	0.53
1:A:199:ALA:HB1	1:A:200:GLU:OE1	2.08	0.53
1:A:310:GLU:O	1:A:313:THR:HG22	2.09	0.53
1:C:242:HIS:ND1	1:C:433:LEU:HG	2.24	0.53
1:D:270:ILE:HG23	1:D:275:MET:HE1	1.91	0.53
1:A:156:LEU:HD11	1:A:174:VAL:HG13	1.90	0.52
1:B:456:ASP:HB3	1:B:461:ILE:HD11	1.91	0.52
1:C:76:GLU:OE2	1:C:436:ARG:NH2	2.42	0.52
1:D:9:ALA:O	1:D:53:PHE:HA	2.09	0.52
1:B:250:GLU:HG2	1:B:271:ALA:HB3	1.92	0.52
1:B:108:TYR:HB3	1:B:174:VAL:HG21	1.90	0.52
1:B:385:GLU:CG	1:B:415:LEU:HD22	2.38	0.52
1:A:159:ARG:HB2	1:A:175:GLU:OE1	2.09	0.52
1:D:68:ARG:HA	1:D:71:THR:HG22	1.91	0.52
1:D:384:THR:HG22	1:D:415:LEU:HD23	1.91	0.52
1:C:308:MET:HE2	1:C:338:MET:H	1.74	0.52
1:A:458:MET:HE3	1:A:484:VAL:HG12	1.90	0.52
1:A:273:GLY:CA	1:A:306:THR:HG21	2.40	0.52
1:C:380:ARG:NH2	1:C:389:SER:OG	2.43	0.52
1:D:456:ASP:N	1:D:456:ASP:OD1	2.42	0.52
1:B:449:THR:HB	1:B:465:LYS:HE2	1.92	0.51
1:D:308:MET:HB3	1:D:326:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLU:OE1	1:A:498:ARG:NH1	2.44	0.51
1:C:481:VAL:HG12	1:C:492:THR:CG2	2.41	0.51
1:C:305:ALA:HA	1:C:338:MET:HB3	1.92	0.51
1:A:200:GLU:H	1:A:200:GLU:CD	2.13	0.51
1:B:284:VAL:CG2	1:B:285:PRO:HD3	2.40	0.51
1:A:320:ARG:NH1	1:B:276:GLY:HA3	2.25	0.51
1:D:158:LEU:HA	1:D:173:GLU:O	2.10	0.51
1:B:67:GLU:O	1:B:70:ALA:HB3	2.11	0.51
1:C:12:GLY:HA3	1:C:344:ALA:O	2.11	0.51
1:C:406:LEU:HD13	1:C:428:LEU:HB2	1.91	0.51
1:A:266:ASP:O	1:A:300:LYS:HB3	2.11	0.51
1:C:145:VAL:HG23	1:C:160:VAL:HG12	1.93	0.51
1:A:196:PRO:HG2	1:A:199:ALA:HA	1.93	0.50
1:B:496:ARG:HG3	1:D:493:ASN:O	2.12	0.50
1:D:415:LEU:O	1:D:418:LYS:HB3	2.11	0.50
1:D:69:MET:O	1:D:72:VAL:HG22	2.11	0.50
1:A:157:GLY:O	1:A:158:LEU:HD13	2.11	0.50
1:B:497:ILE:HG13	1:D:387:MET:CE	2.41	0.50
1:C:292:ILE:HG23	1:C:302:VAL:HG11	1.93	0.50
1:B:198:LEU:HD21	1:B:234:ILE:HD11	1.92	0.50
1:C:190:ASN:N	1:C:190:ASN:HD22	2.10	0.50
1:C:288:GLN:O	1:C:292:ILE:HG13	2.12	0.50
1:C:395:THR:HG21	1:C:421:PRO:HB2	1.94	0.50
1:B:285:PRO:O	1:B:289:LYS:HD3	2.12	0.50
1:B:460:GLU:OE2	1:B:464:ARG:HG2	2.11	0.50
1:D:68:ARG:O	1:D:72:VAL:HG13	2.12	0.50
1:B:208:PHE:O	1:B:211:GLU:HB2	2.12	0.50
1:D:339:LEU:HD22	1:D:342:GLU:HB2	1.93	0.50
1:D:375:SER:OG	1:D:392:LYS:NZ	2.45	0.50
1:D:282:GLU:OE2	1:D:282:GLU:N	2.33	0.49
1:A:431:ASP:OD1	1:A:434:THR:HG23	2.11	0.49
1:C:307:ASN:HA	1:C:310:GLU:OE1	2.12	0.49
1:D:435:GLU:HG3	1:D:446:PRO:HB2	1.93	0.49
1:C:46:ILE:CD1	1:C:83:VAL:HG11	2.42	0.49
1:D:327:PHE:CD2	1:D:363:ALA:HB2	2.48	0.49
1:B:92:PRO:HG2	1:B:221:PHE:HB3	1.94	0.49
1:B:91:GLY:HA2	1:B:202:ASP:OD2	2.12	0.49
1:A:45:LEU:CD2	1:A:350:LEU:HA	2.42	0.49
1:A:406:LEU:HD13	1:A:482:ALA:HB2	1.94	0.49
1:B:400:ILE:HG21	1:B:479:VAL:HG23	1.95	0.49
1:A:187:ASN:HB3	1:A:278:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:MET:HG3	1:B:446:PRO:HG2	1.95	0.49
1:C:140:TYR:OH	1:C:165:ASP:HA	2.12	0.49
1:C:385:GLU:HG2	1:C:415:LEU:HD12	1.94	0.49
1:B:206:ILE:HD13	1:B:231:VAL:HG13	1.95	0.49
1:A:31:GLU:HA	1:A:31:GLU:OE2	2.11	0.48
1:B:10:THR:HA	1:B:54:ARG:HB3	1.95	0.48
1:D:252:GLN:HG3	1:D:256:ASP:OD2	2.13	0.48
1:B:162:ALA:O	1:B:171:GLU:N	2.46	0.48
1:C:372:ARG:NH1	1:D:370:TYR:O	2.45	0.48
1:A:320:ARG:NH1	1:B:272:ARG:O	2.46	0.48
1:D:17:ILE:H	1:D:38:SER:HB3	1.78	0.48
1:A:316:PRO:HB3	1:A:348:TYR:CZ	2.48	0.48
1:B:196:PRO:HG2	1:B:199:ALA:HB2	1.95	0.48
1:C:310:GLU:O	1:C:313:THR:HG23	2.14	0.48
1:D:35:VAL:CG1	1:D:36:GLU:N	2.76	0.48
1:D:454:SER:HA	1:D:486:VAL:HG13	1.95	0.48
1:A:52:THR:HB	1:A:440:LEU:HD21	1.95	0.48
1:A:495:MET:HE2	1:C:495:MET:HE2	1.95	0.48
1:A:145:VAL:HG23	1:A:160:VAL:HG22	1.96	0.48
1:A:13:PRO:HB2	1:A:23:PHE:CD1	2.48	0.48
1:B:493:ASN:OD1	1:B:493:ASN:N	2.45	0.48
1:D:158:LEU:HD13	1:D:174:VAL:HA	1.95	0.48
1:D:206:ILE:HD11	1:D:234:ILE:HG21	1.96	0.48
1:A:383:LYS:HA	1:A:386:VAL:HG12	1.95	0.48
1:B:109:LYS:NZ	1:B:177:ASP:HB3	2.28	0.48
1:B:272:ARG:NH1	1:B:288:GLN:OE1	2.47	0.48
1:C:198:LEU:HG	1:C:198:LEU:O	2.14	0.48
1:C:320:ARG:HD2	1:D:272:ARG:HB3	1.95	0.48
1:C:62:HIS:NE2	1:C:204:ASP:OD1	2.46	0.48
1:A:275:MET:CE	1:A:284:VAL:HG13	2.41	0.47
1:C:233:ALA:HA	1:C:236:GLU:OE2	2.15	0.47
1:D:156:LEU:HD23	1:D:158:LEU:HD21	1.96	0.47
1:C:433:LEU:HD12	1:C:433:LEU:HA	1.64	0.47
1:D:35:VAL:CG1	1:D:36:GLU:H	2.27	0.47
1:A:69:MET:O	1:A:73:LYS:HG3	2.14	0.47
1:A:196:PRO:C	1:A:198:LEU:N	2.72	0.47
1:A:309:LEU:O	1:A:342:GLU:HG2	2.14	0.47
1:A:409:THR:OG1	2:A:601:FBP:O3P	2.25	0.47
1:C:409:THR:N	2:C:601:FBP:O1P	2.44	0.47
1:D:269:MET:SD	1:D:338:MET:HE1	2.55	0.47
1:B:88:ASP:OD1	1:B:248:LYS:NZ	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ARG:HD3	1:A:288:GLN:OE1	2.14	0.47
1:C:272:ARG:NH2	1:C:308:MET:HG2	2.30	0.47
1:C:317:ARG:HH12	1:C:355:THR:HG22	1.80	0.47
1:C:309:LEU:HD12	1:C:339:LEU:HD21	1.97	0.47
1:A:320:ARG:CZ	1:B:276:GLY:HA3	2.45	0.46
1:B:82:LYS:HE2	1:B:432:GLU:OE1	2.16	0.46
1:A:320:ARG:NH1	1:B:273:GLY:O	2.45	0.46
1:C:449:THR:HG22	1:C:450:ASP:H	1.79	0.46
1:C:10:THR:HG22	1:C:344:ALA:HB2	1.98	0.46
1:C:202:ASP:O	1:C:206:ILE:HG13	2.15	0.46
1:D:198:LEU:HD11	1:D:203:ASN:HB2	1.98	0.46
1:A:314:GLU:O	1:A:348:TYR:HE2	1.98	0.46
1:C:317:ARG:NH1	1:C:355:THR:HG22	2.31	0.46
1:B:460:GLU:HG2	1:B:498:ARG:NH1	2.29	0.46
1:C:52:THR:HB	1:C:440:LEU:HD21	1.98	0.46
1:C:164:ASP:O	1:C:166:ALA:N	2.49	0.46
1:D:375:SER:HA	1:D:378:PHE:CE2	2.50	0.46
1:C:167:THR:CB	1:C:169:GLU:CD	2.89	0.46
1:A:94:ILE:HG23	1:A:133:VAL:HG12	1.98	0.46
1:A:249:ILE:CG2	1:A:255:ILE:HG13	2.45	0.46
1:C:15:VAL:HB	1:C:41:ASN:HB3	1.98	0.46
1:C:69:MET:O	1:C:73:LYS:HD2	2.16	0.46
1:C:384:THR:OG1	2:C:601:FBP:O6P	2.21	0.46
1:D:163:LYS:HA	1:D:163:LYS:HE2	1.98	0.46
1:D:197:ALA:HA	1:D:227:ASP:OD1	2.16	0.46
1:A:493:ASN:OD1	1:A:494:THR:HG23	2.17	0.45
1:D:459:PHE:CD1	1:D:496:ARG:HD2	2.50	0.45
1:A:67:GLU:O	1:A:70:ALA:HB3	2.16	0.45
1:A:40:LYS:HA	1:A:43:ALA:HB3	1.99	0.45
1:A:404:VAL:HG11	1:A:462:ALA:HB1	1.98	0.45
1:A:145:VAL:HA	1:A:160:VAL:HG13	1.99	0.45
1:A:150:LEU:HB3	1:A:154:GLY:HA2	1.97	0.45
1:A:200:GLU:N	1:A:200:GLU:CD	2.72	0.45
1:C:251:ASN:HD21	1:C:253:GLN:HB2	1.82	0.45
1:B:426:LEU:HG	1:B:428:LEU:HD21	1.98	0.45
1:C:133:VAL:HG11	1:C:137:LEU:HB2	1.97	0.45
1:C:198:LEU:HD22	1:C:230:GLU:OE2	2.17	0.45
1:C:357:ALA:O	1:C:361:LYS:HG3	2.17	0.45
1:D:246:PHE:CD1	1:D:267:GLY:HA3	2.51	0.45
1:D:246:PHE:HD1	1:D:267:GLY:HA3	1.81	0.45
1:B:72:VAL:HG23	1:B:85:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:HB2	1:B:223:ARG:NH2	2.31	0.45
1:C:316:PRO:CG	1:D:155:LYS:HE2	2.47	0.45
1:C:320:ARG:HA	1:C:323:VAL:HG12	1.99	0.45
1:C:459:PHE:HB3	1:C:498:ARG:HH11	1.82	0.45
1:D:284:VAL:HG22	1:D:285:PRO:HD3	1.99	0.45
1:C:463:GLU:OE1	1:C:501:ARG:N	2.34	0.45
1:D:354:THR:O	1:D:358:THR:HG23	2.17	0.45
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.81	0.44
1:D:65:GLN:HA	1:D:68:ARG:HG2	1.99	0.44
1:A:496:ARG:CG	1:C:494:THR:HG22	2.46	0.44
1:D:39:ALA:HB1	1:D:74:LEU:HD12	1.99	0.44
1:D:436:ARG:O	1:D:439:MET:HG3	2.17	0.44
1:B:452:PRO:CG	1:B:458:MET:HE3	2.46	0.44
1:C:73:LYS:HA	1:C:76:GLU:OE1	2.18	0.44
1:C:447:MET:HE1	1:C:469:ALA:HB2	1.99	0.44
1:D:311:THR:HG21	1:D:319:THR:HG23	1.99	0.44
1:B:56:ASN:ND2	1:B:58:SER:H	2.15	0.44
1:B:197:ALA:HA	1:B:227:ASP:OD1	2.17	0.44
1:C:82:LYS:HE2	1:C:82:LYS:HB3	1.80	0.44
1:C:481:VAL:HG12	1:C:492:THR:HG22	2.00	0.44
1:D:149:VAL:HG12	1:D:158:LEU:HB2	1.98	0.44
1:B:58:SER:HA	1:B:90:LYS:HB3	1.98	0.44
1:B:345:ASN:O	1:B:345:ASN:ND2	2.50	0.44
1:C:327:PHE:CD2	1:C:363:ALA:HB2	2.52	0.44
1:C:459:PHE:CD2	1:C:496:ARG:NH2	2.74	0.44
1:D:64:GLU:O	1:D:68:ARG:HG2	2.17	0.44
1:D:330:VAL:O	1:D:367:LEU:HD21	2.18	0.44
1:D:463:GLU:OE2	1:D:498:ARG:HD3	2.17	0.44
1:C:225:ALA:HB3	1:C:226:LYS:HE2	2.00	0.44
1:C:284:VAL:CG2	1:C:285:PRO:HD3	2.47	0.44
1:D:258:LEU:HD23	1:D:294:LYS:HD2	1.99	0.44
1:A:384:THR:OG1	2:A:601:FBP:O4P	2.34	0.44
1:C:148:GLN:CD	1:C:150:LEU:HD21	2.43	0.44
1:C:484:VAL:O	1:C:493:ASN:ND2	2.51	0.44
1:D:183:GLN:C	1:D:184:LYS:HD2	2.43	0.44
1:D:285:PRO:O	1:D:289:LYS:HG3	2.18	0.44
1:A:484:VAL:HG22	1:A:494:THR:CG2	2.43	0.44
1:B:299:GLY:HA2	1:B:418:LYS:HD2	2.00	0.44
1:B:311:THR:HG23	1:B:322:GLU:OE1	2.18	0.44
1:B:375:SER:HB2	1:B:419:TYR:CD1	2.53	0.44
1:C:391:VAL:O	1:C:395:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLU:OE2	1:A:419:TYR:OH	2.28	0.43
1:A:398:MET:HE2	1:A:398:MET:HB2	1.79	0.43
1:D:301:VAL:HG13	1:D:335:ASP:CB	2.48	0.43
1:A:244:GLN:HA	1:A:266:ASP:OD2	2.18	0.43
1:A:408:LYS:HD2	1:A:408:LYS:O	2.17	0.43
1:B:92:PRO:HB3	1:B:195:PHE:CD2	2.54	0.43
1:B:161:VAL:HG11	1:B:173:GLU:OE1	2.18	0.43
1:C:484:VAL:HG22	1:C:494:THR:HG21	2.00	0.43
1:A:378:PHE:O	1:A:380:ARG:NH2	2.51	0.43
1:A:362:ASN:HD21	1:B:283:MET:HE3	1.83	0.43
1:B:223:ARG:HB2	1:B:253:GLN:HB3	1.99	0.43
1:C:156:LEU:HD11	1:C:174:VAL:HG13	2.01	0.43
1:C:425:ILE:HB	1:C:444:VAL:HA	2.00	0.43
1:C:484:VAL:HG22	1:C:494:THR:CG2	2.49	0.43
1:D:193:ILE:O	1:D:195:PHE:N	2.47	0.43
1:D:312:MET:HE2	1:D:312:MET:HB3	1.75	0.43
1:C:292:ILE:HD12	1:C:332:ASP:HB3	2.00	0.43
1:D:447:MET:HE1	1:D:469:ALA:HB2	2.00	0.43
1:C:65:GLN:O	1:C:69:MET:HG3	2.18	0.43
1:C:221:PHE:CD2	1:C:250:GLU:OE2	2.72	0.43
1:C:406:LEU:HD21	1:C:462:ALA:HB2	2.01	0.43
1:C:483:GLY:HA2	1:C:493:ASN:HB2	2.00	0.43
1:C:6:LYS:O	1:C:336:ALA:HA	2.19	0.43
1:C:478:ILE:CD1	1:C:480:ILE:HD11	2.45	0.43
1:D:56:ASN:C	1:D:58:SER:H	2.27	0.43
1:C:11:LEU:HD21	1:C:53:PHE:CE1	2.54	0.43
1:C:152:ASP:O	1:C:155:LYS:HB2	2.19	0.43
1:C:158:LEU:HD13	1:C:172:VAL:HG21	2.01	0.43
1:C:501:ARG:HD3	1:C:501:ARG:HA	1.79	0.43
1:A:339:LEU:HD23	1:A:342:GLU:HB2	2.00	0.42
1:B:147:ARG:HD3	1:B:147:ARG:HA	1.84	0.42
1:A:383:LYS:HB2	1:A:491:ARG:CD	2.48	0.42
1:C:157:GLY:C	1:C:158:LEU:HD23	2.44	0.42
1:D:16:GLU:OE2	1:D:68:ARG:NH2	2.52	0.42
1:A:22:LYS:HD2	1:A:22:LYS:N	2.34	0.42
1:C:309:LEU:O	1:C:342:GLU:HG2	2.19	0.42
1:B:417:SER:O	1:B:418:LYS:C	2.60	0.42
1:C:272:ARG:HB2	1:C:306:THR:HB	2.00	0.42
1:A:65:GLN:O	1:A:69:MET:HG3	2.20	0.42
1:A:398:MET:HG2	1:C:386:VAL:HG11	2.01	0.42
1:C:45:LEU:CD2	1:C:350:LEU:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:GLN:OE1	1:D:68:ARG:HD2	2.19	0.42
1:C:140:TYR:C	1:C:142:ASP:H	2.28	0.42
1:C:441:ASN:HB2	1:C:444:VAL:HG11	2.01	0.42
1:B:158:LEU:HD13	1:B:172:VAL:HG21	2.01	0.42
1:C:118:THR:HG21	1:C:140:TYR:CD2	2.54	0.42
1:C:284:VAL:HG21	1:D:320:ARG:HG2	2.01	0.42
1:D:179:ILE:HD12	1:D:179:ILE:N	2.34	0.42
1:D:316:PRO:HB3	1:D:348:TYR:CZ	2.55	0.42
1:B:83:VAL:HA	1:B:439:MET:SD	2.59	0.42
1:C:499:THR:O	1:C:501:ARG:NH1	2.53	0.42
1:D:46:ILE:HG12	1:D:83:VAL:HG11	2.01	0.42
1:C:200:GLU:HA	1:C:203:ASN:HB2	2.02	0.41
1:C:290:MET:SD	1:C:294:LYS:HD2	2.60	0.41
1:C:311:THR:C	1:C:313:THR:H	2.28	0.41
1:D:160:VAL:HA	1:D:172:VAL:HG12	2.02	0.41
1:B:93:GLU:C	1:B:94:ILE:HG13	2.45	0.41
1:C:42:ILE:HG23	1:C:53:PHE:CZ	2.55	0.41
1:D:305:ALA:HB2	1:D:338:MET:HE3	2.02	0.41
1:A:463:GLU:O	1:A:467:VAL:HG23	2.19	0.41
1:B:337:THR:HB	1:B:356:MET:HE2	2.02	0.41
1:C:459:PHE:HD2	1:C:496:ARG:NH1	2.17	0.41
1:D:152:ASP:C	1:D:154:GLY:N	2.75	0.41
1:C:72:VAL:O	1:C:75:ALA:HB3	2.20	0.41
1:C:401:LYS:HG3	1:C:476:ASP:CG	2.45	0.41
1:D:375:SER:HB2	1:D:419:TYR:CD1	2.55	0.41
1:B:258:LEU:HG	1:B:262:ILE:HD12	2.02	0.41
1:B:312:MET:HE2	1:B:312:MET:HB3	1.91	0.41
1:C:54:ARG:HA	1:C:86:LEU:O	2.19	0.41
1:A:481:VAL:HG13	1:A:492:THR:CG2	2.51	0.41
1:B:14:ALA:HB2	1:B:345:ASN:HA	2.01	0.41
1:C:93:GLU:OE2	1:C:95:ARG:HD2	2.21	0.41
1:C:440:LEU:HD23	1:C:440:LEU:HA	1.82	0.41
1:D:199:ALA:HB3	1:D:202:ASP:OD2	2.20	0.41
1:A:44:LYS:HA	1:A:44:LYS:HE2	2.03	0.41
1:A:494:THR:HG22	1:C:496:ARG:HG3	2.01	0.41
1:B:54:ARG:NE	1:B:88:ASP:OD2	2.44	0.41
1:C:16:GLU:HG2	1:C:38:SER:HB3	2.03	0.41
1:D:1:MET:HE1	1:D:361:LYS:HG2	2.03	0.41
1:D:58:SER:CB	1:D:90:LYS:HG3	2.50	0.41
1:D:58:SER:OG	1:D:90:LYS:HG3	2.21	0.41
1:B:149:VAL:HB	1:B:158:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.86	0.40
1:C:74:LEU:O	1:C:78:ILE:HG22	2.20	0.40
1:C:311:THR:OG1	1:C:322:GLU:OE2	2.36	0.40
1:A:6:LYS:HD2	1:A:51:ASN:ND2	2.35	0.40
1:A:447:MET:HE3	1:A:447:MET:HB2	2.01	0.40
1:B:150:LEU:HD23	1:B:157:GLY:HA2	2.03	0.40
1:C:221:PHE:HD2	1:C:250:GLU:OE2	2.05	0.40
1:D:284:VAL:N	1:D:285:PRO:CD	2.84	0.40
1:A:158:LEU:HB3	1:A:172:VAL:HG21	2.04	0.40
1:B:387:MET:HE2	1:D:495:MET:CE	2.51	0.40
1:C:74:LEU:HD13	1:C:74:LEU:HA	1.94	0.40
1:C:291:ILE:O	1:C:295:VAL:HG23	2.22	0.40
1:D:150:LEU:O	1:D:186:VAL:HA	2.21	0.40
1:D:198:LEU:CD1	1:D:203:ASN:HB2	2.52	0.40
1:D:275:MET:O	1:D:279:VAL:HG22	2.21	0.40
1:A:481:VAL:CG1	1:A:492:THR:HG21	2.52	0.40
1:C:382:SER:HB2	2:C:601:FBP:P2	2.62	0.40
1:C:432:GLU:HG3	1:C:448:LEU:CD2	2.51	0.40
1:D:447:MET:HE3	1:D:447:MET:HB2	1.85	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	443/521 (85%)	419 (95%)	20 (4%)	4 (1%)	14	30
1	B	433/521 (83%)	412 (95%)	17 (4%)	4 (1%)	14	30
1	C	450/521 (86%)	400 (89%)	42 (9%)	8 (2%)	6	14
1	D	452/521 (87%)	410 (91%)	36 (8%)	6 (1%)	9	21
All	All	1778/2084 (85%)	1641 (92%)	115 (6%)	22 (1%)	10	23

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	112	GLU
1	D	166	ALA
1	A	199	ALA
1	B	110	THR
1	B	273	GLY
1	C	110	THR
1	C	165	ASP
1	D	152	ASP
1	D	490	VAL
1	B	152	ASP
1	C	136	ALA
1	C	147	ARG
1	C	345	ASN
1	D	306	THR
1	A	152	ASP
1	A	306	THR
1	B	306	THR
1	C	168	ARG
1	D	35	VAL
1	C	306	THR
1	C	196	PRO
1	A	270	ILE

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	371/428 (87%)	358 (96%)	13 (4%)	32	59
1	B	367/428 (86%)	356 (97%)	11 (3%)	36	64
1	C	379/428 (89%)	356 (94%)	23 (6%)	17	37
1	D	379/428 (89%)	360 (95%)	19 (5%)	22	46
All	All	1496/1712 (87%)	1430 (96%)	66 (4%)	25	50

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	200	GLU
1	A	211	GLU
1	A	221	PHE
1	A	236	GLU
1	A	324	SER
1	A	345	ASN
1	A	372	ARG
1	A	398	MET
1	A	401	LYS
1	A	415	LEU
1	A	429	THR
1	A	484	VAL
1	B	22	LYS
1	B	81	LYS
1	B	89	THR
1	B	317	ARG
1	B	386	VAL
1	B	408	LYS
1	B	453	SER
1	B	455	THR
1	B	484	VAL
1	B	490	VAL
1	B	492	THR
1	C	1	MET
1	C	32	LYS
1	C	45	LEU
1	C	74	LEU
1	C	82	LYS
1	C	147	ARG
1	C	156	LEU
1	C	163	LYS
1	C	165	ASP
1	C	168	ARG
1	C	169	GLU
1	C	190	ASN
1	C	221	PHE
1	C	302	VAL
1	C	323	VAL
1	C	354	THR
1	C	403	VAL
1	C	456	ASP
1	C	458	MET

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Mol	Chain	Res	Type
1	C	484	VAL
1	C	486	VAL
1	C	491	ARG
1	C	492	THR
1	D	44	LYS
1	D	74	LEU
1	D	81	LYS
1	D	139	ILE
1	D	151	VAL
1	D	161	VAL
1	D	167	THR
1	D	192	LYS
1	D	221	PHE
1	D	286	VAL
1	D	303	ILE
1	D	313	THR
1	D	317	ARG
1	D	386	VAL
1	D	412	THR
1	D	415	LEU
1	D	456	ASP
1	D	457	ASP
1	D	467	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	187	ASN
1	A	345	ASN
1	A	362	ASN
1	B	56	ASN
1	B	65	GLN
1	B	253	GLN
1	B	307	ASN
1	B	441	ASN
1	C	65	GLN
1	C	190	ASN
1	C	229	ASN
1	D	2	ASN
1	D	62	HIS
1	D	148	GLN

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Mol	Chain	Res	Type
1	D	240	ASN
1	D	251	ASN
1	D	252	GLN
1	D	307	ASN
1	D	345	ASN
1	D	381	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	FBP	A	601	-	18,20,20	0.75	1 (5%)	21,32,32	1.18	2 (9%)
2	FBP	B	601	-	18,20,20	0.64	0	21,32,32	1.25	4 (19%)
2	FBP	D	601	-	18,20,20	0.69	0	21,32,32	1.30	2 (9%)
2	FBP	C	601	-	18,20,20	0.77	1 (5%)	21,32,32	1.19	2 (9%)

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	FBP	A	601	-	-	9/13/32/32	0/1/1/1
2	FBP	B	601	-	-	7/13/32/32	0/1/1/1
2	FBP	D	601	-	-	7/13/32/32	0/1/1/1
2	FBP	C	601	-	-	8/13/32/32	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FBP	O2-C2	2.11	1.44	1.40
2	C	601	FBP	O2-C2	2.09	1.44	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FBP	O6P-P2-O6	-3.11	98.55	106.67
2	D	601	FBP	O3-C3-C4	-2.71	103.68	113.25
2	A	601	FBP	O5P-P2-O6	2.57	113.38	106.67
2	B	601	FBP	O3P-P1-O2P	2.46	117.01	107.80
2	A	601	FBP	O6P-P2-O4P	2.44	120.36	110.83
2	B	601	FBP	O6P-P2-O5P	2.39	116.78	107.80
2	D	601	FBP	O3P-P1-O2P	2.38	116.74	107.80
2	B	601	FBP	O5P-P2-O6	-2.27	100.76	106.67
2	C	601	FBP	O6P-P2-O5P	2.15	115.88	107.80
2	B	601	FBP	C6-C5-C4	-2.02	107.93	115.21

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	A	601	FBP	C6-O6-P2-O4P
2	A	601	FBP	C6-O6-P2-O6P
2	B	601	FBP	C1-O1-P1-O2P
2	B	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	O1-C1-C2-C3

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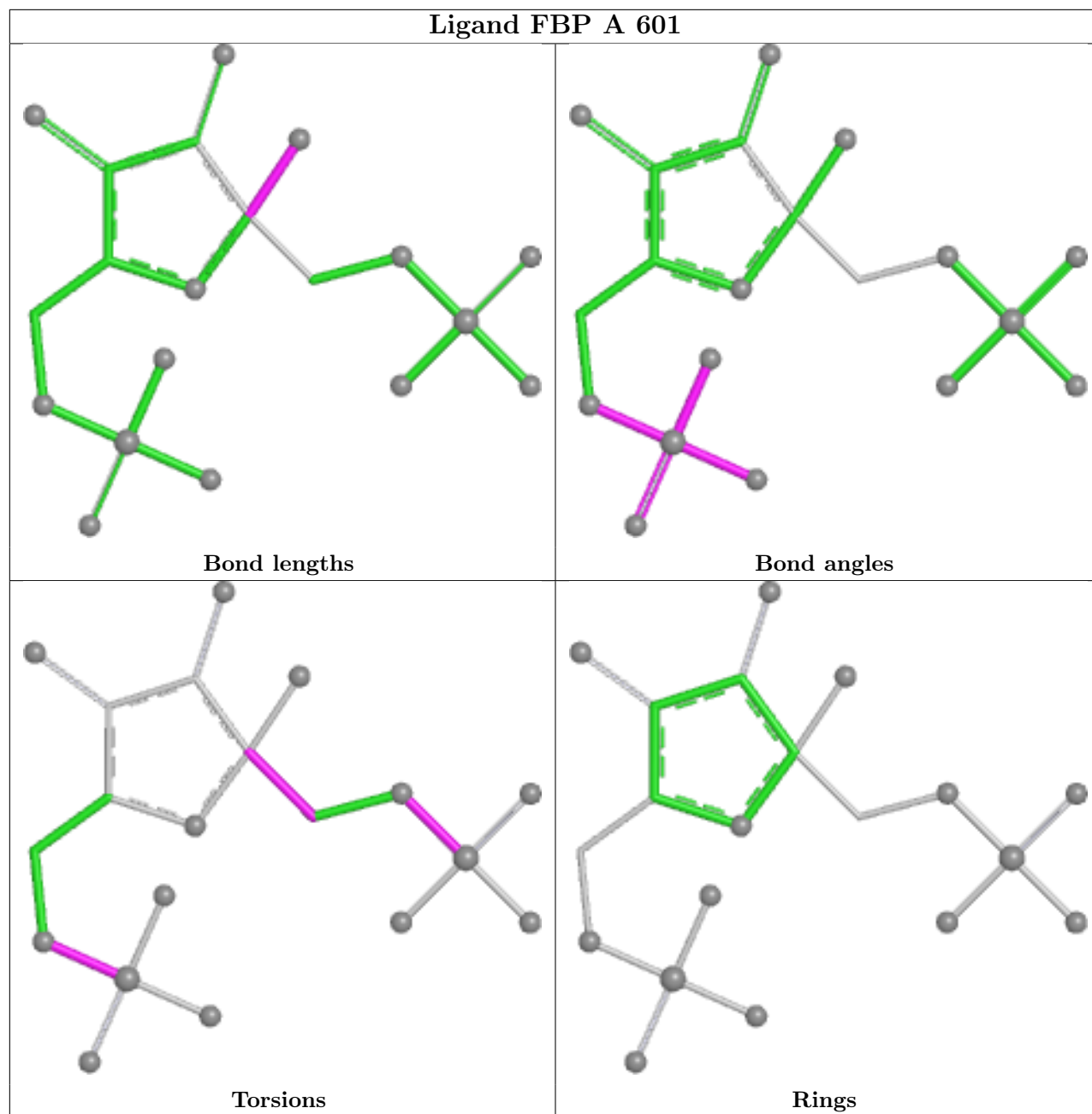
Mol	Chain	Res	Type	Atoms
2	B	601	FBP	O1-C1-C2-O5
2	C	601	FBP	C1-O1-P1-O1P
2	C	601	FBP	C1-O1-P1-O2P
2	C	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	O1-C1-C2-C3
2	C	601	FBP	O1-C1-C2-O5
2	D	601	FBP	C1-O1-P1-O2P
2	D	601	FBP	O1-C1-C2-C3
2	D	601	FBP	O1-C1-C2-O5
2	C	601	FBP	C4-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	A	601	FBP	C1-O1-P1-O1P
2	B	601	FBP	C6-O6-P2-O4P
2	D	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	O1-C1-C2-O2
2	C	601	FBP	O1-C1-C2-O2
2	D	601	FBP	O1-C1-C2-O2
2	D	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C6-O6-P2-O4P
2	B	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C6-O6-P2-O5P

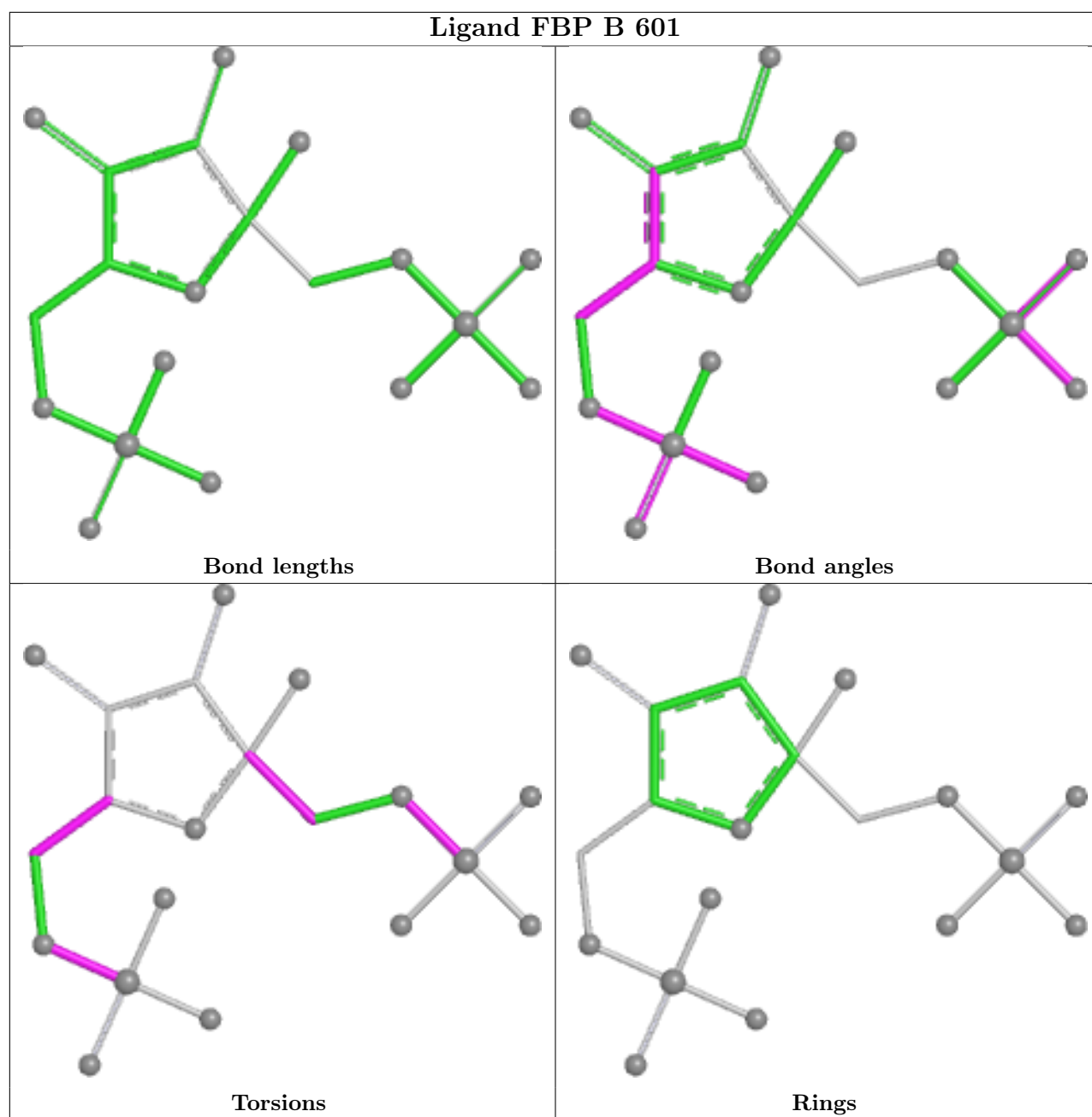
There are no ring outliers.

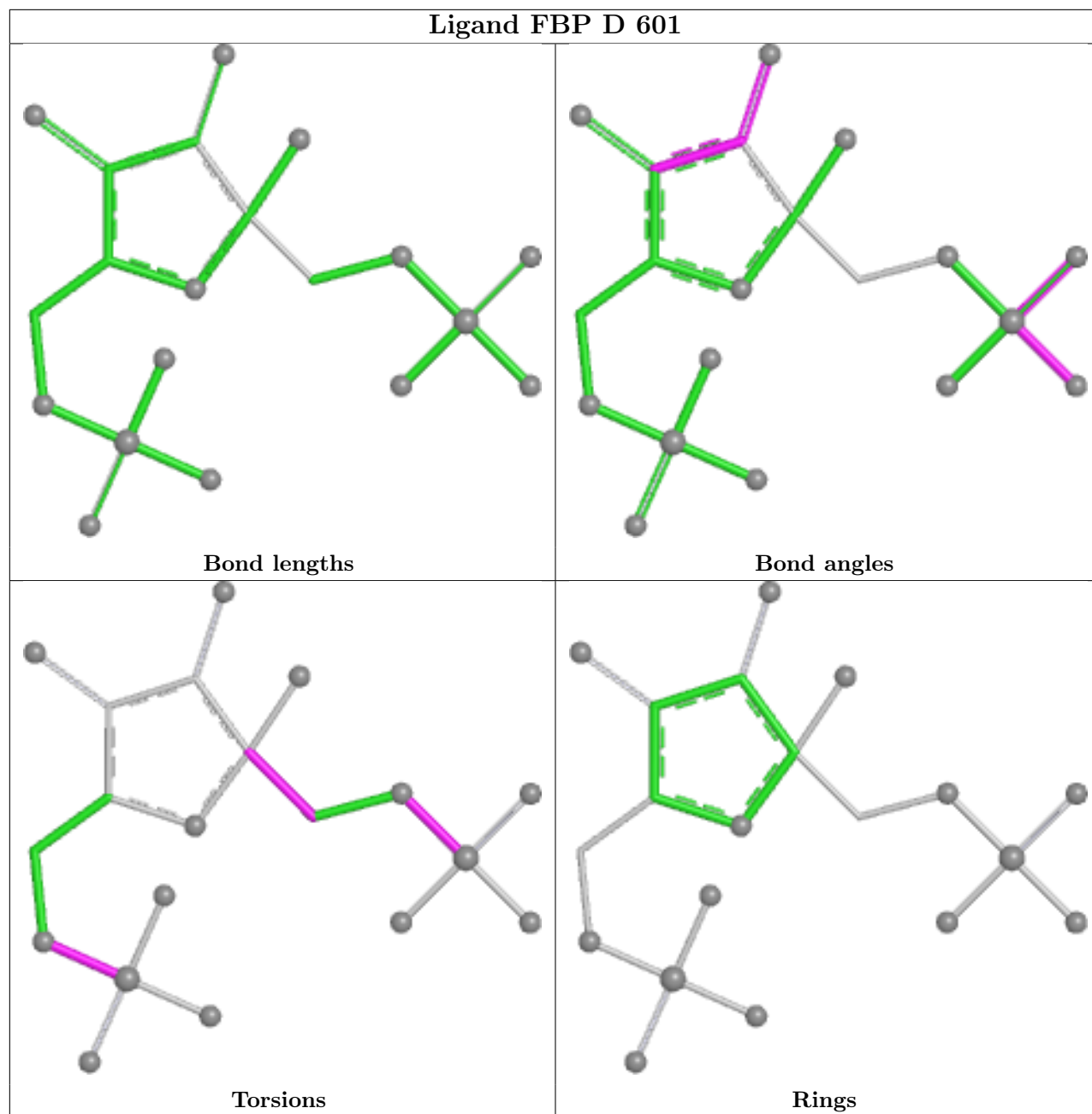
3 monomers are involved in 6 short contacts:

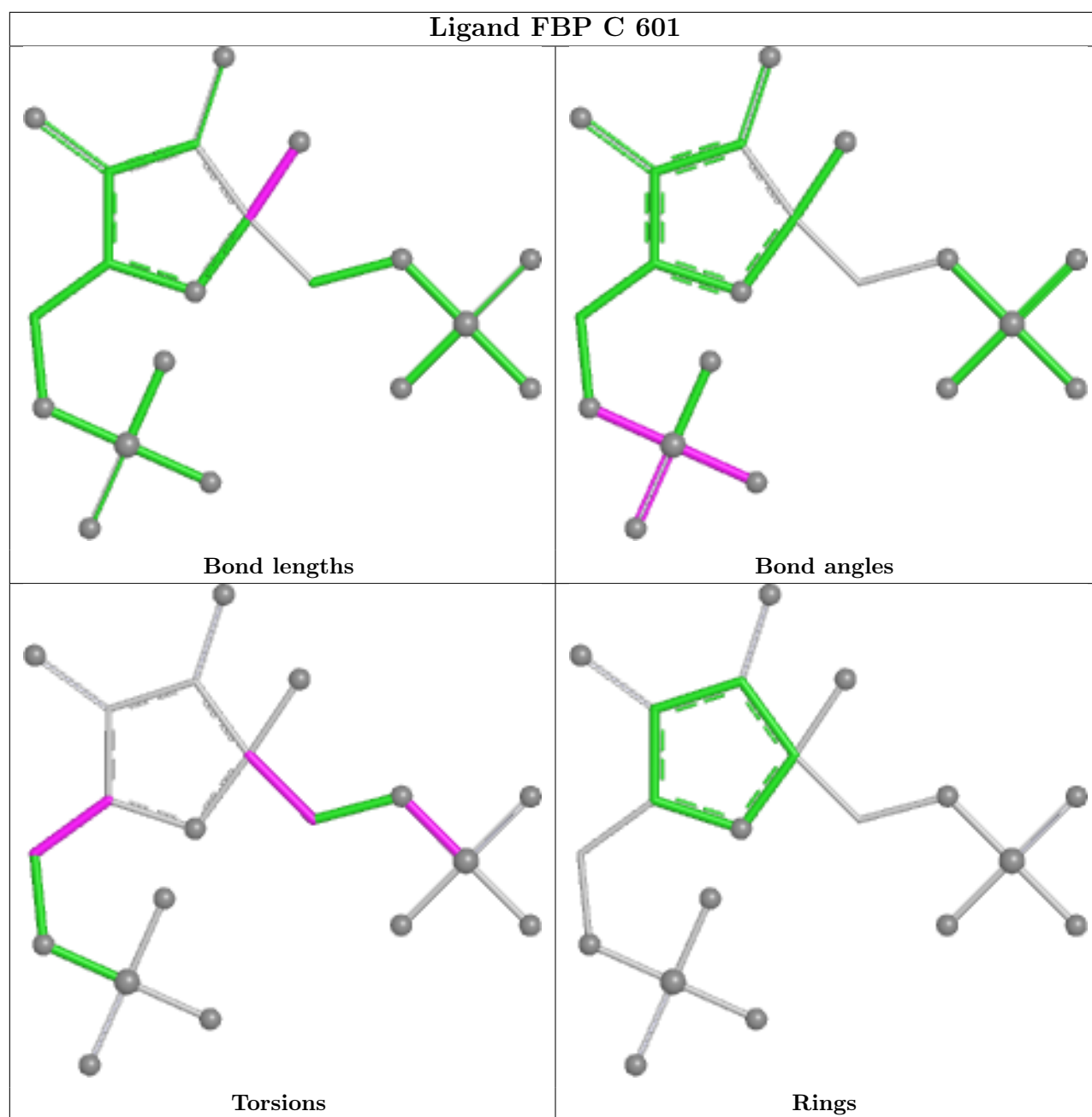
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FBP	2	0
2	D	601	FBP	1	0
2	C	601	FBP	3	0

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	451/521 (86%)	0.07	8 (1%) 67 63	62, 93, 145, 186	0
1	B	445/521 (85%)	0.18	16 (3%) 46 40	62, 92, 148, 172	0
1	C	460/521 (88%)	0.54	33 (7%) 21 17	75, 119, 167, 196	0
1	D	460/521 (88%)	0.19	13 (2%) 55 49	64, 102, 155, 210	0
All	All	1816/2084 (87%)	0.24	70 (3%) 43 38	62, 104, 156, 210	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	445	ILE	4.6
1	B	245	LEU	4.4
1	A	96	THR	4.3
1	C	33	LEU	4.2
1	C	301	VAL	4.2
1	D	117	ALA	4.2
1	D	216	PHE	4.0
1	D	94	ILE	3.8
1	B	305	ALA	3.5
1	C	116	VAL	3.5
1	C	426	LEU	3.5
1	C	446	PRO	3.4
1	C	17	ILE	3.3
1	C	9	ALA	3.2
1	C	199	ALA	3.2
1	A	140	TYR	3.1
1	C	216	PHE	3.1
1	D	87	LEU	3.1
1	B	114	ILE	3.1
1	C	151	VAL	2.9
1	C	96	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	239	GLY	2.9
1	C	437	GLY	2.9
1	D	58	SER	2.8
1	D	199	ALA	2.8
1	A	131	LEU	2.7
1	D	440	LEU	2.7
1	C	48	ALA	2.7
1	B	94	ILE	2.7
1	C	402	LEU	2.6
1	C	239	GLY	2.6
1	C	8	VAL	2.6
1	C	130	ALA	2.6
1	D	21	LYS	2.6
1	C	185	GLY	2.5
1	B	338	MET	2.5
1	B	162	ALA	2.5
1	B	306	THR	2.5
1	C	261	ILE	2.5
1	C	440	LEU	2.5
1	B	235	CYS	2.4
1	C	245	LEU	2.4
1	B	35	VAL	2.4
1	A	193	ILE	2.4
1	C	117	ALA	2.4
1	D	154	GLY	2.3
1	B	156	LEU	2.3
1	B	116	VAL	2.3
1	C	353	VAL	2.3
1	D	137	LEU	2.3
1	D	59	HIS	2.3
1	D	139	ILE	2.3
1	C	428	LEU	2.2
1	A	170	PHE	2.2
1	C	479	VAL	2.2
1	B	197	ALA	2.2
1	B	240	ASN	2.2
1	C	11	LEU	2.2
1	C	60	GLY	2.1
1	C	122	ILE	2.1
1	C	281	PHE	2.1
1	A	500	VAL	2.1
1	D	116	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	413	ALA	2.1
1	A	490	VAL	2.1
1	C	15	VAL	2.1
1	C	68	ARG	2.1
1	A	139	ILE	2.1
1	C	438	LEU	2.0
1	B	242	HIS	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](#)

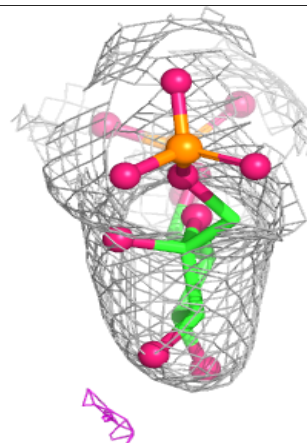
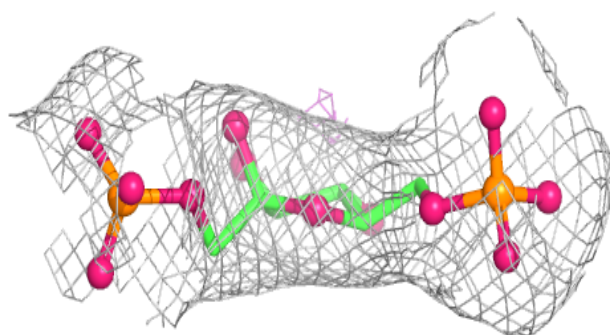
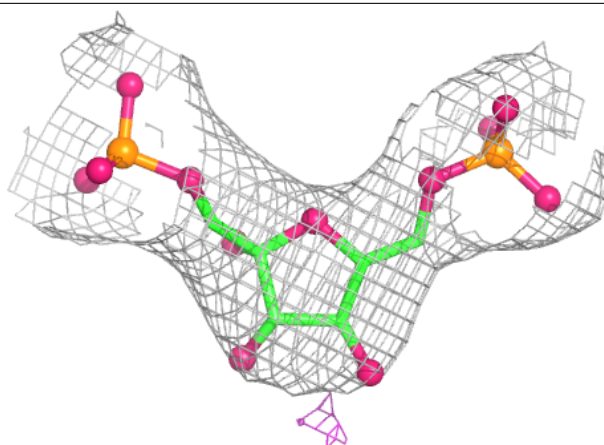
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FBP	A	601	20/20	0.96	0.06	68,84,91,94	0
2	FBP	C	601	20/20	0.96	0.05	94,111,125,135	0
2	FBP	B	601	20/20	0.97	0.05	64,76,87,89	0
2	FBP	D	601	20/20	0.97	0.05	66,73,78,83	0

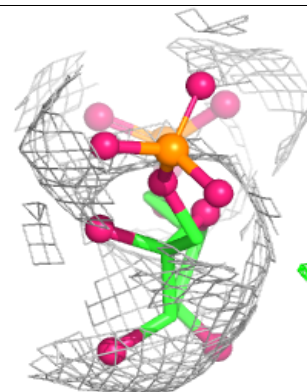
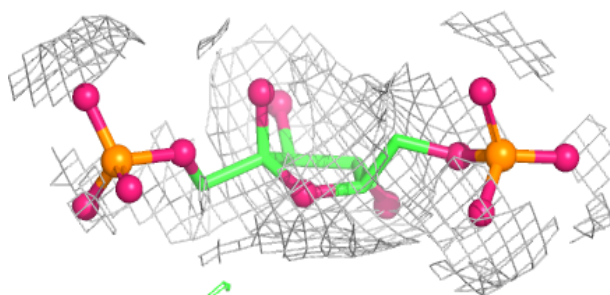
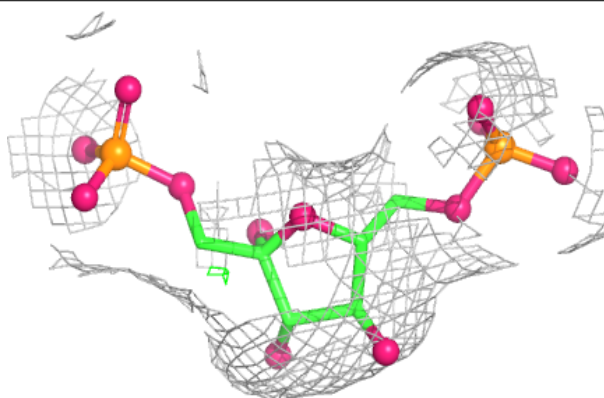
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP A 601:

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

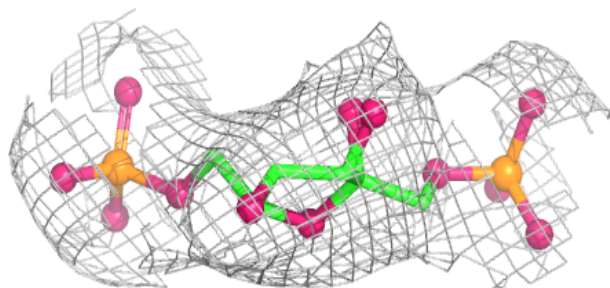
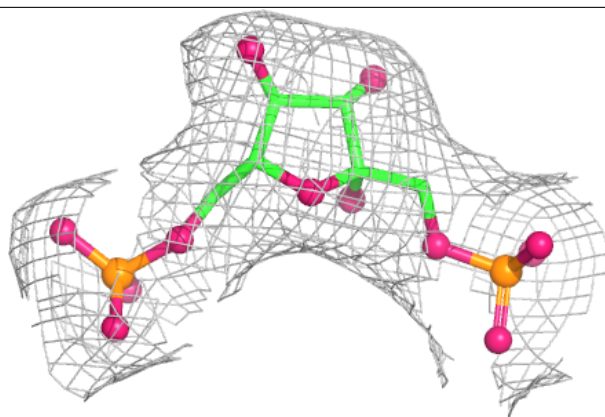
**Electron density around FBP C 601:**

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

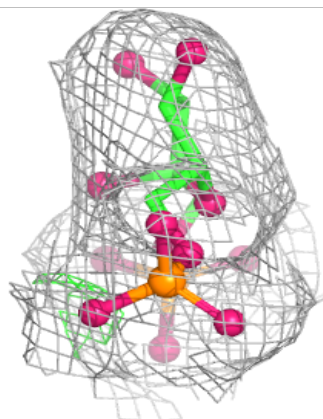
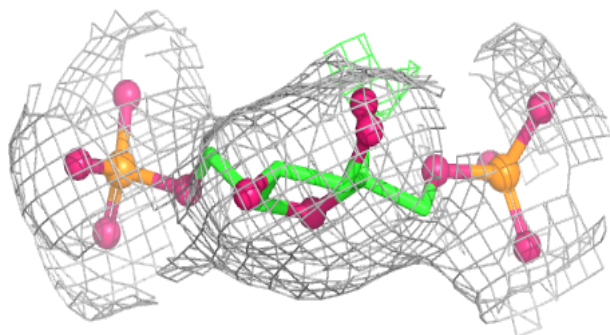
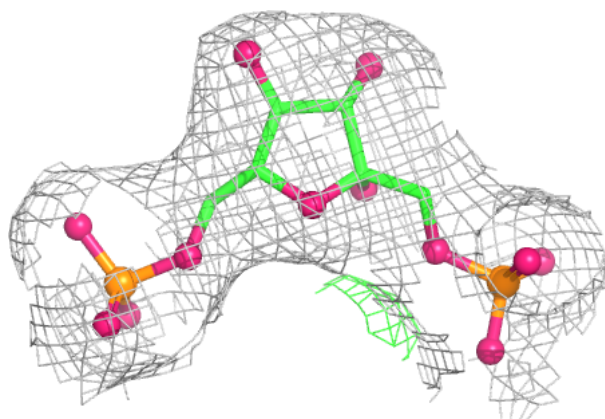


Electron density around FBP B 601:

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

**Electron density around FBP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.