



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:59 AM EDT

PDB ID : 2VGB / pdb_00002vgb
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE
Authors : Valentini, G.; Chiarelli, L.; Fortin, R.; Dolzan, M.; Galizzi, A.; Abraham, D.J.;
Wang, C.; Bianchi, P.; Zanella, A.; Mattevi, A.
Deposited on : 2007-11-12
Resolution : 2.73 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

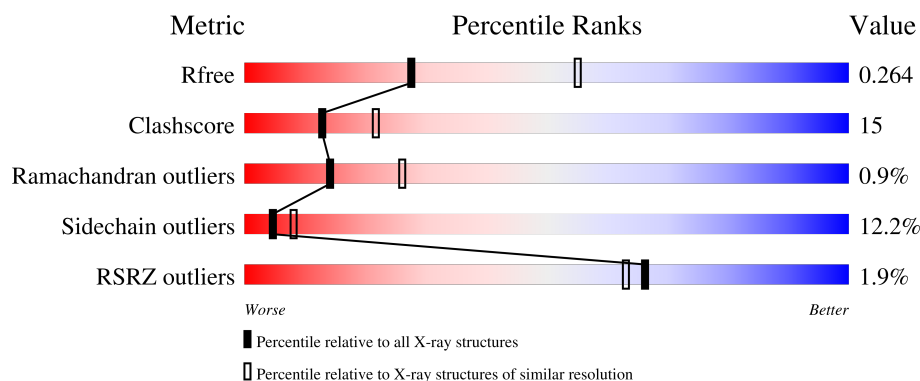
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	528	 2% 62% 31% 5% 5%
1	B	528	 4% 61% 27% 5% 7%
1	C	528	 66% 27% 5% 5%
1	D	528	 65% 27% 5% 5%

2 Entry composition [i](#)

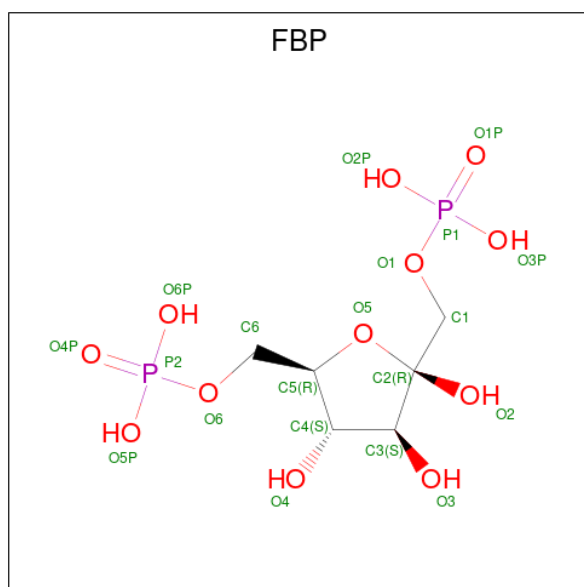
There are 6 unique types of molecules in this entry. The entry contains 15612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ISOZYMES R/L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3912	2457	709	728	18			
1	B	491	Total	C	N	O	S	0	0	0
			3719	2339	673	689	18			
1	C	517	Total	C	N	O	S	0	0	0
			3912	2457	709	728	18			
1	D	512	Total	C	N	O	S	0	0	0
			3880	2437	703	722	18			

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



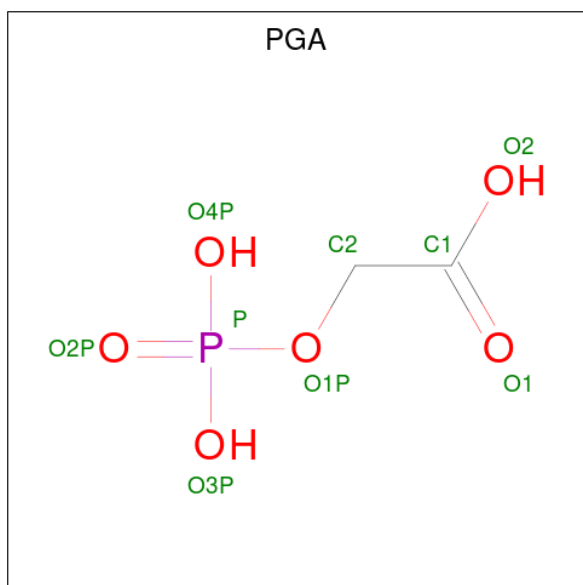
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		

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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 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			9	2	6	1		
3	B	1	Total	C	O	P	0	0
			9	2	6	1		
3	C	1	Total	C	O	P	0	0
			9	2	6	1		
3	D	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		

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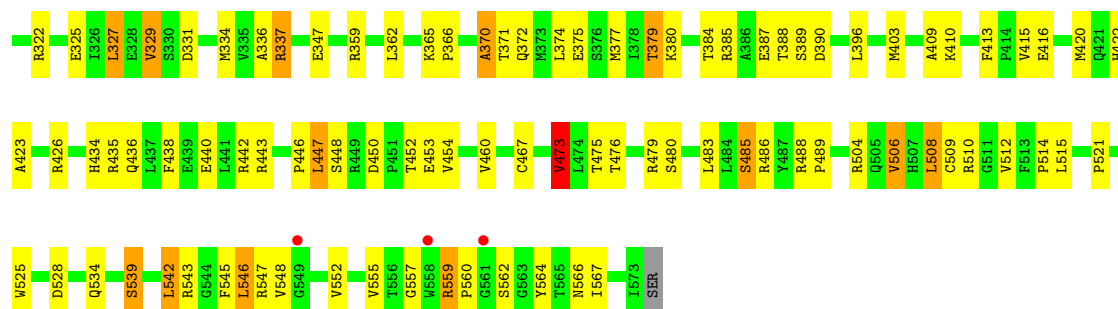
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total K 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	B	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0
5	D	1	Total Mn 1 1	0	0

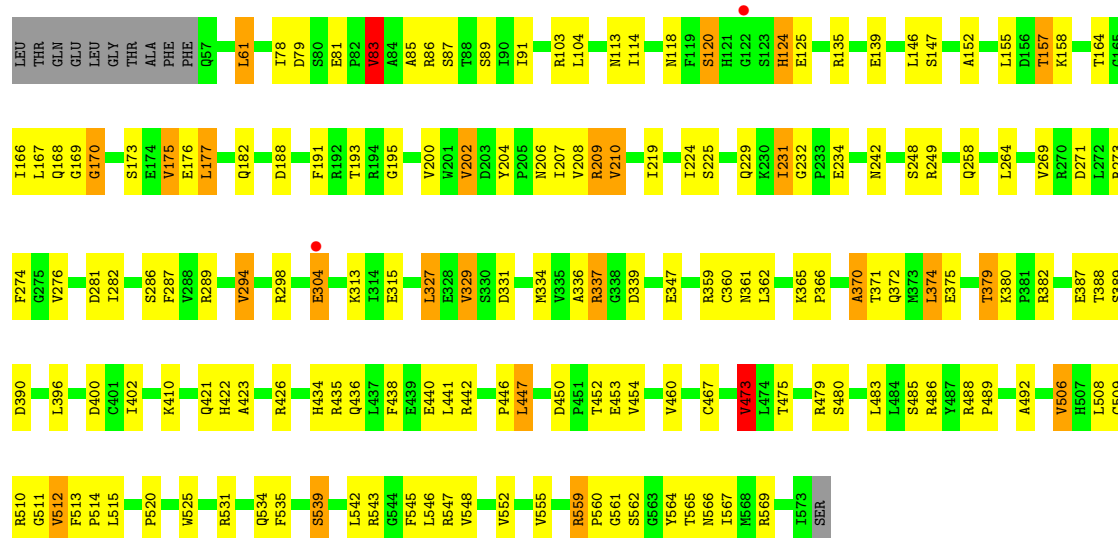
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	12	Total O 12 12	0	0
6	B	16	Total O 16 16	0	0
6	C	20	Total O 20 20	0	0
6	D	17	Total O 17 17	0	0



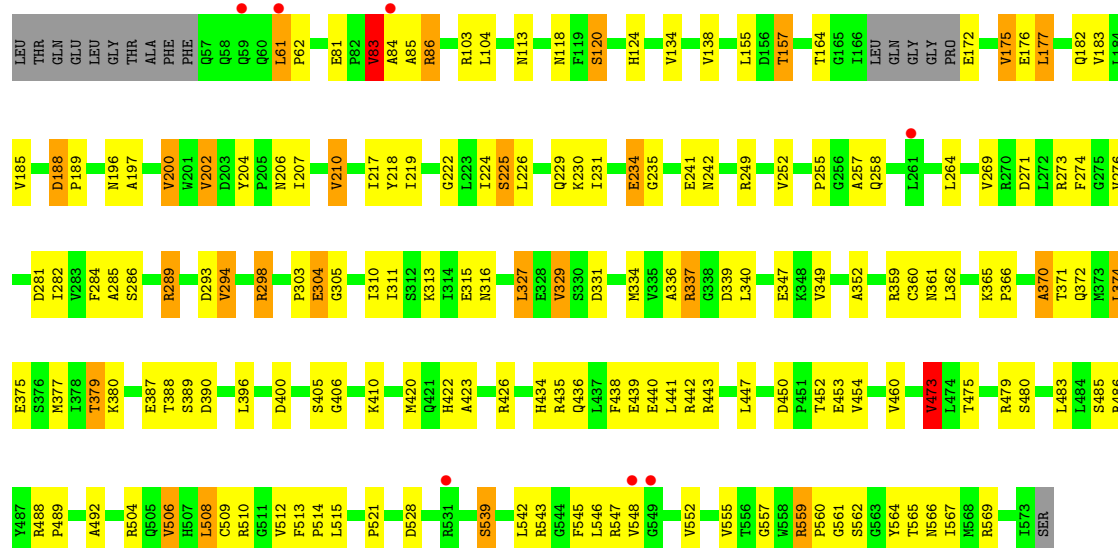
• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

Chain C: 66% 27% 5% .



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

Chain D: 65% 27% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.41Å 172.06Å 85.51Å 90.00° 92.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.73 20.00 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.3 (20.00-2.73) 96.4 (20.00-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.227 , 0.271 0.221 , 0.264	Depositor DCC
R_{free} test set	2784 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15612	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: MN, FBP, K, PGA

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	0.83	4/3976 (0.1%)	1.00	6/5390 (0.1%)
1	B	0.85	3/3776 (0.1%)	1.00	5/5115 (0.1%)
1	C	0.83	2/3976 (0.1%)	1.05	6/5390 (0.1%)
1	D	0.86	0/3942	1.04	7/5342 (0.1%)
All	All	0.84	9/15670 (0.1%)	1.02	24/21237 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	SER	CB-OG	18.05	1.78	1.42
1	A	410	LYS	CE-NZ	11.18	1.82	1.49
1	B	260	ASP	CG-OD1	6.43	1.37	1.25
1	A	189	PRO	C-O	6.02	1.31	1.24
1	A	410	LYS	CD-CE	-5.76	1.35	1.52
1	C	83	VAL	CA-CB	5.63	1.62	1.54
1	A	189	PRO	C-N	5.36	1.41	1.33
1	B	83	VAL	CA-CB	5.29	1.61	1.54
1	C	512	VAL	CA-CB	-5.22	1.48	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	VAL	CB-CA-C	-8.88	97.37	110.33
1	A	473	VAL	CB-CA-C	-7.97	98.69	110.33
1	B	144	SER	CA-CB-OG	-7.96	95.19	111.10
1	A	187	VAL	N-CA-C	-7.89	105.17	112.43
1	D	473	VAL	CB-CA-C	-7.63	99.33	110.63
1	B	473	VAL	CB-CA-C	-7.53	99.48	110.63
1	A	316	ASN	N-CA-C	5.95	116.94	108.74
1	C	561	GLY	N-CA-C	-5.71	105.48	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ASP	CA-C-N	5.66	126.92	119.84
1	A	188	ASP	C-N-CA	5.66	126.92	119.84
1	D	235	GLY	N-CA-C	5.59	118.32	110.38
1	D	316	ASN	N-CA-C	5.59	115.92	108.38
1	C	520	PRO	O-C-N	5.57	123.77	121.15
1	D	210	VAL	N-CA-C	5.41	119.75	113.42
1	D	561	GLY	N-CA-C	-5.35	105.94	112.68
1	C	195	GLY	N-CA-C	5.33	118.79	111.54
1	B	263	GLY	N-CA-C	-5.32	107.72	114.16
1	C	370	ALA	N-CA-C	5.29	117.42	109.23
1	A	287	PHE	N-CA-C	5.26	118.69	111.54
1	D	241	GLU	N-CA-C	-5.25	106.56	113.12
1	D	370	ALA	N-CA-C	5.20	117.71	109.50
1	B	287	PHE	N-CA-C	5.20	118.61	111.54
1	C	287	PHE	N-CA-C	5.14	118.48	111.39
1	B	370	ALA	N-CA-C	5.04	117.04	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3912	0	3992	136	6
1	B	3719	0	3802	125	6
1	C	3912	0	3992	114	1
1	D	3880	0	3959	127	1
2	A	20	0	10	1	0
2	B	20	0	10	3	0
2	C	20	0	10	2	0
2	D	20	0	10	2	0
3	A	9	0	2	0	0
3	B	9	0	2	0	0
3	C	9	0	2	0	0
3	D	9	0	2	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	0	3	0
6	B	16	0	0	2	0
6	C	20	0	0	3	0
6	D	17	0	0	0	0
All	All	15612	0	15793	471	7

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 15.

All (471) 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:A:410:LYS:CE	1:A:410:LYS:NZ	1.82	1.41
1:B:144:SER:CB	1:B:144:SER:OG	1.78	1.32
1:A:488:ARG:NH1	1:A:510:ARG:HB3	1.56	1.20
1:B:488:ARG:NH1	1:B:510:ARG:HB3	1.56	1.18
1:D:488:ARG:NH1	1:D:510:ARG:HB3	1.58	1.17
1:C:488:ARG:NH1	1:C:510:ARG:HB3	1.64	1.11
1:C:86:ARG:HB3	1:C:426:ARG:HG2	1.41	0.99
1:A:86:ARG:HB3	1:A:426:ARG:HG2	1.42	0.99
1:B:86:ARG:HB3	1:B:426:ARG:HG2	1.45	0.97
1:D:86:ARG:HB3	1:D:426:ARG:HG2	1.46	0.97
1:A:488:ARG:HH12	1:A:510:ARG:HB3	1.30	0.96
1:A:347:GLU:HG2	1:C:423:ALA:HB1	1.49	0.95
1:D:488:ARG:HH12	1:D:510:ARG:HB3	1.29	0.94
1:A:442:ARG:HH21	1:B:442:ARG:NH2	1.67	0.93
1:A:442:ARG:HH21	1:B:442:ARG:HH21	0.92	0.91
1:A:442:ARG:NH2	1:B:442:ARG:HH21	1.69	0.91
1:B:488:ARG:HH12	1:B:510:ARG:HB3	1.35	0.90
1:C:225:SER:HB3	1:C:242:ASN:HB2	1.53	0.90
1:B:488:ARG:NH1	1:B:510:ARG:CB	2.36	0.88
1:C:170:GLY:HA3	1:C:173:SER:OG	1.74	0.86
1:C:479:ARG:HG3	1:C:479:ARG:HH11	1.40	0.86
1:C:442:ARG:HH21	1:D:442:ARG:HH21	1.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:ARG:NH1	1:C:510:ARG:CB	2.39	0.85
1:D:488:ARG:NH1	1:D:510:ARG:CB	2.40	0.85
1:B:423:ALA:HB1	1:D:347:GLU:HG2	1.58	0.85
1:B:488:ARG:HH11	1:B:510:ARG:HB3	1.42	0.84
1:C:85:ALA:HB2	1:C:545:PHE:CE2	2.13	0.84
1:C:531:ARG:HD2	6:C:2018:HOH:O	1.78	0.83
1:A:488:ARG:HH11	1:A:510:ARG:HB3	1.43	0.83
1:D:506:VAL:CG1	1:D:512:VAL:HG11	2.08	0.83
1:B:347:GLU:HG2	1:D:423:ALA:HB1	1.60	0.83
1:B:506:VAL:CG1	1:B:512:VAL:HG11	2.11	0.80
1:D:488:ARG:HH12	1:D:510:ARG:CB	1.95	0.80
1:C:372:GLN:HG2	1:C:375:GLU:CG	2.11	0.79
1:D:488:ARG:HH11	1:D:510:ARG:HB3	1.48	0.79
1:A:488:ARG:NH1	1:A:510:ARG:CB	2.41	0.79
1:A:479:ARG:HG3	1:A:479:ARG:HH11	1.49	0.78
1:C:488:ARG:HH12	1:C:510:ARG:HB3	1.46	0.78
1:B:488:ARG:HH12	1:B:510:ARG:CB	1.95	0.78
1:D:315:GLU:HG2	1:D:336:ALA:CB	2.14	0.77
1:C:315:GLU:HG2	1:C:336:ALA:CB	2.16	0.76
1:D:86:ARG:HB3	1:D:426:ARG:CG	2.15	0.76
1:A:223:LEU:HD22	1:C:380:LYS:HE2	1.69	0.74
1:A:216:ARG:HD2	1:A:218:TYR:CE1	2.21	0.74
1:C:372:GLN:HG2	1:C:375:GLU:HG3	1.66	0.74
1:C:488:ARG:HH11	1:C:510:ARG:HB3	1.45	0.74
1:D:506:VAL:HG11	1:D:512:VAL:HG11	1.68	0.74
1:B:89:SER:OG	6:B:2001:HOH:O	2.06	0.73
1:A:423:ALA:HB1	1:C:347:GLU:HG2	1.71	0.73
1:C:506:VAL:CG1	1:C:512:VAL:HG11	2.19	0.73
1:C:488:ARG:HH12	1:C:510:ARG:CB	2.01	0.72
1:A:86:ARG:HB3	1:A:426:ARG:CG	2.20	0.72
1:C:315:GLU:HG2	1:C:336:ALA:HB3	1.70	0.72
1:A:86:ARG:HD3	1:A:422:HIS:ND1	2.04	0.71
1:B:86:ARG:HD3	1:B:422:HIS:ND1	2.04	0.71
1:C:86:ARG:HD3	1:C:422:HIS:ND1	2.05	0.71
1:A:506:VAL:CG1	1:A:512:VAL:HG11	2.20	0.71
1:B:506:VAL:CG1	1:B:512:VAL:CG1	2.69	0.71
1:A:315:GLU:HG2	1:A:336:ALA:CB	2.20	0.71
1:B:479:ARG:HH11	1:B:479:ARG:HG3	1.55	0.70
1:D:86:ARG:HD3	1:D:422:HIS:ND1	2.07	0.70
1:D:315:GLU:HG2	1:D:336:ALA:HB3	1.71	0.70
1:A:379:THR:HG22	1:A:380:LYS:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:506:VAL:CG1	1:D:512:VAL:CG1	2.69	0.70
1:A:488:ARG:HH12	1:A:510:ARG:CB	2.01	0.69
1:A:157:THR:HG22	1:A:286:SER:H	1.58	0.69
1:B:506:VAL:HG11	1:B:512:VAL:HG11	1.74	0.69
1:B:86:ARG:HB3	1:B:426:ARG:CG	2.21	0.69
1:C:379:THR:HG22	1:C:380:LYS:HG3	1.74	0.69
1:B:514:PRO:O	1:B:515:LEU:HD23	1.94	0.68
1:A:506:VAL:HG11	1:A:512:VAL:HG11	1.76	0.68
1:D:372:GLN:HG2	1:D:375:GLU:CG	2.24	0.67
1:A:225:SER:HB3	1:A:242:ASN:H	1.60	0.67
1:B:506:VAL:HG13	1:B:512:VAL:HG11	1.77	0.67
1:C:225:SER:CB	1:C:242:ASN:HB2	2.24	0.67
1:C:514:PRO:O	1:C:515:LEU:HD23	1.95	0.67
1:B:379:THR:HG22	1:B:380:LYS:HG3	1.77	0.66
1:D:485:SER:HB2	1:D:510:ARG:O	1.96	0.66
1:A:315:GLU:HG2	1:A:336:ALA:HB3	1.76	0.66
1:D:157:THR:HG22	1:D:286:SER:H	1.60	0.66
1:B:315:GLU:HG2	1:B:336:ALA:CB	2.25	0.66
1:D:188:ASP:C	1:D:188:ASP:OD1	2.38	0.66
1:B:177:LEU:HD13	1:B:183:VAL:HG21	1.77	0.66
1:C:442:ARG:NH2	1:D:442:ARG:HH21	1.95	0.66
1:D:514:PRO:O	1:D:515:LEU:HD23	1.96	0.66
1:A:347:GLU:CG	1:C:423:ALA:HB1	2.24	0.65
1:A:485:SER:HB2	1:A:510:ARG:O	1.96	0.65
1:B:144:SER:O	6:B:2004:HOH:O	2.14	0.65
1:C:86:ARG:HB3	1:C:426:ARG:CG	2.20	0.65
1:C:460:VAL:HG22	1:C:489:PRO:HG3	1.79	0.65
1:C:331:ASP:O	1:C:366:PRO:HD2	1.96	0.64
1:A:223:LEU:CD2	1:C:380:LYS:HE2	2.27	0.64
1:B:539:SER:O	1:B:543:ARG:HG3	1.97	0.64
1:B:144:SER:OG	1:B:144:SER:CA	2.46	0.64
1:B:269:VAL:O	1:B:273:ARG:HG2	1.99	0.63
1:C:166:ILE:HA	1:C:248:SER:HB3	1.80	0.63
1:D:372:GLN:HG2	1:D:375:GLU:HG3	1.80	0.63
1:A:506:VAL:CG1	1:A:512:VAL:CG1	2.76	0.63
1:B:315:GLU:HG2	1:B:336:ALA:HB3	1.81	0.63
1:B:164:THR:O	1:B:249:ARG:HA	1.98	0.63
1:D:506:VAL:HG13	1:D:512:VAL:HG11	1.79	0.62
1:D:315:GLU:OE2	1:D:339:ASP:OD2	2.17	0.62
1:B:485:SER:HB2	1:B:510:ARG:O	1.99	0.62
1:C:567:ILE:HG12	1:D:569:ARG:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:O	1:A:273:ARG:HG2	2.00	0.62
1:C:506:VAL:HG11	1:C:512:VAL:HG11	1.81	0.62
1:A:479:ARG:HG3	1:A:479:ARG:NH1	2.13	0.62
1:B:281:ASP:OD2	1:B:504:ARG:NE	2.32	0.62
1:B:331:ASP:O	1:B:366:PRO:HD2	2.00	0.62
1:C:269:VAL:O	1:C:273:ARG:HG2	2.00	0.61
1:D:177:LEU:HD12	1:D:183:VAL:HG21	1.82	0.61
1:C:479:ARG:HG3	1:C:479:ARG:NH1	2.09	0.61
1:D:379:THR:HG22	1:D:380:LYS:HG3	1.82	0.61
1:A:331:ASP:O	1:A:366:PRO:HD2	2.01	0.61
1:D:172:GLU:CD	1:D:172:GLU:N	2.59	0.61
1:B:337:ARG:HD3	1:B:370:ALA:O	2.01	0.60
1:D:506:VAL:HG11	1:D:512:VAL:CG1	2.31	0.60
1:A:170:GLY:HA3	1:A:173:SER:OG	2.01	0.60
1:B:290:LYS:HB3	1:B:322:ARG:NH1	2.16	0.60
1:C:315:GLU:OE2	1:C:339:ASP:OD2	2.20	0.60
1:C:506:VAL:CG1	1:C:512:VAL:CG1	2.80	0.60
1:A:337:ARG:HD3	1:A:370:ALA:O	2.01	0.60
1:B:337:ARG:HH22	1:B:390:ASP:CG	2.09	0.60
1:A:460:VAL:HG22	1:A:489:PRO:HG3	1.83	0.59
1:A:447:LEU:HD13	1:B:467:CYS:SG	2.41	0.59
1:C:313:LYS:HD2	1:C:334:MET:SD	2.42	0.59
1:B:372:GLN:HG2	1:B:375:GLU:CG	2.31	0.59
1:D:337:ARG:HH22	1:D:390:ASP:CG	2.11	0.59
1:D:175:VAL:HG21	1:D:196:ASN:HA	1.85	0.59
1:D:175:VAL:CG1	1:D:197:ALA:HA	2.33	0.59
1:B:313:LYS:HD2	1:B:334:MET:SD	2.43	0.58
1:D:539:SER:O	1:D:543:ARG:HG3	2.02	0.58
1:B:479:ARG:HG3	1:B:479:ARG:NH1	2.17	0.58
1:C:219:ILE:HB	1:C:224:ILE:HB	1.85	0.58
1:D:204:TYR:CE1	1:D:206:ASN:HB2	2.39	0.58
1:C:157:THR:HG22	1:C:286:SER:H	1.69	0.58
1:A:450:ASP:O	1:A:454:VAL:HG23	2.03	0.58
1:B:327:LEU:HD22	1:B:365:LYS:HD2	1.86	0.58
1:A:506:VAL:HG11	1:A:512:VAL:CG1	2.34	0.58
1:B:372:GLN:HA	1:B:375:GLU:HG2	1.84	0.58
1:D:269:VAL:O	1:D:273:ARG:HG2	2.04	0.58
1:A:539:SER:O	1:A:543:ARG:HG3	2.03	0.58
1:C:146:LEU:HD23	1:C:535:PHE:CE1	2.38	0.58
1:C:485:SER:HB2	1:C:510:ARG:O	2.04	0.58
1:A:514:PRO:O	1:A:515:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD23	1:A:155:LEU:C	2.28	0.57
1:D:436:GLN:O	1:D:440:GLU:HG3	2.03	0.57
1:A:442:ARG:NH2	1:B:442:ARG:NH2	2.38	0.57
1:D:83:VAL:HG12	1:D:83:VAL:O	2.03	0.57
1:A:372:GLN:HA	1:A:375:GLU:HG2	1.87	0.57
1:B:557:GLY:HA3	2:B:580:FBP:O3	2.04	0.57
1:D:327:LEU:HD22	1:D:365:LYS:HD2	1.86	0.57
1:A:194:ARG:HH11	1:A:194:ARG:HB3	1.70	0.57
1:C:506:VAL:HG13	1:C:512:VAL:HG11	1.85	0.57
1:B:473:VAL:HG13	1:B:555:VAL:HB	1.87	0.57
1:B:506:VAL:HG11	1:B:512:VAL:CG1	2.32	0.56
1:D:177:LEU:CD1	1:D:183:VAL:HG21	2.34	0.56
1:D:83:VAL:O	1:D:83:VAL:CG1	2.54	0.56
1:A:337:ARG:HH22	1:A:390:ASP:CG	2.13	0.56
1:A:83:VAL:HG12	1:A:83:VAL:O	2.04	0.56
1:A:210:VAL:HG12	1:A:257:ALA:HB1	1.88	0.56
1:A:157:THR:CG2	1:A:286:SER:H	2.18	0.56
1:D:460:VAL:HG22	1:D:489:PRO:HG3	1.88	0.55
1:D:134:VAL:O	1:D:138:VAL:HG23	2.06	0.55
1:A:83:VAL:O	1:A:83:VAL:CG1	2.53	0.55
1:B:157:THR:HG22	1:B:286:SER:H	1.72	0.55
1:B:134:VAL:O	1:B:138:VAL:HG23	2.06	0.55
1:D:479:ARG:HG3	1:D:479:ARG:HH11	1.72	0.55
1:D:331:ASP:O	1:D:366:PRO:HD2	2.06	0.55
1:A:276:VAL:HG11	1:A:304:GLU:HB2	1.89	0.55
1:B:157:THR:HG22	1:B:286:SER:HB2	1.88	0.55
1:B:204:TYR:CE1	1:B:206:ASN:HB2	2.42	0.55
1:C:276:VAL:HG11	1:C:304:GLU:HB2	1.89	0.55
1:C:372:GLN:HA	1:C:375:GLU:HG2	1.89	0.55
1:C:442:ARG:HH21	1:D:442:ARG:NH2	2.01	0.55
1:C:539:SER:O	1:C:543:ARG:HG3	2.07	0.55
1:A:162:ILE:HG22	1:A:252:VAL:HB	1.88	0.55
1:D:559:ARG:HD2	1:D:564:TYR:CD1	2.42	0.54
1:D:118:ASN:OD1	1:D:120:SER:HB2	2.06	0.54
1:B:385:ARG:HH11	1:B:385:ARG:HG2	1.72	0.54
1:A:347:GLU:HG2	1:C:423:ALA:CB	2.31	0.54
1:A:208:VAL:HA	1:A:236:LEU:HD21	1.90	0.54
1:C:327:LEU:HD22	1:C:365:LYS:HD2	1.88	0.54
1:B:281:ASP:C	1:B:282:ILE:HG13	2.33	0.54
1:B:420:MET:HE1	1:D:347:GLU:HG3	1.90	0.54
1:C:164:THR:O	1:C:249:ARG:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:VAL:HG13	1:A:512:VAL:HG11	1.91	0.53
1:C:168:GLN:O	1:C:169:GLY:C	2.51	0.53
1:C:231:ILE:HD13	1:C:232:GLY:H	1.73	0.53
1:A:118:ASN:OD1	1:A:120:SER:HB2	2.08	0.53
1:A:465:LYS:HE3	1:B:448:SER:HB3	1.90	0.53
1:A:125:GLU:CD	1:A:125:GLU:H	2.16	0.53
1:D:164:THR:O	1:D:249:ARG:HA	2.09	0.53
1:B:436:GLN:O	1:B:440:GLU:HG3	2.08	0.53
1:C:209:ARG:HG2	1:C:209:ARG:O	2.09	0.53
1:D:219:ILE:HG12	1:D:252:VAL:HG22	1.90	0.53
1:B:460:VAL:HG22	1:B:489:PRO:HG3	1.91	0.52
1:B:118:ASN:OD1	1:B:120:SER:HB2	2.09	0.52
1:B:327:LEU:CD2	1:B:365:LYS:HD2	2.39	0.52
1:C:337:ARG:HH22	1:C:390:ASP:CG	2.18	0.52
1:B:86:ARG:NH2	1:B:113:ASN:OD1	2.41	0.52
1:C:188:ASP:HB3	1:C:191:PHE:HD1	1.74	0.52
1:B:124:HIS:HE1	1:B:271:ASP:OD1	1.93	0.52
1:C:86:ARG:NH2	1:C:113:ASN:OD1	2.42	0.52
1:D:438:PHE:O	1:D:442:ARG:HG3	2.09	0.52
1:A:85:ALA:HB2	1:A:545:PHE:CE2	2.44	0.52
1:C:81:GLU:OE1	1:C:81:GLU:HA	2.08	0.52
1:C:124:HIS:HE1	1:C:271:ASP:OD1	1.93	0.52
1:B:347:GLU:HG3	1:D:420:MET:HE1	1.92	0.51
1:C:475:THR:HA	2:C:580:FBP:H61	1.92	0.51
1:D:479:ARG:HG3	1:D:479:ARG:NH1	2.26	0.51
1:C:114:ILE:HG12	1:C:152:ALA:HB3	1.93	0.51
1:D:185:VAL:HG22	1:D:200:VAL:HG22	1.93	0.51
1:A:436:GLN:O	1:A:440:GLU:HG3	2.10	0.51
1:D:124:HIS:HE1	1:D:271:ASP:OD1	1.93	0.51
1:A:559:ARG:HD2	1:A:564:TYR:CD1	2.46	0.51
1:A:337:ARG:CD	1:A:370:ALA:O	2.58	0.51
1:B:559:ARG:HD2	1:B:564:TYR:CD1	2.46	0.51
1:D:366:PRO:HB3	1:D:508:LEU:O	2.10	0.51
1:D:366:PRO:HA	1:D:400:ASP:OD2	2.11	0.51
1:A:124:HIS:HE1	1:A:271:ASP:OD1	1.94	0.50
1:C:89:SER:OG	6:C:2001:HOH:O	2.19	0.50
1:A:185:VAL:HA	1:A:200:VAL:O	2.12	0.50
1:D:219:ILE:HB	1:D:224:ILE:HB	1.94	0.50
1:D:315:GLU:HG2	1:D:336:ALA:HB1	1.91	0.50
1:A:134:VAL:O	1:A:138:VAL:HG23	2.12	0.50
1:A:327:LEU:HD22	1:A:365:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:GLY:HA3	2:D:580:FBP:O3	2.12	0.50
1:D:81:GLU:HA	1:D:81:GLU:OE1	2.11	0.50
1:D:175:VAL:HG13	1:D:197:ALA:HA	1.94	0.50
1:D:289:ARG:HG3	1:D:293:ASP:OD2	2.12	0.50
1:D:327:LEU:CD2	1:D:365:LYS:HD2	2.42	0.50
1:C:135:ARG:O	1:C:139:GLU:HG2	2.12	0.49
1:B:275:GLY:O	1:B:280:VAL:HG22	2.11	0.49
1:A:372:GLN:HG2	1:A:375:GLU:CG	2.43	0.49
1:B:276:VAL:HG11	1:B:304:GLU:HB2	1.94	0.49
1:B:372:GLN:HG2	1:B:375:GLU:HG3	1.94	0.49
1:C:87:SER:CB	1:C:511:GLY:HA2	2.42	0.49
1:A:286:SER:HA	1:A:313:LYS:HE2	1.93	0.49
1:B:85:ALA:HB2	1:B:545:PHE:CE2	2.48	0.49
1:D:303:PRO:C	1:D:305:GLY:H	2.19	0.49
1:A:168:GLN:HB2	1:A:195:GLY:O	2.12	0.49
1:B:255:PRO:C	1:B:257:ALA:H	2.19	0.49
1:C:402:ILE:HG13	1:C:421:GLN:NE2	2.28	0.49
1:D:86:ARG:NH2	1:D:113:ASN:OD1	2.45	0.49
1:D:372:GLN:HA	1:D:375:GLU:HG2	1.93	0.49
1:C:436:GLN:O	1:C:440:GLU:HG3	2.13	0.49
1:C:453:GLU:HG2	1:C:483:LEU:HD13	1.95	0.49
1:B:420:MET:CE	1:D:347:GLU:HG3	2.43	0.48
1:A:313:LYS:HD2	1:A:334:MET:SD	2.53	0.48
1:B:366:PRO:HB3	1:B:508:LEU:O	2.13	0.48
1:A:186:THR:HB	1:A:188:ASP:H	1.78	0.48
1:A:206:ASN:O	1:A:210:VAL:HG23	2.14	0.48
1:A:441:LEU:O	1:A:442:ARG:C	2.57	0.48
1:A:229:GLN:NE2	1:A:239:GLN:HB2	2.29	0.48
1:C:438:PHE:O	1:C:442:ARG:HG3	2.13	0.48
1:C:569:ARG:HG2	1:D:567:ILE:HG12	1.95	0.48
1:B:384:THR:OG1	1:B:387:GLU:HG3	2.13	0.48
1:D:206:ASN:O	1:D:207:ILE:C	2.55	0.48
1:D:441:LEU:O	1:D:442:ARG:C	2.56	0.48
1:C:125:GLU:CD	1:C:125:GLU:H	2.21	0.48
1:C:337:ARG:CD	1:C:370:ALA:O	2.62	0.48
1:C:452:THR:HG23	1:C:565:THR:HB	1.95	0.47
1:A:87:SER:CB	1:A:511:GLY:HA2	2.44	0.47
1:A:281:ASP:C	1:A:282:ILE:HG13	2.39	0.47
1:D:339:ASP:O	1:D:340:LEU:C	2.57	0.47
1:D:475:THR:HA	2:D:580:FBP:H61	1.96	0.47
1:A:209:ARG:O	1:A:209:ARG:HG2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:VAL:O	1:B:84:ALA:HB2	2.15	0.47
1:B:125:GLU:CD	1:B:125:GLU:H	2.22	0.47
1:B:476:THR:HB	2:B:580:FBP:O4P	2.13	0.47
1:A:225:SER:HB3	1:A:242:ASN:N	2.27	0.47
1:A:438:PHE:O	1:A:442:ARG:HG3	2.14	0.47
1:A:521:PRO:HA	1:A:528:ASP:OD1	2.13	0.47
1:A:230:LYS:HB2	1:A:237:VAL:HB	1.95	0.47
1:B:303:PRO:C	1:B:305:GLY:H	2.23	0.47
1:D:225:SER:HB3	1:D:242:ASN:HD22	1.79	0.47
1:A:315:GLU:HG2	1:A:336:ALA:HB1	1.96	0.47
1:B:207:ILE:HD11	1:B:254:LEU:HD21	1.96	0.47
1:B:347:GLU:HG3	1:D:420:MET:CE	2.44	0.47
1:B:506:VAL:HG13	1:B:512:VAL:CG1	2.40	0.47
1:C:157:THR:HG22	1:C:286:SER:HB2	1.97	0.47
1:A:434:HIS:O	1:A:435:ARG:C	2.57	0.47
1:D:271:ASP:O	1:D:274:PHE:HB3	2.15	0.47
1:A:226:LEU:HD23	1:A:240:VAL:HA	1.96	0.47
1:B:297:VAL:CG1	1:B:310:ILE:HD13	2.45	0.47
1:B:452:THR:HG22	1:B:483:LEU:HD12	1.96	0.47
1:D:452:THR:HG23	1:D:565:THR:HB	1.96	0.47
1:C:177:LEU:N	1:C:177:LEU:HD23	2.30	0.47
1:D:521:PRO:HA	1:D:528:ASP:OD1	2.15	0.47
1:B:156:ASP:C	1:B:156:ASP:OD1	2.58	0.46
1:C:366:PRO:HA	1:C:400:ASP:OD2	2.14	0.46
1:A:222:GLY:O	1:C:382:ARG:HG3	2.14	0.46
1:A:452:THR:HG22	1:A:483:LEU:HD12	1.96	0.46
1:C:506:VAL:HG11	1:C:512:VAL:CG1	2.44	0.46
1:D:255:PRO:C	1:D:257:ALA:H	2.23	0.46
1:B:146:LEU:CB	1:B:542:LEU:HD12	2.45	0.46
1:C:155:LEU:HD23	1:C:155:LEU:C	2.41	0.46
1:A:384:THR:OG1	1:A:387:GLU:HG3	2.16	0.46
1:C:467:CYS:SG	1:D:447:LEU:HD13	2.56	0.46
1:D:281:ASP:C	1:D:282:ILE:HG13	2.41	0.46
1:D:313:LYS:HD2	1:D:334:MET:SD	2.55	0.46
1:A:297:VAL:CG1	1:A:310:ILE:HD13	2.45	0.46
1:D:294:VAL:HG11	1:D:329:VAL:HG12	1.98	0.46
1:B:413:PHE:HB3	1:B:416:GLU:HB2	1.97	0.46
1:B:488:ARG:HH11	1:B:510:ARG:CB	2.19	0.46
1:C:231:ILE:HD13	1:C:232:GLY:N	2.31	0.46
1:C:337:ARG:HD3	1:C:370:ALA:O	2.16	0.46
1:A:473:VAL:HG13	1:A:555:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASP:O	1:C:454:VAL:HG23	2.15	0.46
1:B:450:ASP:O	1:B:454:VAL:HG23	2.15	0.46
1:C:360:CYS:O	1:C:361:ASN:C	2.57	0.46
1:A:177:LEU:HD13	1:A:183:VAL:HG21	1.98	0.45
1:A:340:LEU:O	1:A:344:ILE:HG12	2.16	0.45
1:A:374:LEU:HD12	1:A:387:GLU:HB3	1.97	0.45
1:B:294:VAL:HG11	1:B:329:VAL:HG12	1.99	0.45
1:C:225:SER:HB3	1:C:242:ASN:H	1.81	0.45
1:B:83:VAL:O	1:B:83:VAL:HG12	2.16	0.45
1:C:206:ASN:O	1:C:210:VAL:HG23	2.16	0.45
1:C:488:ARG:HH12	1:C:510:ARG:HB2	1.80	0.45
1:B:521:PRO:HA	1:B:528:ASP:OD1	2.16	0.45
1:C:87:SER:HB3	1:C:511:GLY:HA2	1.99	0.45
1:A:188:ASP:HA	1:A:189:PRO:HD2	1.67	0.45
1:B:69:PHE:O	1:B:72:HIS:HB3	2.16	0.45
1:B:515:LEU:HD13	1:B:539:SER:CB	2.46	0.45
1:D:234:GLU:C	1:D:234:GLU:CD	2.84	0.45
1:A:515:LEU:HD13	1:A:539:SER:CB	2.47	0.45
1:C:118:ASN:OD1	1:C:120:SER:HB2	2.17	0.45
1:C:327:LEU:CD2	1:C:365:LYS:HD2	2.46	0.45
1:D:155:LEU:C	1:D:155:LEU:HD23	2.41	0.45
1:D:405:SER:O	1:D:406:GLY:C	2.60	0.45
1:A:61:LEU:O	1:A:62:PRO:C	2.59	0.45
1:A:360:CYS:O	1:A:361:ASN:C	2.59	0.45
1:C:202:VAL:HG13	1:C:204:TYR:H	1.81	0.45
1:C:515:LEU:HD13	1:C:539:SER:CB	2.47	0.45
1:A:86:ARG:NH2	1:A:113:ASN:OD1	2.49	0.45
1:A:184:LEU:HD11	1:A:235:GLY:HA3	1.98	0.45
1:A:192:ARG:O	1:A:192:ARG:HG2	2.15	0.45
1:D:473:VAL:HG13	1:D:555:VAL:HB	1.99	0.45
1:A:177:LEU:CD1	1:A:183:VAL:HG21	2.47	0.45
1:B:337:ARG:CD	1:B:370:ALA:O	2.64	0.45
1:D:286:SER:HA	1:D:313:LYS:HE2	1.99	0.45
1:A:216:ARG:O	1:A:217:ILE:HG13	2.17	0.45
1:C:559:ARG:HD2	1:C:564:TYR:CD1	2.51	0.45
1:D:85:ALA:HB2	1:D:545:PHE:CE2	2.51	0.45
1:D:276:VAL:HG11	1:D:304:GLU:HB2	1.98	0.45
1:D:229:GLN:O	1:D:230:LYS:HG2	2.17	0.45
1:A:164:THR:O	1:A:249:ARG:HA	2.16	0.44
1:B:438:PHE:O	1:B:442:ARG:HG3	2.17	0.44
1:C:559:ARG:HD3	1:C:560:PRO:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:PRO:C	1:C:447:LEU:O	2.58	0.44
1:C:509:CYS:O	1:C:510:ARG:C	2.56	0.44
1:D:450:ASP:O	1:D:454:VAL:HG23	2.18	0.44
1:A:68:THR:HB	1:C:440:GLU:OE2	2.18	0.44
1:C:434:HIS:O	1:C:435:ARG:C	2.61	0.44
1:C:473:VAL:HG13	1:C:555:VAL:HB	1.98	0.44
1:A:249:ARG:NH1	6:A:2005:HOH:O	2.25	0.44
1:B:434:HIS:O	1:B:435:ARG:C	2.59	0.44
1:D:377:MET:C	1:D:379:THR:N	2.76	0.44
1:C:294:VAL:HG11	1:C:329:VAL:HG12	2.00	0.43
1:B:135:ARG:O	1:B:139:GLU:HG2	2.19	0.43
1:D:506:VAL:HG13	1:D:512:VAL:CG1	2.45	0.43
1:A:175:VAL:CG1	1:A:197:ALA:HA	2.48	0.43
1:B:228:VAL:HA	1:B:238:THR:HA	2.01	0.43
1:D:337:ARG:CD	1:D:370:ALA:O	2.67	0.43
1:A:191:PHE:C	1:A:193:THR:H	2.27	0.43
1:A:480:SER:OG	2:A:580:FBP:O6P	2.33	0.43
1:B:347:GLU:H	1:B:347:GLU:CD	2.26	0.43
1:D:285:ALA:O	1:D:313:LYS:HG3	2.18	0.43
1:D:509:CYS:O	1:D:510:ARG:C	2.59	0.43
1:A:276:VAL:CG1	1:A:304:GLU:HB2	2.49	0.43
1:D:202:VAL:HG13	1:D:204:TYR:H	1.83	0.43
1:A:275:GLY:O	1:A:280:VAL:HG22	2.18	0.43
1:C:374:LEU:HD12	1:C:387:GLU:HB3	2.00	0.43
1:B:377:MET:C	1:B:379:THR:N	2.74	0.43
1:B:559:ARG:HD3	1:B:560:PRO:O	2.19	0.43
1:D:439:GLU:O	1:D:443:ARG:HB2	2.17	0.43
1:A:166:ILE:N	1:A:166:ILE:HD12	2.34	0.43
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.92	0.43
1:B:83:VAL:O	1:B:83:VAL:CG1	2.65	0.43
1:C:83:VAL:O	1:C:83:VAL:CG1	2.67	0.43
1:D:374:LEU:HD12	1:D:387:GLU:HB3	2.00	0.43
1:A:253:ASN:O	1:A:254:LEU:HD23	2.19	0.43
1:A:372:GLN:HG2	1:A:375:GLU:HG3	2.00	0.43
1:C:207:ILE:CG2	1:C:208:VAL:N	2.81	0.43
1:B:102:GLU:OE1	1:B:102:GLU:HA	2.18	0.43
1:B:475:THR:HA	2:B:580:FBP:H61	2.00	0.43
1:D:281:ASP:OD2	1:D:504:ARG:NE	2.48	0.42
1:D:453:GLU:HG2	1:D:483:LEU:HD13	2.02	0.42
1:A:135:ARG:O	1:A:139:GLU:HG2	2.19	0.42
1:C:271:ASP:O	1:C:274:PHE:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:HG2	1:B:385:ARG:NH1	2.33	0.42
1:A:184:LEU:CD1	1:A:235:GLY:HA3	2.50	0.42
1:A:405:SER:O	1:A:406:GLY:C	2.61	0.42
1:B:337:ARG:NH2	1:B:390:ASP:OD1	2.52	0.42
1:C:175:VAL:HG22	6:C:2008:HOH:O	2.19	0.42
1:D:284:PHE:HD1	1:D:311:ILE:HB	1.84	0.42
1:B:81:GLU:HA	1:B:81:GLU:OE1	2.20	0.42
1:C:441:LEU:O	1:C:442:ARG:C	2.61	0.42
1:C:562:SER:HB2	2:C:580:FBP:O4P	2.18	0.42
1:D:157:THR:CG2	1:D:286:SER:H	2.31	0.42
1:D:303:PRO:C	1:D:305:GLY:N	2.77	0.42
1:D:349:VAL:O	1:D:352:ALA:N	2.53	0.42
1:A:175:VAL:HG11	1:A:197:ALA:HA	2.02	0.42
1:A:230:LYS:HA	1:A:230:LYS:HD3	1.82	0.42
1:B:107:MET:HG3	1:B:415:VAL:HG22	2.02	0.42
1:B:446:PRO:C	1:B:447:LEU:O	2.61	0.42
1:A:157:THR:HG22	1:A:286:SER:CB	2.50	0.42
1:D:347:GLU:H	1:D:347:GLU:CD	2.27	0.42
1:B:315:GLU:HG2	1:B:336:ALA:HB1	1.99	0.42
1:C:435:ARG:NH1	1:D:443:ARG:HE	2.18	0.42
1:D:175:VAL:HG11	1:D:197:ALA:HA	2.01	0.42
1:D:337:ARG:HD3	1:D:370:ALA:O	2.20	0.42
1:D:360:CYS:O	1:D:361:ASN:C	2.63	0.42
1:A:219:ILE:HB	1:A:224:ILE:HB	2.01	0.42
1:B:377:MET:C	1:B:379:THR:H	2.28	0.42
1:C:61:LEU:HD12	1:C:61:LEU:HA	1.95	0.42
1:A:104:LEU:O	1:A:108:ILE:HG13	2.19	0.41
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.98	0.41
1:D:83:VAL:O	1:D:84:ALA:HB2	2.20	0.41
1:D:377:MET:HA	1:D:380:LYS:O	2.20	0.41
1:A:207:ILE:HD11	1:A:254:LEU:HD21	2.02	0.41
1:A:347:GLU:H	1:A:347:GLU:CD	2.28	0.41
1:A:348:LYS:HD3	1:C:78:ILE:O	2.21	0.41
1:C:492:ALA:HB1	1:C:513:PHE:CE1	2.55	0.41
1:C:157:THR:HG22	1:C:286:SER:CB	2.49	0.41
1:D:452:THR:HG22	1:D:483:LEU:HD12	2.03	0.41
1:B:146:LEU:HB3	1:B:542:LEU:HD12	2.01	0.41
1:B:545:PHE:C	1:B:546:LEU:HD23	2.45	0.41
1:C:525:TRP:CE2	1:C:560:PRO:HG3	2.56	0.41
1:D:61:LEU:HD12	1:D:61:LEU:HA	1.88	0.41
1:D:492:ALA:HB1	1:D:513:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:LEU:HD13	1:D:539:SER:CB	2.51	0.41
1:A:220:ASP:CG	1:A:250:LYS:HD3	2.46	0.41
1:B:204:TYR:CE1	1:B:261:LEU:HD13	2.55	0.41
1:B:322:ARG:O	1:B:325:GLU:HG2	2.20	0.41
1:A:377:MET:HA	1:A:380:LYS:O	2.20	0.41
1:A:559:ARG:HD3	1:A:560:PRO:O	2.21	0.41
1:B:155:LEU:C	1:B:155:LEU:HD23	2.46	0.41
1:C:91:ILE:HG12	1:C:114:ILE:HB	2.02	0.41
1:D:61:LEU:O	1:D:62:PRO:C	2.61	0.41
1:B:114:ILE:HG12	1:B:152:ALA:HB3	2.03	0.41
1:B:313:LYS:HD2	1:B:334:MET:CE	2.51	0.41
1:D:230:LYS:HA	1:D:230:LYS:HD3	1.80	0.41
1:A:144:SER:HB3	6:A:2003:HOH:O	2.21	0.41
1:A:327:LEU:CD2	1:A:365:LYS:HD2	2.51	0.41
1:A:545:PHE:C	1:A:546:LEU:HD23	2.46	0.41
1:B:96:PRO:HD2	1:B:409:ALA:O	2.21	0.41
1:B:102:GLU:OE1	1:B:105:LYS:HD2	2.21	0.41
1:B:157:THR:HG22	1:B:286:SER:CB	2.50	0.41
1:B:219:ILE:HB	1:B:224:ILE:HB	2.02	0.41
1:B:525:TRP:CE2	1:B:560:PRO:HG3	2.56	0.41
1:C:281:ASP:C	1:C:282:ILE:HG13	2.45	0.41
1:D:218:TYR:HB3	1:D:222:GLY:HA2	2.02	0.41
1:D:434:HIS:O	1:D:435:ARG:C	2.64	0.41
1:D:559:ARG:HD3	1:D:560:PRO:O	2.20	0.41
1:A:133:ASN:ND2	6:A:2002:HOH:O	2.54	0.41
1:B:509:CYS:O	1:B:510:ARG:C	2.62	0.41
1:A:69:PHE:O	1:A:72:HIS:HB3	2.21	0.40
1:A:271:ASP:O	1:A:274:PHE:HB3	2.21	0.40
1:A:569:ARG:HG2	1:B:567:ILE:HG12	2.03	0.40
1:B:61:LEU:O	1:B:62:PRO:C	2.64	0.40
1:A:488:ARG:HH11	1:A:510:ARG:CB	2.23	0.40
1:B:370:ALA:HB1	1:B:403:MET:HE2	2.03	0.40
1:D:315:GLU:CG	1:D:336:ALA:HB3	2.48	0.40
1:D:337:ARG:NH2	1:D:390:ASP:OD1	2.54	0.40
1:A:297:VAL:HG12	1:A:310:ILE:HD13	2.04	0.40
1:A:317:HIS:HE2	1:C:79:ASP:CG	2.30	0.40
1:A:465:LYS:HE3	1:B:448:SER:CB	2.51	0.40
1:D:188:ASP:HA	1:D:189:PRO:HD3	1.83	0.40
1:D:217:ILE:HB	1:D:226:LEU:HB2	2.02	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:HIS:CE1	1:B:322:ARG:NH1[1_655]	1.57	0.63
1:A:306:HIS:CE1	1:B:322:ARG:NH2[1_655]	1.63	0.57
1:A:306:HIS:NE2	1:B:322:ARG:NH1[1_655]	1.65	0.55
1:A:306:HIS:CE1	1:B:322:ARG:CZ[1_655]	1.67	0.53
1:A:306:HIS:NE2	1:B:322:ARG:CZ[1_655]	2.09	0.11
1:C:258:GLN:NE2	1:D:298:ARG:O[1_556]	2.17	0.03
1:A:306:HIS:ND1	1:B:322:ARG:NH2[1_655]	2.19	0.01

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	515/528 (98%)	476 (92%)	35 (7%)	4 (1%)	16	29
1	B	483/528 (92%)	452 (94%)	25 (5%)	6 (1%)	10	19
1	C	515/528 (98%)	482 (94%)	28 (5%)	5 (1%)	12	22
1	D	508/528 (96%)	479 (94%)	26 (5%)	3 (1%)	21	36
All	All	2021/2112 (96%)	1889 (94%)	114 (6%)	18 (1%)	14	26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	B	83	VAL
1	C	83	VAL
1	D	83	VAL
1	A	566	ASN
1	C	447	LEU
1	C	566	ASN
1	A	371	THR
1	B	447	LEU
1	B	566	ASN
1	D	371	THR

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Mol	Chain	Res	Type
1	D	566	ASN
1	B	84	ALA
1	B	371	THR
1	C	371	THR
1	A	486	ARG
1	C	170	GLY
1	B	213	VAL

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	414/423 (98%)	367 (89%)	47 (11%)	5	10
1	B	394/423 (93%)	342 (87%)	52 (13%)	4	6
1	C	414/423 (98%)	363 (88%)	51 (12%)	4	8
1	D	411/423 (97%)	362 (88%)	49 (12%)	5	9
All	All	1633/1692 (96%)	1434 (88%)	199 (12%)	5	8

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	83	VAL
1	A	99	ARG
1	A	103	ARG
1	A	104	LEU
1	A	120	SER
1	A	157	THR
1	A	177	LEU
1	A	182	GLN
1	A	194	ARG
1	A	200	VAL
1	A	202	VAL
1	A	209	ARG
1	A	221	ASP

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Mol	Chain	Res	Type
1	A	227	VAL
1	A	231	ILE
1	A	234	GLU
1	A	264	LEU
1	A	289	ARG
1	A	294	VAL
1	A	298	ARG
1	A	304	GLU
1	A	310	ILE
1	A	327	LEU
1	A	329	VAL
1	A	337	ARG
1	A	359	ARG
1	A	362	LEU
1	A	374	LEU
1	A	379	THR
1	A	388	THR
1	A	389	SER
1	A	396	LEU
1	A	410	LYS
1	A	443	ARG
1	A	473	VAL
1	A	480	SER
1	A	486	ARG
1	A	506	VAL
1	A	508	LEU
1	A	539	SER
1	A	542	LEU
1	A	546	LEU
1	A	547	ARG
1	A	548	VAL
1	A	552	VAL
1	A	559	ARG
1	B	61	LEU
1	B	83	VAL
1	B	103	ARG
1	B	104	LEU
1	B	120	SER
1	B	124	HIS
1	B	144	SER
1	B	157	THR
1	B	175	VAL

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Mol	Chain	Res	Type
1	B	176	GLU
1	B	177	LEU
1	B	182	GLN
1	B	202	VAL
1	B	207	ILE
1	B	210	VAL
1	B	258	GLN
1	B	260	ASP
1	B	264	LEU
1	B	289	ARG
1	B	294	VAL
1	B	298	ARG
1	B	301	LEU
1	B	304	GLU
1	B	310	ILE
1	B	327	LEU
1	B	329	VAL
1	B	337	ARG
1	B	359	ARG
1	B	362	LEU
1	B	374	LEU
1	B	379	THR
1	B	388	THR
1	B	389	SER
1	B	396	LEU
1	B	410	LYS
1	B	443	ARG
1	B	453	GLU
1	B	473	VAL
1	B	480	SER
1	B	485	SER
1	B	486	ARG
1	B	506	VAL
1	B	508	LEU
1	B	534	GLN
1	B	539	SER
1	B	542	LEU
1	B	546	LEU
1	B	547	ARG
1	B	548	VAL
1	B	552	VAL
1	B	559	ARG

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Mol	Chain	Res	Type
1	B	562	SER
1	C	61	LEU
1	C	83	VAL
1	C	103	ARG
1	C	104	LEU
1	C	120	SER
1	C	124	HIS
1	C	147	SER
1	C	157	THR
1	C	158	LYS
1	C	167	LEU
1	C	175	VAL
1	C	176	GLU
1	C	177	LEU
1	C	182	GLN
1	C	193	THR
1	C	200	VAL
1	C	202	VAL
1	C	209	ARG
1	C	210	VAL
1	C	229	GLN
1	C	231	ILE
1	C	234	GLU
1	C	264	LEU
1	C	289	ARG
1	C	294	VAL
1	C	298	ARG
1	C	304	GLU
1	C	327	LEU
1	C	329	VAL
1	C	337	ARG
1	C	359	ARG
1	C	362	LEU
1	C	374	LEU
1	C	379	THR
1	C	388	THR
1	C	389	SER
1	C	396	LEU
1	C	410	LYS
1	C	473	VAL
1	C	480	SER
1	C	486	ARG

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Mol	Chain	Res	Type
1	C	506	VAL
1	C	508	LEU
1	C	534	GLN
1	C	539	SER
1	C	542	LEU
1	C	546	LEU
1	C	547	ARG
1	C	548	VAL
1	C	552	VAL
1	C	559	ARG
1	D	61	LEU
1	D	83	VAL
1	D	86	ARG
1	D	103	ARG
1	D	104	LEU
1	D	120	SER
1	D	157	THR
1	D	175	VAL
1	D	176	GLU
1	D	177	LEU
1	D	182	GLN
1	D	188	ASP
1	D	200	VAL
1	D	202	VAL
1	D	210	VAL
1	D	225	SER
1	D	231	ILE
1	D	234	GLU
1	D	258	GLN
1	D	264	LEU
1	D	289	ARG
1	D	294	VAL
1	D	298	ARG
1	D	304	GLU
1	D	310	ILE
1	D	327	LEU
1	D	329	VAL
1	D	337	ARG
1	D	359	ARG
1	D	362	LEU
1	D	374	LEU
1	D	379	THR

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Mol	Chain	Res	Type
1	D	388	THR
1	D	389	SER
1	D	396	LEU
1	D	410	LYS
1	D	473	VAL
1	D	480	SER
1	D	486	ARG
1	D	506	VAL
1	D	508	LEU
1	D	539	SER
1	D	542	LEU
1	D	546	LEU
1	D	547	ARG
1	D	548	VAL
1	D	552	VAL
1	D	559	ARG
1	D	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	133	ASN
1	A	168	GLN
1	A	198	ASN
1	A	229	GLN
1	A	253	ASN
1	A	267	GLN
1	A	421	GLN
1	B	124	HIS
1	B	133	ASN
1	B	198	ASN
1	B	258	GLN
1	B	421	GLN
1	B	436	GLN
1	B	534	GLN
1	C	124	HIS
1	C	133	ASN
1	C	229	GLN
1	C	421	GLN
1	C	534	GLN
1	D	124	HIS

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Mol	Chain	Res	Type
1	D	133	ASN
1	D	182	GLN
1	D	229	GLN
1	D	242	ASN
1	D	253	ASN
1	D	258	GLN
1	D	421	GLN

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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
3	PGA	B	581	5,4	8,8,8	1.17	1 (12%)	10,11,11	1.08	0
2	FBP	B	580	-	18,20,20	1.01	1 (5%)	21,32,32	0.78	0
3	PGA	C	581	5,4	8,8,8	1.43	1 (12%)	10,11,11	1.51	1 (10%)
3	PGA	A	581	5,4	8,8,8	1.37	1 (12%)	10,11,11	1.30	1 (10%)
2	FBP	D	580	-	18,20,20	1.07	1 (5%)	21,32,32	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGA	D	581	5,4	8,8,8	1.12	1 (12%)	10,11,11	0.98	0
2	FBP	C	580	-	18,20,20	1.18	1 (5%)	21,32,32	0.85	0
2	FBP	A	580	-	18,20,20	1.07	1 (5%)	21,32,32	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGA	B	581	5,4	-	3/6/6/6	-
2	FBP	B	580	-	-	3/13/32/32	0/1/1/1
3	PGA	C	581	5,4	-	3/6/6/6	-
3	PGA	A	581	5,4	-	4/6/6/6	-
2	FBP	D	580	-	-	6/13/32/32	0/1/1/1
3	PGA	D	581	5,4	-	3/6/6/6	-
2	FBP	C	580	-	-	6/13/32/32	0/1/1/1
2	FBP	A	580	-	-	3/13/32/32	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	581	PGA	O1P-C2	-3.09	1.40	1.43
3	A	581	PGA	O1P-C2	-2.86	1.40	1.43
2	A	580	FBP	O2-C2	2.63	1.45	1.40
3	D	581	PGA	O1P-C2	-2.46	1.40	1.43
2	D	580	FBP	O2-C2	2.42	1.44	1.40
2	B	580	FBP	O2-C2	2.30	1.44	1.40
3	B	581	PGA	O1P-C2	-2.21	1.41	1.43
2	C	580	FBP	O2-C2	2.07	1.44	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	581	PGA	O1P-C2-C1	-3.74	104.90	110.54
3	A	581	PGA	O1P-C2-C1	-2.86	106.22	110.54

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	580	FBP	C1-O1-P1-O3P
2	C	580	FBP	C6-O6-P2-O5P
2	C	580	FBP	C6-O6-P2-O6P
2	D	580	FBP	C1-O1-P1-O3P
2	D	580	FBP	C6-O6-P2-O4P
2	D	580	FBP	C6-O6-P2-O5P
2	D	580	FBP	C6-O6-P2-O6P
3	A	581	PGA	C2-O1P-P-O2P
3	A	581	PGA	C2-O1P-P-O3P
3	A	581	PGA	C2-O1P-P-O4P
3	B	581	PGA	C2-O1P-P-O2P
3	B	581	PGA	C2-O1P-P-O3P
3	B	581	PGA	C2-O1P-P-O4P
3	C	581	PGA	C2-O1P-P-O2P
3	C	581	PGA	C2-O1P-P-O3P
3	C	581	PGA	C2-O1P-P-O4P
3	D	581	PGA	C2-O1P-P-O3P
3	D	581	PGA	C2-O1P-P-O4P
2	D	580	FBP	O5-C5-C6-O6
2	A	580	FBP	O5-C5-C6-O6
2	C	580	FBP	O5-C5-C6-O6
2	D	580	FBP	C4-C5-C6-O6
2	A	580	FBP	C4-C5-C6-O6
2	C	580	FBP	C4-C5-C6-O6
2	C	580	FBP	C6-O6-P2-O4P
3	D	581	PGA	C2-O1P-P-O2P
2	B	580	FBP	C6-O6-P2-O4P
2	C	580	FBP	C1-O1-P1-O1P
2	B	580	FBP	O5-C5-C6-O6
2	B	580	FBP	C4-C5-C6-O6
3	A	581	PGA	O1-C1-C2-O1P

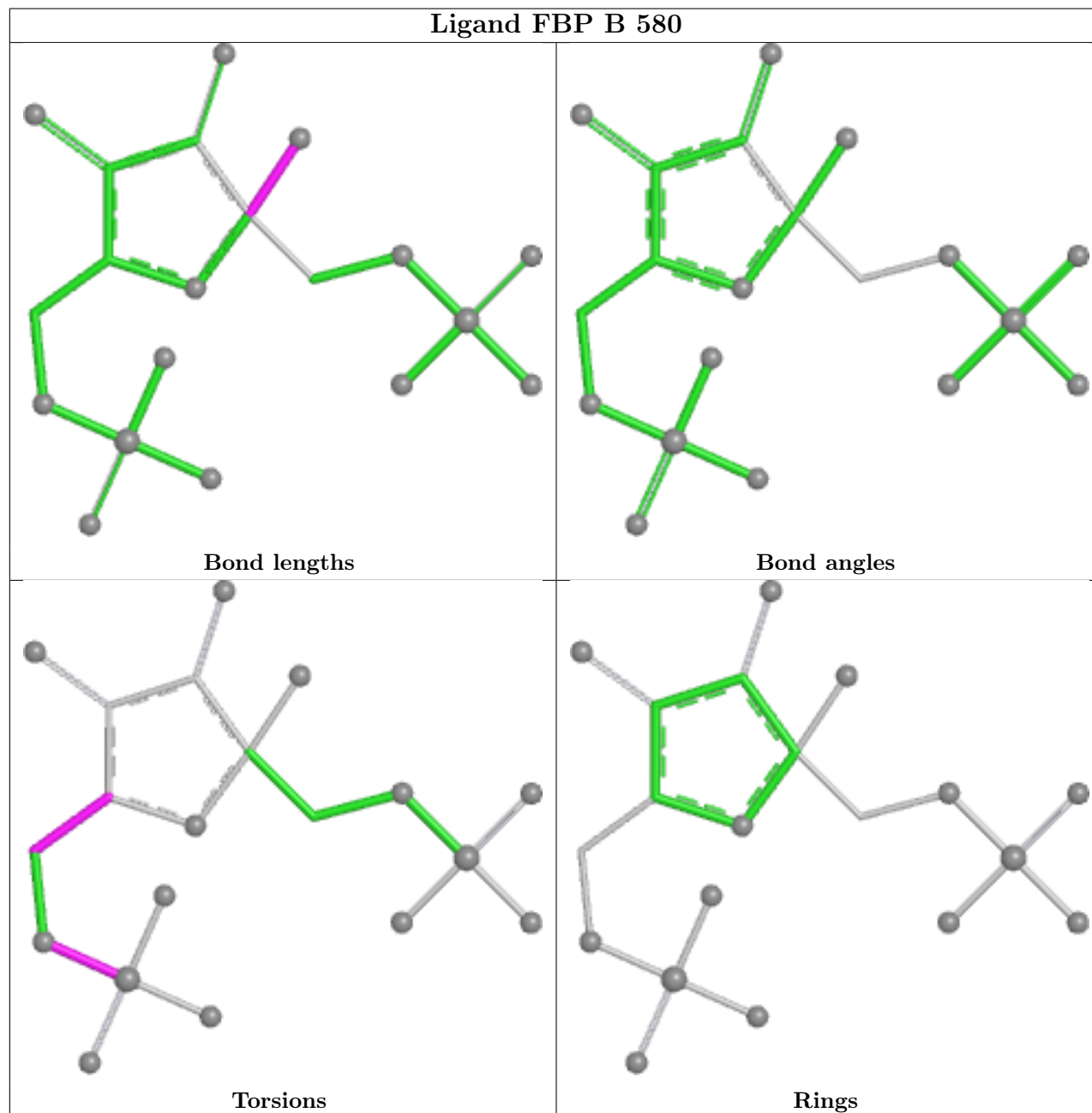
There are no ring outliers.

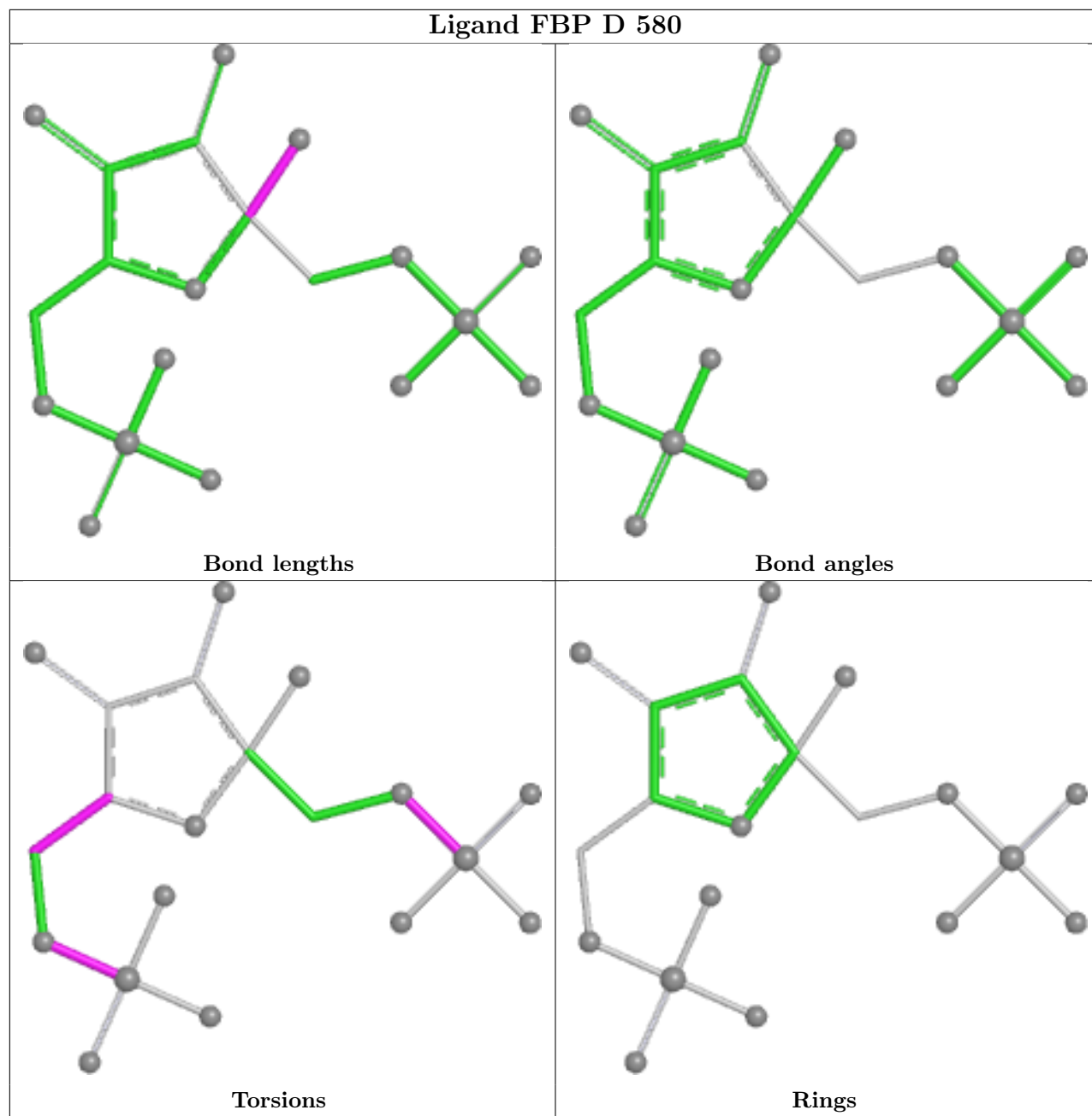
4 monomers are involved in 8 short contacts:

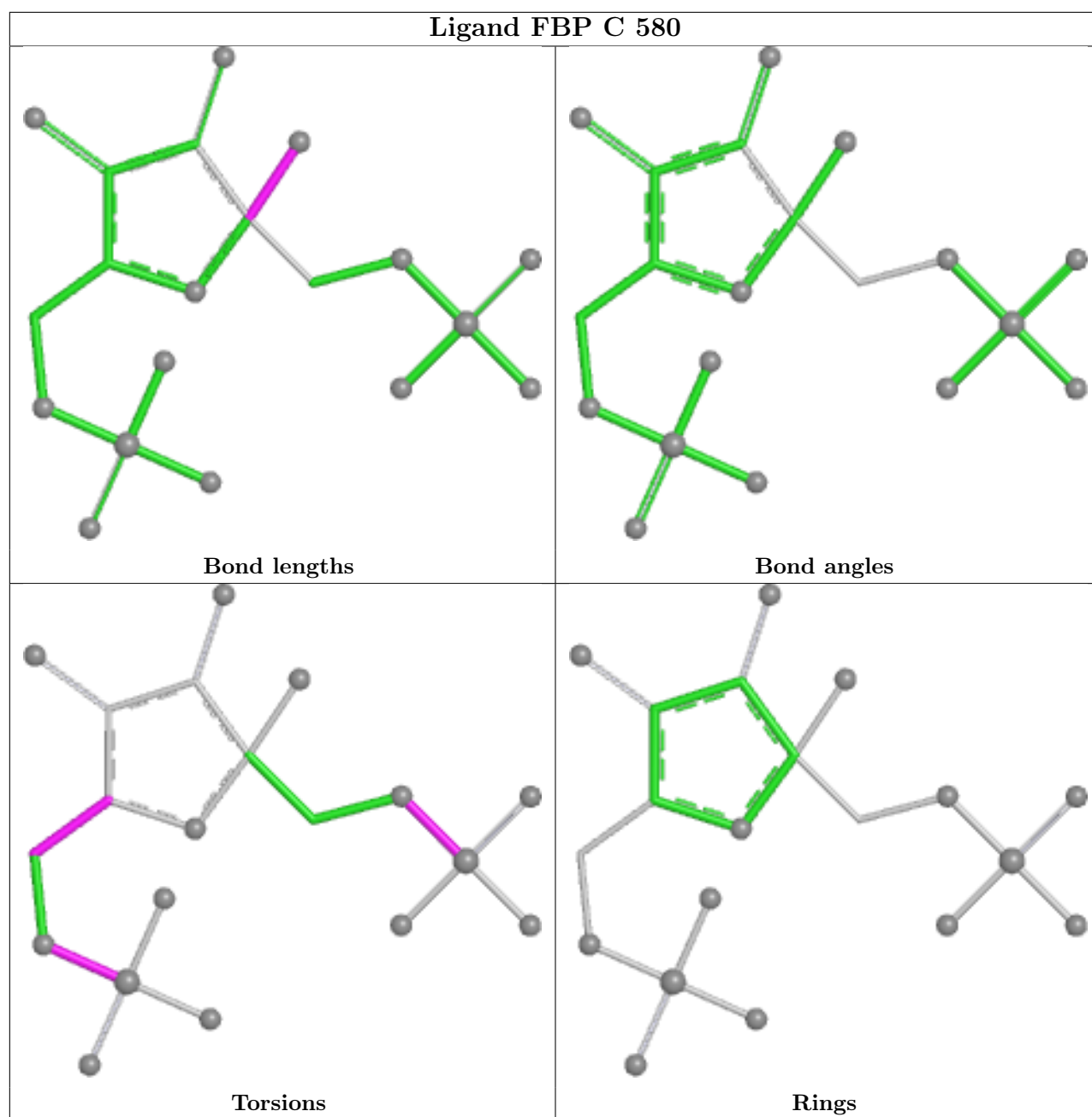
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	580	FBP	3	0
2	D	580	FBP	2	0
2	C	580	FBP	2	0
2	A	580	FBP	1	0

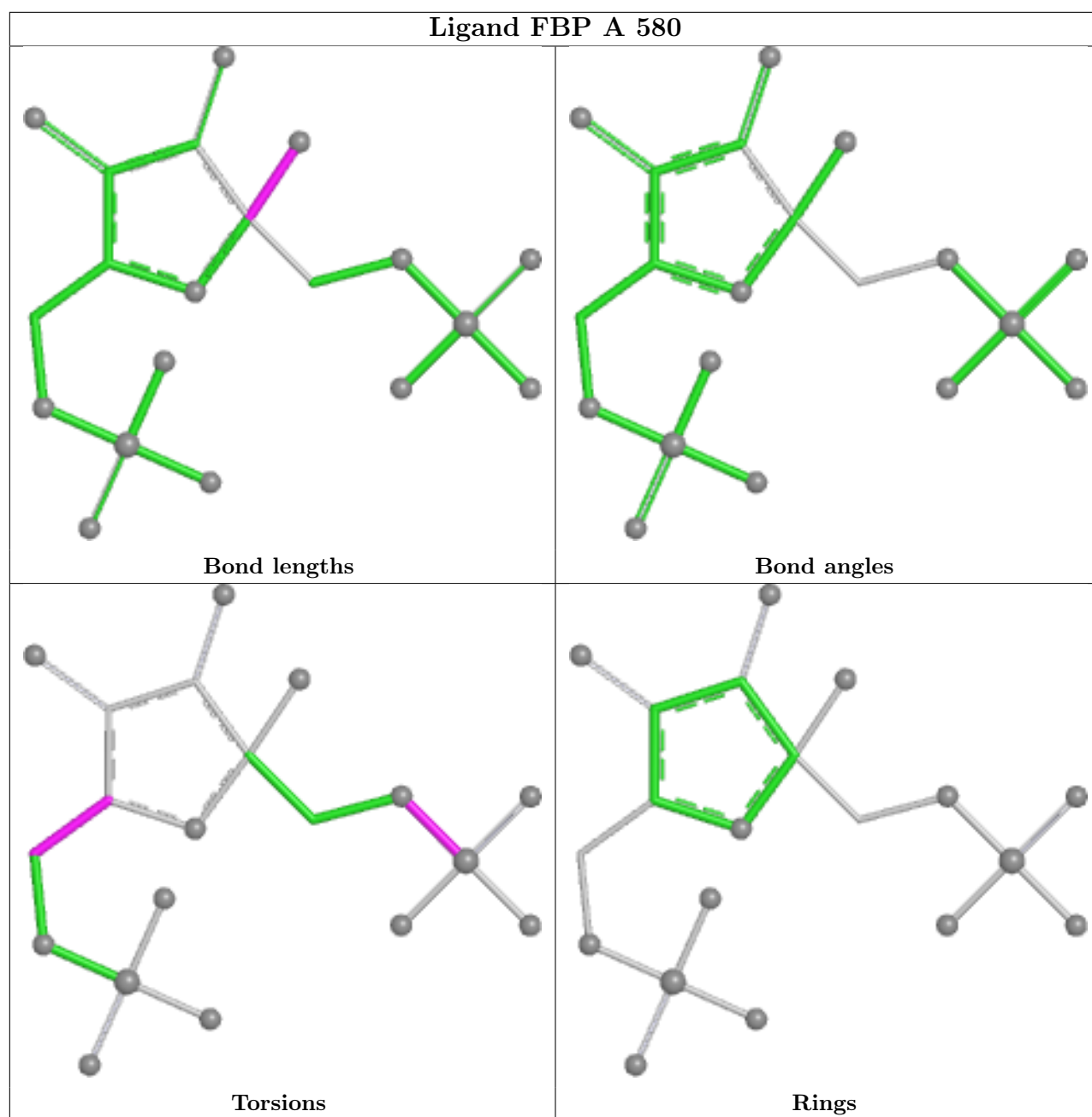
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

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	517/528 (97%)	0.24	10 (1%) 66 63	33, 40, 47, 57	0
1	B	491/528 (92%)	0.30	20 (4%) 41 40	33, 39, 47, 57	0
1	C	517/528 (97%)	-0.08	2 (0%) 88 89	33, 40, 47, 57	0
1	D	512/528 (96%)	-0.03	7 (1%) 73 72	33, 40, 47, 57	0
All	All	2037/2112 (96%)	0.11	39 (1%) 66 63	33, 40, 47, 57	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	GLY	7.1
1	A	303	PRO	3.7
1	A	302	GLY	3.5
1	B	142	ALA	3.5
1	B	258	GLN	3.5
1	A	223	LEU	2.9
1	B	120	SER	2.9
1	B	166	ILE	2.8
1	D	549	GLY	2.7
1	B	83	VAL	2.7
1	B	66	ALA	2.7
1	A	307	GLY	2.6
1	A	561	GLY	2.6
1	D	261	LEU	2.4
1	A	520	PRO	2.4
1	B	57	GLN	2.4
1	C	304	GLU	2.4
1	B	254	LEU	2.3
1	B	213	VAL	2.3
1	A	59	GLN	2.3
1	B	306	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	262	PRO	2.2
1	C	122	GLY	2.2
1	A	261	LEU	2.2
1	D	59	GLN	2.2
1	B	561	GLY	2.2
1	B	558	TRP	2.2
1	D	61	LEU	2.2
1	B	221	ASP	2.2
1	B	257	ALA	2.1
1	D	531	ARG	2.1
1	A	231	ILE	2.1
1	D	548	VAL	2.1
1	B	216	ARG	2.1
1	D	84	ALA	2.1
1	A	222	GLY	2.0
1	B	209	ARG	2.0
1	B	549	GLY	2.0
1	B	208	VAL	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(Å ²)	Q<0.9
3	PGA	A	581	9/9	0.86	0.20	104,106,107,108	0
4	K	B	586	1/1	0.86	0.09	81,81,81,81	0
3	PGA	C	581	9/9	0.89	0.23	103,105,107,108	0
2	FBP	B	580	20/20	0.90	0.12	71,75,77,78	0
3	PGA	B	581	9/9	0.90	0.17	104,106,108,108	0

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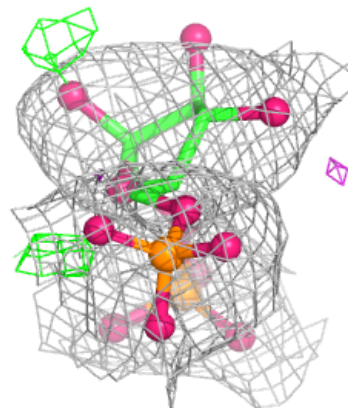
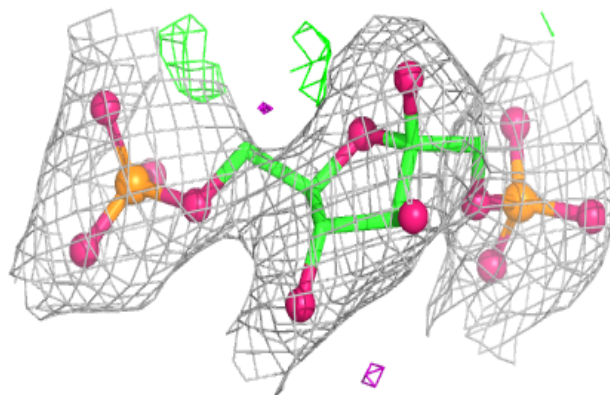
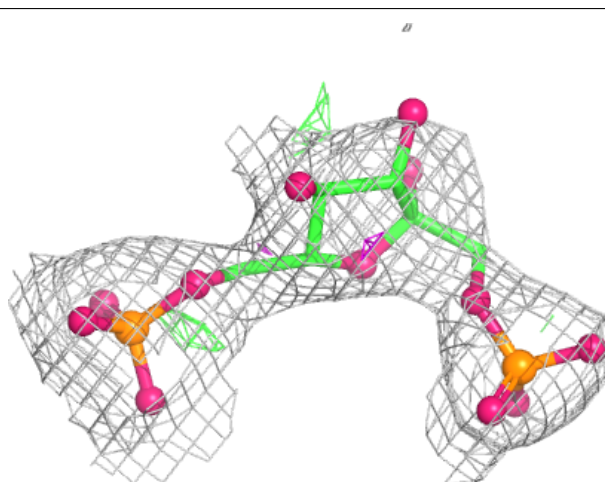
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FBP	D	580	20/20	0.91	0.14	69,73,76,77	0
3	PGA	D	581	9/9	0.92	0.19	103,106,107,108	0
2	FBP	A	580	20/20	0.92	0.11	70,75,77,78	0
4	K	A	582	1/1	0.93	0.06	78,78,78,78	0
2	FBP	C	580	20/20	0.95	0.10	68,73,76,77	0
4	K	C	590	1/1	0.95	0.07	67,67,67,67	0
4	K	D	594	1/1	0.96	0.05	60,60,60,60	0
5	MN	A	583	1/1	0.97	0.05	70,70,70,70	0
5	MN	D	595	1/1	0.97	0.04	59,59,59,59	0
5	MN	B	587	1/1	0.98	0.03	64,64,64,64	0
5	MN	C	591	1/1	0.99	0.04	58,58,58,58	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.

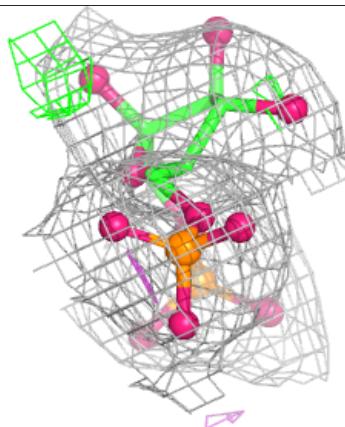
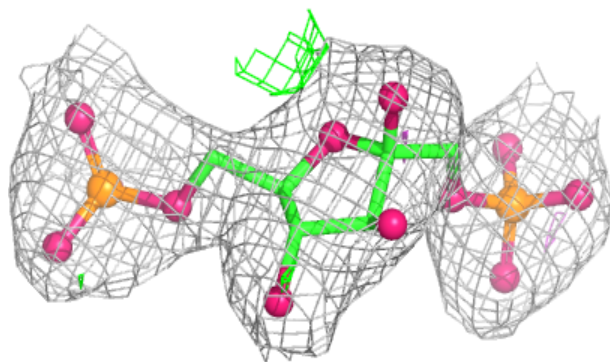
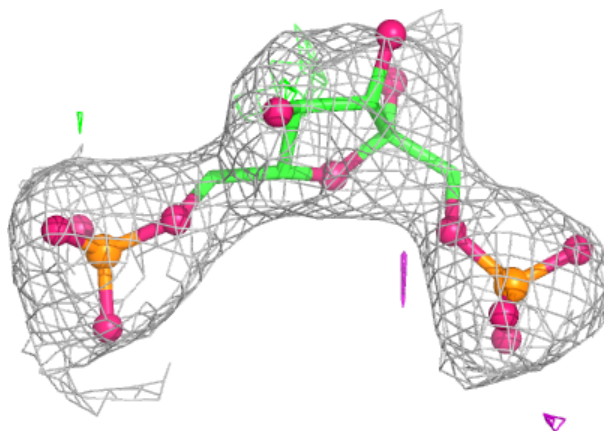
Electron density around FBP B 580:

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

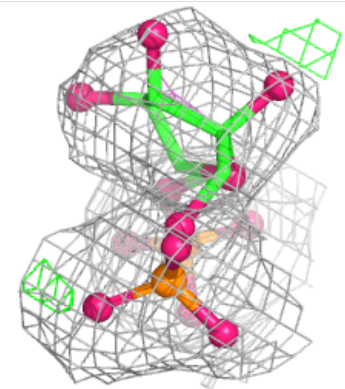
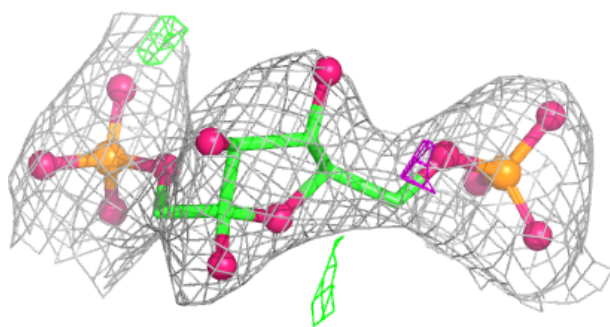
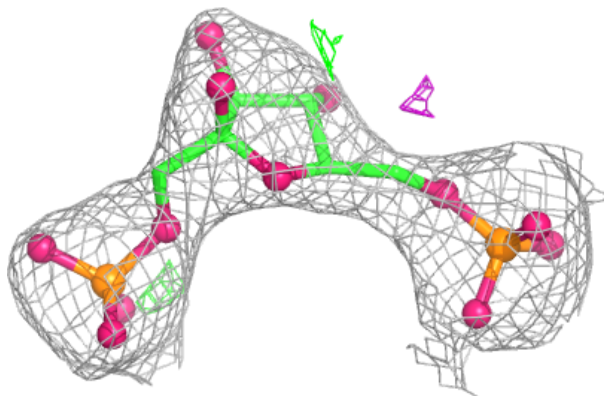


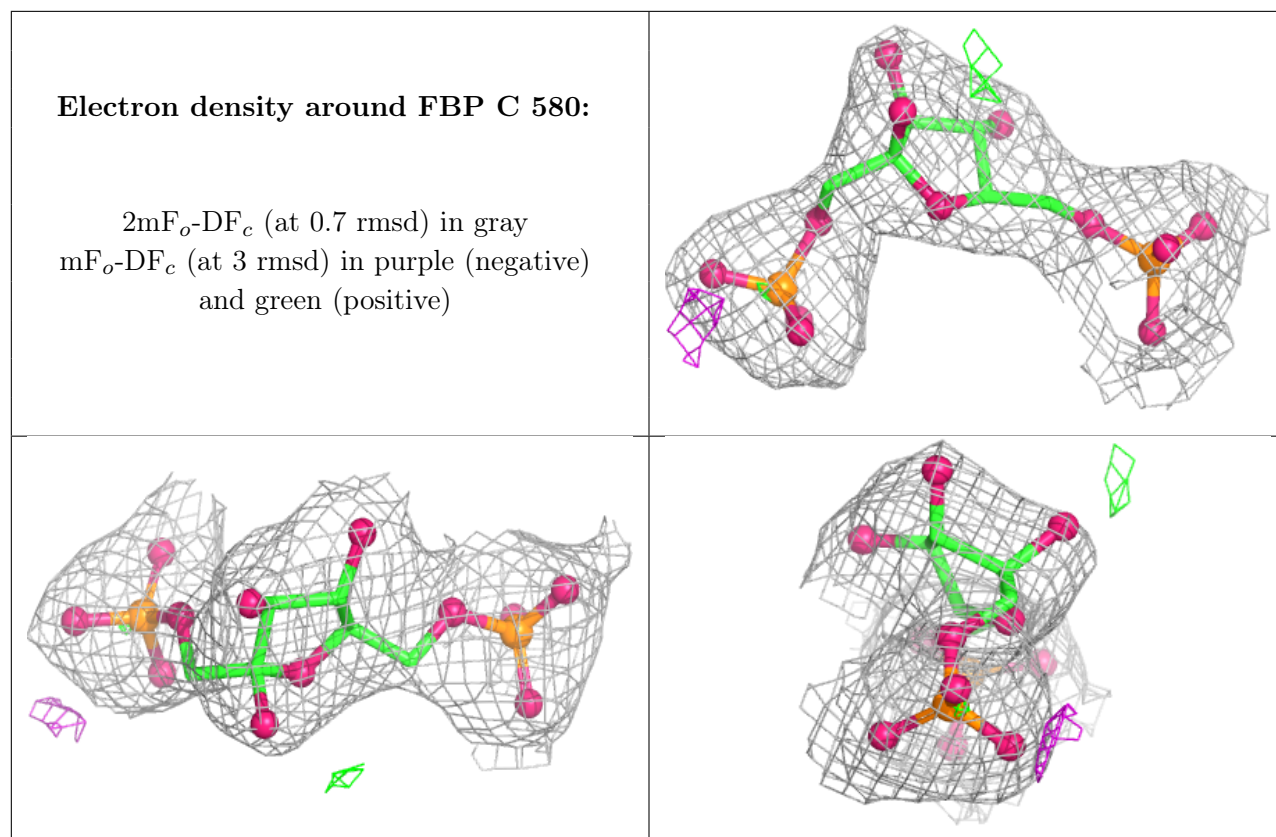
Electron density around FBP D 580:

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

**Electron density around FBP A 580:**

$2mF_o-DF_c$ (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.