



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:21 AM BST

PDB ID : 2VGG
Title : HUMAN ERYTHROCYTE PYRUVATE KINASE: R479H MUTANT
Authors : Valentini, G.; Chiarelli, L.R.; Fortin, R.; Dolzan, M.; Galizzi, A.; Abraham, D.J.; Wang, C.; Bianchi, P.; Zanella, A.; Mattevi, A.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

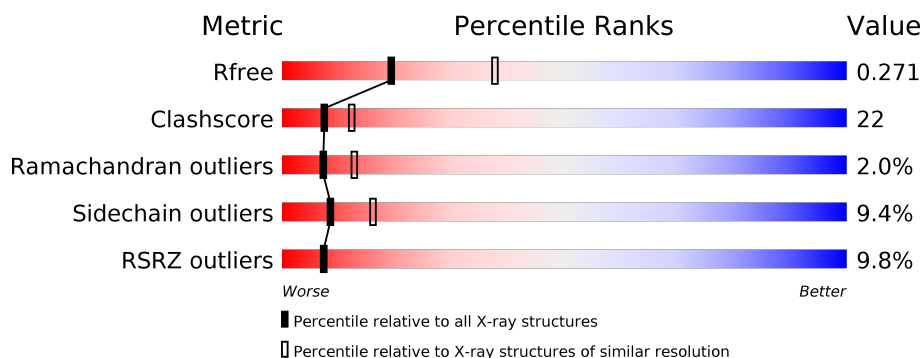
1 Overall quality at a glance

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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 on 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	<div> <div>11%</div> <div> <div></div> <div>55%</div> <div>33%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	528	<div> <div>10%</div> <div> <div></div> <div>53%</div> <div>31%</div> <div>6%</div> <div>• 9%</div> </div> </div>
1	C	528	<div> <div>7%</div> <div> <div></div> <div>55%</div> <div>36%</div> <div>5%</div> <div>• •</div> </div> </div>
1	D	528	<div> <div>8%</div> <div> <div></div> <div>55%</div> <div>31%</div> <div>8%</div> <div>• 5%</div> </div> </div>

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 crite-

ria:

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	D	581	-	-	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.

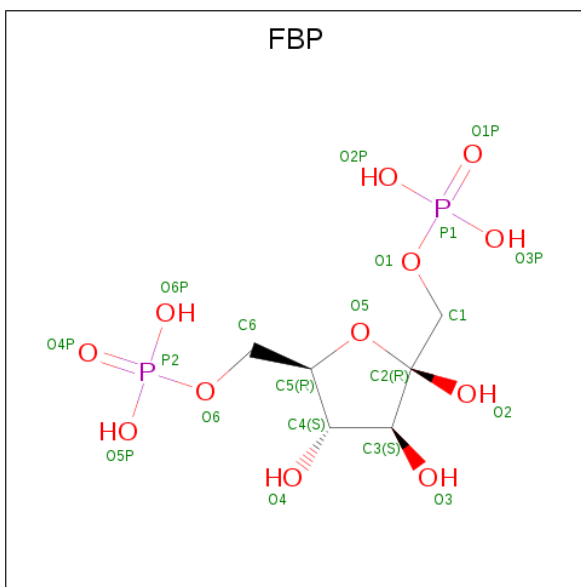
- Molecule 1 is a protein called PYRUVATE KINASE ISOZYMES R/L.

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:

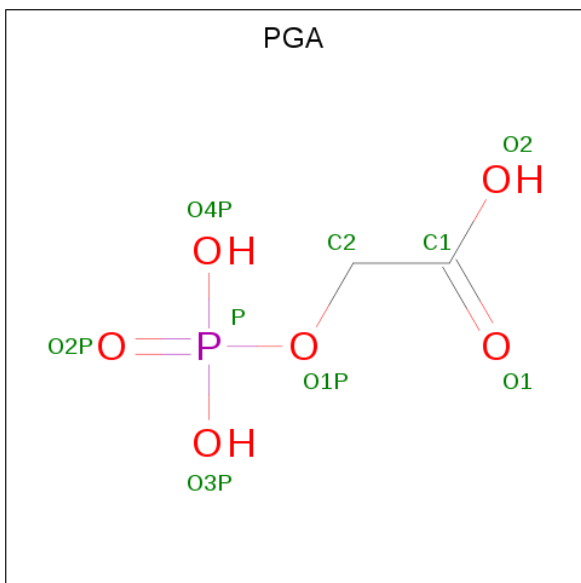
Chain	Residue	Modelled	Actual	Comment	Reference
A	479	HIS	ARG	engineered mutation	UNP P30613
B	479	HIS	ARG	engineered mutation	UNP P30613
C	479	HIS	ARG	engineered mutation	UNP P30613
D	479	HIS	ARG	engineered mutation	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: 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 (three-letter code: 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 (three-letter code: K) (formula: K).

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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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.

Chain A:

11% 55% 33% 7% . .

LEU THR GLN GLU GLY THR ALA PHE PRE GLN GLN GLN LEU PRO ALA A64 A65 A66 D67 T68 T69 T70 T71 T72 T73 T74 T75 T76 T77 T78 T79 T80 T81 T82 T83 T84 T85 T86 T87 T88 T89 T90 T91 T92 T93 T94 T95 T96 T97 T98 T99 T100

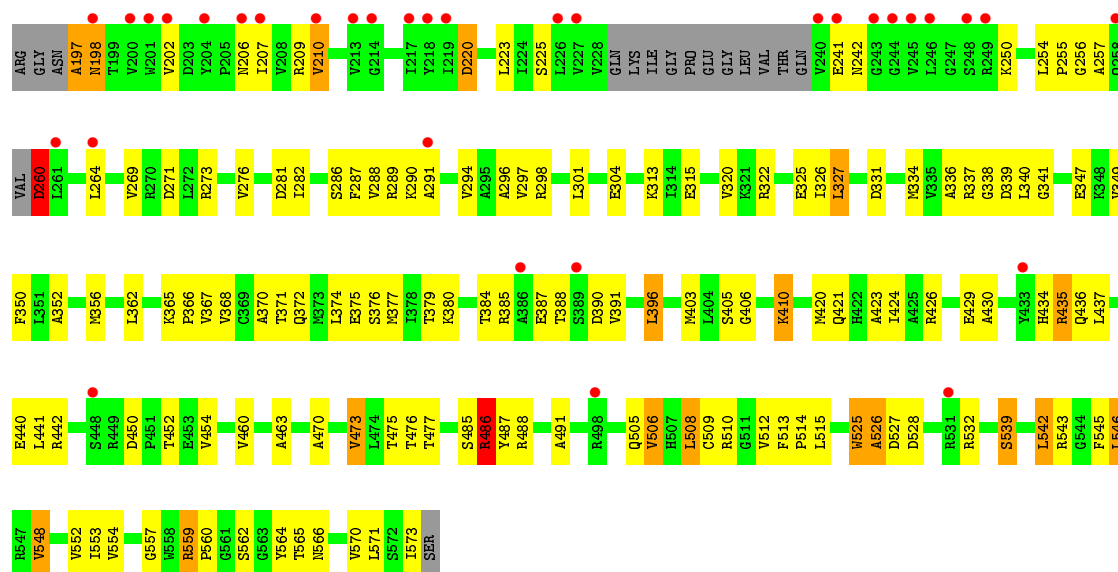
E129 E130 E131 E132 E133 E134 E135 E136 E137 E138 E139 E140 E141 E142 E143 E144 E145 E146 E147 E148 E149 E150 E151 E152 E153 E154 E155 E156 E157 E158 E159 E160 E161 E162 E163 E164 E165 E166 E167 E168 E169 E170 E171 E172 E173 E174 E175 E176 E177 E178 E179 E180 E181 E182 E183 E184 E185 E186 E187 E188 E189 E190 E191 E192 E193 E194 E195 E196 E197 E198 E199 E200

N206 N207 N208 N209 N210 N211 N212 N213 N214 N215 N216 N217 N218 N219 N220 N221 N222 N223 N224 N225 N226 N227 N228 N229 N230 N231 N232 N233 N234 N235 N236 N237 N238 N239 N240 N241 N242 N243 N244 N245 N246 N247 N248 N249 N250 N251 N252 N253 N254 N255 N256 N257 N258 N259 N260 N261 N262 N263 N264 N265 N266 N267 N268 N269 N270 N271 N272 N273 N274 N275 N276 N277 N278 N279 N280 N281 N282 N283 N284 N285 N286 N287 N288 N289 N290 N291 N292 N293 N294 N295 N296 N297 N298 N299 N300

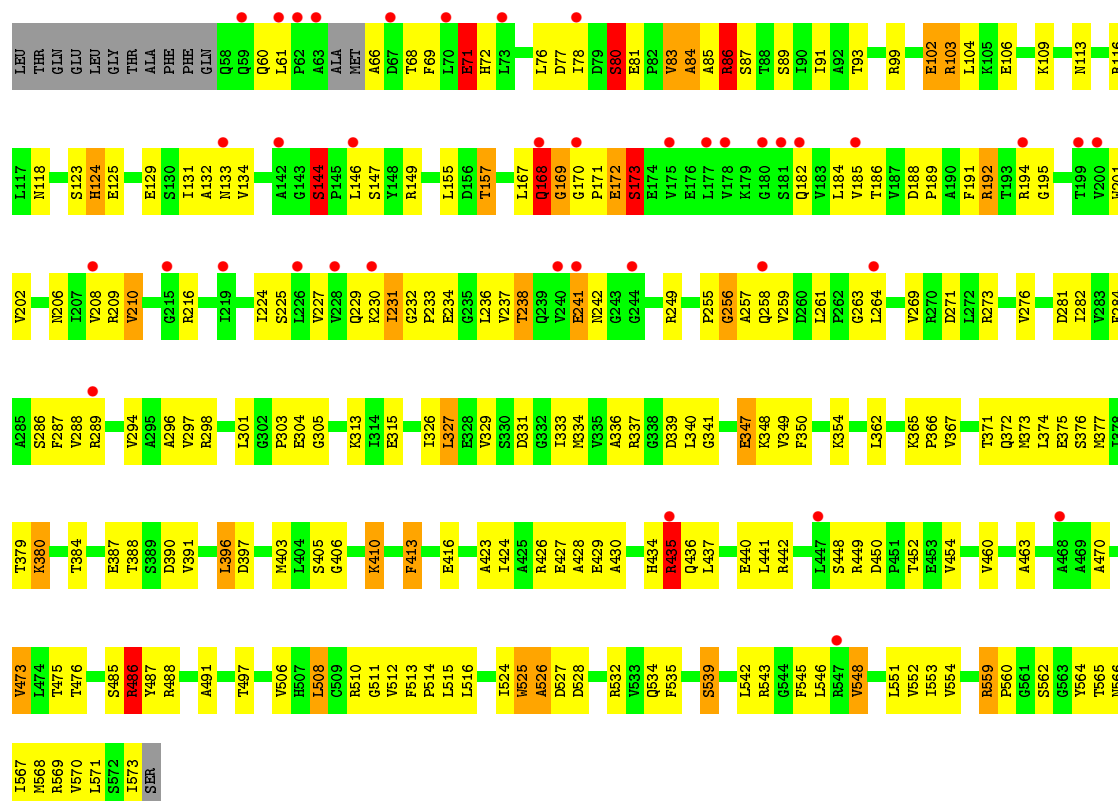
R382 P383 T384 R385 A386 E387 T388 S389 D390 V391 A392 L396 D397 G398 A399 D400 C401 M402 M403 L404 S405 G406 K410 F413 P414 V415 E416 M420 Q421 H422 A423 R426 E429 Y433 H434 R435 Q436 L437 E440 L441 R442 R449 D450 P451 T452 E453 V454 A456 V460 G557 W558 R559 P560 V561 L562 G563 Y564 L565 V570 L571 S572 I573 SER

Chain B:

Category	Percentage
Red	10%
Green	53%
Yellow	31%
Orange	6%
Grey	9%

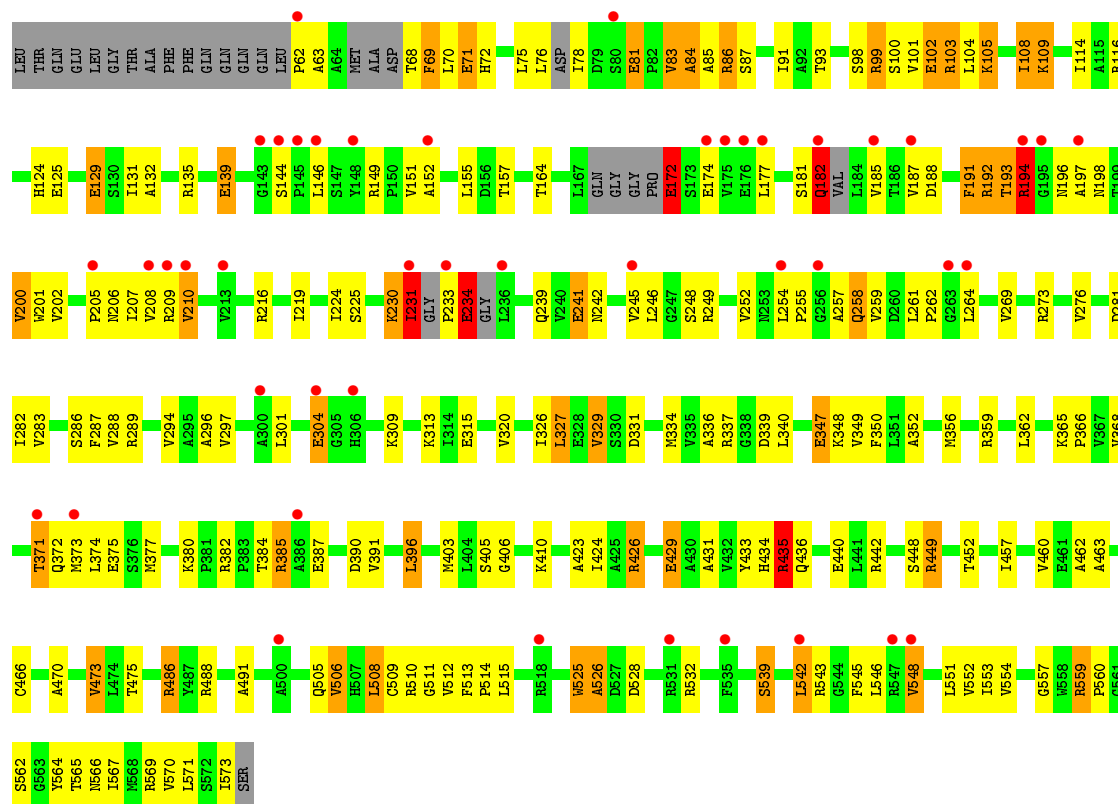


• Molecule 1: PYRUVATE KINASE ISOZYMES R/L



• 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 46.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.6 (20.00-2.74) 91.9 (46.49-2.60)	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 (1.32%)	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)	0.27 , 66.3	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: K, FBP, PGA, 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	1.27	40/3889 (1.0%)	1.01	23/5271 (0.4%)
1	B	1.25	24/3721 (0.6%)	0.94	14/5036 (0.3%)
1	C	1.41	36/3953 (0.9%)	1.08	26/5359 (0.5%)
1	D	1.43	44/3857 (1.1%)	1.19	22/5219 (0.4%)
All	All	1.34	144/15420 (0.9%)	1.06	85/20885 (0.4%)

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 (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	GLU	CD-OE1	44.98	1.75	1.25
1	B	144	SER	CB-OG	27.59	1.78	1.42
1	D	182	GLN	C-O	22.30	1.65	1.23
1	A	102	GLU	CG-CD	21.17	1.83	1.51
1	C	144	SER	CB-OG	21.03	1.69	1.42
1	D	230	LYS	CE-NZ	20.61	2.00	1.49
1	C	102	GLU	CD-OE1	20.35	1.48	1.25
1	A	382	ARG	CZ-NH2	19.35	1.58	1.33
1	A	103	ARG	CZ-NH2	-18.89	1.08	1.33
1	B	176	GLU	CD-OE1	18.52	1.46	1.25
1	D	194	ARG	CZ-NH1	-18.11	1.09	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	GLU	CD-OE2	17.75	1.45	1.25
1	B	198	ASN	CG-OD1	-17.50	0.85	1.24
1	D	231	ILE	C-O	16.99	1.55	1.23
1	D	109	LYS	CD-CE	16.74	1.93	1.51
1	D	234	GLU	CD-OE1	16.02	1.43	1.25
1	D	71	GLU	CD-OE1	-15.12	1.09	1.25
1	C	80	SER	CB-OG	15.08	1.61	1.42
1	D	382	ARG	CZ-NH2	14.35	1.51	1.33
1	D	71	GLU	CD-OE2	14.08	1.41	1.25
1	B	147	SER	CB-OG	13.97	1.60	1.42
1	C	123	SER	CB-OG	13.88	1.60	1.42
1	B	260	ASP	N-CA	13.68	1.73	1.46
1	A	382	ARG	NE-CZ	-13.50	1.15	1.33
1	B	129	GLU	CD-OE2	-13.06	1.11	1.25
1	B	139	GLU	CD-OE2	11.87	1.38	1.25
1	D	241	GLU	CD-OE1	11.70	1.38	1.25
1	A	192	ARG	CZ-NH1	11.69	1.48	1.33
1	B	198	ASN	CG-ND2	11.64	1.61	1.32
1	D	382	ARG	NE-CZ	11.44	1.48	1.33
1	D	149	ARG	CZ-NH2	10.92	1.47	1.33
1	A	426	ARG	CZ-NH1	10.91	1.47	1.33
1	C	192	ARG	CZ-NH1	10.74	1.47	1.33
1	A	109	LYS	CD-CE	10.41	1.77	1.51
1	B	176	GLU	CG-CD	10.39	1.67	1.51
1	A	130	SER	CB-OG	10.38	1.55	1.42
1	A	71	GLU	CD-OE1	10.33	1.37	1.25
1	A	158	LYS	CE-NZ	-10.11	1.23	1.49
1	C	102	GLU	CD-OE2	10.09	1.36	1.25
1	A	102	GLU	CD-OE1	-10.08	1.14	1.25
1	C	71	GLU	CB-CG	9.86	1.70	1.52
1	C	106	GLU	CD-OE1	9.82	1.36	1.25
1	C	103	ARG	CZ-NH1	9.82	1.45	1.33
1	A	103	ARG	NE-CZ	9.72	1.45	1.33
1	A	209	ARG	CZ-NH1	-9.63	1.20	1.33
1	A	169	GLY	C-N	9.54	1.50	1.33
1	C	410	LYS	CE-NZ	9.49	1.72	1.49
1	A	147	SER	CB-OG	9.39	1.54	1.42
1	A	229	GLN	CD-NE2	9.38	1.56	1.32
1	A	382	ARG	CD-NE	9.28	1.62	1.46
1	A	209	ARG	CZ-NH2	9.24	1.45	1.33
1	D	105	LYS	CE-NZ	9.20	1.72	1.49
1	B	410	LYS	CD-CE	9.09	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	234	GLU	CD-OE2	9.09	1.35	1.25
1	B	136	GLU	CD-OE2	-9.05	1.15	1.25
1	B	71	GLU	CB-CG	9.00	1.69	1.52
1	D	233	PRO	N-CA	8.96	1.62	1.47
1	B	106	GLU	CD-OE2	8.80	1.35	1.25
1	C	241	GLU	CD-OE1	8.70	1.35	1.25
1	A	258	GLN	CD-NE2	8.67	1.54	1.32
1	B	105	LYS	CE-NZ	8.48	1.70	1.49
1	A	258	GLN	CD-OE1	8.44	1.42	1.24
1	D	382	ARG	CZ-NH1	-8.41	1.22	1.33
1	C	125	GLU	CD-OE2	8.39	1.34	1.25
1	C	149	ARG	CZ-NH1	8.38	1.44	1.33
1	A	106	GLU	CG-CD	8.23	1.64	1.51
1	C	172	GLU	CD-OE2	8.01	1.34	1.25
1	A	83	VAL	CB-CG2	7.98	1.69	1.52
1	A	125	GLU	CD-OE1	7.95	1.34	1.25
1	D	194	ARG	NE-CZ	7.86	1.43	1.33
1	C	103	ARG	NE-CZ	7.82	1.43	1.33
1	A	410	LYS	CE-NZ	7.67	1.68	1.49
1	A	176	GLU	CD-OE2	7.47	1.33	1.25
1	C	216	ARG	CZ-NH1	7.38	1.42	1.33
1	C	125	GLU	CD-OE1	7.33	1.33	1.25
1	A	73	LEU	CG-CD2	7.27	1.78	1.51
1	C	149	ARG	CZ-NH2	-7.26	1.23	1.33
1	D	81	GLU	CD-OE1	7.11	1.33	1.25
1	D	181	SER	C-O	7.07	1.36	1.23
1	D	181	SER	CB-OG	7.06	1.51	1.42
1	B	161	GLU	CB-CG	7.02	1.65	1.52
1	B	176	GLU	CB-CG	6.99	1.65	1.52
1	B	67	ASP	CG-OD2	6.91	1.41	1.25
1	C	413	PHE	CD2-CE2	6.88	1.53	1.39
1	A	179	LYS	CE-NZ	6.85	1.66	1.49
1	A	103	ARG	CD-NE	6.83	1.58	1.46
1	D	125	GLU	CG-CD	6.81	1.62	1.51
1	D	239	GLN	CD-NE2	6.79	1.49	1.32
1	C	258	GLN	CG-CD	6.73	1.66	1.51
1	D	149	ARG	CZ-NH1	-6.59	1.24	1.33
1	A	136	GLU	CD-OE1	6.50	1.32	1.25
1	D	429	GLU	CD-OE1	6.50	1.32	1.25
1	C	189	PRO	CG-CD	6.49	1.72	1.50
1	D	230	LYS	CB-CG	6.48	1.70	1.52
1	D	216	ARG	CZ-NH2	6.48	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	233	PRO	N-CD	6.48	1.56	1.47
1	D	129	GLU	CB-CG	6.46	1.64	1.52
1	A	81	GLU	CD-OE2	6.44	1.32	1.25
1	A	401	CYS	CB-SG	-6.41	1.71	1.82
1	C	124	HIS	CE1-NE2	6.41	1.47	1.32
1	B	130	SER	CB-OG	6.40	1.50	1.42
1	C	129	GLU	CD-OE1	-6.29	1.18	1.25
1	B	62	PRO	CG-CD	6.23	1.71	1.50
1	C	173	SER	CB-OG	6.20	1.50	1.42
1	C	169	GLY	C-O	-6.20	1.13	1.23
1	D	193	THR	CB-OG1	6.14	1.55	1.43
1	D	62	PRO	CG-CD	6.12	1.70	1.50
1	A	123	SER	CB-OG	6.11	1.50	1.42
1	D	109	LYS	CE-NZ	6.01	1.64	1.49
1	D	192	ARG	CG-CD	5.95	1.66	1.51
1	A	106	GLU	CD-OE1	5.93	1.32	1.25
1	A	416	GLU	CG-CD	5.93	1.60	1.51
1	D	258	GLN	CD-NE2	5.93	1.47	1.32
1	B	100	SER	CB-OG	5.84	1.49	1.42
1	D	233	PRO	CA-CB	5.82	1.65	1.53
1	C	169	GLY	C-N	5.80	1.43	1.33
1	D	149	ARG	NE-CZ	5.77	1.40	1.33
1	C	109	LYS	CE-NZ	5.66	1.63	1.49
1	D	172	GLU	CD-OE1	5.66	1.31	1.25
1	C	168	GLN	CD-NE2	5.63	1.47	1.32
1	B	136	GLU	CD-OE1	5.57	1.31	1.25
1	B	149	ARG	CZ-NH1	5.56	1.40	1.33
1	A	161	GLU	CB-CG	5.55	1.62	1.52
1	A	125	GLU	CD-OE2	-5.51	1.19	1.25
1	D	139	GLU	CD-OE1	5.49	1.31	1.25
1	D	241	GLU	CD-OE2	5.45	1.31	1.25
1	C	168	GLN	CD-OE1	5.44	1.35	1.24
1	D	139	GLU	CD-OE2	-5.42	1.19	1.25
1	C	172	GLU	CD-OE1	5.39	1.31	1.25
1	D	69	PHE	CG-CD2	5.35	1.46	1.38
1	A	176	GLU	CB-CG	5.33	1.62	1.52
1	D	216	ARG	CZ-NH1	5.32	1.40	1.33
1	C	256	GLY	C-O	5.30	1.32	1.23
1	D	410	LYS	CE-NZ	5.27	1.62	1.49
1	C	241	GLU	CD-OE2	5.25	1.31	1.25
1	A	169	GLY	C-O	5.20	1.31	1.23
1	A	102	GLU	CD-OE2	5.17	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	ARG	CD-NE	5.12	1.55	1.46
1	D	233	PRO	C-N	5.11	1.45	1.34
1	B	175	VAL	C-O	5.07	1.32	1.23
1	C	216	ARG	NE-CZ	5.05	1.39	1.33
1	B	105	LYS	CD-CE	5.05	1.63	1.51
1	C	125	GLU	CG-CD	5.02	1.59	1.51
1	C	124	HIS	CG-ND1	5.01	1.49	1.38

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	ARG	NE-CZ-NH2	31.49	136.04	120.30
1	C	103	ARG	NE-CZ-NH1	23.29	131.94	120.30
1	D	359	ARG	NE-CZ-NH1	17.88	129.24	120.30
1	D	149	ARG	NE-CZ-NH2	-15.03	112.79	120.30
1	C	71	GLU	OE1-CD-OE2	-14.00	106.50	123.30
1	A	102	GLU	OE1-CD-OE2	-13.75	106.81	123.30
1	D	216	ARG	NE-CZ-NH1	-13.10	113.75	120.30
1	D	194	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	A	103	ARG	NE-CZ-NH2	12.55	126.58	120.30
1	D	81	GLU	OE1-CD-OE2	-12.50	108.30	123.30
1	C	103	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	D	149	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	D	382	ARG	NH1-CZ-NH2	-11.46	106.79	119.40
1	A	426	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	C	106	GLU	OE1-CD-OE2	-9.99	111.31	123.30
1	D	234	GLU	OE1-CD-OE2	9.99	135.29	123.30
1	C	149	ARG	NE-CZ-NH2	9.71	125.16	120.30
1	A	102	GLU	CG-CD-OE2	9.71	137.71	118.30
1	D	382	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	C	192	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	C	125	GLU	OE1-CD-OE2	9.23	134.38	123.30
1	D	194	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	158	LYS	CD-CE-NZ	8.62	131.53	111.70
1	B	175	VAL	N-CA-CB	-8.55	92.68	111.50
1	A	103	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	B	129	GLU	OE1-CD-OE2	-8.05	113.64	123.30
1	C	192	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	C	413	PHE	CG-CD2-CE2	-7.76	112.26	120.80
1	C	109	LYS	CD-CE-NZ	-7.73	93.93	111.70
1	C	102	GLU	OE1-CD-OE2	7.59	132.40	123.30
1	C	413	PHE	CZ-CE2-CD2	7.55	129.16	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	GLU	OE1-CD-OE2	7.41	132.19	123.30
1	C	413	PHE	CD1-CE1-CZ	7.41	129.00	120.10
1	D	81	GLU	CG-CD-OE2	7.39	133.09	118.30
1	B	71	GLU	OE1-CD-OE2	-7.34	114.49	123.30
1	D	139	GLU	OE1-CD-OE2	-7.30	114.53	123.30
1	A	382	ARG	CD-NE-CZ	-7.12	113.64	123.60
1	B	198	ASN	CB-CG-ND2	-7.01	99.87	116.70
1	C	103	ARG	CD-NE-CZ	-6.96	113.86	123.60
1	B	198	ASN	OD1-CG-ND2	6.89	137.74	121.90
1	D	191	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	A	73	LEU	CB-CG-CD1	-6.80	99.44	111.00
1	D	385	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	103	ARG	NH1-CZ-NH2	-6.70	112.03	119.40
1	A	382	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	473	VAL	CB-CA-C	-6.68	98.71	111.40
1	A	426	ARG	NH1-CZ-NH2	-6.54	112.20	119.40
1	C	216	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	473	VAL	CB-CA-C	-6.47	99.11	111.40
1	A	125	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	A	169	GLY	CA-C-O	6.45	132.21	120.60
1	A	169	GLY	C-N-CA	-6.23	109.21	122.30
1	C	86	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	D	382	ARG	CG-CD-NE	6.19	124.79	111.80
1	B	396	LEU	CA-CB-CG	6.12	129.39	115.30
1	D	234	GLU	CG-CD-OE1	-6.02	106.26	118.30
1	A	359	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	249	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	109	LYS	CD-CE-NZ	5.89	125.25	111.70
1	A	192	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	A	396	LEU	CA-CB-CG	5.87	128.81	115.30
1	D	359	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	169	GLY	CA-C-O	5.86	131.14	120.60
1	B	144	SER	CA-CB-OG	-5.82	95.49	111.20
1	C	410	LYS	CB-CG-CD	-5.80	96.51	111.60
1	A	106	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	D	359	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	D	473	VAL	CB-CA-C	-5.72	100.52	111.40
1	A	147	SER	CB-CA-C	-5.60	99.46	110.10
1	B	260	ASP	N-CA-C	5.53	125.94	111.00
1	C	413	PHE	CE1-CZ-CE2	-5.53	110.05	120.00
1	C	125	GLU	CG-CD-OE2	-5.42	107.46	118.30
1	C	396	LEU	CA-CB-CG	5.40	127.72	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	TYR	CZ-CE2-CD2	-5.34	114.99	119.80
1	A	473	VAL	CB-CA-C	-5.34	101.26	111.40
1	B	197	ALA	N-CA-CB	5.17	117.33	110.10
1	A	382	ARG	CG-CD-NE	-5.16	100.96	111.80
1	B	71	GLU	CB-CG-CD	-5.14	100.33	114.20
1	D	396	LEU	CB-CG-CD1	5.07	119.63	111.00
1	D	426	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	62	PRO	N-CD-CG	-5.06	95.61	103.20
1	A	261	LEU	CA-CB-CG	5.04	126.89	115.30
1	C	71	GLU	CG-CD-OE1	5.03	128.35	118.30
1	C	410	LYS	CB-CA-C	-5.03	100.35	110.40
1	A	103	ARG	CD-NE-CZ	-5.02	116.57	123.60

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 [i](#)

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	186	1
1	B	3666	0	3738	162	2
1	C	3889	0	3963	193	3
1	D	3799	0	3880	180	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	3	0
3	A	9	0	2	3	0
3	B	9	0	2	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	9	0	2	2	0
3	D	9	0	2	13	0
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	15525	683	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 22.

All (683) 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:CD2	1:A:73:LEU:CG	1.78	1.59
1:A:109:LYS:CE	1:A:109:LYS:CD	1.77	1.58
1:D:105:LYS:CE	1:D:105:LYS:NZ	1.72	1.51
1:A:410:LYS:NZ	1:A:410:LYS:CE	1.68	1.51
1:B:105:LYS:NZ	1:B:105:LYS:CE	1.70	1.51
1:C:410:LYS:NZ	1:C:410:LYS:CE	1.72	1.47
1:D:109:LYS:CD	1:D:109:LYS:CE	1.93	1.47
1:B:260:ASP:N	1:B:260:ASP:CA	1.73	1.46
1:A:102:GLU:CG	1:A:102:GLU:CD	1.83	1.45
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	1.32
1:B:144:SER:OG	1:B:144:SER:CB	1.78	1.31
3:D:581:PGA:O1P	3:D:581:PGA:C2	1.78	1.30
1:D:230:LYS:NZ	1:D:230:LYS:CE	2.00	1.25
1:C:71:GLU:CD	1:C:71:GLU:OE1	1.75	1.23
1:C:488:ARG:NH1	1:C:510:ARG:HB3	1.77	1.00
1:A:73:LEU:CD1	1:A:73:LEU:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:PRO:O	1:D:515:LEU:HD23	1.68	0.92
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:P	3:D:581:PGA:C2	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:O4P	3:D:581:PGA:C2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:HD11	1:A:235:GLY:HA3	1.65	0.79
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:NH1	1:A:194:ARG:HB3	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:O2	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: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:CB	1:A:73:LEU:CD2	2.65	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:C:288:VAL:HG12	1:C:326:ILE:HD13	1.71	0.73
1:A:385:ARG:HH11	1:A:385:ARG:HG2	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:A:514:PRO:C	1:A:515:LEU:HD23	2.11	0.71
1:D:269:VAL:O	1:D:273:ARG:HG2	1.91	0.71
1:A:194:ARG:HB3	1:A:194:ARG:HH11	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:514:PRO:C	1:D:515:LEU:HD23	2.12	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:B:514:PRO:C	1:B:515:LEU:HD23	2.12	0.68
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:A:554:VAL:HG21	1:A:571:LEU:HD11	1.76	0.67
1:C:449:ARG:HG3	1:D:551:LEU:HD11	1.77	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:HA	1:A:102:GLU:OE1	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: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: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
1:D:86:ARG:CB	1:D:426:ARG:HG2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:B:102:GLU:HA	1.98	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:B:223:LEU:CD1	1:D:380:LYS:HZ3	2.11	0.64
1:A:385:ARG:NH1	1:A:385:ARG:HG2	2.12	0.64
1:D:554:VAL:HG21	1:D:571:LEU:HD11	1.79	0.64
1:D:83:VAL:O	1:D:84:ALA:CB	2.45	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: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:C:514:PRO:C	1:C:515:LEU:HD23	2.18	0.63
1:A:525:TRP:O	1:A:527:ASP:N	2.32	0.62
1:C:410:LYS:CD	1:C:410:LYS:NZ	2.61	0.62
1:C:87:SER:HB2	1:C:511:GLY:HA2	1.79	0.62
1:D:105:LYS:CD	1:D:105:LYS:NZ	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:A:405:SER:O	1:A:406:GLY:C	2.37	0.62
1:B:525:TRP:O	1:B:526:ALA:C	2.38	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: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:C:525:TRP:O	1:C:526:ALA:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:276:VAL:HG11	1:A:304:GLU:HB2	1.82	0.60
1:D:81:GLU:OE1	1:D:81:GLU:HA	2.00	0.60
1:B:337:ARG:HH22	1:B:390:ASP:CG	2.05	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:81:GLU:HA	1:A:81:GLU:OE1	2.01	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: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:HD13	1:A:73:LEU:CD2	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:C:168:GLN:C	1:C:170:GLY:H	2.07	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
1:D:286:SER:HA	1:D:313:LYS:HE2	1.85	0.58
1:D:63:ALA:O	1:D:72:HIS:ND1	2.31	0.58
1:A:525:TRP:O	1:A:526:ALA:C	2.42	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:D:337:ARG:HH22	1:D:390:ASP:CG	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:525:TRP:O	1:D:526:ALA:C	2.42	0.57
1:A:373:MET:O	1:A:387:GLU:HB3	2.03	0.57
1:A:339:ASP:OD2	3:A:581:PGA:O4P	2.21	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:C:337:ARG:HH22	1:C:390:ASP:CG	2.07	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:188:ASP:C	1:D:188:ASP:OD1	2.43	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:D:281:ASP:C	1:D:282:ILE:HG13	2.24	0.57
1:B:78:ILE:HD13	1:D:320:VAL:HG11	1.88	0.56
1:A:192:ARG:HA	1:A:201:TRP:CD2	2.41	0.56
1:A:67:ASP:N	1:A:71:GLU:OE1	2.38	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: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: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
1:B:347:GLU:HG2	1:D:423:ALA:HB1	1.86	0.56
1:B:155:LEU:C	1:B:155:LEU:HD23	2.27	0.55
1:B:57:GLN:HB2	1:B:62:PRO:HD3	1.88	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:CB	1:A:194:ARG:HH11	2.19	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:A:434:HIS:O	1:A:435:ARG:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LEU:HD11	1:D:246:LEU:HD22	1.87	0.55
1:A:155:LEU:HD23	1:A:155:LEU:C	2.27	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:B:367:VAL:O	1:B:367:VAL:HG13	2.07	0.55
1:A:223:LEU:CD2	1:C:380:LYS:HE2	2.36	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:D:371:THR:OG1	3:D:581:PGA:O1	2.11	0.55
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:434:HIS:O	1:B:435:ARG:C	2.44	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: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: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:264:LEU:HD22	1:D:296:ALA:HB1	1.89	0.54
1:D:87:SER:HB2	1:D:511:GLY:CA	2.38	0.54
1:A:337:ARG:HH22	1:A:390:ASP:CG	2.11	0.53
1:C:144:SER:CB	1:C:144:SER:HG	2.12	0.53
1:A:91:ILE:HB	1:A:403:MET:HG3	1.90	0.53
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: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:A:525:TRP:CE2	1:A:560:PRO:HG3	2.43	0.53
1:A:102:GLU:OE1	1:A:105:LYS:HD2	2.09	0.53
1:A:281:ASP:C	1:A:282:ILE:HG13	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TYR:CZ	1:A:206:ASN:HB2	2.44	0.52
1:A:83:VAL:HG12	1:A:83:VAL:O	2.08	0.52
1:C:206:ASN:O	1:C:210:VAL:HG23	2.09	0.52
1:C:434:HIS:O	1:C:435:ARG:C	2.47	0.52
1:D:109:LYS:CG	1:D:109:LYS:CE	2.82	0.52
1:C:372:GLN:HG2	1:C:375:GLU:HG3	1.89	0.52
1:A:118:ASN:OD1	1:A:118:ASN:C	2.48	0.51
1:D:327:LEU:HD22	1:D:365:LYS:HD2	1.92	0.51
1:A:100:SER:O	1:A:101:VAL:C	2.49	0.51
1:A:442:ARG:NH2	1:B:442:ARG:NH2	2.47	0.51
1:C:327:LEU:CD2	1:C:365:LYS:HD2	2.40	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:125:GLU:H	1:A:125:GLU:CD	2.13	0.51
1:A:167:LEU:CD1	1:A:195:GLY:O	2.58	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
1:C:510:ARG:HG2	1:C:511:GLY:N	2.26	0.51
1:A:348:LYS:HE2	1:C:427:GLU:OE2	2.11	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: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:B:77:ASP:C	1:B:77:ASP:OD1	2.48	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: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:506:VAL:CG1	1:D:512:VAL:HG11	2.40	0.50
1:D:146:LEU:HB2	1:D:542:LEU:HD12	1.94	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:192:ARG:HG3	1:D:201:TRP:CH2	2.46	0.50
1:D:87:SER:HB2	1:D:511:GLY:HA2	1.94	0.50
1:A:255:PRO:C	1:A:257:ALA:H	2.14	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:B:281:ASP:C	1:B:282:ILE:HG13	2.31	0.50
1:C:81:GLU:OE1	1:C:81:GLU:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:405:SER:O	1:B:406:GLY:C	2.48	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:OE1	1:C:172:GLU:N	2.43	0.50
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.92	0.49
1:C:485:SER:O	1:C:486:ARG:C	2.49	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:D:352:ALA:HB1	1:D:356:MET:HE2	1.93	0.49
1:A:168:GLN:HB2	1:A:195:GLY:O	2.12	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:255:PRO:C	1:B:257:ALA:H	2.15	0.49
1:B:313:LYS:HD2	1:B:334:MET:SD	2.53	0.49
1:C:86:ARG:CB	1:C:426:ARG:HG2	2.28	0.49
1:A:360:CYS:O	1:A:361:ASN:C	2.51	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:A:223:LEU:HD11	1:C:380:LYS:NZ	2.28	0.49
1:D:405:SER:O	1:D:406:GLY:C	2.50	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:281:ASP:C	1:C:282:ILE:HG13	2.32	0.48
1:D:470:ALA:HA	1:D:491:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:VAL:HG11	1:B:424:ILE:HB	1.96	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:A:329:VAL:O	1:A:329:VAL:HG13	2.13	0.48
1:B:120:SER:OG	1:B:161:GLU:OE2	2.25	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:D:172:GLU:N	1:D:172:GLU:CD	2.66	0.48
1:A:202:VAL:HG13	1:A:204:TYR:H	1.78	0.48
1:A:87:SER:OG	1:A:510:ARG:HG2	2.13	0.48
1:B:146:LEU:HB2	1:B:542:LEU:HD12	1.94	0.48
1:B:81:GLU:HA	1:B:81:GLU:OE1	2.12	0.48
1:C:488:ARG:HH11	1:C:510:ARG:HD2	1.77	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:B:485:SER:O	1:B:486:ARG:C	2.51	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: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: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:B:441:LEU:O	1:B:442:ARG:C	2.52	0.47
1:C:539:SER:O	1:C:543:ARG:HG3	2.14	0.47
1:C:87:SER:HB2	1:C:511:GLY:H	1.76	0.47
1:A:206:ASN:O	1:A:210:VAL:HG23	2.14	0.47
1:A:68:THR:OG1	1:A:71:GLU:HB2	2.14	0.47
1:B:379:THR:HG22	1:B:380:LYS:HG3	1.96	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:C:348:LYS:O	1:C:349:VAL:C	2.53	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:D:155:LEU:C	1:D:155:LEU:HD23	2.35	0.47
1:D:525:TRP:NE1	1:D:560:PRO:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:GLU:CD	3:D:581:PGA:O4P	2.50	0.47
1:D:83:VAL:CG1	1:D:83:VAL:O	2.63	0.47
1:A:441:LEU:O	1:A:442:ARG:C	2.52	0.47
1:B:91:ILE:HB	1:B:403:MET:HG3	1.95	0.47
1:D:191:PHE:CD2	1:D:194:ARG:CD	2.98	0.47
1:D:255:PRO:C	1:D:257:ALA:H	2.18	0.47
1:D:377:MET:HA	1:D:380:LYS:O	2.15	0.47
1:B:434:HIS:O	1:B:435:ARG:O	2.32	0.47
1:B:87:SER:H	1:B:429:GLU:CD	2.17	0.47
1:C:124:HIS:HE1	1:C:271:ASP:OD1	1.98	0.47
1:C:405:SER:O	1:C:406:GLY:C	2.53	0.47
1:A:167:LEU:HD23	1:A:173:SER:O	2.15	0.47
1:A:456:ALA:O	1:A:460:VAL:HG23	2.15	0.47
1:C:301:LEU:HA	1:C:301:LEU:HD12	1.60	0.47
1:A:320:VAL:HG11	1:C:78:ILE:HD13	1.97	0.47
1:D:207:ILE:HD11	1:D:254:LEU:HD21	1.97	0.47
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:545:PHE:C	1:A:546:LEU:HD23	2.35	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:131:ILE:O	1:C:132:ALA:C	2.54	0.46
1:C:155:LEU:HD23	1:C:155:LEU:C	2.35	0.46
1:D:434:HIS:O	1:D:435:ARG:C	2.53	0.46
1:C:264:LEU:HD22	1:C:296:ALA:HB1	1.97	0.46
1:C:349:VAL:O	1:C:350:PHE:C	2.53	0.46
1:C:441:LEU:O	1:C:442:ARG:C	2.53	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:131:ILE:O	1:D:132:ALA:C	2.53	0.46
1:A:420:MET:O	1:A:421:GLN:C	2.54	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:448:SER:OG	1:C:449:ARG:N	2.46	0.46
1:D:349:VAL:O	1:D:350:PHE:C	2.53	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:C:157:THR:HG22	1:C:286:SER:HB2	1.97	0.46
1:C:87:SER:HB3	1:C:511:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:63:ALA:HA	1:D:75:LEU:HB2	1.97	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:487:TYR:O	1:C:488:ARG:HB2	2.16	0.45
1:D:69:PHE:O	1:D:72:HIS:HB3	2.16	0.45
1:C:454:VAL:CG1	1:D:462:ALA:HB1	2.46	0.45
1:B:362:LEU:HD12	1:D:70:LEU:HD21	1.98	0.45
1:C:413:PHE:HB3	1:C:416:GLU:HB2	1.99	0.45
1:B:131:ILE:O	1:B:132:ALA:C	2.53	0.45
1:B:99:ARG:NH2	1:B:129:GLU:OE1	2.39	0.45
1:A:385:ARG:HE	1:C:341:GLY:HA3	1.80	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:B:352:ALA:HB1	1:B:356:MET:HE2	1.99	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:367:VAL:HG13	1:C:367:VAL:O	2.17	0.45
1:D:339:ASP:O	1:D:340:LEU:C	2.51	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:559:ARG:HD2	1:A:564:TYR:CE1	2.52	0.45
1:A:86:ARG:NH2	1:A:113:ASN:OD1	2.50	0.45
1:B:156:ASP:OD1	1:B:156:ASP:C	2.56	0.45
1:B:87:SER:N	1:B:429:GLU:OE1	2.47	0.45
1:B:85:ALA:HB2	1:B:545:PHE:CE2	2.52	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:A:347:GLU:H	1:A:347:GLU:CD	2.18	0.45
1:A:509:CYS:O	1:A:510:ARG:C	2.55	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:A:354:LYS:NZ	1:A:397:ASP:OD1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:TRP:CE2	1:B:560:PRO:HG3	2.52	0.44
1:B:83:VAL:CG1	1:B:83:VAL:O	2.64	0.44
1:B:297:VAL:O	1:B:301:LEU:HB2	2.17	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
1:A:167:LEU:HD21	1:A:175:VAL:H	1.83	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:B:339:ASP:O	1:B:340:LEU:C	2.55	0.44
1:B:434:HIS:O	1:B:437:LEU:N	2.51	0.44
1:B:85:ALA:HB2	1:B:545:PHE:HE2	1.82	0.44
1:A:347:GLU:CG	1:C:423:ALA:HB1	2.44	0.44
1:C:548:VAL:HA	1:C:573:ILE:HG22	1.99	0.44
1:C:553:ILE:HD12	1:C:570:VAL:HG22	1.98	0.44
1:D:231:ILE:C	1:D:231:ILE:CD1	2.86	0.44
1:A:515:LEU:CD1	1:A:539:SER:HB2	2.48	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:B:320:VAL:HG11	1:D:78:ILE:HD13	1.98	0.44
1:A:87:SER:N	1:A:429:GLU:OE1	2.50	0.44
1:C:168:GLN:C	1:C:170:GLY:N	2.71	0.44
1:D:100:SER:O	1:D:101:VAL:C	2.55	0.44
1:D:509:CYS:O	1:D:510:ARG:C	2.56	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:118:ASN:OD1	1:C:118:ASN:C	2.56	0.44
1:C:329:VAL:HG13	1:C:329:VAL:O	2.18	0.44
1:D:506:VAL:CG1	1:D:512:VAL:CG1	2.96	0.43
1:D:114:ILE:HG12	1:D:152:ALA:HB3	2.00	0.43
1:A:73:LEU:HD22	1:A:73:LEU:HD13	1.98	0.43
1:A:85:ALA:HB3	1:A:513:PHE:CZ	2.54	0.43
1:B:118:ASN:OD1	1:B:118:ASN:C	2.57	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:B:100:SER:O	1:B:101:VAL:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:581:PGA:O3P	3:A:581:PGA:O1	2.36	0.43
1:B:260:ASP:CB	1:B:260:ASP:N	2.73	0.43
1:C:434:HIS:O	1:C:437:LEU:N	2.52	0.43
1:D:185:VAL:HA	1:D:200:VAL:O	2.18	0.43
1:D:348:LYS:O	1:D:349:VAL:C	2.56	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:C:442:ARG:NH2	1:D:442:ARG:NH2	2.55	0.43
1:D:234:GLU:O	1:D:234:GLU:OE1	2.36	0.43
1:D:85:ALA:HB2	1:D:545:PHE:CE2	2.54	0.43
1:B:515:LEU:CD1	1:B:539:SER:HB2	2.48	0.43
1:C:144:SER:CA	1:C:144:SER:OG	2.58	0.43
1:B:505:GLN:O	1:B:508:LEU:HB2	2.19	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: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:210:VAL:HG11	1:D:258:GLN:O	2.19	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:C:339:ASP:O	1:C:340:LEU:C	2.57	0.42
1:A:488:ARG:NH1	1:A:510:ARG:HD2	2.34	0.42
1:B:349:VAL:O	1:B:350:PHE:C	2.56	0.42
1:B:542:LEU:HD22	1:B:542:LEU:O	2.20	0.42
1:B:545:PHE:C	1:B:546:LEU:HD23	2.40	0.42
1:C:232:GLY:HA2	1:C:233:PRO:HD3	1.83	0.42
1:C:375:GLU:O	1:C:376:SER:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:D:116:ARG:HH11	1.69	0.42
1:D:329:VAL:O	1:D:329:VAL:HG13	2.20	0.42
1:A:301:LEU:HA	1:A:301:LEU:HD12	1.64	0.42
1:A:545:PHE:CB	1:A:546:LEU:HD23	2.49	0.42
1:D:553:ILE:CD1	1:D:570:VAL:HG22	2.49	0.42
1:B:175:VAL:HG13	1:B:197:ALA:HA	2.01	0.42
1:B:420:MET:O	1:B:421:GLN:C	2.57	0.42
1:B:525:TRP:NE1	1:B:560:PRO:HG3	2.34	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:59:GLN:CD	1:B:83:VAL:HG12	2.40	0.42
1:C:116:ARG:HD3	1:C:116:ARG:HH11	1.63	0.42
1:D:301:LEU:HA	1:D:301:LEU:HD12	1.64	0.42
1:A:434:HIS:O	1:A:435:ARG:O	2.37	0.42
1:A:70:LEU:O	1:A:73:LEU:HB2	2.19	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:A:545:PHE:HB3	1:A:546:LEU:HD23	2.02	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.86	0.41
1:A:423:ALA:HB1	1:C:347:GLU:HG2	2.01	0.41
1:A:131:ILE:O	1:A:132:ALA:C	2.59	0.41
1:B:322:ARG:NH2	1:B:325:GLU:OE2	2.53	0.41
1:B:385:ARG:HG2	1:B:385:ARG:NH1	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:C:303:PRO:C	1:C:305:GLY:H	2.24	0.41
1:C:87:SER:H	1:C:429:GLU:CD	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ILE:HG22	1:C:225:SER:N	2.34	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:C:449:ARG:NH1	1:D:466:CYS:O	2.53	0.41
1:B:509:CYS:O	1:B:510:ARG:C	2.59	0.41
1:A:91:ILE:HD13	1:A:284:PHE:CZ	2.55	0.41
1:A:542:LEU:O	1:A:542:LEU:HD22	2.21	0.41
1:A:225:SER:HB3	1:A:242:ASN:H	1.85	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:A:157:THR:HG22	1:A:286:SER:HB2	2.02	0.41
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.90	0.41
1:B:372:GLN:HG2	1:B:375:GLU:HG3	2.03	0.41
1:C:188:ASP:C	1:C:188:ASP:OD1	2.59	0.41
1:C:263:GLY:O	1:C:264:LEU:HD12	2.21	0.41
1:C:296:ALA:O	1:C:297:VAL:C	2.59	0.41
1:C:77:ASP:O	1:C:80:SER:HB2	2.21	0.41
1:A:116:ARG:NH2	1:A:156:ASP:OD2	2.46	0.41
1:B:375:GLU:O	1:B:376:SER:C	2.59	0.41
1:C:133:ASN:O	1:C:134:VAL:C	2.57	0.41
1:C:333:ILE:HG22	1:C:334:MET:N	2.35	0.41
1:D:372:GLN:HA	1:D:375:GLU:HG2	2.03	0.41
1:B:209:ARG:HG2	1:B:209:ARG:O	2.21	0.41
1:B:124:HIS:HE1	1:B:271:ASP:OD1	2.04	0.41
1:C:372:GLN:HA	1:C:375:GLU:HG2	2.02	0.41
1:C:66:ALA:HB1	1:C:71:GLU:HB3	2.02	0.41
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.76	0.40
1:C:144:SER:N	1:C:144:SER:OG	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:196:ASN:C	1:D:198:ASN:N	2.72	0.40
1:D:72:HIS:NE2	1:D:431:ALA:O	2.54	0.40
1:B:70:LEU:HD12	1:B:70:LEU:HA	1.84	0.40
1:C:485:SER:O	1:C:487:TYR:N	2.54	0.40
1:C:255:PRO:C	1:C:257:ALA:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:THR:HG22	1:B:286:SER:HB2	2.04	0.40
1:B:290:LYS:O	1:B:291:ALA:C	2.59	0.40
1:B:334:MET:HA	1:B:368:VAL:HB	2.04	0.40
1:C:380:LYS:HB3	1:C:380:LYS:HE2	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%)	8	15
1	B	470/528 (89%)	426 (91%)	32 (7%)	12 (3%)	5	8
1	C	510/528 (97%)	465 (91%)	36 (7%)	9 (2%)	8	15
1	D	487/528 (92%)	442 (91%)	36 (7%)	9 (2%)	8	15
All	All	1969/2112 (93%)	1780 (90%)	150 (8%)	39 (2%)	7	13

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

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Mol	Chain	Res	Type
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
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%)	368 (91%)	37 (9%)	9	17
1	B	389/423 (92%)	355 (91%)	34 (9%)	10	19
1	C	412/423 (97%)	370 (90%)	42 (10%)	7	13
1	D	403/423 (95%)	364 (90%)	39 (10%)	8	14
All	All	1609/1692 (95%)	1457 (91%)	152 (9%)	8	16

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	86	ARG
1	A	87	SER
1	A	99	ARG
1	A	103	ARG
1	A	104	LEU
1	A	144	SER
1	A	157	THR
1	A	167	LEU
1	A	182	GLN
1	A	186	THR
1	A	202	VAL
1	A	209	ARG
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	327	LEU
1	A	347	GLU
1	A	374	LEU
1	A	382	ARG
1	A	388	THR
1	A	396	LEU
1	A	402	ILE
1	A	449	ARG
1	A	473	VAL
1	A	486	ARG
1	A	508	LEU
1	A	539	SER

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Mol	Chain	Res	Type
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
1	B	182	GLN
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	327	LEU
1	B	374	LEU
1	B	388	THR
1	B	396	LEU
1	B	410	LYS
1	B	473	VAL
1	B	486	ARG
1	B	506	VAL
1	B	508	LEU
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

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Mol	Chain	Res	Type
1	C	80	SER
1	C	83	VAL
1	C	86	ARG
1	C	99	ARG
1	C	103	ARG
1	C	104	LEU
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	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	327	LEU
1	C	347	GLU
1	C	374	LEU
1	C	380	LYS
1	C	388	THR
1	C	396	LEU
1	C	435	ARG
1	C	473	VAL
1	C	486	ARG
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	D	83	VAL
1	D	86	ARG

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Mol	Chain	Res	Type
1	D	99	ARG
1	D	103	ARG
1	D	104	LEU
1	D	108	ILE
1	D	124	HIS
1	D	144	SER
1	D	157	THR
1	D	172	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	289	ARG
1	D	294	VAL
1	D	304	GLU
1	D	327	LEU
1	D	329	VAL
1	D	347	GLU
1	D	374	LEU
1	D	396	LEU
1	D	435	ARG
1	D	449	ARG
1	D	473	VAL
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	548	VAL
1	D	552	VAL
1	D	559	ARG
1	D	562	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS

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Mol	Chain	Res	Type
1	A	133	ASN
1	A	168	GLN
1	A	182	GLN
1	A	229	GLN
1	A	258	GLN
1	A	361	ASN
1	A	421	GLN
1	B	124	HIS
1	B	133	ASN
1	B	361	ASN
1	B	421	GLN
1	C	124	HIS
1	C	133	ASN
1	C	182	GLN
1	C	198	ASN
1	C	253	ASN
1	C	361	ASN
1	C	421	GLN
1	C	534	GLN
1	D	124	HIS
1	D	133	ASN
1	D	182	GLN
1	D	253	ASN
1	D	421	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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
3	PGA	C	581	5	5,8,8	1.97	2 (40%)	6,11,11	3.01	2 (33%)
3	PGA	A	581	1,5	5,8,8	2.66	3 (60%)	6,11,11	2.29	4 (66%)
2	FBP	B	580	-	18,20,20	1.44	3 (16%)	23,32,32	0.76	1 (4%)
2	FBP	A	580	-	18,20,20	1.02	1 (5%)	23,32,32	0.98	1 (4%)
2	FBP	D	580	-	18,20,20	1.02	2 (11%)	23,32,32	0.99	1 (4%)
2	FBP	C	580	-	18,20,20	0.97	1 (5%)	23,32,32	0.90	0
3	PGA	D	581	1,5	5,8,8	4.12	1 (20%)	6,11,11	1.77	3 (50%)
3	PGA	B	581	5	5,8,8	0.98	0	6,11,11	1.97	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGA	C	581	5	-	3/4/6/6	-
3	PGA	A	581	1,5	-	4/4/6/6	-
2	FBP	B	580	-	-	5/13/32/32	0/1/1/1
2	FBP	A	580	-	-	5/13/32/32	0/1/1/1
2	FBP	D	580	-	-	8/13/32/32	0/1/1/1
2	FBP	C	580	-	-	5/13/32/32	0/1/1/1
3	PGA	D	581	1,5	-	3/4/6/6	-
3	PGA	B	581	5	-	3/4/6/6	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	581	PGA	O1P-C2	9.08	1.78	1.45
2	B	580	FBP	O2-C2	4.88	1.49	1.40
3	A	581	PGA	O1P-C2	4.61	1.62	1.45
2	A	580	FBP	O2-C2	3.42	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	580	FBP	O2-C2	3.19	1.46	1.40
3	C	581	PGA	P-O2P	2.97	1.60	1.50
2	D	580	FBP	O2-C2	2.83	1.45	1.40
3	A	581	PGA	P-O2P	2.67	1.59	1.50
2	B	580	FBP	P1-O1	2.20	1.67	1.60
3	A	581	PGA	P-O1P	2.14	1.67	1.60
3	C	581	PGA	P-O3P	-2.12	1.46	1.54
2	B	580	FBP	P1-O1P	2.05	1.57	1.50
2	D	580	FBP	P1-O1	2.03	1.66	1.60

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	581	PGA	O3P-P-O1P	-6.27	90.05	106.73
3	B	581	PGA	O3P-P-O1P	-3.89	96.38	106.73
3	C	581	PGA	O3P-P-O2P	3.29	123.56	110.68
3	A	581	PGA	O1P-P-O2P	3.10	115.17	106.47
3	A	581	PGA	O3P-P-O1P	-3.04	98.63	106.73
3	D	581	PGA	O3P-P-O1P	2.90	114.44	106.73
2	A	580	FBP	P2-O6-C6	2.80	126.02	118.30
3	D	581	PGA	O4P-P-O1P	-2.38	100.40	106.73
3	B	581	PGA	O3P-P-O2P	2.36	119.92	110.68
2	D	580	FBP	O6-C6-C5	-2.36	100.88	108.99
3	A	581	PGA	O3P-P-O2P	-2.15	102.26	110.68
3	D	581	PGA	O1P-P-O2P	2.11	112.40	106.47
3	A	581	PGA	O4P-P-O1P	2.08	112.27	106.73
2	B	580	FBP	O3P-P1-O1	2.02	112.11	106.73

There are no chirality outliers.

All (36) torsion outliers are listed below:

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

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

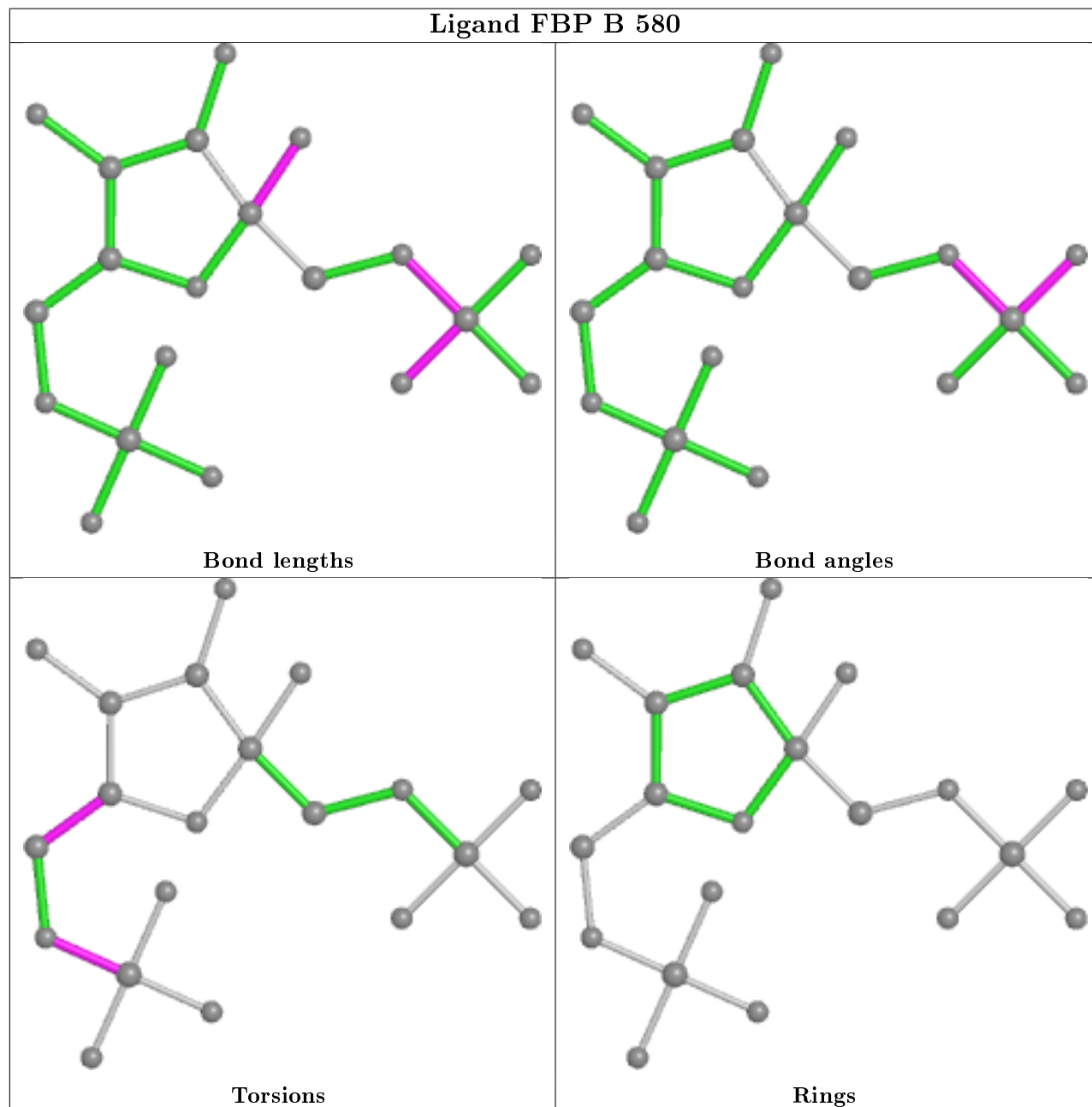
There are no ring outliers.

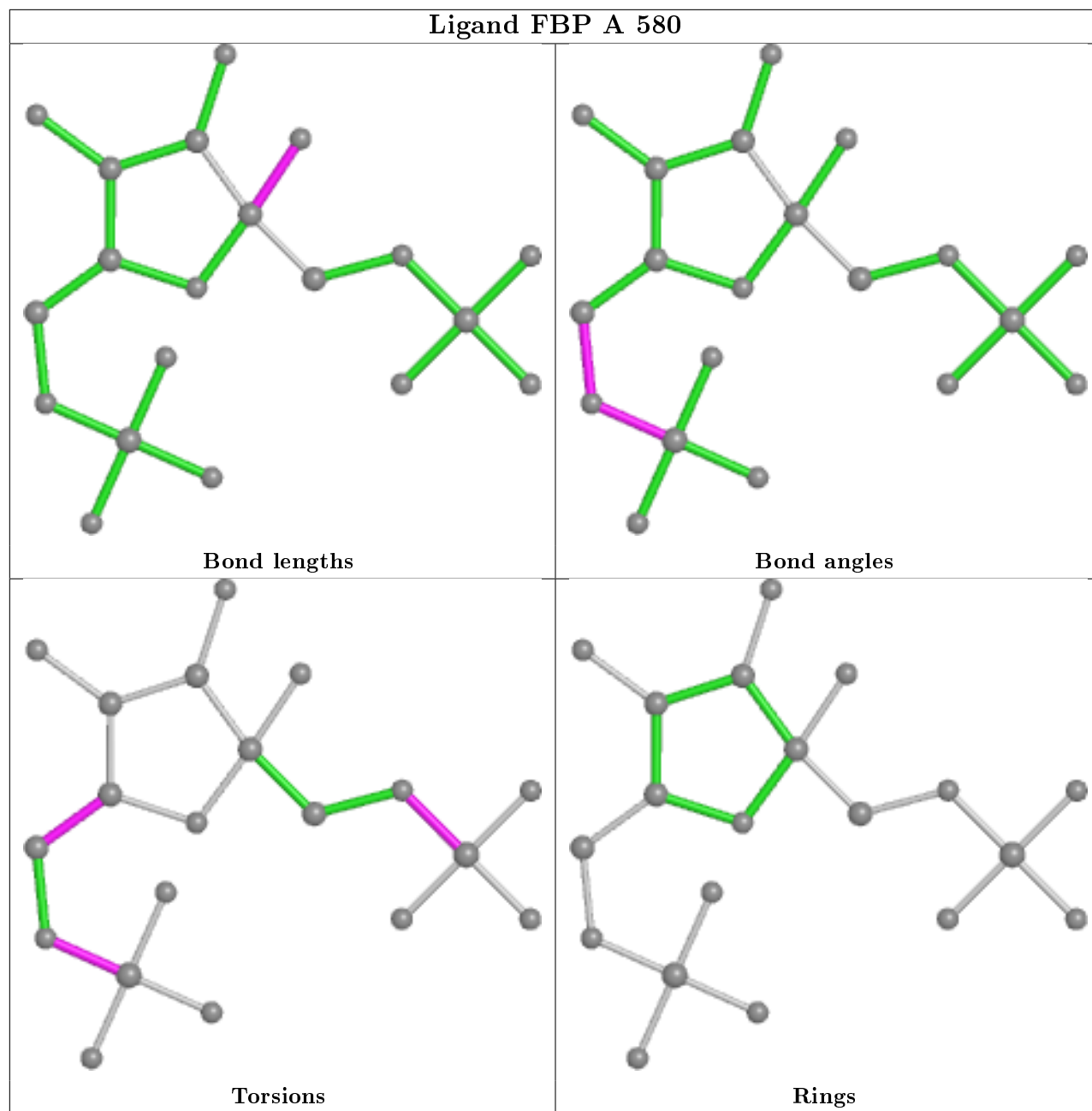
8 monomers are involved in 38 short contacts:

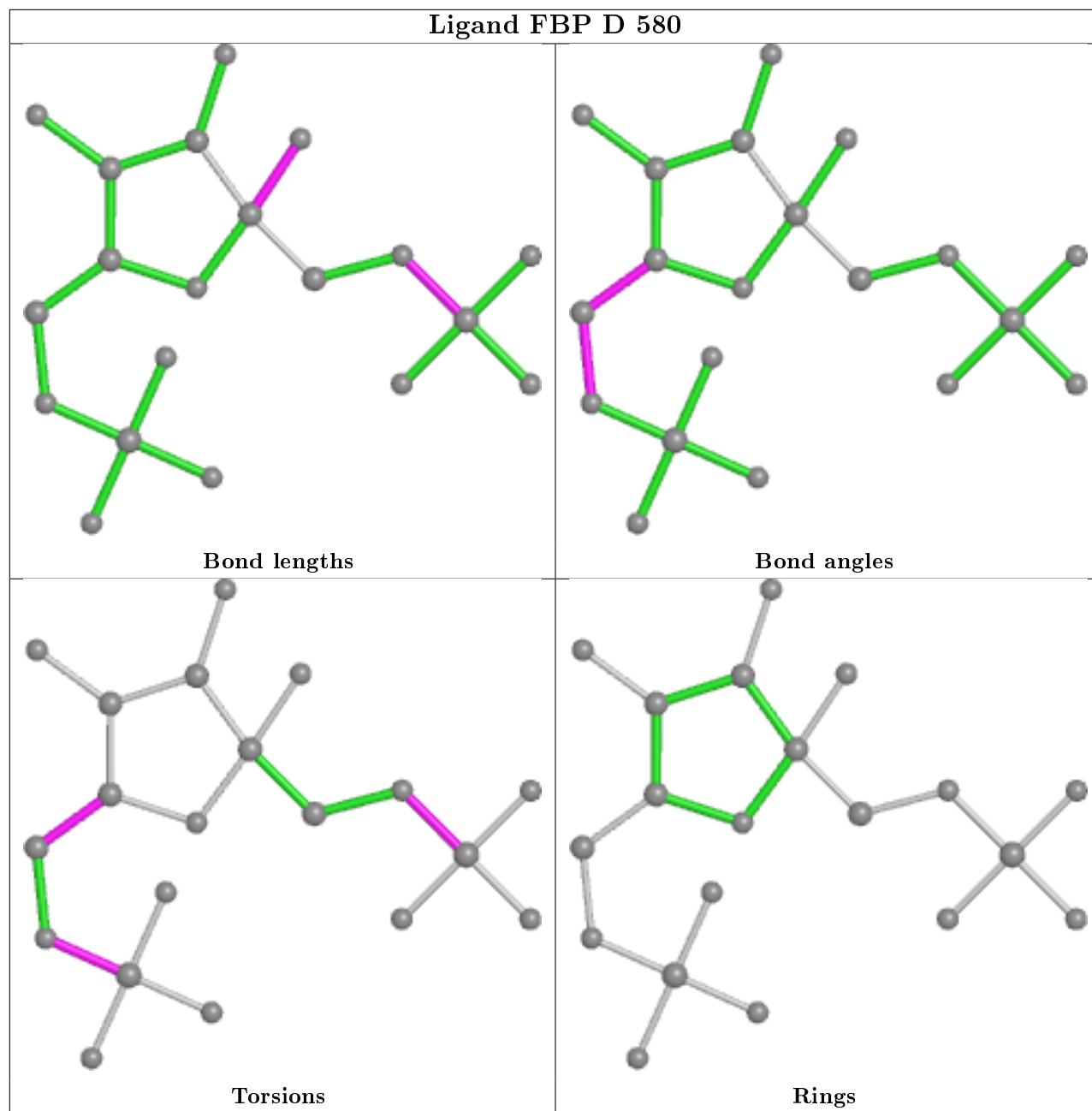
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	581	PGA	2	0
3	A	581	PGA	3	0
2	B	580	FBP	7	0
2	A	580	FBP	3	0
2	D	580	FBP	3	0
2	C	580	FBP	3	0
3	D	581	PGA	13	0
3	B	581	PGA	4	0

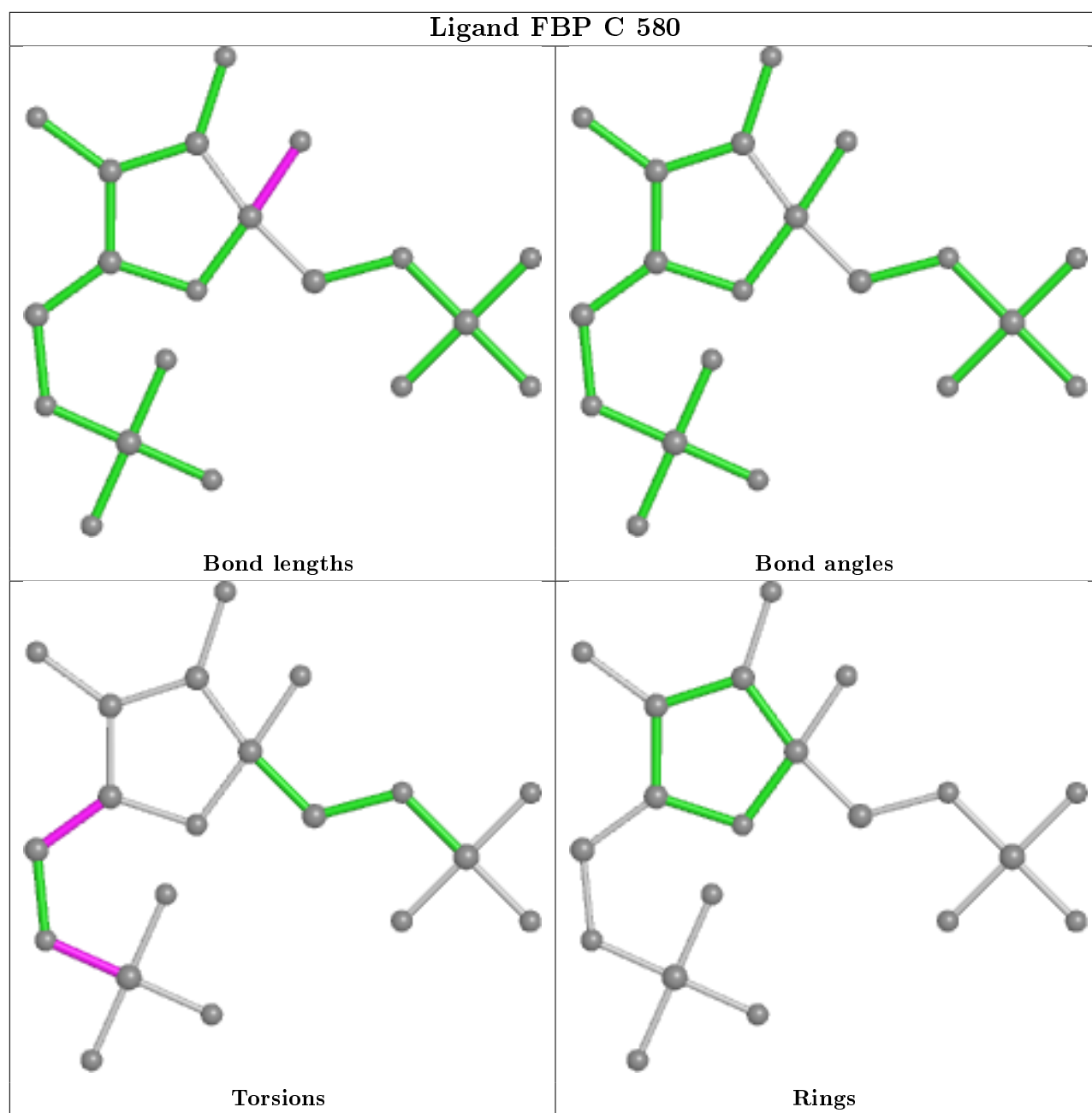
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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%)	0.64	60 (11%) 4 4	44, 56, 70, 94	0
1	B	483/528 (91%)	0.67	54 (11%) 5 5	43, 56, 71, 113	0
1	C	514/528 (97%)	0.43	39 (7%) 13 15	43, 56, 71, 128	0
1	D	501/528 (94%)	0.53	44 (8%) 10 10	44, 56, 70, 133	0
All	All	2004/2112 (94%)	0.57	197 (9%) 7 7	43, 56, 71, 133	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	VAL	9.1
1	B	177	LEU	8.3
1	A	237	VAL	8.2
1	D	146	LEU	7.9
1	B	185	VAL	7.3
1	A	146	LEU	6.6
1	B	227	VAL	6.6
1	C	67	ASP	6.4
1	B	60	GLN	6.4
1	A	236	LEU	6.4
1	B	210	VAL	6.1
1	D	535	PHE	6.1
1	B	240	VAL	5.9
1	C	240	VAL	5.9
1	C	61	LEU	5.9
1	C	62	PRO	5.9
1	A	209	ARG	5.9
1	D	195	GLY	5.7
1	B	201	TRP	5.7
1	D	231	ILE	5.7
1	A	520	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	162	ILE	5.5
1	B	214	GLY	5.4
1	D	233	PRO	5.2
1	A	64	ALA	5.2
1	B	180	GLY	5.2
1	B	202	VAL	5.0
1	A	204	TYR	4.9
1	C	194	ARG	4.9
1	B	213	VAL	4.9
1	C	177	LEU	4.9
1	A	548	VAL	4.9
1	B	258	GLN	4.8
1	B	248	SER	4.8
1	D	236	LEU	4.8
1	B	246	LEU	4.7
1	D	210	VAL	4.7
1	B	245	VAL	4.6
1	B	142	ALA	4.5
1	D	185	VAL	4.5
1	A	238	THR	4.4
1	D	194	ARG	4.4
1	B	175	VAL	4.3
1	D	182	GLN	4.2
1	C	289	ARG	4.2
1	D	245	VAL	4.1
1	B	57	GLN	4.1
1	B	226	LEU	4.1
1	A	547	ARG	4.1
1	A	180	GLY	4.0
1	A	147	SER	4.0
1	A	210	VAL	3.9
1	B	186	THR	3.9
1	C	258	GLN	3.9
1	B	217	ILE	3.9
1	A	207	ILE	3.8
1	C	78	ILE	3.8
1	A	211	VAL	3.8
1	A	519	GLU	3.7
1	D	205	PRO	3.7
1	B	66	ALA	3.7
1	C	168	GLN	3.7
1	A	261	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	263	GLY	3.6
1	C	175	VAL	3.6
1	B	249	ARG	3.6
1	B	143	GLY	3.5
1	B	261	LEU	3.5
1	B	207	ILE	3.5
1	B	219	ILE	3.4
1	A	449	ARG	3.4
1	A	185	VAL	3.4
1	B	183	VAL	3.4
1	C	73	LEU	3.4
1	A	68	THR	3.3
1	B	176	GLU	3.3
1	C	244	GLY	3.3
1	A	175	VAL	3.3
1	A	535	PHE	3.3
1	A	258	GLN	3.2
1	D	177	LEU	3.2
1	A	239	GLN	3.2
1	D	547	ARG	3.2
1	A	256	GLY	3.2
1	D	174	GLU	3.2
1	C	215	GLY	3.2
1	B	243	GLY	3.1
1	A	173	SER	3.1
1	D	306	HIS	3.1
1	D	143	GLY	3.1
1	C	435	ARG	3.0
1	C	178	VAL	3.0
1	D	209	ARG	3.0
1	B	244	GLY	3.0
1	A	229	GLN	3.0
1	C	170	GLY	2.9
1	B	204	TYR	2.9
1	A	263	GLY	2.9
1	D	373	MET	2.9
1	A	165	GLY	2.9
1	B	448	SER	2.9
1	D	144	SER	2.9
1	D	145	PRO	2.9
1	C	226	LEU	2.8
1	D	197	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	264	LEU	2.8
1	B	164	THR	2.8
1	D	213	VAL	2.8
1	D	256	GLY	2.8
1	B	146	LEU	2.8
1	C	182	GLN	2.8
1	D	518	ARG	2.8
1	D	548	VAL	2.7
1	A	177	LEU	2.7
1	A	65	MET	2.7
1	B	291	ALA	2.7
1	C	59	GLN	2.7
1	D	500	ALA	2.7
1	A	228	VAL	2.7
1	A	542	LEU	2.7
1	B	83	VAL	2.6
1	C	185	VAL	2.6
1	D	254	LEU	2.6
1	A	168	GLN	2.6
1	A	166	ILE	2.6
1	A	169	GLY	2.6
1	B	179	LYS	2.6
1	C	181	SER	2.6
1	D	62	PRO	2.6
1	B	206	ASN	2.6
1	D	304	GLU	2.6
1	D	264	LEU	2.5
1	C	199	THR	2.5
1	B	218	TYR	2.5
1	B	184	LEU	2.5
1	A	216	ARG	2.5
1	C	241	GLU	2.5
1	D	300	ALA	2.5
1	B	61	LEU	2.5
1	D	80	SER	2.5
1	D	176	GLU	2.5
1	A	262	PRO	2.5
1	C	547	ARG	2.5
1	A	176	GLU	2.5
1	A	326	ILE	2.5
1	D	187	VAL	2.5
1	A	67	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	166	ILE	2.4
1	B	198	ASN	2.4
1	B	433	TYR	2.4
1	A	234	GLU	2.4
1	D	531	ARG	2.4
1	A	369	CYS	2.3
1	C	468	ALA	2.3
1	D	152	ALA	2.3
1	B	498	ARG	2.3
1	B	178	VAL	2.3
1	A	546	LEU	2.3
1	D	386	ALA	2.3
1	A	523	ALA	2.3
1	A	399	ALA	2.3
1	C	200	VAL	2.3
1	C	264	LEU	2.2
1	A	531	ARG	2.2
1	C	70	LEU	2.2
1	C	133	ASN	2.2
1	C	180	GLY	2.2
1	B	531	ARG	2.2
1	C	63	ALA	2.2
1	C	230	LYS	2.2
1	D	175	VAL	2.2
1	A	205	PRO	2.2
1	D	148	TYR	2.2
1	A	160	PRO	2.2
1	A	144	SER	2.1
1	A	227	VAL	2.1
1	D	208	VAL	2.1
1	B	241	GLU	2.1
1	C	228	VAL	2.1
1	C	146	LEU	2.1
1	A	392	ALA	2.1
1	A	522	GLU	2.1
1	C	219	ILE	2.1
1	B	389	SER	2.1
1	A	391	VAL	2.1
1	B	58	GLN	2.1
1	A	164	THR	2.1
1	C	447	LEU	2.1
1	D	542	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	400	ASP	2.1
1	C	208	VAL	2.0
1	C	142	ALA	2.0
1	A	90	ILE	2.0
1	A	500	ALA	2.0
1	B	386	ALA	2.0
1	D	371	THR	2.0
1	A	255	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FBP	B	580	20/20	0.74	0.32	87,104,107,108	0
2	FBP	A	580	20/20	0.76	0.31	85,102,104,104	0
2	FBP	D	580	20/20	0.79	0.30	72,86,90,92	0
2	FBP	C	580	20/20	0.87	0.26	80,90,94,95	0
4	K	D	594	1/1	0.88	0.09	91,91,91,91	0
3	PGA	A	581	9/9	0.90	0.21	91,92,92,92	0
3	PGA	D	581	9/9	0.91	0.16	92,92,92,92	0
3	PGA	C	581	9/9	0.92	0.14	92,92,93,94	0
4	K	C	590	1/1	0.92	0.13	91,91,91,91	0
5	MN	A	583	1/1	0.92	0.09	91,91,91,91	0
4	K	B	586	1/1	0.93	0.07	91,91,91,91	0
4	K	A	582	1/1	0.94	0.05	91,91,91,91	0
3	PGA	B	581	9/9	0.94	0.11	95,97,98,98	0
5	MN	B	587	1/1	0.96	0.03	93,93,93,93	0
5	MN	D	595	1/1	0.96	0.03	90,90,90,90	0

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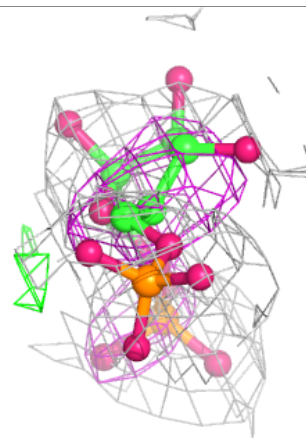
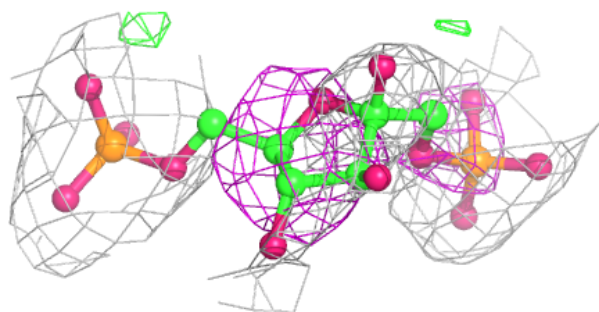
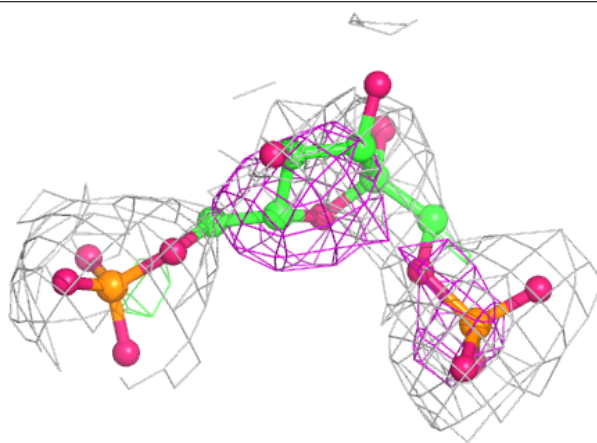
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MN	C	591	1/1	0.96	0.04	91,91,91,91	0

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.

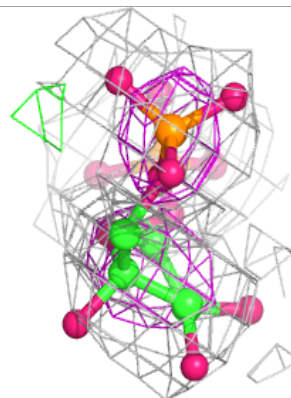
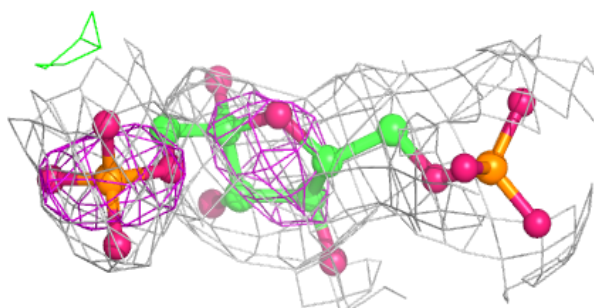
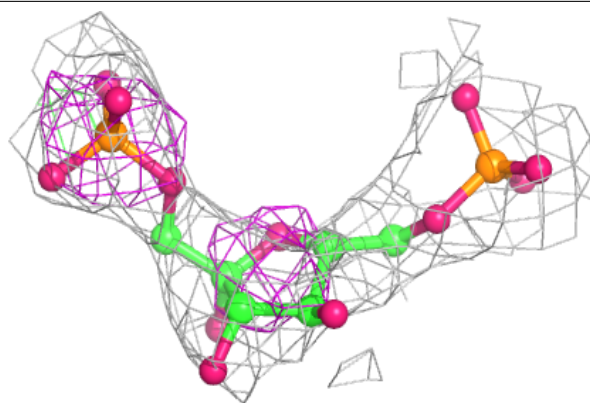
Electron density around FBP B 580:

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

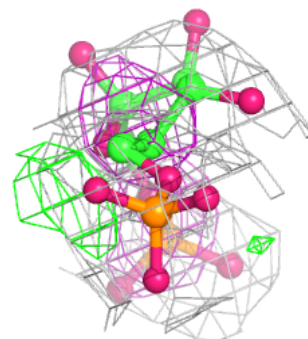
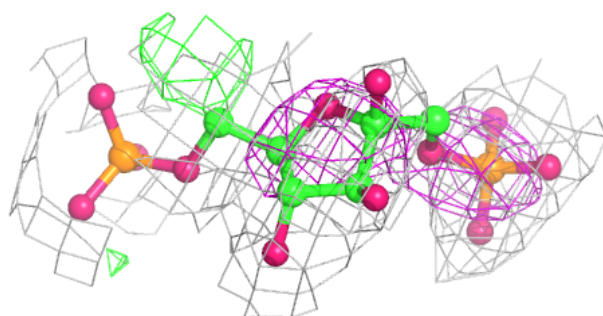
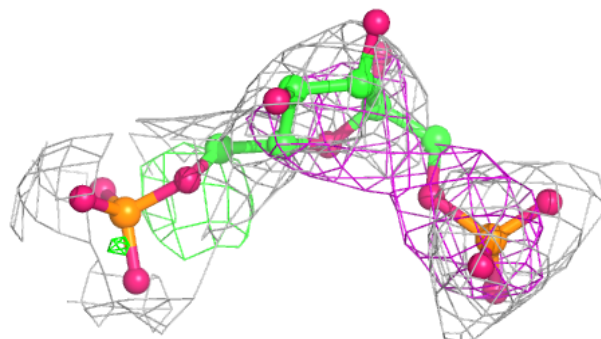


Electron density around FBP A 580:

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

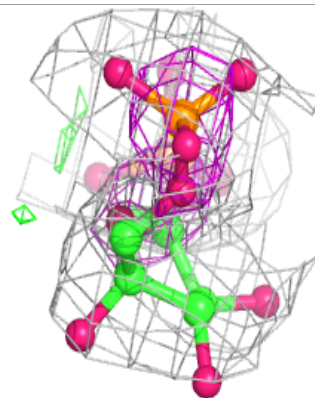
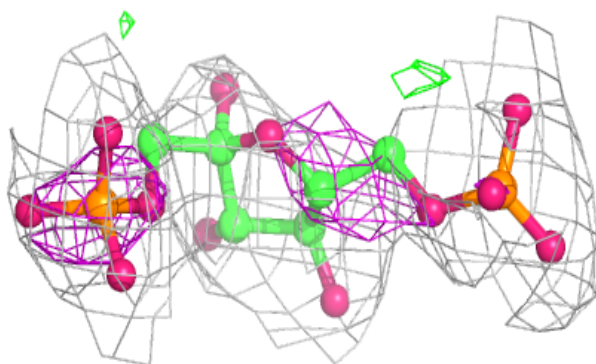
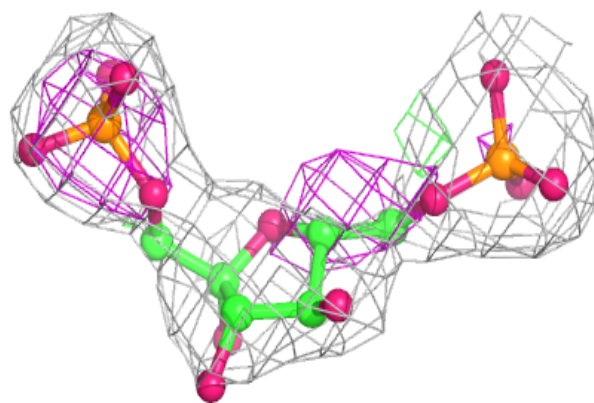
**Electron density around FBP D 580:**

$2mF_o-DF_c$ (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.