



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:19 AM UTC

PDB ID : 2VGG / pdb_00002vgg
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE: R479H MUTANT
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Deposited on : 2007-11-13
Resolution : 2.74 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

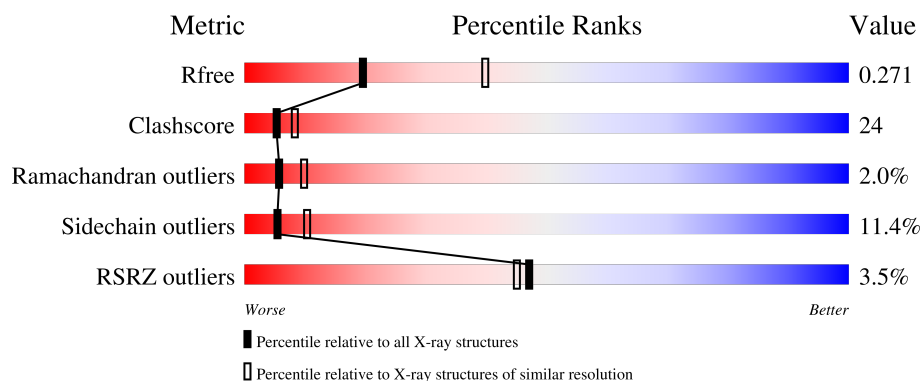
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	 4% 53% 34% 7% • •
1	B	528	 3% 51% 33% 7% • 9%
1	C	528	 4% 50% 39% 7% • •
1	D	528	 2% 49% 37% 8% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FBP	B	580	-	-	X	-
3	PGA	A	581	-	X	-	-
3	PGA	B	581	-	-	X	-
3	PGA	C	581	-	X	-	-
3	PGA	D	581	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15305 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.

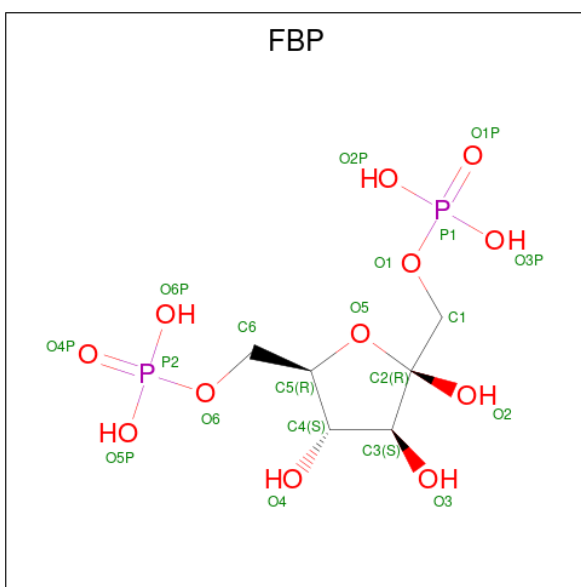
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3827	2404	692	713	18			
1	B	483	Total	C	N	O	S	0	0	0
			3666	2307	663	679	17			
1	C	514	Total	C	N	O	S	0	0	0
			3889	2444	704	724	17			
1	D	501	Total	C	N	O	S	0	0	0
			3799	2392	687	703	17			

There are 4 discrepancies between the modelled and reference sequences:

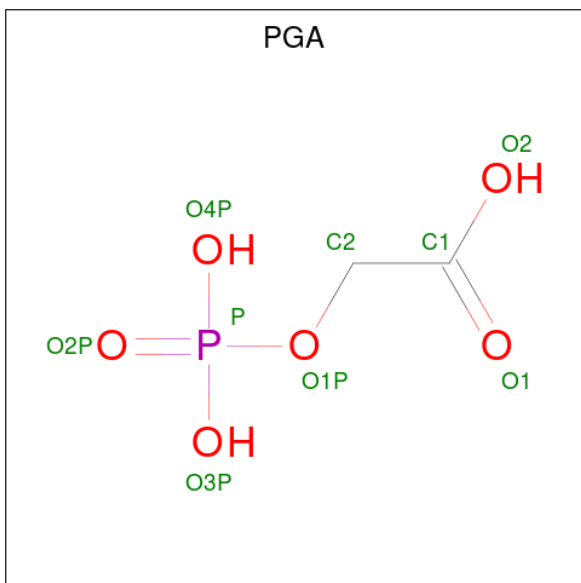
Chain	Residue	Modelled	Actual	Comment	Reference
A	479	HIS	ARG	engineered mutation	UNP P30613
B	479	HIS	ARG	engineered mutation	UNP P30613
C	479	HIS	ARG	engineered mutation	UNP P30613
D	479	HIS	ARG	engineered mutation	UNP P30613

- 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		
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 9 2 6 1	0	0
3	B	1	Total C O P 9 2 6 1	0	0
3	C	1	Total C O P 9 2 6 1	0	0
3	D	1	Total C O P 9 2 6 1	0	0

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

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

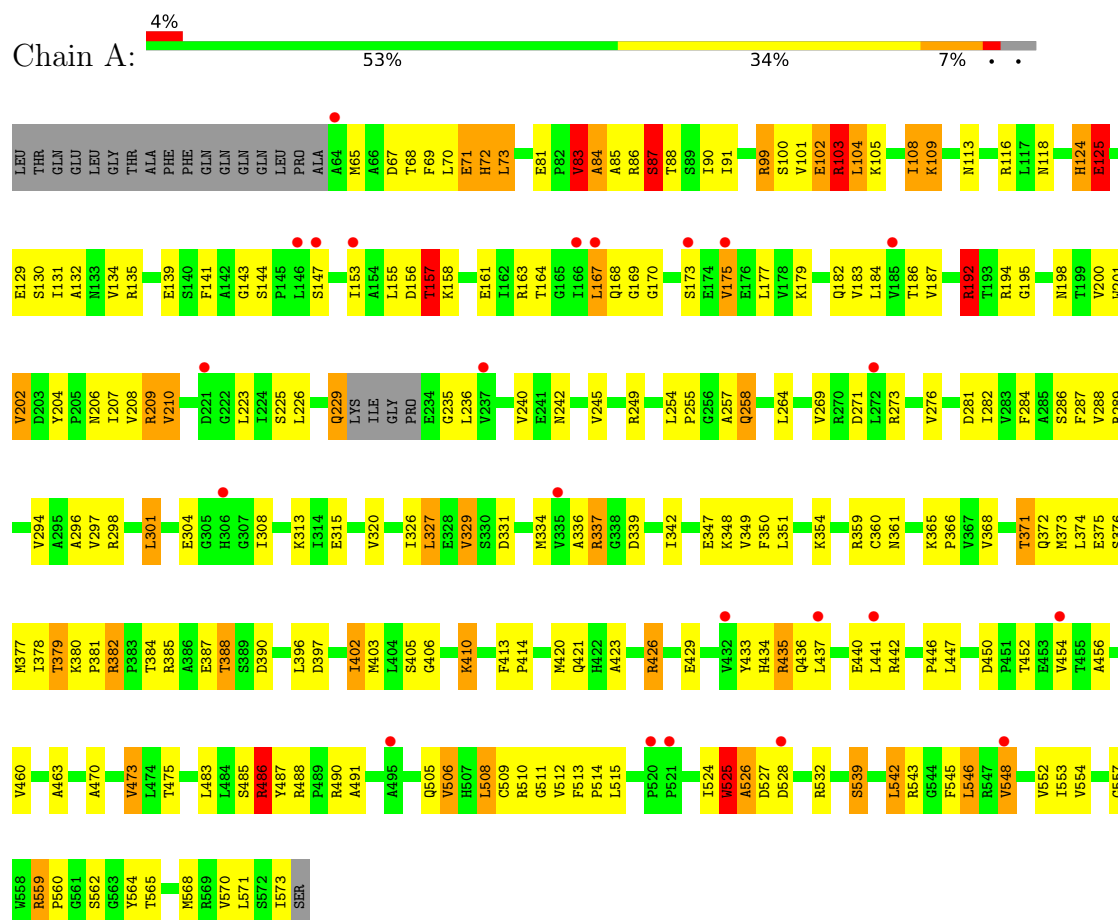
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

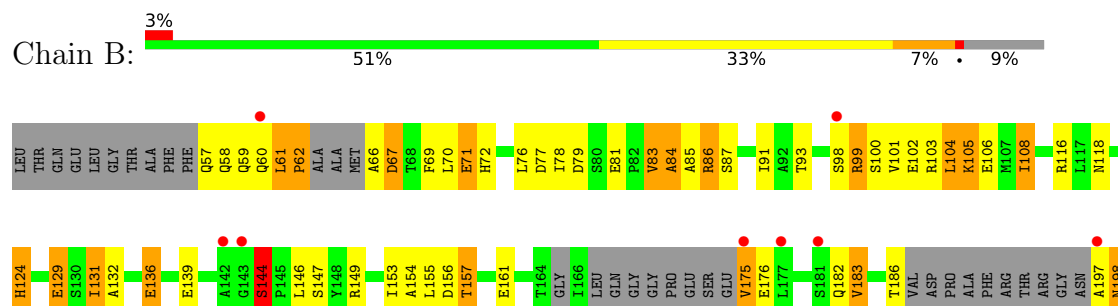
3 Residue-property plots

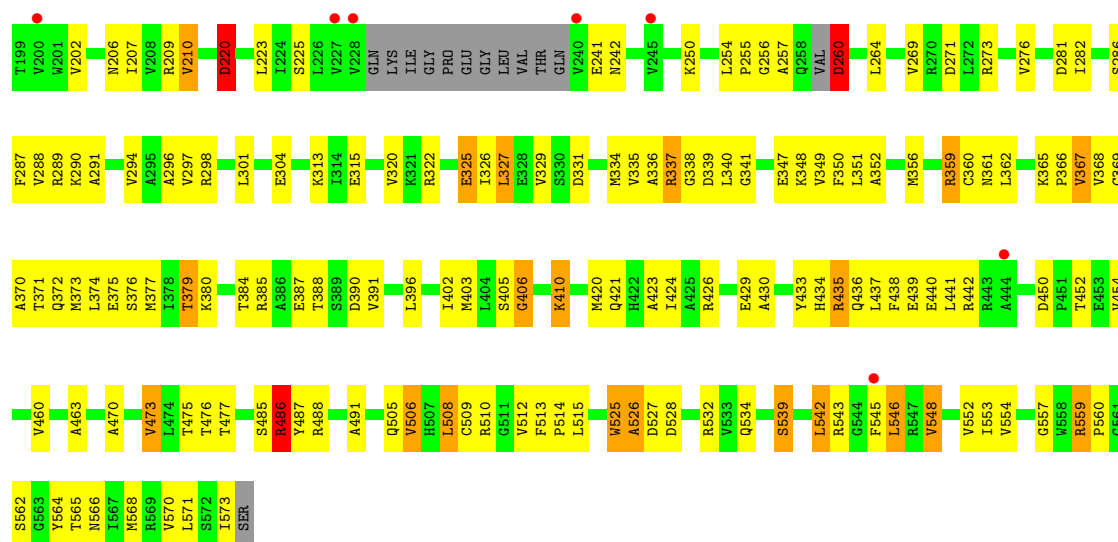
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PYRUVATE KINASE ISOZYMES R/L

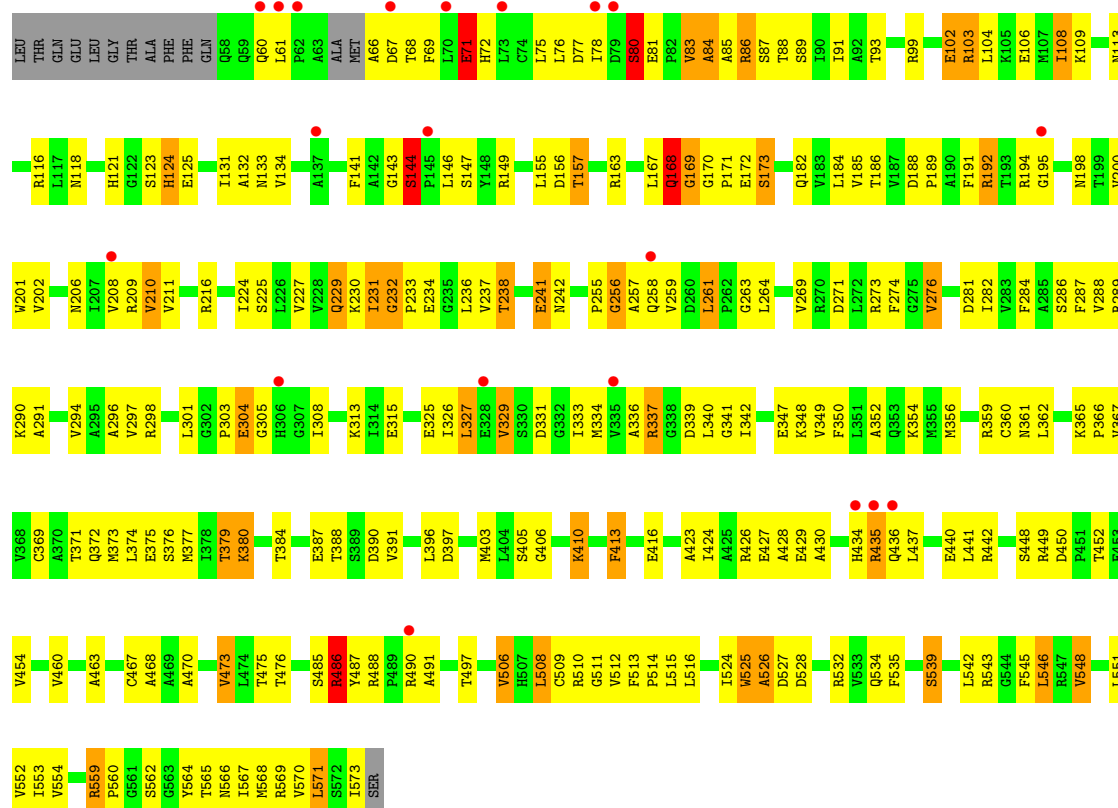


• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



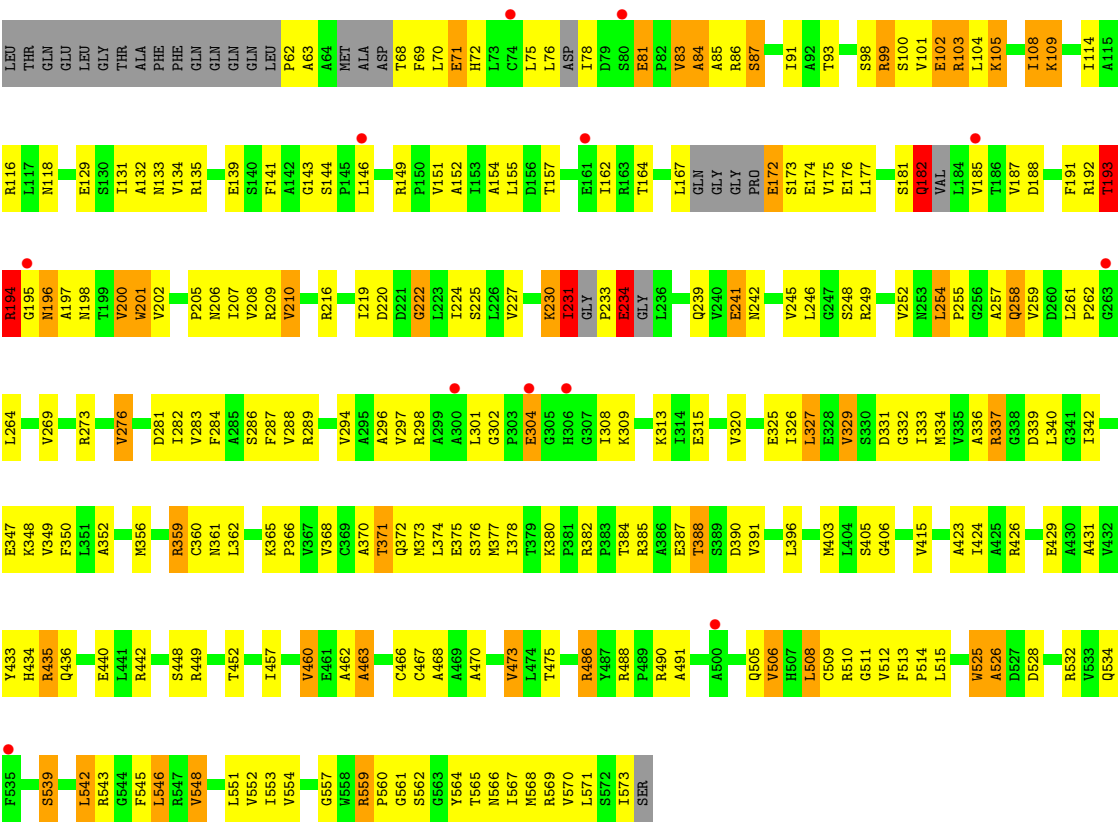


• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



• Molecule 1: PYRUVATE KINASE ISOZYMES R/L





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.04Å 171.79Å 85.09Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.74 20.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	92.6 (20.00-2.74) 92.4 (20.00-2.74)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.253 , 0.294 0.238 , 0.271	Depositor DCC
R_{free} test set	792 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15305	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.33	32/3889 (0.8%)	1.25	26/5271 (0.5%)
1	B	1.25	24/3721 (0.6%)	1.23	17/5036 (0.3%)
1	C	1.35	33/3953 (0.8%)	1.27	26/5359 (0.5%)
1	D	1.45	40/3857 (1.0%)	1.29	29/5219 (0.6%)
All	All	1.35	129/15420 (0.8%)	1.26	98/20885 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
All	All	0	5

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	GLU	CD-OE1	26.20	1.75	1.25
1	D	182	GLN	C-O	21.08	1.65	1.23
1	B	198	ASN	CG-OD1	-20.05	0.85	1.23
1	A	103	ARG	CZ-NH2	-19.19	1.08	1.33
1	A	382	ARG	CZ-NH2	19.04	1.58	1.33
1	B	144	SER	CB-OG	17.99	1.78	1.42
1	D	230	LYS	CE-NZ	17.07	2.00	1.49
1	D	194	ARG	CZ-NH1	-16.61	1.09	1.32
1	D	231	ILE	C-O	16.04	1.55	1.23
1	A	382	ARG	NE-CZ	-15.95	1.15	1.33
1	C	124	HIS	CE1-NE2	14.84	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	260	ASP	N-CA	14.46	1.73	1.46
1	D	382	ARG	CZ-NH2	14.04	1.51	1.33
1	C	144	SER	CB-OG	13.72	1.69	1.42
1	B	198	ASN	CG-ND2	13.66	1.61	1.33
1	D	109	LYS	CD-CE	13.55	1.93	1.52
1	D	382	ARG	NE-CZ	13.52	1.48	1.33
1	A	102	GLU	CG-CD	12.66	1.83	1.52
1	C	102	GLU	CD-OE1	11.94	1.48	1.25
1	A	103	ARG	NE-CZ	11.49	1.45	1.33
1	A	382	ARG	CD-NE	11.41	1.62	1.46
1	A	169	GLY	C-N	11.23	1.50	1.33
1	A	192	ARG	CZ-NH1	11.06	1.48	1.32
1	A	229	GLN	CD-NE2	10.98	1.56	1.33
1	B	176	GLU	CD-OE1	10.88	1.46	1.25
1	D	181	SER	C-O	10.86	1.36	1.23
1	D	149	ARG	CZ-NH2	10.62	1.47	1.33
1	C	124	HIS	CG-ND1	10.48	1.49	1.38
1	D	102	GLU	CD-OE2	10.44	1.45	1.25
1	A	426	ARG	CZ-NH1	10.34	1.47	1.32
1	D	233	PRO	N-CA	10.28	1.62	1.47
1	C	192	ARG	CZ-NH1	10.19	1.47	1.32
1	A	258	GLN	CD-NE2	10.13	1.54	1.33
1	A	258	GLN	CD-OE1	9.98	1.42	1.23
1	C	80	SER	CB-OG	9.85	1.61	1.42
1	D	234	GLU	CD-OE1	9.43	1.43	1.25
1	C	103	ARG	CZ-NH1	9.33	1.45	1.32
1	D	194	ARG	NE-CZ	9.29	1.43	1.33
1	C	103	ARG	NE-CZ	9.24	1.43	1.33
1	B	147	SER	CB-OG	9.13	1.60	1.42
1	C	123	SER	CB-OG	9.07	1.60	1.42
1	A	209	ARG	CZ-NH2	8.93	1.45	1.33
1	D	233	PRO	C-N	8.89	1.45	1.33
1	A	209	ARG	CZ-NH1	-8.73	1.20	1.32
1	D	71	GLU	CD-OE1	-8.60	1.09	1.25
1	A	158	LYS	CE-NZ	-8.53	1.23	1.49
1	A	103	ARG	CD-NE	8.44	1.58	1.46
1	B	67	ASP	CG-OD2	8.37	1.41	1.25
1	D	71	GLU	CD-OE2	8.31	1.41	1.25
1	A	109	LYS	CD-CE	8.28	1.77	1.52
1	B	124	HIS	CE1-NE2	-8.11	1.24	1.32
1	C	149	ARG	CZ-NH1	7.99	1.44	1.32
1	A	73	LEU	CG-CD2	7.94	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	GLN	CD-NE2	7.89	1.49	1.33
1	C	410	LYS	CE-NZ	7.80	1.72	1.49
1	D	181	SER	C-N	7.79	1.44	1.33
1	C	256	GLY	C-N	7.61	1.44	1.33
1	D	382	ARG	CZ-NH1	-7.59	1.22	1.32
1	D	105	LYS	CE-NZ	7.57	1.72	1.49
1	C	149	ARG	CZ-NH2	-7.57	1.23	1.33
1	C	169	GLY	C-O	-7.54	1.13	1.23
1	B	129	GLU	CD-OE2	-7.40	1.11	1.25
1	D	193	THR	CB-OG1	7.36	1.55	1.43
1	A	525	TRP	C-N	7.28	1.43	1.33
1	B	410	LYS	CD-CE	7.17	1.74	1.52
1	D	460	VAL	CA-CB	-7.16	1.46	1.54
1	C	216	ARG	CZ-NH1	7.06	1.42	1.32
1	B	124	HIS	CD2-NE2	7.04	1.45	1.37
1	B	139	GLU	CD-OE2	7.03	1.38	1.25
1	B	105	LYS	CE-NZ	6.97	1.70	1.49
1	D	241	GLU	CD-OE1	6.93	1.38	1.25
1	D	258	GLN	CD-NE2	6.87	1.47	1.33
1	B	367	VAL	CA-CB	-6.84	1.46	1.54
1	D	149	ARG	NE-CZ	6.81	1.40	1.33
1	A	130	SER	CB-OG	6.80	1.55	1.42
1	C	169	GLY	C-N	6.71	1.43	1.33
1	A	175	VAL	C-O	6.59	1.32	1.24
1	D	233	PRO	N-CD	6.55	1.56	1.47
1	C	168	GLN	CD-NE2	6.52	1.47	1.33
1	C	121	HIS	CE1-NE2	6.51	1.39	1.32
1	C	168	GLN	CD-OE1	6.50	1.35	1.23
1	C	241	GLU	C-O	6.43	1.32	1.24
1	A	124	HIS	CE1-NE2	6.37	1.39	1.32
1	A	209	ARG	CD-NE	6.35	1.55	1.46
1	A	410	LYS	CE-NZ	6.29	1.68	1.49
1	C	189	PRO	CG-CD	6.27	1.72	1.50
1	B	176	GLU	CG-CD	6.19	1.67	1.52
1	D	216	ARG	CZ-NH2	6.17	1.41	1.33
1	A	147	SER	CB-OG	6.16	1.54	1.42
1	C	71	GLU	CB-CG	6.14	1.70	1.52
1	A	71	GLU	CD-OE1	6.14	1.37	1.25
1	D	463	ALA	CA-CB	-6.14	1.43	1.53
1	C	256	GLY	C-O	6.08	1.32	1.23
1	B	153	ILE	CA-CB	-6.03	1.46	1.54
1	B	62	PRO	CG-CD	6.02	1.71	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	102	GLU	CD-OE2	6.00	1.36	1.25
1	C	216	ARG	NE-CZ	5.97	1.39	1.33
1	A	169	GLY	C-O	5.96	1.31	1.23
1	D	62	PRO	CG-CD	5.91	1.70	1.50
1	D	149	ARG	CZ-NH1	-5.90	1.24	1.32
1	D	233	PRO	CA-CB	5.87	1.65	1.53
1	D	230	LYS	CB-CG	5.87	1.70	1.52
1	A	525	TRP	C-O	5.86	1.31	1.24
1	C	106	GLU	CD-OE1	5.84	1.36	1.25
1	C	67	ASP	CG-OD2	5.84	1.36	1.25
1	D	175	VAL	C-O	5.83	1.30	1.24
1	B	61	LEU	C-O	5.82	1.30	1.24
1	C	258	GLN	CG-CD	5.79	1.66	1.52
1	D	258	GLN	CD-OE1	5.78	1.34	1.23
1	B	220	ASP	CG-OD2	5.73	1.36	1.25
1	A	102	GLU	CD-OE1	-5.68	1.14	1.25
1	D	231	ILE	CB-CG1	5.66	1.64	1.53
1	A	179	LYS	CE-NZ	5.61	1.66	1.49
1	B	71	GLU	CB-CG	5.60	1.69	1.52
1	A	72	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	154	ALA	CA-CB	-5.55	1.45	1.53
1	C	75	LEU	CG-CD2	-5.47	1.34	1.52
1	D	175	VAL	C-N	5.45	1.41	1.33
1	D	342	ILE	CA-CB	-5.43	1.47	1.54
1	D	234	GLU	CD-OE2	5.42	1.35	1.25
1	B	149	ARG	CZ-NH1	5.38	1.40	1.32
1	B	106	GLU	CD-OE2	5.25	1.35	1.25
1	D	173	SER	C-O	5.23	1.30	1.23
1	C	198	ASN	CG-OD1	5.22	1.33	1.23
1	C	241	GLU	CD-OE1	5.20	1.35	1.25
1	A	83	VAL	CB-CG2	5.17	1.69	1.52
1	D	216	ARG	CZ-NH1	5.15	1.40	1.32
1	B	136	GLU	CD-OE2	-5.08	1.15	1.25
1	C	125	GLU	CD-OE2	5.01	1.34	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	ARG	NE-CZ-NH2	18.72	136.04	119.20
1	B	198	ASN	OD1-CG-ND2	15.14	137.74	122.60
1	B	175	VAL	N-CA-CB	-11.07	92.68	111.50
1	B	198	ASN	CB-CG-ND2	-11.02	99.87	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ARG	NE-CZ-NH1	10.45	131.94	121.50
1	D	382	ARG	NH1-CZ-NH2	-9.62	106.79	119.30
1	A	102	GLU	CG-CD-OE2	8.40	137.71	118.40
1	B	473	VAL	CB-CA-C	-8.34	98.71	111.31
1	A	103	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	C	473	VAL	CB-CA-C	-8.08	99.11	111.31
1	A	169	GLY	CA-C-N	-8.06	109.21	121.87
1	A	169	GLY	C-N-CA	-8.06	109.21	121.87
1	B	144	SER	CA-CB-OG	-7.81	95.49	111.10
1	D	473	VAL	CB-CA-C	-7.80	100.52	111.21
1	D	216	ARG	NE-CZ-NH1	-7.75	113.75	121.50
1	D	359	ARG	NE-CZ-NH1	7.74	129.24	121.50
1	A	382	ARG	CD-NE-CZ	-7.69	113.64	124.40
1	C	232	GLY	CA-C-N	7.61	127.28	119.82
1	C	232	GLY	C-N-CA	7.61	127.28	119.82
1	A	258	GLN	OE1-CD-NE2	7.54	130.14	122.60
1	C	103	ARG	CD-NE-CZ	-7.53	113.86	124.40
1	B	131	ILE	N-CA-C	-7.22	103.81	110.82
1	B	71	GLU	CB-CG-CD	-7.22	100.33	112.60
1	D	149	ARG	NE-CZ-NH2	-7.13	112.79	119.20
1	A	473	VAL	CB-CA-C	-6.89	101.26	110.98
1	C	71	GLU	OE1-CD-OE2	-6.83	106.50	122.90
1	B	176	GLU	CB-CG-CD	-6.78	101.08	112.60
1	A	73	LEU	CD1-CG-CD2	-6.76	95.93	110.80
1	A	102	GLU	OE1-CD-OE2	-6.71	106.81	122.90
1	A	169	GLY	CA-C-O	6.69	132.21	120.57
1	C	149	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	B	335	VAL	CB-CA-C	-6.51	105.26	112.68
1	B	406	GLY	N-CA-C	-6.46	104.82	112.64
1	C	410	LYS	CB-CG-CD	-6.43	96.51	111.30
1	B	161	GLU	CB-CG-CD	-6.42	101.69	112.60
1	D	81	GLU	CG-CD-OE2	6.39	133.09	118.40
1	A	187	VAL	N-CA-C	-6.37	106.57	112.43
1	A	388	THR	N-CA-C	-6.34	104.29	111.07
1	C	80	SER	CA-CB-OG	-6.28	98.55	111.10
1	C	342	ILE	CB-CA-C	-6.15	105.65	111.06
1	A	158	LYS	CD-CE-NZ	6.13	131.53	111.90
1	D	276	VAL	CB-CA-C	-6.13	104.12	111.97
1	D	81	GLU	OE1-CD-OE2	-6.08	108.30	122.90
1	C	169	GLY	CA-C-O	6.08	131.14	120.57
1	D	382	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	147	SER	CB-CA-C	-6.00	99.46	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	ILE	N-CA-C	-5.91	104.87	110.42
1	D	194	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	A	490	ARG	N-CA-C	-5.82	105.28	112.90
1	D	382	ARG	CG-CD-NE	5.81	124.79	112.00
1	D	102	GLU	CB-CG-CD	5.80	122.46	112.60
1	D	378	ILE	N-CA-C	-5.80	103.84	111.09
1	D	162	ILE	N-CA-C	-5.79	99.42	108.86
1	C	261	LEU	CA-C-N	5.74	125.69	119.78
1	C	261	LEU	C-N-CA	5.74	125.69	119.78
1	D	196	ASN	N-CA-C	5.71	116.91	108.86
1	B	108	ILE	N-CA-C	-5.68	105.19	110.53
1	C	109	LYS	CD-CE-NZ	-5.62	93.93	111.90
1	D	201	TRP	N-CA-C	-5.60	100.76	109.72
1	A	103	ARG	CD-NE-CZ	-5.59	116.57	124.40
1	C	103	ARG	NH1-CZ-NH2	-5.59	112.03	119.30
1	B	61	LEU	O-C-N	5.57	124.78	120.38
1	C	103	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	D	231	ILE	CA-C-O	-5.53	111.39	120.80
1	C	229	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	C	413	PHE	CE1-CZ-CE2	-5.53	110.05	120.00
1	A	378	ILE	N-CA-C	-5.49	104.36	112.04
1	D	227	VAL	CB-CA-C	-5.48	103.47	110.98
1	A	426	ARG	NH1-CZ-NH2	-5.46	112.20	119.30
1	A	103	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	245	VAL	N-CA-C	5.38	116.10	107.98
1	A	382	ARG	CB-CG-CD	-5.36	98.97	111.30
1	D	222	GLY	N-CA-C	-5.36	107.85	115.30
1	B	260	ASP	N-CA-C	5.34	125.94	111.00
1	C	123	SER	CA-CB-OG	-5.34	100.43	111.10
1	C	211	VAL	N-CA-C	5.33	112.41	107.56
1	C	163	ARG	N-CA-C	5.31	117.46	109.23
1	A	153	ILE	N-CA-C	5.28	115.46	107.75
1	D	234	GLU	CG-CD-OE1	-5.28	106.26	118.40
1	C	490	ARG	N-CA-C	-5.27	106.00	112.90
1	A	342	ILE	CB-CA-C	-5.24	105.77	110.91
1	D	415	VAL	N-CA-C	-5.20	105.31	110.62
1	D	490	ARG	N-CA-C	-5.17	106.12	112.90
1	D	234	GLU	OE1-CD-OE2	5.16	135.29	122.90
1	D	302	GLY	CA-C-N	5.14	124.31	118.97
1	D	302	GLY	C-N-CA	5.14	124.31	118.97
1	D	370	ALA	N-CA-C	5.13	116.98	109.24
1	C	189	PRO	CB-CG-CD	-5.11	89.74	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ILE	N-CA-C	5.11	115.21	107.75
1	C	413	PHE	CZ-CE2-CD2	5.09	129.16	120.00
1	A	87	SER	CB-CA-C	5.08	118.19	109.15
1	D	460	VAL	CB-CA-C	-5.06	105.49	111.97
1	B	62	PRO	N-CD-CG	-5.06	95.61	103.20
1	C	276	VAL	CB-CA-C	-5.06	105.50	111.97
1	D	154	ALA	N-CA-C	5.05	116.64	108.41
1	B	154	ALA	N-CA-C	5.02	116.71	108.52
1	A	382	ARG	CG-CD-NE	-5.02	100.96	112.00
1	A	157	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	GLU	Sidechain
1	A	382	ARG	Sidechain
1	B	136	GLU	Sidechain
1	C	102	GLU	Sidechain
1	C	71	GLU	Sidechain

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	3827	0	3896	199	1
1	B	3666	0	3738	174	2
1	C	3889	0	3963	207	3
1	D	3799	0	3880	203	0
2	A	20	0	10	3	0
2	B	20	0	10	7	0
2	C	20	0	10	3	0
2	D	20	0	10	4	0
3	A	9	0	3	2	0
3	B	9	0	2	4	0
3	C	9	0	2	2	0
3	D	9	0	2	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
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
All	All	15305	0	15526	744	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (744) 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:73:LEU:CG	1:A:73:LEU:CD2	1.78	1.59
1:A:109:LYS:CE	1:A:109:LYS:CD	1.77	1.58
1:D:105:LYS:NZ	1:D:105:LYS:CE	1.72	1.51
1:A:410:LYS:CE	1:A:410:LYS:NZ	1.68	1.51
1:B:105:LYS:NZ	1:B:105:LYS:CE	1.70	1.51
1:A:102:GLU:CD	1:A:102:GLU:CG	1.83	1.50
1:C:410:LYS:CE	1:C:410:LYS:NZ	1.72	1.47
1:D:109:LYS:CE	1:D:109:LYS:CD	1.93	1.47
1:B:260:ASP:N	1:B:260:ASP:CA	1.73	1.46
1:C:144:SER:CB	1:C:144:SER:OG	1.69	1.40
1:D:182:GLN:O	1:D:182:GLN:C	1.65	1.37
1:B:144:SER:CB	1:B:144:SER:OG	1.78	1.31
3:D:581:PGA:C2	3:D:581:PGA:O1P	1.78	1.30
1:C:71:GLU:OE1	1:C:71:GLU:CD	1.75	1.27
1:D:230:LYS:CE	1:D:230:LYS:NZ	2.00	1.25
1:D:315:GLU:OE2	3:D:581:PGA:O4P	1.65	1.14
1:C:488:ARG:NH1	1:C:510:ARG:HB3	1.77	1.00
1:A:73:LEU:CD2	1:A:73:LEU:CD1	2.40	0.98
1:C:86:ARG:HB3	1:C:426:ARG:HG2	1.42	0.98
1:D:336:ALA:HB1	3:D:581:PGA:H22	1.46	0.97
1:B:86:ARG:HB3	1:B:426:ARG:HG2	1.47	0.97
1:D:225:SER:HB3	1:D:242:ASN:HB2	1.47	0.95
1:C:488:ARG:HH12	1:C:510:ARG:CB	1.79	0.95
1:D:86:ARG:HB3	1:D:426:ARG:HG2	1.46	0.94
1:D:514:PRO:O	1:D:515:LEU:HD23	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:HH21	1:B:442:ARG:HH21	1.14	0.91
1:A:488:ARG:HH12	1:A:510:ARG:HB3	1.37	0.90
1:B:488:ARG:NH1	1:B:510:ARG:HB3	1.86	0.90
1:B:488:ARG:HH12	1:B:510:ARG:HB3	1.35	0.90
1:B:514:PRO:O	1:B:515:LEU:HD23	1.70	0.90
1:C:488:ARG:HH12	1:C:510:ARG:HB3	1.29	0.90
1:C:85:ALA:HB2	1:C:545:PHE:CE2	2.07	0.89
1:D:488:ARG:HH12	1:D:510:ARG:HB3	1.36	0.89
1:A:442:ARG:HH21	1:B:442:ARG:NH2	1.71	0.89
1:C:83:VAL:O	1:C:84:ALA:HB2	1.71	0.89
1:D:488:ARG:NH1	1:D:510:ARG:HB3	1.86	0.89
1:A:86:ARG:HB3	1:A:426:ARG:HG2	1.54	0.88
1:B:488:ARG:HH12	1:B:510:ARG:CB	1.85	0.88
1:C:315:GLU:HG2	1:C:336:ALA:HB3	1.55	0.87
1:A:488:ARG:NH1	1:A:510:ARG:HB3	1.89	0.87
1:C:442:ARG:HH21	1:D:442:ARG:HH21	1.21	0.87
1:D:339:ASP:OD2	3:D:581:PGA:O2P	1.90	0.87
1:B:315:GLU:HG2	1:B:336:ALA:HB3	1.57	0.86
1:C:559:ARG:HD2	1:C:564:TYR:CD1	2.11	0.86
1:A:514:PRO:O	1:A:515:LEU:HD23	1.75	0.85
1:A:83:VAL:O	1:A:84:ALA:HB2	1.75	0.85
1:D:192:ARG:O	1:D:192:ARG:HG2	1.76	0.85
1:D:488:ARG:HH12	1:D:510:ARG:CB	1.89	0.85
3:D:581:PGA:C2	3:D:581:PGA:P	2.64	0.84
1:B:559:ARG:HD2	1:B:564:TYR:CD1	2.12	0.84
1:C:339:ASP:OD2	3:C:581:PGA:O4P	1.95	0.84
1:D:315:GLU:HG2	1:D:336:ALA:HB3	1.57	0.84
1:A:559:ARG:HD2	1:A:564:TYR:CD1	2.13	0.83
1:D:559:ARG:HD2	1:D:564:TYR:CD1	2.13	0.83
1:B:83:VAL:O	1:B:84:ALA:HB2	1.77	0.83
3:D:581:PGA:C2	3:D:581:PGA:O4P	2.27	0.82
1:D:288:VAL:HG12	1:D:326:ILE:HD13	1.61	0.82
1:A:99:ARG:NH2	1:A:129:GLU:OE1	2.11	0.81
1:A:167:LEU:HD12	1:A:168:GLN:H	1.46	0.80
1:B:223:LEU:CD1	1:D:380:LYS:NZ	2.45	0.80
1:A:488:ARG:HH12	1:A:510:ARG:CB	1.93	0.80
1:B:475:THR:HA	2:B:580:FBP:H61	1.64	0.80
1:D:87:SER:N	1:D:429:GLU:OE1	2.15	0.80
1:A:223:LEU:HD22	1:C:380:LYS:HE2	1.62	0.80
1:B:384:THR:OG1	1:B:387:GLU:HG3	1.82	0.79
1:A:184:LEU:HD11	1:A:235:GLY:HA3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HB3	1:C:426:ARG:CG	2.13	0.79
1:D:83:VAL:O	1:D:84:ALA:HB2	1.81	0.79
1:A:194:ARG:HB3	1:A:194:ARG:NH1	1.98	0.79
1:A:442:ARG:NH2	1:B:442:ARG:HH21	1.79	0.79
1:A:371:THR:OG1	3:A:581:PGA:O1	2.00	0.78
1:B:336:ALA:HB1	3:B:581:PGA:C2	2.14	0.78
1:B:223:LEU:HD13	1:D:380:LYS:NZ	1.99	0.77
1:B:339:ASP:OD2	3:B:581:PGA:O4P	2.02	0.77
1:B:336:ALA:HB1	3:B:581:PGA:H22	1.64	0.77
1:B:223:LEU:HD13	1:D:380:LYS:HZ1	1.46	0.77
1:B:86:ARG:HB3	1:B:426:ARG:CG	2.15	0.77
1:D:86:ARG:HB3	1:D:426:ARG:CG	2.15	0.77
1:C:85:ALA:HB2	1:C:545:PHE:HE2	1.49	0.77
1:C:442:ARG:NH2	1:D:442:ARG:HH21	1.83	0.76
1:D:532:ARG:NH2	2:D:580:FBP:O1P	2.16	0.76
1:C:506:VAL:CG1	1:C:512:VAL:HG11	2.16	0.76
1:D:87:SER:HB3	1:D:511:GLY:HA2	1.67	0.76
1:A:525:TRP:O	1:A:528:ASP:N	2.19	0.76
1:A:514:PRO:C	1:A:515:LEU:HD23	2.11	0.76
1:A:109:LYS:CE	1:A:109:LYS:CG	2.64	0.75
1:D:475:THR:HA	2:D:580:FBP:H61	1.68	0.75
1:C:442:ARG:HH21	1:D:442:ARG:NH2	1.85	0.75
1:C:83:VAL:O	1:C:84:ALA:CB	2.35	0.74
1:A:86:ARG:HB3	1:A:426:ARG:CG	2.16	0.74
1:A:347:GLU:HG2	1:C:423:ALA:HB1	1.70	0.74
1:A:73:LEU:CD2	1:A:73:LEU:CB	2.65	0.74
1:D:514:PRO:C	1:D:515:LEU:HD23	2.12	0.74
1:B:288:VAL:HG12	1:B:326:ILE:HD13	1.68	0.74
1:C:225:SER:HB3	1:C:242:ASN:HB2	1.70	0.73
1:B:514:PRO:C	1:B:515:LEU:HD23	2.12	0.73
1:C:288:VAL:HG12	1:C:326:ILE:HD13	1.71	0.73
1:A:385:ARG:HG2	1:A:385:ARG:HH11	1.52	0.73
1:A:315:GLU:HG2	1:A:336:ALA:HB3	1.70	0.72
3:D:581:PGA:O4P	3:D:581:PGA:H22	1.89	0.72
1:A:85:ALA:HB1	1:A:513:PHE:CE2	2.24	0.72
1:A:83:VAL:O	1:A:84:ALA:CB	2.37	0.72
1:C:514:PRO:O	1:C:515:LEU:HD23	1.88	0.72
1:D:87:SER:CB	1:D:511:GLY:HA2	2.20	0.72
1:C:551:LEU:HD11	1:D:449:ARG:HG3	1.72	0.71
1:B:66:ALA:HB1	1:B:71:GLU:HG2	1.71	0.71
1:D:269:VAL:O	1:D:273:ARG:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HB3	1:A:194:ARG:HH11	1.54	0.70
1:B:532:ARG:NH2	2:B:580:FBP:O1P	2.21	0.70
1:C:488:ARG:NH1	1:C:510:ARG:CB	2.47	0.70
1:D:525:TRP:O	1:D:528:ASP:N	2.23	0.70
1:B:223:LEU:CD1	1:D:380:LYS:HZ1	2.03	0.70
1:D:336:ALA:HB1	3:D:581:PGA:C2	2.19	0.70
1:A:384:THR:OG1	1:A:387:GLU:HG3	1.91	0.69
1:C:170:GLY:HA3	1:C:173:SER:HB3	1.74	0.69
1:B:557:GLY:HA3	2:B:580:FBP:O3	1.92	0.69
1:D:557:GLY:HA3	2:D:580:FBP:O3	1.92	0.69
1:A:286:SER:HA	1:A:313:LYS:HE2	1.73	0.69
1:C:60:GLN:HB2	1:C:430:ALA:O	1.93	0.68
1:C:85:ALA:HB1	1:C:513:PHE:CE2	2.28	0.68
1:A:554:VAL:HG21	1:A:571:LEU:CD1	2.23	0.68
1:B:83:VAL:O	1:B:84:ALA:CB	2.41	0.68
1:C:554:VAL:HG21	1:C:571:LEU:HD11	1.75	0.68
1:B:532:ARG:NH1	2:B:580:FBP:O2P	2.27	0.68
1:C:452:THR:HG23	1:C:565:THR:HB	1.76	0.68
1:A:86:ARG:CB	1:A:426:ARG:HG2	2.25	0.67
1:C:170:GLY:HA3	1:C:173:SER:CB	2.24	0.67
1:A:167:LEU:HD12	1:A:195:GLY:O	1.94	0.67
1:C:514:PRO:C	1:C:515:LEU:HD23	2.18	0.67
1:A:554:VAL:HG21	1:A:571:LEU:HD11	1.76	0.67
1:B:525:TRP:O	1:B:526:ALA:C	2.38	0.67
1:C:449:ARG:HG3	1:D:551:LEU:HD11	1.77	0.67
1:A:405:SER:O	1:A:406:GLY:C	2.37	0.67
1:B:105:LYS:NZ	1:B:105:LYS:CD	2.57	0.67
1:C:384:THR:OG1	1:C:387:GLU:HG3	1.94	0.67
1:A:102:GLU:OE1	1:A:102:GLU:HA	1.95	0.67
1:C:146:LEU:HD23	1:C:535:PHE:CE1	2.30	0.67
1:D:554:VAL:HG21	1:D:571:LEU:CD1	2.25	0.67
1:A:288:VAL:HG12	1:A:326:ILE:HD13	1.77	0.66
1:C:525:TRP:O	1:C:526:ALA:C	2.36	0.66
1:D:208:VAL:O	1:D:231:ILE:HD11	1.94	0.66
1:C:372:GLN:HG2	1:C:375:GLU:CG	2.24	0.66
1:D:371:THR:OG1	3:D:581:PGA:O1	2.11	0.66
1:C:525:TRP:O	1:C:528:ASP:N	2.29	0.66
1:A:225:SER:HB3	1:A:242:ASN:HB2	1.77	0.65
1:C:230:LYS:HB2	1:C:237:VAL:HB	1.78	0.65
3:D:581:PGA:O4P	3:D:581:PGA:O2	2.15	0.65
1:C:87:SER:CB	1:C:511:GLY:HA2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ARG:CB	1:D:426:ARG:HG2	2.24	0.65
1:B:337:ARG:HH22	1:B:390:ASP:CG	2.05	0.65
1:A:315:GLU:HG2	1:A:336:ALA:CB	2.26	0.64
1:D:85:ALA:HB1	1:D:513:PHE:CE2	2.32	0.64
1:C:410:LYS:NZ	1:C:410:LYS:CG	2.60	0.64
1:D:460:VAL:O	1:D:463:ALA:HB3	1.96	0.64
1:C:475:THR:HA	2:C:580:FBP:H61	1.79	0.64
1:B:102:GLU:HA	1:B:102:GLU:OE1	1.98	0.64
1:B:223:LEU:CD1	1:D:380:LYS:HZ3	2.11	0.64
1:B:554:VAL:HG21	1:B:571:LEU:HD11	1.79	0.64
1:C:506:VAL:CG1	1:C:512:VAL:CG1	2.76	0.64
1:A:385:ARG:HG2	1:A:385:ARG:NH1	2.12	0.64
1:D:83:VAL:O	1:D:84:ALA:CB	2.45	0.64
1:D:554:VAL:HG21	1:D:571:LEU:HD11	1.79	0.64
1:C:315:GLU:HG2	1:C:336:ALA:CB	2.28	0.64
1:C:506:VAL:HG11	1:C:512:VAL:HG11	1.79	0.63
1:B:223:LEU:HD11	1:D:380:LYS:NZ	2.12	0.63
1:B:286:SER:HA	1:B:313:LYS:HE2	1.78	0.63
1:B:85:ALA:HB1	1:B:513:PHE:CE2	2.33	0.63
1:C:525:TRP:O	1:C:527:ASP:N	2.32	0.63
1:B:77:ASP:OD1	1:B:79:ASP:N	2.25	0.63
1:B:525:TRP:O	1:B:528:ASP:N	2.30	0.63
1:C:168:GLN:C	1:C:170:GLY:H	2.07	0.63
1:B:377:MET:HA	1:B:380:LYS:O	1.99	0.63
1:B:485:SER:O	1:B:488:ARG:N	2.27	0.63
1:A:525:TRP:O	1:A:527:ASP:N	2.32	0.62
1:A:525:TRP:O	1:A:526:ALA:C	2.42	0.62
1:C:410:LYS:NZ	1:C:410:LYS:CD	2.61	0.62
1:D:281:ASP:C	1:D:282:ILE:HG13	2.24	0.62
1:C:87:SER:HB2	1:C:511:GLY:HA2	1.79	0.62
1:D:337:ARG:HH22	1:D:390:ASP:CG	2.07	0.62
1:D:105:LYS:NZ	1:D:105:LYS:CD	2.59	0.62
1:C:286:SER:HA	1:C:313:LYS:HE2	1.79	0.62
1:D:91:ILE:HB	1:D:403:MET:HG3	1.82	0.62
1:A:161:GLU:OE1	1:A:163:ARG:NE	2.27	0.62
1:B:369:CYS:SG	1:B:373:MET:HE3	2.39	0.62
1:D:525:TRP:O	1:D:526:ALA:C	2.42	0.62
1:A:269:VAL:O	1:A:273:ARG:HG2	1.98	0.62
1:D:87:SER:HB2	1:D:511:GLY:N	2.14	0.62
1:B:183:VAL:HG22	1:B:198:ASN:HA	1.81	0.62
1:C:337:ARG:HH22	1:C:390:ASP:CG	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:VAL:O	1:C:273:ARG:HG2	1.99	0.62
1:C:259:VAL:HG12	1:C:261:LEU:HB2	1.81	0.61
1:B:66:ALA:HB1	1:B:71:GLU:CG	2.29	0.61
1:C:331:ASP:O	1:C:366:PRO:HD2	2.01	0.61
1:D:336:ALA:CB	3:D:581:PGA:H22	2.27	0.61
1:B:269:VAL:O	1:B:273:ARG:HG2	2.01	0.61
1:B:315:GLU:HG2	1:B:336:ALA:CB	2.29	0.61
1:B:86:ARG:CB	1:B:426:ARG:HG2	2.26	0.61
1:C:554:VAL:HG21	1:C:571:LEU:CD1	2.30	0.61
1:A:208:VAL:HG12	1:A:236:LEU:HG	1.82	0.61
1:D:99:ARG:NH2	1:D:129:GLU:OE1	2.29	0.61
1:D:188:ASP:C	1:D:188:ASP:OD1	2.43	0.60
1:C:91:ILE:HB	1:C:403:MET:HG3	1.83	0.60
1:C:391:VAL:HG11	1:C:424:ILE:HB	1.83	0.60
1:B:554:VAL:HG21	1:B:571:LEU:CD1	2.31	0.60
1:B:155:LEU:C	1:B:155:LEU:HD23	2.27	0.60
1:A:276:VAL:HG11	1:A:304:GLU:HB2	1.82	0.60
1:D:81:GLU:HA	1:D:81:GLU:OE1	2.00	0.60
1:B:423:ALA:HB1	1:D:347:GLU:HG2	1.83	0.60
1:B:452:THR:HG23	1:B:565:THR:HB	1.82	0.60
1:A:70:LEU:HB2	1:C:440:GLU:OE1	2.02	0.60
1:C:169:GLY:O	1:C:171:PRO:HD3	2.02	0.60
1:A:434:HIS:O	1:A:435:ARG:C	2.44	0.60
1:A:81:GLU:OE1	1:A:81:GLU:HA	2.01	0.59
1:A:155:LEU:HD23	1:A:155:LEU:C	2.27	0.59
1:D:372:GLN:HG2	1:D:375:GLU:CG	2.33	0.59
1:C:506:VAL:HG13	1:C:512:VAL:HG11	1.84	0.59
1:D:191:PHE:CE2	1:D:194:ARG:HD3	2.37	0.59
1:B:434:HIS:O	1:B:435:ARG:C	2.44	0.59
1:B:506:VAL:CG1	1:B:512:VAL:HG11	2.32	0.59
1:A:167:LEU:HD12	1:A:168:GLN:N	2.15	0.59
1:A:377:MET:HA	1:A:380:LYS:O	2.02	0.59
1:B:525:TRP:O	1:B:527:ASP:N	2.36	0.59
1:A:351:LEU:HD23	1:C:76:LEU:HD13	1.85	0.58
1:D:206:ASN:O	1:D:210:VAL:HG23	2.03	0.58
1:A:73:LEU:CD2	1:A:73:LEU:HD13	2.33	0.58
1:D:191:PHE:CD2	1:D:194:ARG:HD3	2.38	0.58
1:B:144:SER:OG	1:B:144:SER:CA	2.48	0.58
1:A:281:ASP:C	1:A:282:ILE:HG13	2.29	0.58
1:B:372:GLN:HG2	1:B:375:GLU:CG	2.33	0.58
1:D:68:THR:OG1	1:D:71:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HH22	1:A:390:ASP:CG	2.11	0.58
1:D:63:ALA:O	1:D:72:HIS:ND1	2.31	0.58
1:D:286:SER:HA	1:D:313:LYS:HE2	1.85	0.58
1:A:460:VAL:O	1:A:463:ALA:HB3	2.03	0.58
1:A:539:SER:O	1:A:543:ARG:HG3	2.03	0.58
1:B:477:THR:N	2:B:580:FBP:O4P	2.25	0.58
1:C:185:VAL:HG23	1:C:238:THR:HG21	1.86	0.58
1:D:315:GLU:HG2	1:D:336:ALA:CB	2.30	0.58
1:C:87:SER:HB2	1:C:511:GLY:CA	2.34	0.57
1:D:327:LEU:CD2	1:D:365:LYS:HD2	2.34	0.57
1:B:488:ARG:HH11	1:B:510:ARG:HD2	1.67	0.57
1:C:170:GLY:CA	1:C:173:SER:HB3	2.34	0.57
1:B:225:SER:HB3	1:B:242:ASN:HB2	1.85	0.57
1:B:460:VAL:O	1:B:463:ALA:HB3	2.05	0.57
1:A:339:ASP:OD2	3:A:581:PGA:O4P	2.21	0.57
1:A:373:MET:O	1:A:387:GLU:HB3	2.03	0.57
1:B:487:TYR:O	1:B:488:ARG:HB2	2.04	0.57
3:D:581:PGA:O1P	3:D:581:PGA:C1	2.50	0.57
1:A:402:ILE:HG13	1:A:421:GLN:NE2	2.20	0.57
1:A:436:GLN:O	1:A:440:GLU:HG3	2.05	0.57
1:A:506:VAL:CG1	1:A:512:VAL:HG11	2.35	0.57
1:D:505:GLN:O	1:D:508:LEU:HB2	2.05	0.57
1:C:276:VAL:HG11	1:C:304:GLU:HB2	1.86	0.57
1:B:336:ALA:CB	3:B:581:PGA:H22	2.33	0.57
1:C:434:HIS:O	1:C:435:ARG:C	2.47	0.57
1:A:67:ASP:N	1:A:71:GLU:OE1	2.38	0.56
1:A:118:ASN:C	1:A:118:ASN:OD1	2.48	0.56
1:A:192:ARG:HA	1:A:201:TRP:CD2	2.41	0.56
1:B:78:ILE:HD13	1:D:320:VAL:HG11	1.88	0.56
1:C:192:ARG:HA	1:C:201:TRP:CD2	2.40	0.56
1:A:207:ILE:HD11	1:A:254:LEU:HD21	1.87	0.56
1:B:276:VAL:HG11	1:B:304:GLU:HB2	1.87	0.56
1:A:100:SER:O	1:A:101:VAL:C	2.49	0.56
1:C:231:ILE:HD13	1:C:232:GLY:H	1.71	0.56
1:B:223:LEU:HD11	1:D:380:LYS:HZ3	1.69	0.56
1:D:164:THR:O	1:D:249:ARG:HA	2.05	0.56
1:A:125:GLU:CD	1:A:125:GLU:H	2.13	0.56
1:B:220:ASP:OD1	1:B:250:LYS:HD3	2.05	0.56
1:B:315:GLU:OE2	1:B:339:ASP:OD2	2.23	0.56
1:C:170:GLY:HA3	1:C:173:SER:OG	2.06	0.56
1:C:379:THR:HG22	1:C:380:LYS:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLU:HG2	1:D:423:ALA:HB1	1.86	0.56
1:B:57:GLN:HB2	1:B:62:PRO:HD3	1.88	0.55
1:B:77:ASP:OD1	1:B:77:ASP:C	2.48	0.55
1:C:208:VAL:HA	1:C:236:LEU:HD21	1.88	0.55
1:C:373:MET:O	1:C:387:GLU:HB3	2.06	0.55
1:A:70:LEU:HD21	1:C:362:LEU:HD12	1.88	0.55
1:A:194:ARG:HH11	1:A:194:ARG:CB	2.19	0.55
1:C:144:SER:CB	1:C:144:SER:HG	2.13	0.55
1:C:354:LYS:NZ	1:C:397:ASP:OD1	2.39	0.55
1:A:70:LEU:HD21	1:C:362:LEU:CD1	2.37	0.55
1:C:87:SER:HB2	1:C:511:GLY:N	2.21	0.55
1:B:281:ASP:C	1:B:282:ILE:HG13	2.31	0.55
1:D:177:LEU:HD11	1:D:246:LEU:HD22	1.87	0.55
1:A:255:PRO:C	1:A:257:ALA:H	2.14	0.55
1:A:553:ILE:CD1	1:A:570:VAL:HG22	2.37	0.55
1:C:377:MET:HA	1:C:380:LYS:O	2.07	0.55
1:D:259:VAL:HG12	1:D:261:LEU:CB	2.37	0.55
1:A:223:LEU:CD2	1:C:380:LYS:HE2	2.36	0.55
1:B:367:VAL:O	1:B:367:VAL:HG13	2.07	0.55
1:C:454:VAL:HG12	1:D:462:ALA:HB1	1.88	0.55
1:D:362:LEU:O	1:D:486:ARG:NH2	2.40	0.55
1:B:405:SER:O	1:B:406:GLY:C	2.48	0.54
1:D:436:GLN:O	1:D:440:GLU:HG3	2.07	0.54
1:A:331:ASP:O	1:A:366:PRO:HD2	2.08	0.54
1:B:488:ARG:NH1	1:B:510:ARG:HD2	2.22	0.54
1:D:452:THR:HG23	1:D:565:THR:HB	1.90	0.54
1:A:85:ALA:HB2	1:A:545:PHE:CE2	2.42	0.54
1:C:68:THR:OG1	1:C:71:GLU:OE1	2.22	0.54
1:C:485:SER:O	1:C:486:ARG:C	2.49	0.54
1:D:352:ALA:HB1	1:D:356:MET:HE2	1.89	0.54
1:A:85:ALA:HB2	1:A:545:PHE:HE2	1.73	0.54
1:D:331:ASP:O	1:D:366:PRO:HD2	2.08	0.54
1:B:255:PRO:C	1:B:257:ALA:H	2.15	0.54
1:B:539:SER:O	1:B:543:ARG:HG3	2.08	0.54
1:B:331:ASP:O	1:B:366:PRO:HD2	2.08	0.54
1:C:559:ARG:HD3	1:C:560:PRO:O	2.08	0.54
1:D:87:SER:HB2	1:D:511:GLY:CA	2.38	0.54
1:D:264:LEU:HD22	1:D:296:ALA:HB1	1.89	0.54
1:A:360:CYS:O	1:A:361:ASN:C	2.51	0.53
1:D:405:SER:O	1:D:406:GLY:C	2.50	0.53
1:A:91:ILE:HB	1:A:403:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:THR:HB	1:C:440:GLU:OE2	2.09	0.53
1:D:313:LYS:HD2	1:D:334:MET:SD	2.48	0.53
1:A:379:THR:HG22	1:A:380:LYS:HG3	1.90	0.53
1:C:281:ASP:C	1:C:282:ILE:HG13	2.32	0.53
1:A:475:THR:HA	2:A:580:FBP:H61	1.89	0.53
1:C:488:ARG:HH12	1:C:510:ARG:HB2	1.67	0.53
1:D:172:GLU:CD	1:D:172:GLU:N	2.66	0.53
1:A:525:TRP:CE2	1:A:560:PRO:HG3	2.43	0.53
1:B:485:SER:O	1:B:486:ARG:C	2.51	0.53
1:A:102:GLU:OE1	1:A:105:LYS:HD2	2.09	0.53
1:B:450:ASP:O	1:B:454:VAL:HG23	2.09	0.52
1:B:327:LEU:CD2	1:B:365:LYS:HD2	2.39	0.52
1:B:441:LEU:O	1:B:442:ARG:C	2.52	0.52
1:C:327:LEU:HD22	1:C:365:LYS:HD2	1.91	0.52
1:C:460:VAL:O	1:C:463:ALA:HB3	2.09	0.52
1:B:77:ASP:OD1	1:B:78:ILE:N	2.41	0.52
1:D:108:ILE:HD13	1:D:151:VAL:HG21	1.91	0.52
1:A:204:TYR:CZ	1:A:206:ASN:HB2	2.44	0.52
1:C:348:LYS:O	1:C:349:VAL:C	2.53	0.52
1:A:83:VAL:O	1:A:83:VAL:HG12	2.08	0.52
1:C:206:ASN:O	1:C:210:VAL:HG23	2.09	0.52
1:D:109:LYS:CE	1:D:109:LYS:CG	2.82	0.52
1:C:372:GLN:HG2	1:C:375:GLU:HG3	1.89	0.52
1:D:155:LEU:C	1:D:155:LEU:HD23	2.35	0.52
1:D:315:GLU:CD	3:D:581:PGA:O4P	2.50	0.52
1:D:347:GLU:H	1:D:347:GLU:CD	2.17	0.52
1:A:441:LEU:O	1:A:442:ARG:C	2.52	0.52
1:D:255:PRO:C	1:D:257:ALA:H	2.18	0.51
1:D:327:LEU:HD22	1:D:365:LYS:HD2	1.92	0.51
1:A:442:ARG:NH2	1:B:442:ARG:NH2	2.47	0.51
1:B:87:SER:H	1:B:429:GLU:CD	2.17	0.51
1:C:327:LEU:CD2	1:C:365:LYS:HD2	2.40	0.51
1:C:405:SER:O	1:C:406:GLY:C	2.53	0.51
1:C:209:ARG:HG2	1:C:209:ARG:O	2.11	0.51
1:D:488:ARG:NH1	1:D:510:ARG:CB	2.58	0.51
1:A:102:GLU:CD	1:A:102:GLU:CB	2.80	0.51
1:A:167:LEU:CD1	1:A:195:GLY:O	2.58	0.51
1:A:545:PHE:C	1:A:546:LEU:HD23	2.35	0.51
1:D:568:MET:HE3	1:D:570:VAL:HG23	1.92	0.51
1:D:559:ARG:HD3	1:D:560:PRO:O	2.11	0.51
1:A:548:VAL:HA	1:A:573:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:O	1:C:132:ALA:C	2.54	0.51
1:C:155:LEU:HD23	1:C:155:LEU:C	2.35	0.51
1:C:510:ARG:HG2	1:C:511:GLY:N	2.26	0.51
1:D:434:HIS:O	1:D:435:ARG:C	2.53	0.51
1:A:348:LYS:HE2	1:C:427:GLU:OE2	2.11	0.51
1:C:441:LEU:O	1:C:442:ARG:C	2.53	0.51
1:A:452:THR:HG23	1:A:565:THR:HB	1.92	0.51
1:A:553:ILE:HD12	1:A:570:VAL:HG22	1.93	0.51
1:C:349:VAL:O	1:C:350:PHE:C	2.53	0.51
1:D:131:ILE:O	1:D:132:ALA:C	2.53	0.51
1:D:539:SER:O	1:D:543:ARG:HG3	2.11	0.51
1:A:350:PHE:CZ	1:C:428:ALA:HA	2.46	0.51
1:A:420:MET:O	1:A:421:GLN:C	2.54	0.51
1:C:436:GLN:O	1:C:440:GLU:HG3	2.10	0.51
1:C:506:VAL:HG11	1:C:512:VAL:CG1	2.39	0.51
1:D:349:VAL:O	1:D:350:PHE:C	2.53	0.51
1:D:373:MET:O	1:D:387:GLU:HB3	2.11	0.51
1:A:183:VAL:HG22	1:A:198:ASN:HA	1.93	0.50
1:A:524:ILE:O	1:A:525:TRP:O	2.28	0.50
1:B:470:ALA:HA	1:B:491:ALA:HB1	1.93	0.50
1:D:146:LEU:HB2	1:D:542:LEU:HD12	1.94	0.50
1:D:506:VAL:CG1	1:D:512:VAL:HG11	2.40	0.50
1:A:327:LEU:HD22	1:A:365:LYS:HD2	1.92	0.50
1:C:86:ARG:NH2	1:C:113:ASN:OD1	2.44	0.50
1:D:87:SER:HB2	1:D:511:GLY:HA2	1.94	0.50
1:D:192:ARG:HG3	1:D:201:TRP:CH2	2.46	0.50
1:D:192:ARG:O	1:D:192:ARG:CG	2.51	0.50
1:A:557:GLY:HA3	2:A:580:FBP:O3	2.11	0.50
1:C:81:GLU:OE1	1:C:81:GLU:HA	2.10	0.50
1:D:219:ILE:HG21	1:D:246:LEU:HD13	1.93	0.50
1:A:264:LEU:HD22	1:A:296:ALA:HB1	1.91	0.50
1:B:506:VAL:CG1	1:B:512:VAL:CG1	2.90	0.50
1:D:146:LEU:CB	1:D:542:LEU:HD12	2.42	0.50
1:B:506:VAL:HG11	1:B:512:VAL:HG11	1.93	0.50
1:A:208:VAL:HA	1:A:236:LEU:HD11	1.93	0.50
1:A:366:PRO:HB3	1:A:508:LEU:O	2.11	0.50
1:A:488:ARG:HH11	1:A:510:ARG:HD2	1.76	0.50
1:A:505:GLN:O	1:A:508:LEU:HB2	2.12	0.50
1:C:172:GLU:N	1:C:172:GLU:OE1	2.43	0.50
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.92	0.49
1:D:339:ASP:O	1:D:340:LEU:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ILE:O	1:B:132:ALA:C	2.53	0.49
1:D:525:TRP:CE2	1:D:560:PRO:HG3	2.47	0.49
1:D:553:ILE:HD12	1:D:570:VAL:HG22	1.93	0.49
1:A:168:GLN:HB2	1:A:195:GLY:O	2.12	0.49
1:A:347:GLU:H	1:A:347:GLU:CD	2.18	0.49
1:A:509:CYS:O	1:A:510:ARG:C	2.55	0.49
1:B:327:LEU:HD22	1:B:365:LYS:HD2	1.93	0.49
1:C:255:PRO:O	1:C:257:ALA:N	2.44	0.49
1:D:259:VAL:HG12	1:D:261:LEU:HB3	1.93	0.49
1:D:276:VAL:HG11	1:D:304:GLU:HB2	1.94	0.49
1:B:104:LEU:O	1:B:108:ILE:HG13	2.13	0.49
1:B:264:LEU:HD22	1:B:296:ALA:HB1	1.94	0.49
1:B:548:VAL:HA	1:B:573:ILE:HG22	1.95	0.49
1:D:99:ARG:NH2	1:D:129:GLU:HB2	2.27	0.49
1:A:327:LEU:CD2	1:A:365:LYS:HD2	2.43	0.49
1:B:207:ILE:HD11	1:B:254:LEU:HD21	1.94	0.49
1:B:313:LYS:HD2	1:B:334:MET:SD	2.53	0.49
1:B:339:ASP:O	1:B:340:LEU:C	2.55	0.49
1:C:86:ARG:CB	1:C:426:ARG:HG2	2.28	0.49
1:A:223:LEU:HD11	1:C:380:LYS:NZ	2.28	0.49
1:A:559:ARG:HD3	1:A:560:PRO:O	2.13	0.49
1:C:146:LEU:HD23	1:C:535:PHE:HE1	1.77	0.49
1:D:231:ILE:CD1	1:D:231:ILE:C	2.86	0.49
1:A:104:LEU:O	1:A:108:ILE:HG13	2.12	0.49
1:A:223:LEU:HD22	1:C:380:LYS:CE	2.40	0.49
1:D:548:VAL:HA	1:D:573:ILE:HG22	1.94	0.49
1:B:206:ASN:O	1:B:210:VAL:HG23	2.13	0.48
1:C:352:ALA:HB1	1:C:356:MET:HE2	1.95	0.48
1:D:100:SER:O	1:D:101:VAL:C	2.55	0.48
1:D:470:ALA:HA	1:D:491:ALA:HB1	1.95	0.48
1:D:509:CYS:O	1:D:510:ARG:C	2.56	0.48
1:B:391:VAL:HG11	1:B:424:ILE:HB	1.96	0.48
1:C:168:GLN:C	1:C:170:GLY:N	2.71	0.48
1:C:567:ILE:HG12	1:D:569:ARG:HG2	1.95	0.48
1:C:86:ARG:HH21	1:C:89:SER:HA	1.78	0.48
1:C:118:ASN:C	1:C:118:ASN:OD1	2.56	0.48
1:A:329:VAL:O	1:A:329:VAL:HG13	2.13	0.48
1:B:156:ASP:C	1:B:156:ASP:OD1	2.56	0.48
1:B:532:ARG:HH12	2:B:580:FBP:H11	1.77	0.48
1:D:135:ARG:O	1:D:139:GLU:HG2	2.13	0.48
1:A:87:SER:OG	1:A:510:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG13	1:A:204:TYR:H	1.78	0.48
1:B:81:GLU:HA	1:B:81:GLU:OE1	2.12	0.48
1:B:146:LEU:HB2	1:B:542:LEU:HD12	1.94	0.48
1:C:488:ARG:HH11	1:C:510:ARG:HD2	1.77	0.48
1:B:118:ASN:OD1	1:B:118:ASN:C	2.57	0.48
1:C:532:ARG:HH12	2:C:580:FBP:H11	1.79	0.48
1:A:506:VAL:CG1	1:A:512:VAL:CG1	2.91	0.48
1:A:506:VAL:HG11	1:A:512:VAL:HG11	1.94	0.48
1:A:85:ALA:CB	1:A:513:PHE:CZ	2.97	0.48
1:B:93:THR:HA	1:B:116:ARG:HB3	1.95	0.48
1:B:100:SER:O	1:B:101:VAL:C	2.57	0.48
1:C:69:PHE:O	1:C:72:HIS:HB3	2.14	0.48
1:A:91:ILE:HD13	1:A:284:PHE:HZ	1.78	0.48
1:D:348:LYS:O	1:D:349:VAL:C	2.56	0.48
1:D:506:VAL:HG13	1:D:512:VAL:HG11	1.95	0.48
1:B:436:GLN:O	1:B:440:GLU:HG3	2.14	0.48
1:C:68:THR:OG1	1:C:71:GLU:HB2	2.14	0.48
1:A:525:TRP:NE1	1:A:560:PRO:HG3	2.29	0.47
1:C:87:SER:HB2	1:C:511:GLY:H	1.76	0.47
1:C:539:SER:O	1:C:543:ARG:HG3	2.14	0.47
1:A:68:THR:OG1	1:A:71:GLU:HB2	2.14	0.47
1:A:206:ASN:O	1:A:210:VAL:HG23	2.14	0.47
1:B:379:THR:HG22	1:B:380:LYS:HG3	1.96	0.47
1:B:568:MET:HE3	1:B:570:VAL:HG23	1.95	0.47
1:D:102:GLU:HA	1:D:102:GLU:OE1	2.14	0.47
1:A:434:HIS:O	1:A:437:LEU:N	2.47	0.47
1:D:219:ILE:HB	1:D:224:ILE:HB	1.96	0.47
1:D:259:VAL:CG1	1:D:261:LEU:HB2	2.43	0.47
1:B:66:ALA:CB	1:B:71:GLU:HG2	2.40	0.47
1:C:366:PRO:HB3	1:C:508:LEU:O	2.15	0.47
1:C:91:ILE:HD13	1:C:284:PHE:HZ	1.78	0.47
1:C:339:ASP:O	1:C:340:LEU:C	2.57	0.47
1:C:375:GLU:O	1:C:376:SER:C	2.58	0.47
1:D:525:TRP:NE1	1:D:560:PRO:HG3	2.30	0.47
1:B:545:PHE:C	1:B:546:LEU:HD23	2.40	0.47
1:C:255:PRO:C	1:C:257:ALA:H	2.22	0.47
1:D:83:VAL:O	1:D:83:VAL:CG1	2.63	0.47
1:B:91:ILE:HB	1:B:403:MET:HG3	1.95	0.47
1:B:349:VAL:O	1:B:350:PHE:C	2.56	0.47
1:D:191:PHE:CD2	1:D:194:ARG:CD	2.98	0.47
1:D:377:MET:HA	1:D:380:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:HIS:HE1	1:C:271:ASP:OD1	1.98	0.47
1:A:167:LEU:HD23	1:A:173:SER:O	2.15	0.47
1:A:320:VAL:HG11	1:C:78:ILE:HD13	1.97	0.47
1:A:456:ALA:O	1:A:460:VAL:HG23	2.15	0.47
1:C:301:LEU:HD12	1:C:301:LEU:HA	1.60	0.47
1:D:207:ILE:HD11	1:D:254:LEU:HD21	1.97	0.47
1:B:420:MET:O	1:B:421:GLN:C	2.57	0.46
1:B:559:ARG:HD3	1:B:560:PRO:O	2.15	0.46
1:C:337:ARG:NH2	1:C:390:ASP:OD1	2.48	0.46
1:D:297:VAL:O	1:D:301:LEU:HB2	2.15	0.46
1:A:223:LEU:CD1	1:C:380:LYS:NZ	2.79	0.46
1:B:506:VAL:HG13	1:B:512:VAL:HG11	1.96	0.46
1:C:264:LEU:HD22	1:C:296:ALA:HB1	1.97	0.46
1:A:131:ILE:O	1:A:132:ALA:C	2.59	0.46
1:B:59:GLN:CD	1:B:83:VAL:HG12	2.40	0.46
1:B:337:ARG:CD	1:B:370:ALA:O	2.63	0.46
1:B:488:ARG:NH1	1:B:510:ARG:CB	2.56	0.46
1:C:227:VAL:HG23	1:C:241:GLU:HB2	1.97	0.46
1:D:561:GLY:O	2:D:580:FBP:O4	2.29	0.46
1:A:87:SER:H	1:A:429:GLU:CD	2.24	0.46
1:A:450:ASP:O	1:A:454:VAL:HG23	2.16	0.46
1:B:553:ILE:HD12	1:B:570:VAL:HG22	1.96	0.46
1:C:87:SER:H	1:C:429:GLU:CD	2.23	0.46
1:C:303:PRO:C	1:C:305:GLY:H	2.24	0.46
1:C:448:SER:OG	1:C:449:ARG:N	2.46	0.46
1:A:90:ILE:HG23	1:A:421:GLN:NE2	2.31	0.46
1:B:337:ARG:HD2	1:B:370:ALA:O	2.15	0.46
1:B:509:CYS:O	1:B:510:ARG:C	2.59	0.46
1:C:87:SER:HB3	1:C:511:GLY:HA2	1.97	0.46
1:C:157:THR:HG22	1:C:286:SER:HB2	1.97	0.46
1:D:283:VAL:O	1:D:283:VAL:HG12	2.16	0.46
1:A:226:LEU:HD23	1:A:240:VAL:HA	1.97	0.46
1:D:63:ALA:HA	1:D:75:LEU:HB2	1.97	0.46
1:D:225:SER:OG	1:D:241:GLU:OE1	2.33	0.46
3:D:581:PGA:O4P	3:D:581:PGA:C1	2.63	0.46
1:A:334:MET:HA	1:A:368:VAL:HB	1.98	0.46
1:A:510:ARG:HG2	1:A:511:GLY:N	2.29	0.46
1:C:185:VAL:HB	1:C:236:LEU:HB2	1.98	0.46
1:D:554:VAL:HG21	1:D:571:LEU:HD12	1.98	0.46
1:B:146:LEU:CB	1:B:542:LEU:HD12	2.46	0.45
1:C:188:ASP:OD1	1:C:188:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:PHE:O	1:D:72:HIS:HB3	2.16	0.45
1:B:352:ALA:HB1	1:B:356:MET:HE2	1.98	0.45
1:B:362:LEU:HD12	1:D:70:LEU:HD21	1.98	0.45
1:B:375:GLU:O	1:B:376:SER:C	2.59	0.45
1:C:133:ASN:O	1:C:134:VAL:C	2.57	0.45
1:C:454:VAL:CG1	1:D:462:ALA:HB1	2.46	0.45
1:B:434:HIS:O	1:B:435:ARG:O	2.32	0.45
1:C:413:PHE:HB3	1:C:416:GLU:HB2	1.99	0.45
1:C:487:TYR:O	1:C:488:ARG:HB2	2.16	0.45
1:A:385:ARG:HE	1:C:341:GLY:HA3	1.80	0.45
1:B:99:ARG:NH2	1:B:129:GLU:OE1	2.39	0.45
1:C:93:THR:HA	1:C:116:ARG:HB3	1.99	0.45
1:B:225:SER:OG	1:B:241:GLU:HB3	2.17	0.45
1:D:98:SER:HA	1:D:103:ARG:HG2	1.99	0.45
1:A:297:VAL:O	1:A:301:LEU:HB2	2.17	0.45
1:A:413:PHE:N	1:A:414:PRO:CD	2.79	0.45
1:C:296:ALA:O	1:C:297:VAL:C	2.59	0.45
1:C:367:VAL:O	1:C:367:VAL:HG13	2.17	0.45
1:D:196:ASN:C	1:D:198:ASN:N	2.72	0.45
1:B:290:LYS:O	1:B:291:ALA:C	2.59	0.45
1:B:559:ARG:HD2	1:B:564:TYR:CE1	2.52	0.45
1:C:191:PHE:HA	1:C:194:ARG:HB2	1.98	0.45
1:A:86:ARG:NH2	1:A:113:ASN:OD1	2.50	0.45
1:A:559:ARG:HD2	1:A:564:TYR:CE1	2.52	0.45
1:B:85:ALA:HB2	1:B:545:PHE:CE2	2.52	0.45
1:B:87:SER:N	1:B:429:GLU:OE1	2.47	0.45
1:C:171:PRO:HB2	1:C:172:GLU:CD	2.42	0.45
1:C:192:ARG:HA	1:C:201:TRP:CE2	2.52	0.45
1:C:450:ASP:O	1:C:454:VAL:HG23	2.17	0.45
1:D:133:ASN:O	1:D:134:VAL:C	2.60	0.45
1:B:60:GLN:OE1	1:B:76:LEU:HA	2.16	0.45
1:C:184:LEU:HD12	1:C:236:LEU:O	2.16	0.45
1:D:188:ASP:OD2	1:D:191:PHE:HD1	2.00	0.45
1:B:83:VAL:O	1:B:83:VAL:CG1	2.64	0.44
1:B:525:TRP:CE2	1:B:560:PRO:HG3	2.52	0.44
1:A:375:GLU:O	1:A:376:SER:C	2.59	0.44
1:B:297:VAL:O	1:B:301:LEU:HB2	2.17	0.44
1:B:348:LYS:O	1:B:349:VAL:C	2.59	0.44
1:C:524:ILE:O	1:C:525:TRP:O	2.35	0.44
1:C:569:ARG:HG2	1:D:567:ILE:HG12	1.99	0.44
1:A:164:THR:O	1:A:249:ARG:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD21	1:A:175:VAL:H	1.83	0.44
1:A:347:GLU:CG	1:C:423:ALA:HB1	2.44	0.44
1:A:470:ALA:HA	1:A:491:ALA:HB1	1.98	0.44
1:A:554:VAL:HG21	1:A:571:LEU:HD12	2.00	0.44
1:A:568:MET:HE3	1:A:570:VAL:HG23	1.99	0.44
1:B:85:ALA:HB2	1:B:545:PHE:HE2	1.82	0.44
1:B:434:HIS:O	1:B:437:LEU:N	2.51	0.44
1:C:548:VAL:HA	1:C:573:ILE:HG22	1.99	0.44
1:C:273:ARG:O	1:C:274:PHE:C	2.61	0.44
1:C:553:ILE:HD12	1:C:570:VAL:HG22	1.98	0.44
1:D:220:ASP:C	1:D:222:GLY:H	2.25	0.44
1:A:515:LEU:CD1	1:A:539:SER:HB2	2.48	0.44
1:A:141:PHE:C	1:A:143:GLY:H	2.25	0.44
1:B:320:VAL:HG11	1:D:78:ILE:HD13	1.98	0.44
1:C:225:SER:CB	1:C:242:ASN:HB2	2.45	0.44
1:C:535:PHE:O	1:C:539:SER:OG	2.35	0.44
1:D:259:VAL:CG1	1:D:261:LEU:CB	2.95	0.44
1:D:515:LEU:HD11	1:D:539:SER:HB2	1.99	0.44
1:D:554:VAL:CG2	1:D:571:LEU:HD12	2.48	0.44
1:A:87:SER:N	1:A:429:GLU:OE1	2.50	0.44
1:C:509:CYS:O	1:C:510:ARG:C	2.61	0.44
1:D:231:ILE:C	1:D:231:ILE:HD13	2.43	0.44
1:A:320:VAL:HG11	1:C:78:ILE:CD1	2.48	0.44
1:B:301:LEU:HA	1:B:301:LEU:HD12	1.60	0.44
1:C:329:VAL:O	1:C:329:VAL:HG13	2.18	0.44
1:C:360:CYS:O	1:C:361:ASN:C	2.60	0.44
1:D:506:VAL:CG1	1:D:512:VAL:CG1	2.96	0.43
1:B:351:LEU:O	1:B:352:ALA:C	2.61	0.43
1:B:359:ARG:O	1:B:360:CYS:C	2.59	0.43
1:B:433:TYR:O	1:B:434:HIS:C	2.60	0.43
1:D:114:ILE:HG12	1:D:152:ALA:HB3	2.00	0.43
1:A:73:LEU:HD13	1:A:73:LEU:HD22	1.98	0.43
1:A:85:ALA:HB3	1:A:513:PHE:CZ	2.54	0.43
1:D:360:CYS:O	1:D:361:ASN:C	2.62	0.43
1:D:515:LEU:CD1	1:D:539:SER:HB2	2.48	0.43
1:C:434:HIS:O	1:C:435:ARG:O	2.36	0.43
1:D:85:ALA:CB	1:D:513:PHE:CZ	3.02	0.43
1:A:488:ARG:NH1	1:A:510:ARG:CB	2.63	0.43
1:C:545:PHE:C	1:C:546:LEU:HD23	2.43	0.43
1:B:260:ASP:N	1:B:260:ASP:CB	2.73	0.43
1:C:434:HIS:O	1:C:437:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HA	1:D:200:VAL:O	2.18	0.43
1:D:391:VAL:HG11	1:D:424:ILE:HB	2.00	0.43
1:D:442:ARG:HG2	1:D:457:ILE:HD11	1.99	0.43
1:A:69:PHE:O	1:A:72:HIS:HB3	2.18	0.43
1:C:559:ARG:HD2	1:C:564:TYR:CE1	2.51	0.43
1:D:225:SER:OG	1:D:241:GLU:HB3	2.19	0.43
1:A:135:ARG:O	1:A:139:GLU:HG2	2.18	0.43
1:B:360:CYS:O	1:B:361:ASN:C	2.62	0.43
1:C:141:PHE:C	1:C:143:GLY:H	2.26	0.43
1:C:442:ARG:NH2	1:D:442:ARG:NH2	2.55	0.43
1:D:85:ALA:HB2	1:D:545:PHE:CE2	2.54	0.43
1:D:234:GLU:OE1	1:D:234:GLU:O	2.36	0.43
1:D:545:PHE:C	1:D:546:LEU:HD23	2.44	0.43
1:A:125:GLU:CD	1:A:125:GLU:N	2.77	0.43
1:B:515:LEU:CD1	1:B:539:SER:HB2	2.48	0.43
1:C:144:SER:OG	1:C:144:SER:CA	2.58	0.43
1:B:505:GLN:O	1:B:508:LEU:HB2	2.19	0.43
1:C:71:GLU:O	1:C:72:HIS:C	2.61	0.43
1:C:297:VAL:O	1:C:301:LEU:HB2	2.19	0.43
1:C:410:LYS:NZ	1:C:410:LYS:HG3	2.33	0.43
1:C:452:THR:HG23	1:C:565:THR:CB	2.48	0.43
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.72	0.43
1:B:347:GLU:H	1:B:347:GLU:CD	2.25	0.42
1:C:497:THR:O	1:C:516:LEU:HD12	2.19	0.42
1:C:553:ILE:CD1	1:C:570:VAL:HG22	2.49	0.42
1:D:141:PHE:C	1:D:143:GLY:H	2.26	0.42
1:D:210:VAL:HG11	1:D:258:GLN:O	2.19	0.42
1:D:375:GLU:C	1:D:377:MET:N	2.75	0.42
1:D:559:ARG:HD2	1:D:564:TYR:CE1	2.52	0.42
1:A:313:LYS:HD2	1:A:334:MET:SD	2.59	0.42
1:A:371:THR:HG22	1:A:372:GLN:HG3	2.01	0.42
1:A:506:VAL:HG13	1:A:512:VAL:HG11	2.01	0.42
1:C:168:GLN:O	1:C:170:GLY:N	2.52	0.42
1:A:209:ARG:HD3	1:A:210:VAL:HG22	2.01	0.42
1:B:435:ARG:O	1:B:436:GLN:C	2.62	0.42
1:B:438:PHE:O	1:B:439:GLU:C	2.60	0.42
1:C:156:ASP:OD1	1:C:156:ASP:C	2.62	0.42
1:C:369:CYS:SG	1:C:373:MET:HE3	2.59	0.42
1:A:296:ALA:O	1:A:297:VAL:C	2.61	0.42
1:A:488:ARG:NH1	1:A:510:ARG:HD2	2.34	0.42
1:B:70:LEU:O	1:B:71:GLU:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LEU:HD22	1:B:542:LEU:O	2.20	0.42
1:C:232:GLY:HA2	1:C:233:PRO:HD3	1.83	0.42
1:C:525:TRP:CE2	1:C:560:PRO:HG3	2.54	0.42
1:D:488:ARG:HH11	1:D:510:ARG:HD2	1.83	0.42
1:D:566:ASN:OD1	1:D:567:ILE:HG13	2.19	0.42
1:A:460:VAL:HG21	1:A:487:TYR:HB2	2.00	0.42
1:B:488:ARG:NH1	1:B:510:ARG:CD	2.82	0.42
1:C:336:ALA:HB1	3:C:581:PGA:C2	2.50	0.42
1:D:116:ARG:HH11	1:D:116:ARG:HD3	1.69	0.42
1:D:329:VAL:O	1:D:329:VAL:HG13	2.20	0.42
1:A:134:VAL:O	1:A:135:ARG:C	2.62	0.42
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.64	0.42
1:A:545:PHE:CB	1:A:546:LEU:HD23	2.49	0.42
1:C:375:GLU:C	1:C:377:MET:N	2.75	0.42
1:C:467:CYS:O	1:C:468:ALA:C	2.62	0.42
1:D:188:ASP:CG	1:D:191:PHE:HD1	2.27	0.42
1:D:296:ALA:O	1:D:297:VAL:C	2.63	0.42
1:D:553:ILE:CD1	1:D:570:VAL:HG22	2.49	0.42
1:B:60:GLN:HB2	1:B:430:ALA:O	2.20	0.42
1:B:69:PHE:O	1:B:72:HIS:HB3	2.20	0.42
1:B:175:VAL:HG13	1:B:197:ALA:HA	2.01	0.42
1:B:525:TRP:NE1	1:B:560:PRO:HG3	2.34	0.42
1:C:116:ARG:HH11	1:C:116:ARG:HD3	1.63	0.42
1:D:118:ASN:OD1	1:D:118:ASN:C	2.63	0.42
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.64	0.42
1:A:70:LEU:O	1:A:73:LEU:HB2	2.19	0.42
1:A:434:HIS:O	1:A:435:ARG:O	2.37	0.42
1:D:261:LEU:HA	1:D:262:PRO:HD3	1.89	0.42
1:D:334:MET:HA	1:D:368:VAL:HB	2.02	0.42
1:D:384:THR:OG1	1:D:387:GLU:HG3	2.19	0.42
1:A:87:SER:OG	1:A:510:ARG:CG	2.68	0.41
1:C:168:GLN:HB2	1:C:195:GLY:O	2.20	0.41
1:C:566:ASN:OD1	1:C:567:ILE:HG13	2.19	0.41
1:D:187:VAL:HG11	1:D:205:PRO:HA	2.02	0.41
1:D:375:GLU:O	1:D:376:SER:C	2.62	0.41
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.86	0.41
1:A:354:LYS:NZ	1:A:397:ASP:OD1	2.40	0.41
1:A:423:ALA:HB1	1:C:347:GLU:HG2	2.01	0.41
1:A:545:PHE:HB3	1:A:546:LEU:HD23	2.02	0.41
1:A:255:PRO:C	1:A:257:ALA:N	2.78	0.41
1:B:322:ARG:NH2	1:B:325:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:NH1	1:B:385:ARG:HG2	2.36	0.41
1:B:476:THR:N	2:B:580:FBP:O4P	2.54	0.41
1:D:219:ILE:HG12	1:D:252:VAL:HG22	2.02	0.41
1:D:309:LYS:HG2	1:D:505:GLN:NE2	2.35	0.41
1:A:124:HIS:HE1	1:A:271:ASP:OD1	2.03	0.41
1:A:506:VAL:C	1:A:508:LEU:N	2.77	0.41
1:A:372:GLN:HA	1:A:375:GLU:HG2	2.01	0.41
1:A:433:TYR:CD2	1:A:436:GLN:HB2	2.56	0.41
1:A:452:THR:HG22	1:A:483:LEU:HD12	2.02	0.41
1:B:260:ASP:OD1	1:B:260:ASP:C	2.63	0.41
1:B:341:GLY:HA3	1:D:385:ARG:HE	1.85	0.41
1:B:545:PHE:CB	1:B:546:LEU:HD23	2.51	0.41
1:C:224:ILE:HG22	1:C:225:SER:N	2.34	0.41
1:C:435:ARG:O	1:C:436:GLN:C	2.62	0.41
1:C:449:ARG:NH1	1:D:466:CYS:O	2.53	0.41
1:C:470:ALA:HA	1:C:491:ALA:HB1	2.01	0.41
1:C:476:THR:H	2:C:580:FBP:H61	1.85	0.41
1:D:448:SER:OG	1:D:449:ARG:N	2.54	0.41
1:D:387:GLU:O	1:D:388:THR:C	2.61	0.41
1:D:433:TYR:O	1:D:434:HIS:C	2.63	0.41
1:A:91:ILE:HD13	1:A:284:PHE:CZ	2.55	0.41
1:A:542:LEU:HD22	1:A:542:LEU:O	2.21	0.41
1:C:290:LYS:O	1:C:291:ALA:C	2.64	0.41
1:D:284:PHE:CD2	1:D:334:MET:HE1	2.55	0.41
1:A:225:SER:HB3	1:A:242:ASN:H	1.85	0.41
1:A:349:VAL:O	1:A:350:PHE:C	2.61	0.41
1:D:93:THR:HA	1:D:116:ARG:HB3	2.03	0.41
1:D:174:GLU:HB3	1:D:245:VAL:HG13	2.03	0.41
1:D:435:ARG:O	1:D:436:GLN:C	2.64	0.41
1:A:116:ARG:NH2	1:A:156:ASP:OD2	2.46	0.41
1:A:157:THR:HG22	1:A:286:SER:HB2	2.02	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.90	0.41
1:B:296:ALA:O	1:B:297:VAL:C	2.64	0.41
1:B:372:GLN:HG2	1:B:375:GLU:HG3	2.03	0.41
1:C:77:ASP:O	1:C:80:SER:HB2	2.21	0.41
1:C:263:GLY:O	1:C:264:LEU:HD12	2.21	0.41
1:C:333:ILE:HG22	1:C:334:MET:N	2.35	0.41
1:D:220:ASP:C	1:D:222:GLY:N	2.79	0.41
1:D:372:GLN:HA	1:D:375:GLU:HG2	2.03	0.41
1:D:467:CYS:O	1:D:468:ALA:C	2.64	0.41
1:B:124:HIS:HE1	1:B:271:ASP:OD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:O	1:B:209:ARG:HG2	2.21	0.41
1:C:66:ALA:HB1	1:C:71:GLU:HB3	2.02	0.41
1:C:372:GLN:HA	1:C:375:GLU:HG2	2.02	0.41
1:D:332:GLY:C	1:D:333:ILE:HG12	2.46	0.41
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.76	0.40
1:C:144:SER:OG	1:C:144:SER:N	2.55	0.40
1:D:261:LEU:HD12	1:D:262:PRO:HD2	2.02	0.40
1:D:372:GLN:HG2	1:D:375:GLU:HG3	2.03	0.40
1:A:103:ARG:HH11	1:A:103:ARG:HD2	1.71	0.40
1:A:532:ARG:HH22	2:A:580:FBP:P1	2.43	0.40
1:D:72:HIS:NE2	1:D:431:ALA:O	2.54	0.40
1:D:193:THR:C	1:D:195:GLY:H	2.29	0.40
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.84	0.40
1:C:191:PHE:O	1:C:192:ARG:C	2.64	0.40
1:A:446:PRO:O	1:A:447:LEU:C	2.64	0.40
1:A:485:SER:O	1:A:486:ARG:C	2.64	0.40
1:C:515:LEU:CD1	1:C:539:SER:HB2	2.52	0.40
1:D:433:TYR:CD2	1:D:436:GLN:HB2	2.56	0.40
1:A:381:PRO:HB3	1:A:413:PHE:CE2	2.57	0.40
1:B:157:THR:HG22	1:B:286:SER:HB2	2.04	0.40
1:B:334:MET:HA	1:B:368:VAL:HB	2.04	0.40
1:C:380:LYS:HE2	1:C:380:LYS:HB3	1.72	0.40

All (3) 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:209:ARG:NH2	1:C:449:ARG:NH2[1_655]	1.91	0.29
1:B:102:GLU:CD	1:C:534:GLN:NE2[2_545]	2.07	0.13
1:B:102:GLU:OE2	1:C:534:GLN:NE2[2_545]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	502/528 (95%)	447 (89%)	46 (9%)	9 (2%)	6	11
1	B	470/528 (89%)	426 (91%)	32 (7%)	12 (3%)	4	6
1	C	510/528 (97%)	465 (91%)	36 (7%)	9 (2%)	6	11
1	D	487/528 (92%)	442 (91%)	36 (7%)	9 (2%)	6	11
All	All	1969/2112 (93%)	1780 (90%)	150 (8%)	39 (2%)	6	10

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	525	TRP
1	A	526	ALA
1	B	84	ALA
1	B	435	ARG
1	B	525	TRP
1	B	526	ALA
1	C	84	ALA
1	C	435	ARG
1	C	525	TRP
1	C	526	ALA
1	D	84	ALA
1	D	435	ARG
1	D	525	TRP
1	D	526	ALA
1	A	287	PHE
1	A	435	ARG
1	B	220	ASP
1	B	287	PHE
1	B	486	ARG
1	C	168	GLN
1	C	486	ARG
1	D	193	THR
1	B	98	SER
1	D	197	ALA
1	A	371	THR
1	B	338	GLY
1	A	192	ARG
1	B	256	GLY
1	B	566	ASN
1	C	371	THR

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Mol	Chain	Res	Type
1	D	194	ARG
1	D	287	PHE
1	D	371	THR
1	A	486	ARG
1	B	371	THR
1	C	287	PHE
1	A	170	GLY
1	C	256	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/423 (96%)	360 (89%)	45 (11%)	6	11
1	B	389/423 (92%)	347 (89%)	42 (11%)	6	11
1	C	412/423 (97%)	360 (87%)	52 (13%)	4	7
1	D	403/423 (95%)	358 (89%)	45 (11%)	6	11
All	All	1609/1692 (95%)	1425 (89%)	184 (11%)	5	10

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	83	VAL
1	A	87	SER
1	A	88	THR
1	A	99	ARG
1	A	103	ARG
1	A	104	LEU
1	A	108	ILE
1	A	125	GLU
1	A	144	SER
1	A	157	THR
1	A	167	LEU
1	A	177	LEU

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Mol	Chain	Res	Type
1	A	182	GLN
1	A	186	THR
1	A	200	VAL
1	A	202	VAL
1	A	210	VAL
1	A	229	GLN
1	A	258	GLN
1	A	289	ARG
1	A	294	VAL
1	A	298	ARG
1	A	301	LEU
1	A	308	ILE
1	A	327	LEU
1	A	329	VAL
1	A	337	ARG
1	A	359	ARG
1	A	374	LEU
1	A	379	THR
1	A	388	THR
1	A	396	LEU
1	A	402	ILE
1	A	473	VAL
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	548	VAL
1	A	552	VAL
1	A	559	ARG
1	A	562	SER
1	B	58	GLN
1	B	61	LEU
1	B	67	ASP
1	B	83	VAL
1	B	86	ARG
1	B	99	ARG
1	B	103	ARG
1	B	104	LEU
1	B	144	SER
1	B	157	THR

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Mol	Chain	Res	Type
1	B	182	GLN
1	B	183	VAL
1	B	186	THR
1	B	202	VAL
1	B	210	VAL
1	B	260	ASP
1	B	289	ARG
1	B	294	VAL
1	B	298	ARG
1	B	325	GLU
1	B	327	LEU
1	B	329	VAL
1	B	337	ARG
1	B	359	ARG
1	B	374	LEU
1	B	379	THR
1	B	388	THR
1	B	396	LEU
1	B	402	ILE
1	B	410	LYS
1	B	473	VAL
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	548	VAL
1	B	552	VAL
1	B	559	ARG
1	B	562	SER
1	C	61	LEU
1	C	71	GLU
1	C	80	SER
1	C	83	VAL
1	C	86	ARG
1	C	88	THR
1	C	99	ARG
1	C	103	ARG
1	C	104	LEU
1	C	108	ILE

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Mol	Chain	Res	Type
1	C	144	SER
1	C	147	SER
1	C	157	THR
1	C	167	LEU
1	C	173	SER
1	C	182	GLN
1	C	186	THR
1	C	200	VAL
1	C	202	VAL
1	C	210	VAL
1	C	229	GLN
1	C	231	ILE
1	C	234	GLU
1	C	238	THR
1	C	289	ARG
1	C	294	VAL
1	C	298	ARG
1	C	304	GLU
1	C	308	ILE
1	C	325	GLU
1	C	327	LEU
1	C	329	VAL
1	C	337	ARG
1	C	359	ARG
1	C	374	LEU
1	C	379	THR
1	C	380	LYS
1	C	388	THR
1	C	396	LEU
1	C	473	VAL
1	C	486	ARG
1	C	506	VAL
1	C	508	LEU
1	C	539	SER
1	C	542	LEU
1	C	546	LEU
1	C	548	VAL
1	C	552	VAL
1	C	559	ARG
1	C	562	SER
1	C	568	MET
1	C	571	LEU

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Mol	Chain	Res	Type
1	D	83	VAL
1	D	87	SER
1	D	99	ARG
1	D	103	ARG
1	D	104	LEU
1	D	108	ILE
1	D	144	SER
1	D	157	THR
1	D	167	LEU
1	D	172	GLU
1	D	176	GLU
1	D	182	GLN
1	D	200	VAL
1	D	202	VAL
1	D	209	ARG
1	D	210	VAL
1	D	231	ILE
1	D	234	GLU
1	D	248	SER
1	D	254	LEU
1	D	289	ARG
1	D	294	VAL
1	D	298	ARG
1	D	304	GLU
1	D	308	ILE
1	D	325	GLU
1	D	327	LEU
1	D	329	VAL
1	D	337	ARG
1	D	359	ARG
1	D	374	LEU
1	D	388	THR
1	D	396	LEU
1	D	473	VAL
1	D	486	ARG
1	D	506	VAL
1	D	508	LEU
1	D	534	GLN
1	D	539	SER
1	D	542	LEU
1	D	546	LEU
1	D	548	VAL

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Mol	Chain	Res	Type
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	133	ASN
1	A	168	GLN
1	A	182	GLN
1	A	198	ASN
1	A	258	GLN
1	A	421	GLN
1	A	534	GLN
1	B	57	GLN
1	B	124	HIS
1	B	133	ASN
1	B	353	GLN
1	B	421	GLN
1	B	436	GLN
1	C	124	HIS
1	C	133	ASN
1	C	168	GLN
1	C	182	GLN
1	C	353	GLN
1	C	421	GLN
1	C	534	GLN
1	D	121	HIS
1	D	124	HIS
1	D	133	ASN
1	D	182	GLN
1	D	198	ASN
1	D	253	ASN
1	D	421	GLN
1	D	534	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
2	FBP	C	580	-	18,20,20	0.97	1 (5%)	21,32,32	0.90	0
2	FBP	D	580	-	18,20,20	1.02	2 (11%)	21,32,32	0.94	2 (9%)
3	PGA	B	581	5	8,8,8	1.22	1 (12%)	10,11,11	2.31	3 (30%)
3	PGA	A	581	5	8,8,8	6.89	4 (50%)	10,11,11	2.22	5 (50%)
2	FBP	B	580	-	18,20,20	1.44	3 (16%)	21,32,32	0.78	1 (4%)
3	PGA	C	581	5	8,8,8	3.78	5 (62%)	10,11,11	3.18	4 (40%)
3	PGA	D	581	5	8,8,8	12.63	2 (25%)	10,11,11	3.47	4 (40%)
2	FBP	A	580	-	18,20,20	1.01	1 (5%)	21,32,32	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	C	580	-	-	5/13/32/32	0/1/1/1
2	FBP	D	580	-	-	8/13/32/32	0/1/1/1
3	PGA	B	581	5	-	3/6/6/6	-
3	PGA	A	581	5	-	6/6/6/6	-

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	581	PGA	O1P-C2	35.52	1.78	1.43
3	A	581	PGA	O1P-C2	18.82	1.62	1.43
3	C	581	PGA	O2-C1	-6.14	1.10	1.30
3	C	581	PGA	O1-C1	5.58	1.40	1.22
3	C	581	PGA	O1P-C2	-5.22	1.38	1.43
2	B	580	FBP	O2-C2	4.82	1.49	1.40
2	A	580	FBP	O2-C2	3.39	1.46	1.40
2	C	580	FBP	O2-C2	3.17	1.46	1.40
3	C	581	PGA	P-O2P	3.10	1.60	1.50
3	D	581	PGA	C2-C1	2.84	1.59	1.50
2	D	580	FBP	O2-C2	2.81	1.45	1.40
3	A	581	PGA	P-O2P	2.79	1.59	1.50
3	A	581	PGA	O2-C1	2.48	1.39	1.30
2	B	580	FBP	P1-O1	2.22	1.67	1.60
3	C	581	PGA	P-O3P	-2.18	1.46	1.54
3	A	581	PGA	P-O1P	2.15	1.67	1.60
2	B	580	FBP	P1-O1P	2.15	1.57	1.50
3	B	581	PGA	O2-C1	-2.04	1.24	1.30
2	D	580	FBP	P1-O1	2.04	1.66	1.60

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	581	PGA	O1P-C2-C1	-9.86	95.67	110.54
3	C	581	PGA	O3P-P-O1P	-6.38	90.05	106.67
3	C	581	PGA	O1P-C2-C1	-6.29	101.06	110.54
3	B	581	PGA	O1P-C2-C1	-5.24	102.63	110.54
3	B	581	PGA	O3P-P-O1P	-3.94	96.38	106.67
3	A	581	PGA	O1P-C2-C1	-3.54	105.20	110.54
3	C	581	PGA	O3P-P-O2P	3.27	123.56	110.83
3	A	581	PGA	O1P-P-O2P	3.23	115.17	106.44
3	A	581	PGA	O3P-P-O1P	-3.08	98.63	106.67
3	D	581	PGA	O3P-P-O1P	2.98	114.44	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	581	PGA	O4P-P-O1P	-2.40	100.40	106.67
2	D	580	FBP	O6-C6-C5	-2.38	100.88	108.99
3	B	581	PGA	O3P-P-O2P	2.33	119.92	110.83
3	D	581	PGA	O1P-P-O2P	2.20	112.40	106.44
3	A	581	PGA	O3P-P-O2P	-2.20	102.26	110.83
3	A	581	PGA	O4P-P-O1P	2.15	112.27	106.67
2	B	580	FBP	O3P-P1-O1	2.09	112.11	106.67
3	C	581	PGA	O2-C1-O1	2.04	128.59	123.33
2	D	580	FBP	O1-P1-O1P	2.03	111.93	106.44

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	580	FBP	C1-O1-P1-O2P
2	A	580	FBP	C1-O1-P1-O3P
2	B	580	FBP	C6-O6-P2-O5P
2	B	580	FBP	C6-O6-P2-O6P
2	C	580	FBP	C6-O6-P2-O5P
2	C	580	FBP	C6-O6-P2-O6P
2	D	580	FBP	C1-O1-P1-O1P
2	D	580	FBP	C1-O1-P1-O2P
2	D	580	FBP	C1-O1-P1-O3P
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	A	581	PGA	C1-C2-O1P-P
3	B	581	PGA	C2-O1P-P-O3P
3	B	581	PGA	C2-O1P-P-O4P
3	C	581	PGA	C2-O1P-P-O3P
3	C	581	PGA	C2-O1P-P-O4P
3	D	581	PGA	C2-O1P-P-O2P
3	D	581	PGA	C2-O1P-P-O3P
3	D	581	PGA	C2-O1P-P-O4P
3	A	581	PGA	O1-C1-C2-O1P
3	A	581	PGA	O2-C1-C2-O1P
3	D	581	PGA	O2-C1-C2-O1P
2	A	580	FBP	O5-C5-C6-O6
2	B	580	FBP	C4-C5-C6-O6
2	B	580	FBP	O5-C5-C6-O6

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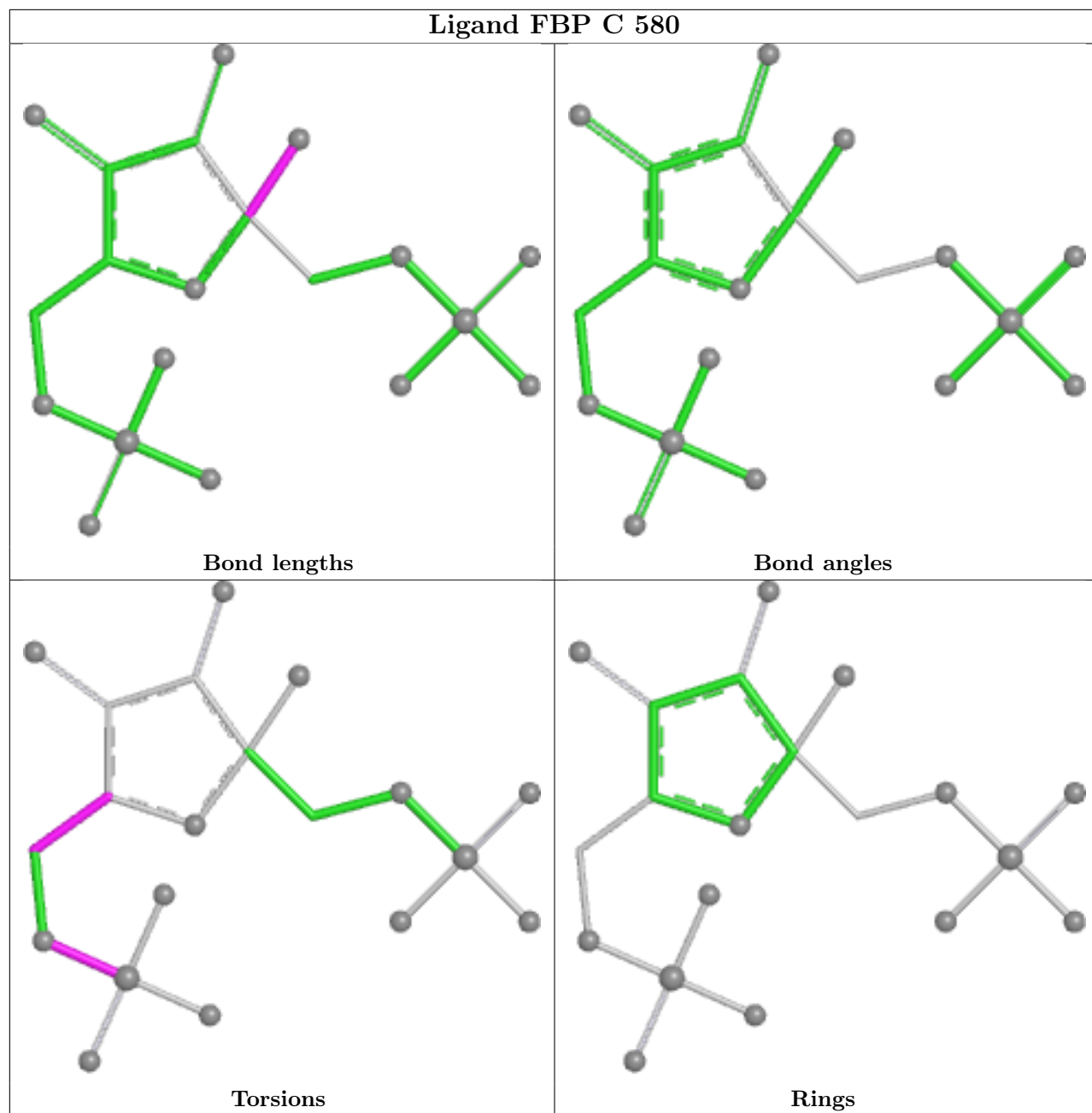
Mol	Chain	Res	Type	Atoms
2	C	580	FBP	O5-C5-C6-O6
2	D	580	FBP	O5-C5-C6-O6
3	D	581	PGA	O1-C1-C2-O1P
2	C	580	FBP	C4-C5-C6-O6
2	D	580	FBP	C4-C5-C6-O6
2	A	580	FBP	C6-O6-P2-O4P
2	B	580	FBP	C6-O6-P2-O4P
2	C	580	FBP	C6-O6-P2-O4P
2	D	580	FBP	C6-O6-P2-O4P
3	B	581	PGA	C2-O1P-P-O2P
3	C	581	PGA	C2-O1P-P-O2P
2	A	580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

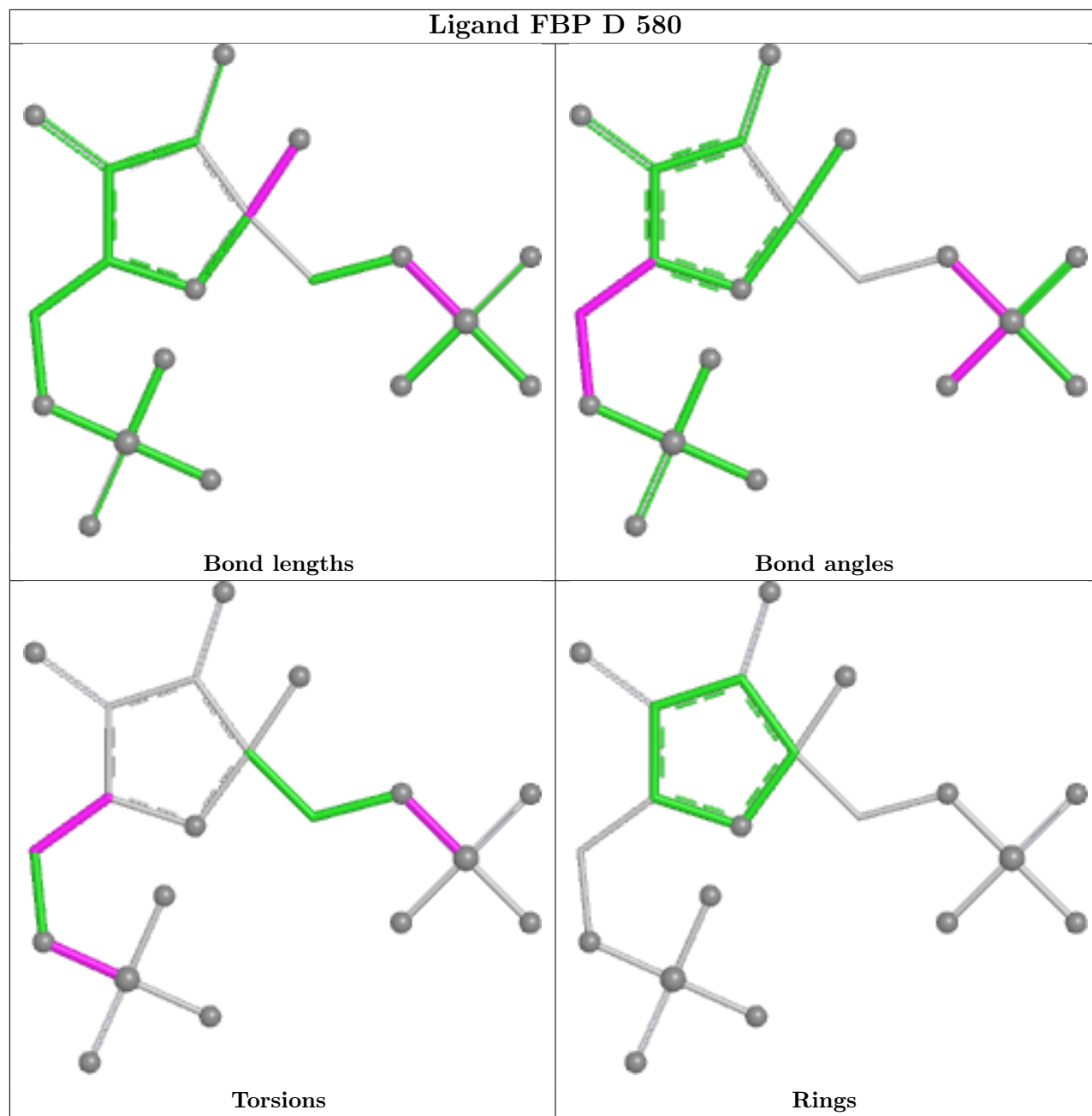
There are no ring outliers.

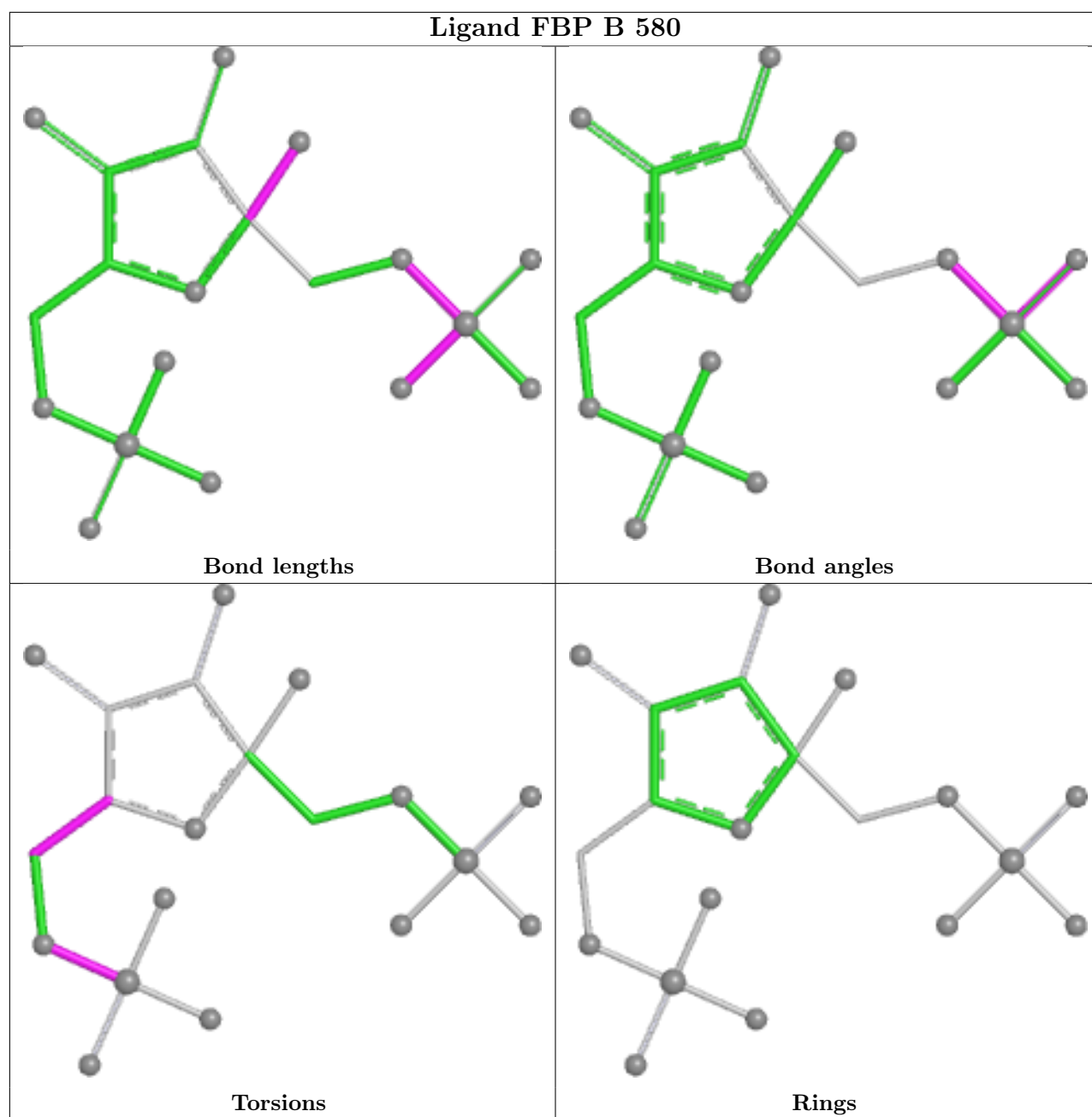
8 monomers are involved in 39 short contacts:

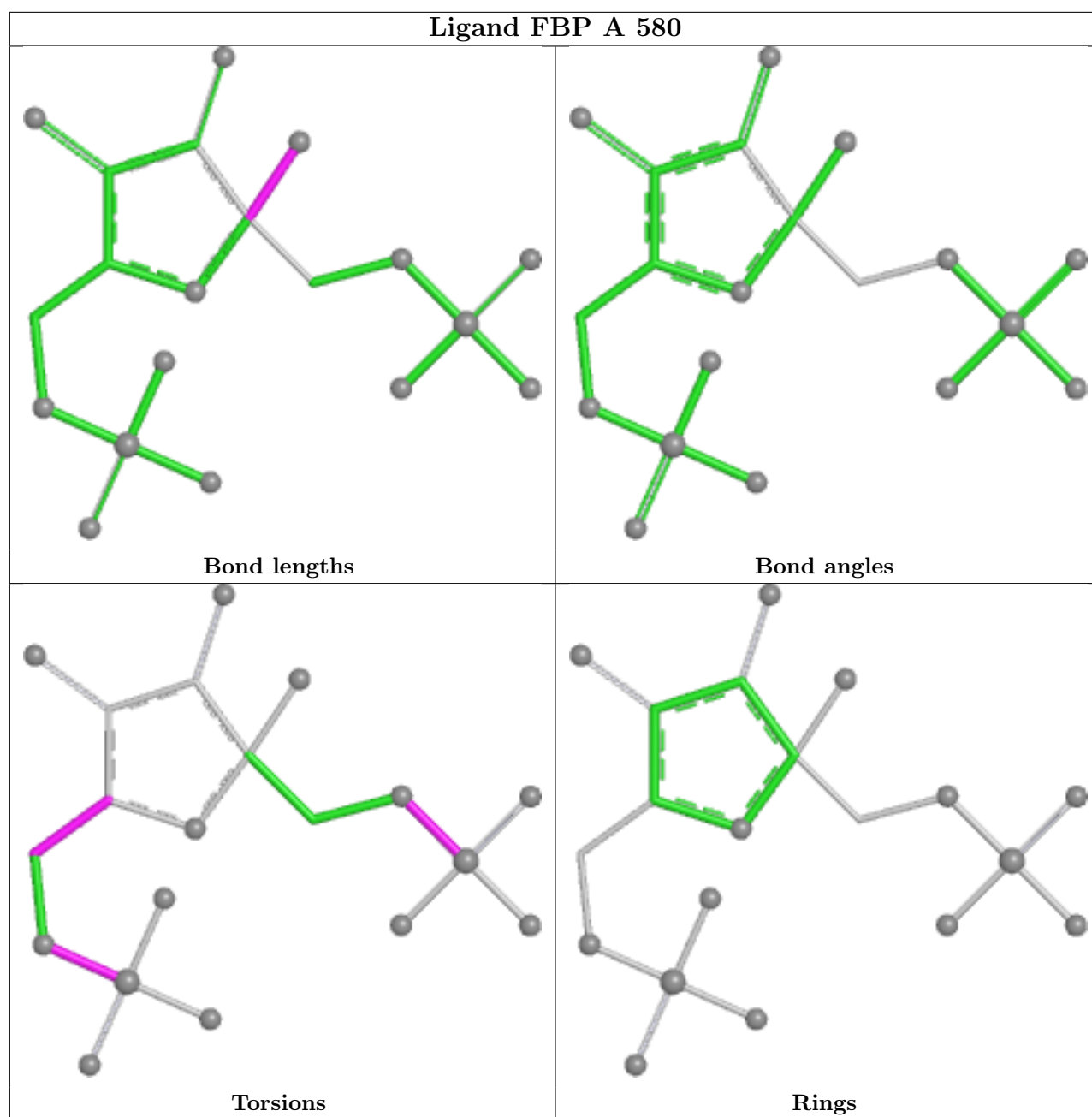
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	580	FBP	3	0
2	D	580	FBP	4	0
3	B	581	PGA	4	0
3	A	581	PGA	2	0
2	B	580	FBP	7	0
3	C	581	PGA	2	0
3	D	581	PGA	14	0
2	A	580	FBP	3	0

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	506/528 (95%)	0.41	23 (4%) 38 37	44, 56, 70, 94	0
1	B	483/528 (91%)	0.29	15 (3%) 51 49	43, 56, 71, 113	0
1	C	514/528 (97%)	0.28	20 (3%) 43 41	43, 56, 71, 128	0
1	D	501/528 (94%)	0.24	12 (2%) 59 56	44, 56, 70, 133	0
All	All	2004/2112 (94%)	0.30	70 (3%) 47 45	43, 56, 71, 133	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	LEU	5.4
1	D	263	GLY	4.8
1	C	78	ILE	4.5
1	D	300	ALA	4.0
1	C	258	GLN	3.8
1	A	237	VAL	3.8
1	B	60	GLN	3.5
1	D	195	GLY	3.5
1	A	441	LEU	3.4
1	D	304	GLU	3.3
1	C	137	ALA	3.3
1	D	306	HIS	3.2
1	B	142	ALA	3.2
1	B	228	VAL	3.1
1	B	197	ALA	3.0
1	D	535	PHE	3.0
1	A	521	PRO	3.0
1	B	143	GLY	2.9
1	C	70	LEU	2.9
1	D	80	SER	2.9
1	D	146	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	173	SER	2.8
1	B	200	VAL	2.8
1	C	306	HIS	2.8
1	B	227	VAL	2.8
1	C	195	GLY	2.7
1	A	167	LEU	2.7
1	C	62	PRO	2.7
1	A	306	HIS	2.7
1	C	61	LEU	2.6
1	A	548	VAL	2.6
1	B	245	VAL	2.6
1	A	432	VAL	2.5
1	B	175	VAL	2.5
1	C	328	GLU	2.5
1	C	145	PRO	2.5
1	D	74	CYS	2.5
1	A	221	ASP	2.5
1	A	146	LEU	2.4
1	A	185	VAL	2.4
1	C	490	ARG	2.4
1	D	161	GLU	2.3
1	A	335	VAL	2.3
1	B	240	VAL	2.3
1	B	177	LEU	2.3
1	C	435	ARG	2.2
1	A	153	ILE	2.2
1	B	444	ALA	2.2
1	D	500	ALA	2.2
1	C	60	GLN	2.2
1	A	528	ASP	2.2
1	A	175	VAL	2.2
1	C	67	ASP	2.1
1	B	98	SER	2.1
1	B	181	SER	2.1
1	C	335	VAL	2.1
1	A	166	ILE	2.1
1	A	437	LEU	2.1
1	C	79	ASP	2.0
1	A	64	ALA	2.0
1	A	520	PRO	2.0
1	C	436	GLN	2.0
1	C	434	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	185	VAL	2.0
1	B	545	PHE	2.0
1	A	495	ALA	2.0
1	A	147	SER	2.0
1	A	272	LEU	2.0
1	A	454	VAL	2.0
1	C	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](#)

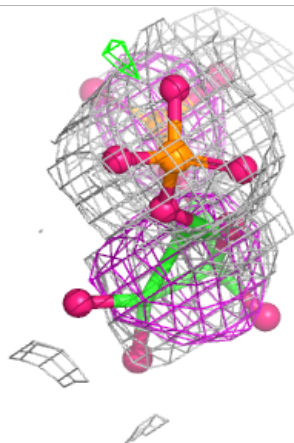
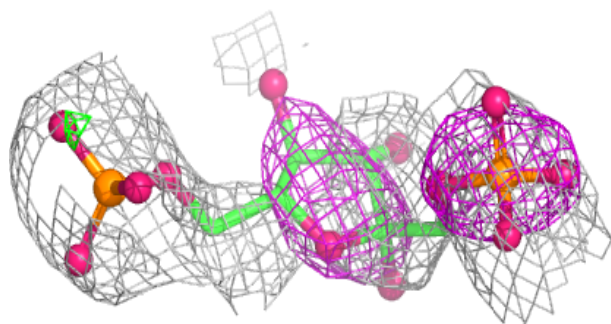
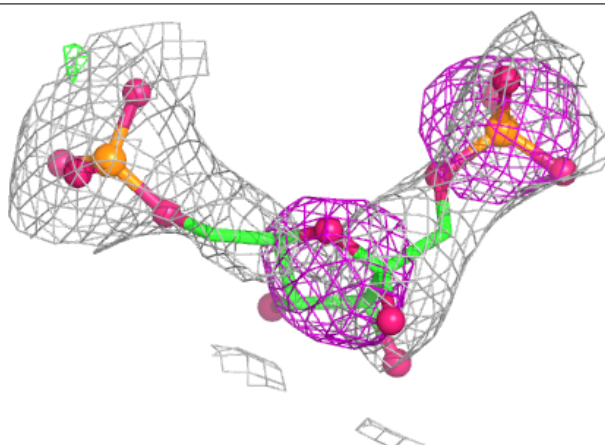
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FBP	A	580	20/20	0.69	0.16	85,102,104,104	0
2	FBP	B	580	20/20	0.69	0.18	87,104,107,108	0
2	FBP	D	580	20/20	0.74	0.18	72,86,90,92	0
2	FBP	C	580	20/20	0.79	0.14	80,90,94,95	0
3	PGA	C	581	9/9	0.80	0.17	92,92,93,94	0
3	PGA	D	581	9/9	0.81	0.15	92,92,92,92	0
3	PGA	A	581	9/9	0.84	0.16	91,92,92,92	0
3	PGA	B	581	9/9	0.84	0.13	95,97,98,98	0
4	K	A	582	1/1	0.86	0.12	91,91,91,91	0
4	K	D	594	1/1	0.91	0.10	91,91,91,91	0
4	K	B	586	1/1	0.92	0.08	91,91,91,91	0
4	K	C	590	1/1	0.96	0.06	91,91,91,91	0
5	MN	A	583	1/1	0.97	0.14	91,91,91,91	0
5	MN	B	587	1/1	0.97	0.10	93,93,93,93	0
5	MN	D	595	1/1	0.97	0.11	90,90,90,90	0
5	MN	C	591	1/1	0.98	0.14	91,91,91,91	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.

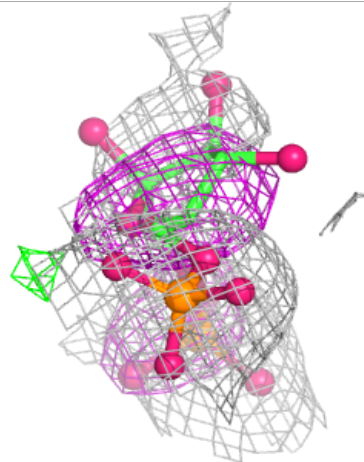
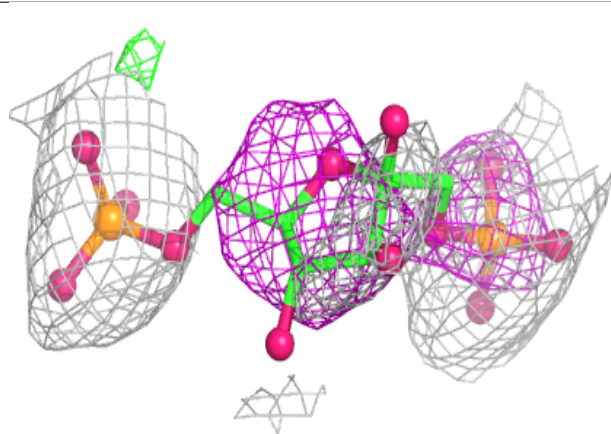
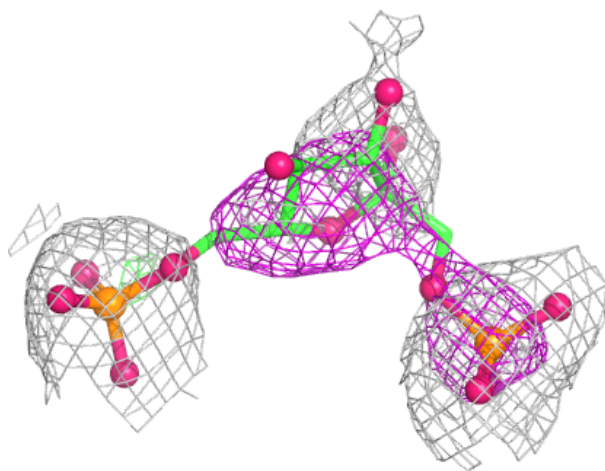
Electron density around FBP A 580:

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



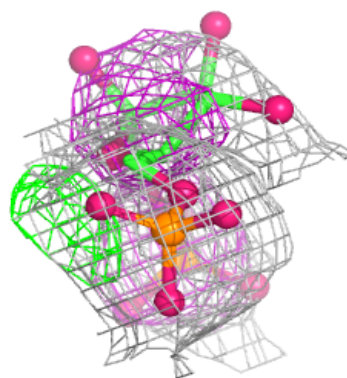
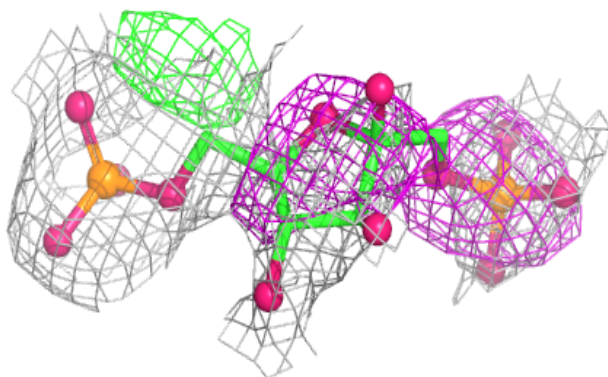
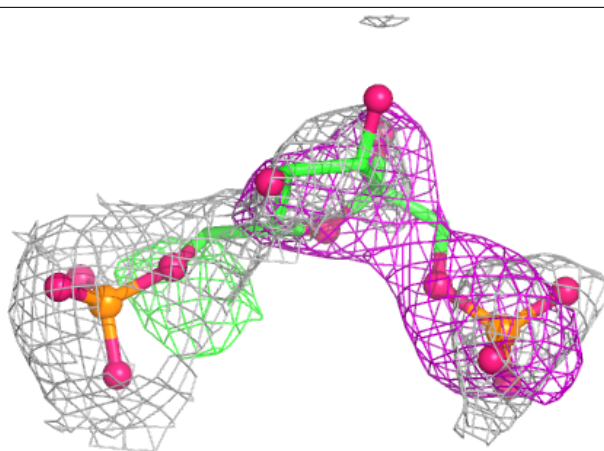
Electron density around FBP B 580:

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

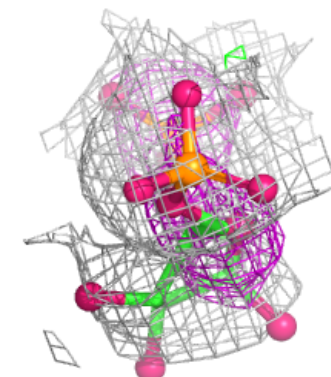
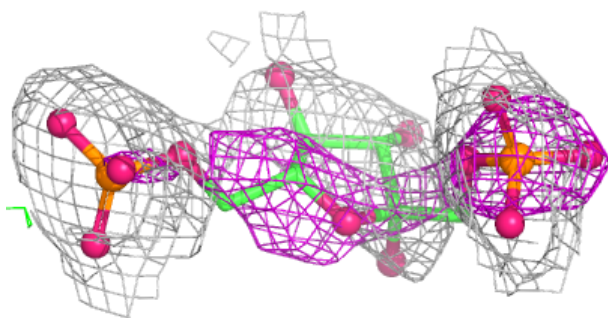
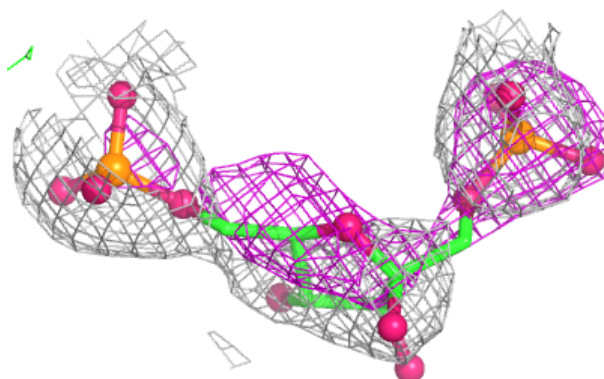


Electron density around FBP D 580:

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

**Electron density around FBP C 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.