



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:31 AM BST

PDB ID : 1A3W  
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-  
PLEXED WITH FBP, PG, MN2+ AND K+  
Authors : Jurica, M.S.; Mesecar, A.; Heath, P.J.; Shi, W.; Nowak, T.; Stoddard, B.L.  
Deposited on : 1998-01-26  
Resolution : 3.00 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](mailto: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.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

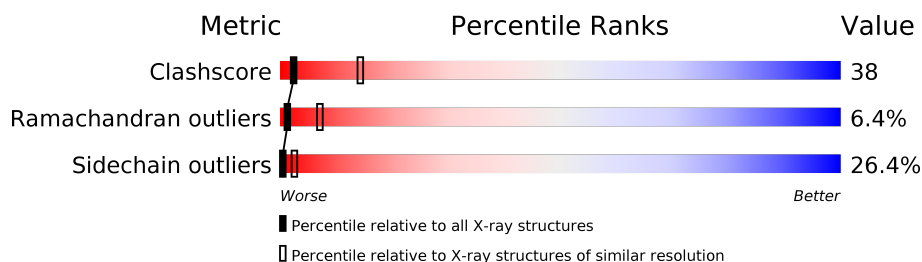
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	

## 2 Entry composition [i](#)

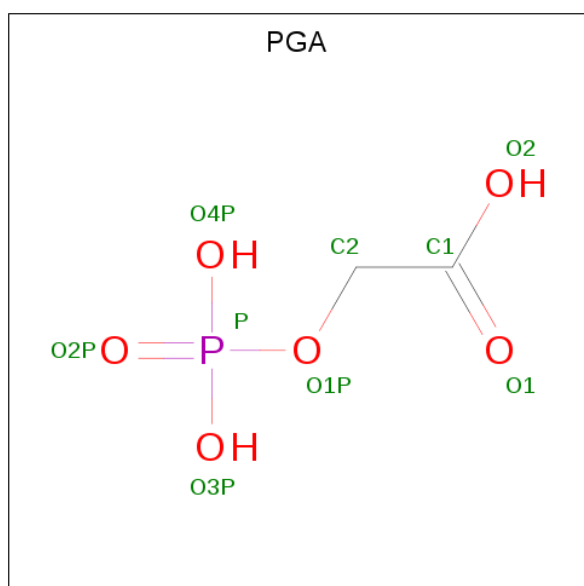
There are 5 unique types of molecules in this entry. The entry contains 7581 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PYRUVATE KINASE.

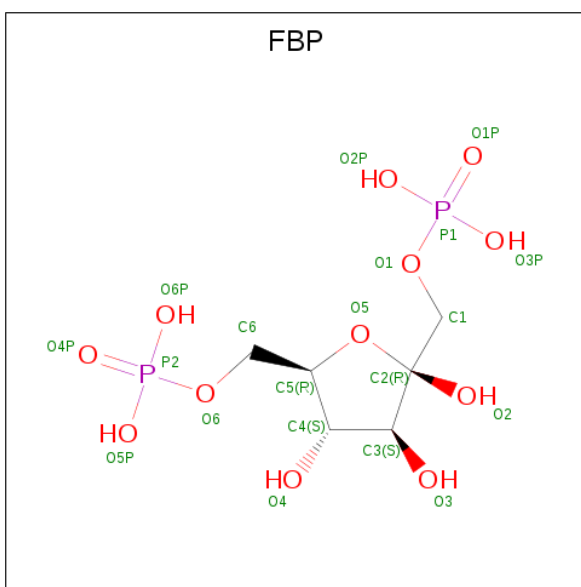
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3773	2380	650	726	17			
1	B	489	Total	C	N	O	S	0	0	0
			3746	2362	647	720	17			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula:  $C_2H_5O_6P$ ).



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

- Molecule 3 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
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

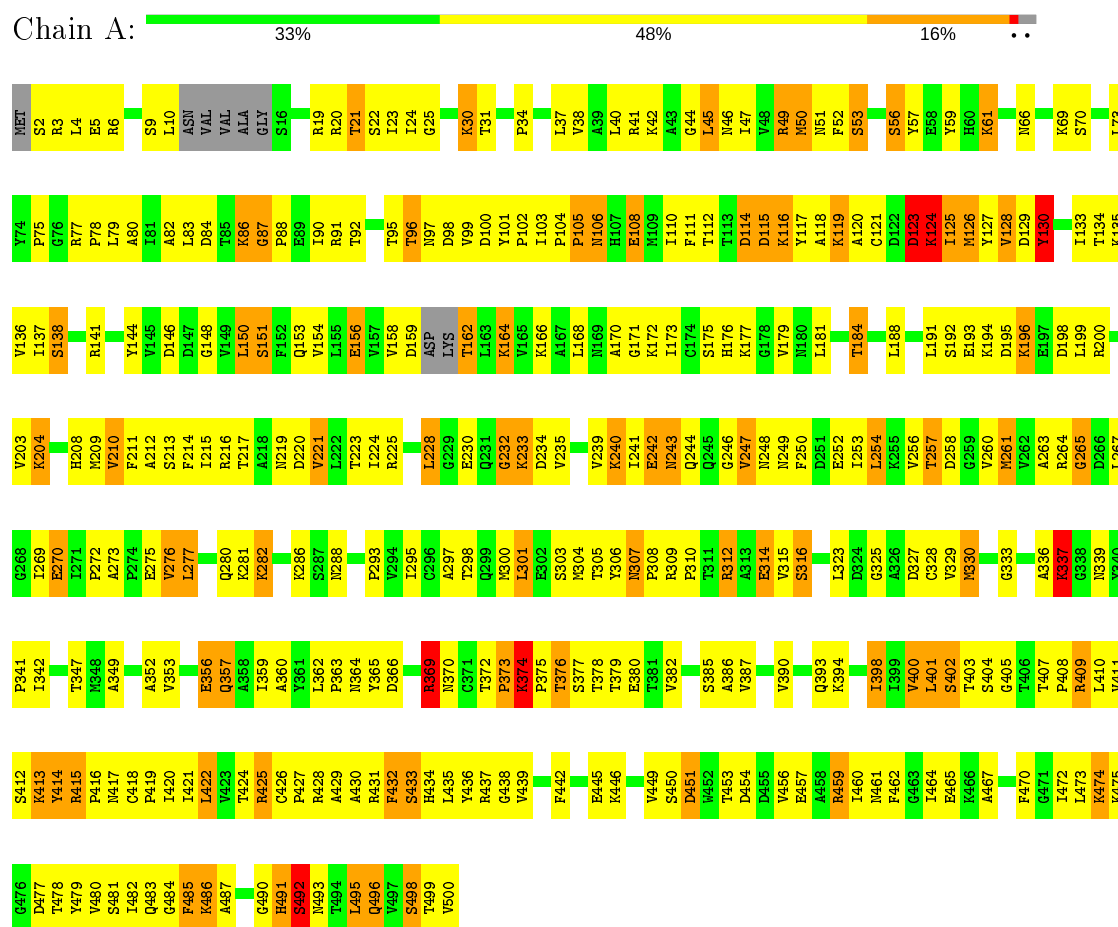
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		

### 3 Residue-property plots

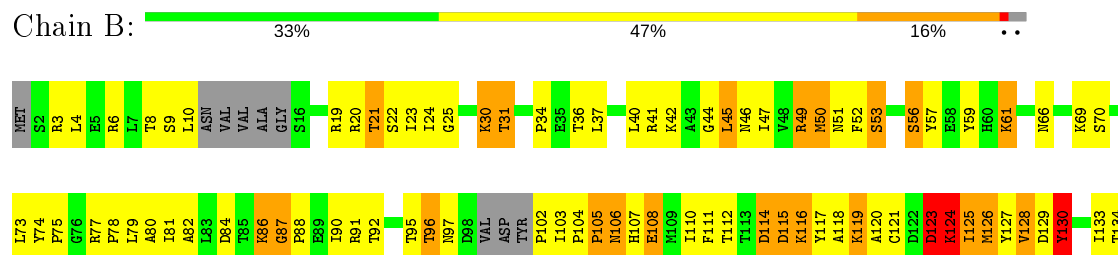
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: PYRUVATE KINASE



#### • Molecule 1: PYRUVATE KINASE



S481	N417	T347	I269	K204	K135
I482	C418	P348	E270	H208	V136
Q483	P419	A349	I271	M209	I137
G484	I420	A352	P272	V210	S138
F485	I421	A353	A273	F211	
K486	I422	V353	P274	A212	R141
A487	V423	E356	E275	S213	Y144
	T424	Q357	V276	F214	V145
G490	R425	A358	L277	I215	D146
H491	R428	I359	Q280	R216	D147
S492	A429	A360	K281	T217	G148
N493	A430	Y361	K282	A218	V149
T494	R431	L362	N288	N219	L150
L495	P432	P363	P293	V221	S151
Q496	S433	N364	P294	L222	F152
S498	H434	Y365	V294	T223	Q153
T499	L435	A366	I295	I224	V154
V500	Y436	R369	C296	R225	L155
	R437	N370	A297		E156
	G438	T372	T298	L228	V157
	V439	T373	Q299	V158	D159
	F442	P373	M300	ASP	
	E445	K374	L301	LYS	
	R446	P375	E302	T162	
	V449	T376	S303	L163	
	D451	S377	M304	K164	
	V450	T378	T305	V165	
	D452	T379	Y306	K166	
	T453	E360	N307	A167	
	D454	T381	P308	L168	
	V455	V382	R309	M169	
	E456	S385	P310	A170	
	E457	A386	T311	G171	
	A458	V387	R312	K172	
	R459		A313	I173	
	I460	Q393	E314	G174	
	N461	R394	V315	S175	
	F462	T398	S316	H176	
	G463	I399	I323	K177	
	I464	V400	I324	G178	
	E465	L401	G325	V179	
	K466	S402	A326	M180	
	A467	T403	D327	L181	
	K468	S404	C328	T184	
	E469	G405	V329	K251	
	F470	T406	N330	E252	
	G471	T407	G333	L254	
	I472	P408		V255	
	L473	R409	A336	T257	
	K474	L410	K337	D258	
	K475	V411	G338	G259	
	G476	S412	N339	V260	
	D477	K413	Y340	M261	
	T478	Y414	P341	V262	
	Y479	R415	I342	A263	
	V480	P416		R264	
				G265	
				D266	
				L267	
				G268	
					V203

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.40 Å   102.70 Å   110.90 Å 90.00°   112.30°   90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	75.9 (100.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.218 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

## 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	0.29	0/3834	0.63	7/5196 (0.1%)
1	B	0.31	0/3805	0.65	8/5153 (0.2%)
All	All	0.30	0/7639	0.64	15/10349 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	B	369	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	369	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	369	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	B	409	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	B	428	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	409	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	B	409	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	B	428	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	A	409	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	428	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	428	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	369	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	409	ARG	CD-NE-CZ	5.08	130.72	123.60
1	A	369	ARG	CD-NE-CZ	5.08	130.71	123.60

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3773	0	3844	296	0
1	B	3746	0	3822	298	0
2	A	9	0	2	1	0
2	B	9	0	2	0	0
3	A	20	0	10	3	0
3	B	20	0	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	7581	0	7690	579	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (579) 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:B:374:LYS:H	1:B:375:PRO:HA	1.16	1.11
1:A:374:LYS:H	1:A:375:PRO:HA	1.19	1.05
1:B:398:ILE:HD11	1:B:482:ILE:HD11	1.43	1.01
1:A:242:GLU:HG3	1:A:263:ALA:CB	1.95	0.96
1:B:242:GLU:HG3	1:B:263:ALA:CB	1.97	0.95
1:B:242:GLU:HG3	1:B:263:ALA:HB1	1.49	0.95
1:B:301:LEU:HA	1:B:314:GLU:HG2	1.47	0.95
1:A:242:GLU:HG3	1:A:263:ALA:HB1	1.49	0.94
1:A:301:LEU:HA	1:A:314:GLU:HG2	1.48	0.94
1:A:398:ILE:HD11	1:A:482:ILE:HD11	1.48	0.92
1:B:24:ILE:HB	1:B:330:MET:HB2	1.53	0.91
1:A:10:LEU:H	1:B:282:LYS:HE2	1.37	0.90
1:A:24:ILE:HB	1:A:330:MET:HB2	1.52	0.89
1:A:119:LYS:HE2	1:A:119:LYS:H	1.40	0.86
1:A:121:CYS:HB2	1:A:126:MET:HA	1.58	0.86
1:A:282:LYS:HE2	1:B:10:LEU:H	1.40	0.86
1:B:119:LYS:HE2	1:B:119:LYS:H	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:LEU:HD22	1:A:500:VAL:HG21	1.57	0.86
1:A:310:PRO:HG3	1:A:347:THR:HG21	1.57	0.86
1:A:240:LYS:HD3	1:A:261:MET:SD	2.16	0.85
1:B:121:CYS:HB2	1:B:126:MET:HA	1.56	0.85
1:B:310:PRO:HG3	1:B:347:THR:HG21	1.58	0.84
1:A:373:PRO:O	1:A:374:LYS:HB2	1.78	0.84
1:B:473:LEU:HD22	1:B:500:VAL:HG21	1.58	0.84
1:A:373:PRO:HB2	1:A:375:PRO:HA	1.59	0.82
1:B:373:PRO:HB2	1:B:375:PRO:HA	1.61	0.82
1:B:110:ILE:HD11	1:B:162:THR:HG22	1.62	0.81
1:B:373:PRO:O	1:B:374:LYS:HB2	1.78	0.81
1:B:23:ILE:H	1:B:46:ASN:HD22	1.28	0.81
1:A:136:VAL:HG22	1:A:184:THR:HG22	1.61	0.81
1:B:136:VAL:HG22	1:B:184:THR:HG22	1.63	0.80
1:A:126:MET:HG3	1:A:173:ILE:HD11	1.63	0.79
1:A:456:VAL:HG12	1:A:459:ARG:HH21	1.46	0.79
1:B:144:TYR:HB3	1:B:148:GLY:HA2	1.65	0.79
1:A:151:SER:HB2	1:A:168:LEU:HD12	1.65	0.78
1:A:23:ILE:H	1:A:46:ASN:HD22	1.28	0.78
1:A:144:TYR:HB3	1:A:148:GLY:HA2	1.66	0.78
1:A:30:LYS:HE3	1:A:30:LYS:H	1.48	0.78
1:A:24:ILE:HB	1:A:330:MET:CB	2.13	0.78
1:B:456:VAL:HG12	1:B:459:ARG:HH21	1.48	0.78
1:B:24:ILE:HB	1:B:330:MET:CB	2.12	0.77
1:B:240:LYS:HD3	1:B:261:MET:SD	2.25	0.77
1:A:429:ALA:HA	1:A:432:PHE:CZ	2.19	0.77
1:B:30:LYS:HE3	1:B:30:LYS:H	1.48	0.77
1:B:374:LYS:H	1:B:375:PRO:CA	1.96	0.77
1:B:95:THR:HA	1:B:121:CYS:O	1.86	0.76
1:A:95:THR:HA	1:A:121:CYS:O	1.85	0.75
1:B:34:PRO:HD3	1:B:66:ASN:HB3	1.68	0.75
1:B:126:MET:HG3	1:B:173:ILE:HD11	1.67	0.75
1:A:110:ILE:HD11	1:A:162:THR:HG22	1.68	0.74
1:A:91:ARG:H	1:A:129:ASP:HB2	1.52	0.74
1:B:373:PRO:HB2	1:B:376:THR:N	2.03	0.74
1:B:429:ALA:HA	1:B:432:PHE:CZ	2.23	0.74
1:A:104:PRO:HD2	1:A:171:GLY:O	1.88	0.72
1:A:456:VAL:HG12	1:A:459:ARG:NH2	2.04	0.72
1:A:374:LYS:H	1:A:375:PRO:CA	1.99	0.72
1:A:244:GLN:O	1:A:247:VAL:HG23	1.90	0.72
1:B:91:ARG:H	1:B:129:ASP:HB2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HG23	1:A:130:TYR:H	1.55	0.72
1:A:34:PRO:HD3	1:A:66:ASN:HB3	1.71	0.72
1:B:301:LEU:HD23	1:B:314:GLU:HG2	1.72	0.71
1:A:301:LEU:HD23	1:A:314:GLU:HG2	1.71	0.71
1:B:241:ILE:O	1:B:263:ALA:HB3	1.91	0.71
1:A:246:GLY:O	1:A:250:PHE:HB2	1.90	0.71
1:B:386:ALA:HA	1:B:495:LEU:HD11	1.72	0.71
1:A:373:PRO:HB2	1:A:376:THR:N	2.06	0.71
1:B:115:ASP:H	1:B:127:TYR:HE2	1.39	0.70
1:A:386:ALA:HA	1:A:495:LEU:HD11	1.72	0.70
1:A:115:ASP:H	1:A:127:TYR:HE2	1.40	0.70
1:B:151:SER:HB2	1:B:168:LEU:HD12	1.73	0.70
1:B:104:PRO:HD2	1:B:171:GLY:O	1.91	0.70
1:B:41:ARG:HE	1:B:79:LEU:HB2	1.57	0.70
1:B:56:SER:N	1:B:59:TYR:HB2	2.07	0.69
1:B:456:VAL:HG12	1:B:459:ARG:NH2	2.06	0.69
1:B:374:LYS:N	1:B:375:PRO:HA	1.98	0.69
1:A:102:PRO:O	1:A:173:ILE:HG22	1.93	0.69
1:A:295:ILE:HG12	1:A:328:CYS:HB2	1.73	0.69
1:A:41:ARG:HE	1:A:79:LEU:HB2	1.58	0.68
1:A:56:SER:N	1:A:59:TYR:HB2	2.09	0.68
1:A:239:VAL:CG2	1:A:260:VAL:HG12	2.23	0.68
1:B:103:ILE:HA	1:B:172:LYS:HA	1.76	0.68
1:A:378:THR:HG21	1:A:486:LYS:HE2	1.75	0.68
1:B:373:PRO:HB2	1:B:376:THR:H	1.59	0.68
1:A:95:THR:HG23	1:A:175:SER:HB3	1.75	0.68
1:B:159:ASP:HA	1:B:162:THR:HB	1.75	0.68
1:B:246:GLY:O	1:B:250:PHE:HB2	1.94	0.68
1:A:374:LYS:N	1:A:375:PRO:HA	2.00	0.68
1:A:19:ARG:HH12	1:A:46:ASN:HD21	1.42	0.67
1:B:239:VAL:CG2	1:B:260:VAL:HG12	2.23	0.67
1:B:432:PHE:O	1:B:435:LEU:HB2	1.95	0.67
1:B:90:ILE:HG23	1:B:130:TYR:H	1.58	0.67
1:B:295:ILE:HG12	1:B:328:CYS:HB2	1.76	0.67
1:A:130:TYR:HB3	1:A:133:ILE:HB	1.77	0.67
1:B:378:THR:HG21	1:B:486:LYS:HE2	1.77	0.67
1:B:19:ARG:HH12	1:B:46:ASN:HD21	1.42	0.67
1:B:263:ALA:O	1:B:267:LEU:HB2	1.95	0.66
1:B:398:ILE:HD11	1:B:482:ILE:CD1	2.23	0.66
1:A:199:LEU:O	1:A:203:VAL:HG13	1.95	0.66
1:A:103:ILE:HA	1:A:172:LYS:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ALA:O	1:A:364:ASN:HB2	1.96	0.66
1:A:413:LYS:C	1:A:415:ARG:H	1.99	0.66
1:B:130:TYR:HB3	1:B:133:ILE:HB	1.78	0.66
1:B:460:ILE:HD11	1:B:483:GLN:HE21	1.61	0.66
1:A:90:ILE:HD12	1:A:130:TYR:HB2	1.77	0.66
1:B:307:ASN:ND2	1:B:308:PRO:HD2	2.10	0.66
1:B:95:THR:HG23	1:B:175:SER:HB3	1.77	0.66
1:A:96:THR:HA	1:A:120:ALA:HA	1.76	0.65
1:A:50:MET:HB2	1:A:82:ALA:O	1.96	0.65
1:B:264:ARG:HH11	1:B:280:GLN:HE22	1.43	0.65
1:A:432:PHE:O	1:A:435:LEU:HB2	1.96	0.65
1:A:307:ASN:ND2	1:A:308:PRO:HD2	2.10	0.65
1:B:96:THR:HA	1:B:120:ALA:HA	1.77	0.65
1:A:110:ILE:HG13	1:A:111:PHE:N	2.12	0.65
1:B:360:ALA:O	1:B:364:ASN:HB2	1.96	0.65
1:B:117:TYR:HB2	1:B:127:TYR:CE1	2.32	0.65
1:B:24:ILE:HD12	1:B:295:ILE:HG21	1.77	0.65
1:B:50:MET:HB2	1:B:82:ALA:O	1.95	0.65
1:A:241:ILE:O	1:A:263:ALA:HB3	1.96	0.65
1:A:30:LYS:HE3	1:A:30:LYS:N	2.12	0.65
1:A:460:ILE:HD11	1:A:483:GLN:HE21	1.62	0.65
1:A:264:ARG:HH11	1:A:280:GLN:HE22	1.43	0.64
1:B:243:ASN:HA	1:B:270:GLU:HG2	1.78	0.64
1:A:258:ASP:O	1:A:293:PRO:HD2	1.97	0.64
1:B:30:LYS:HE3	1:B:30:LYS:N	2.11	0.64
1:B:413:LYS:C	1:B:415:ARG:H	2.00	0.64
1:A:24:ILE:HD12	1:A:295:ILE:HG21	1.79	0.64
1:A:209:MET:HE1	1:A:432:PHE:HA	1.79	0.64
1:A:373:PRO:HB2	1:A:376:THR:H	1.63	0.64
1:B:258:ASP:O	1:B:293:PRO:HD2	1.97	0.64
1:A:263:ALA:O	1:A:267:LEU:HB2	1.97	0.63
1:B:21:THR:HG23	1:B:437:ARG:HG3	1.81	0.63
1:A:51:ASN:OD1	1:A:53:SER:HB2	1.99	0.63
1:A:57:TYR:O	1:A:61:LYS:HB2	1.99	0.63
1:B:451:ASP:C	1:B:453:THR:H	2.02	0.63
1:B:90:ILE:HD12	1:B:130:TYR:HB2	1.80	0.63
1:A:250:PHE:HE1	1:A:260:VAL:HG11	1.63	0.63
1:B:244:GLN:O	1:B:247:VAL:HG23	1.99	0.63
1:B:386:ALA:CA	1:B:495:LEU:HD11	2.30	0.62
1:A:484:GLY:O	1:A:485:PHE:HB2	2.00	0.62
1:B:159:ASP:HA	1:B:162:THR:CB	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:O	1:B:61:LYS:HB2	1.98	0.62
1:B:199:LEU:O	1:B:203:VAL:HG13	2.00	0.62
1:A:215:ILE:HG13	1:A:239:VAL:HG12	1.82	0.62
1:A:386:ALA:CA	1:A:495:LEU:HD11	2.30	0.62
1:B:110:ILE:HG13	1:B:111:PHE:N	2.13	0.62
1:A:451:ASP:C	1:A:453:THR:H	2.02	0.61
1:B:209:MET:HE1	1:B:432:PHE:HA	1.81	0.61
1:A:491:HIS:HA	3:A:1007:FBP:O4	1.99	0.61
1:A:101:TYR:N	1:A:102:PRO:HD3	2.14	0.61
1:A:117:TYR:HB2	1:A:127:TYR:CE1	2.36	0.61
1:A:398:ILE:HD11	1:A:482:ILE:CD1	2.26	0.61
1:B:484:GLY:O	1:B:485:PHE:HB2	1.99	0.61
1:B:382:VAL:HG23	1:B:495:LEU:HD12	1.83	0.61
1:B:250:PHE:HE1	1:B:260:VAL:HG11	1.66	0.60
1:A:301:LEU:HB3	1:A:304:MET:HG3	1.84	0.60
1:B:47:ILE:HA	1:B:80:ALA:HB3	1.84	0.60
1:A:243:ASN:HA	1:A:270:GLU:HG2	1.82	0.60
1:A:21:THR:HG23	1:A:437:ARG:HG3	1.84	0.60
1:A:239:VAL:HG23	1:A:260:VAL:HG12	1.82	0.59
1:A:47:ILE:HA	1:A:80:ALA:HB3	1.83	0.59
1:A:244:GLN:HG3	1:A:248:ASN:ND2	2.17	0.59
1:B:244:GLN:HG3	1:B:248:ASN:ND2	2.18	0.59
1:B:239:VAL:HG23	1:B:260:VAL:HG12	1.83	0.59
1:B:53:SER:HA	1:B:86:LYS:HB2	1.84	0.59
1:A:2:SER:HB2	1:A:5:GLU:HB2	1.86	0.58
1:A:103:ILE:HG12	1:A:172:LYS:HB3	1.85	0.58
1:B:215:ILE:HG13	1:B:239:VAL:HG12	1.85	0.58
1:A:53:SER:HA	1:A:86:LYS:HB2	1.84	0.58
1:B:212:ALA:O	1:B:240:LYS:HB2	2.04	0.58
1:B:407:THR:O	1:B:411:VAL:HG23	2.03	0.58
1:B:250:PHE:CE1	1:B:260:VAL:HG11	2.39	0.58
1:B:301:LEU:HB3	1:B:304:MET:HG3	1.86	0.57
1:A:228:LEU:HG	1:A:235:VAL:HG11	1.86	0.57
1:B:103:ILE:HG12	1:B:172:LYS:HB3	1.86	0.57
1:A:250:PHE:CE1	1:A:260:VAL:HG11	2.39	0.57
1:A:316:SER:HA	1:B:277:LEU:HD12	1.86	0.57
1:A:323:LEU:HD23	1:A:359:ILE:HG12	1.86	0.57
1:A:407:THR:O	1:A:411:VAL:HG23	2.04	0.57
1:A:382:VAL:HG23	1:A:495:LEU:HD12	1.87	0.57
1:B:117:TYR:HB2	1:B:127:TYR:HE1	1.70	0.57
1:B:215:ILE:HD11	1:B:224:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:SER:H	1:B:59:TYR:HB2	1.68	0.57
1:B:323:LEU:HD23	1:B:359:ILE:HG12	1.87	0.57
1:A:402:SER:HA	3:A:1007:FBP:H61	1.85	0.57
1:A:309:ARG:NH2	1:B:269:ILE:HD13	2.19	0.56
1:A:102:PRO:O	1:A:104:PRO:HD3	2.04	0.56
1:A:312:ARG:HG3	1:B:264:ARG:HB3	1.87	0.56
1:B:272:PRO:HD2	1:B:275:GLU:OE2	2.05	0.56
1:A:212:ALA:O	1:A:240:LYS:HB2	2.05	0.56
1:A:215:ILE:HD11	1:A:224:ILE:HD11	1.86	0.56
1:A:272:PRO:HD2	1:A:275:GLU:OE2	2.06	0.56
1:A:373:PRO:HB2	1:A:375:PRO:CA	2.33	0.55
1:B:295:ILE:HG23	1:B:328:CYS:HB2	1.88	0.55
1:B:51:ASN:OD1	1:B:53:SER:HB2	2.07	0.55
1:B:307:ASN:HD22	1:B:308:PRO:HD2	1.70	0.55
1:B:20:ARG:HH12	1:B:417:ASN:HA	1.70	0.55
1:B:228:LEU:HG	1:B:235:VAL:HG11	1.89	0.55
1:A:10:LEU:HB2	1:B:282:LYS:HG3	1.89	0.55
1:A:88:PRO:HD2	1:A:214:PHE:HB2	1.88	0.55
1:B:366:ASP:O	1:B:369:ARG:HG3	2.07	0.55
1:A:56:SER:H	1:A:59:TYR:HB2	1.70	0.55
1:B:373:PRO:HB2	1:B:375:PRO:CA	2.35	0.55
1:B:34:PRO:HD3	1:B:66:ASN:CB	2.37	0.55
1:A:456:VAL:HA	1:A:459:ARG:HE	1.71	0.54
1:B:102:PRO:O	1:B:173:ILE:HG22	2.07	0.54
1:A:405:GLY:O	1:A:408:PRO:HG2	2.08	0.54
1:A:20:ARG:HH12	1:A:417:ASN:HA	1.71	0.54
1:A:307:ASN:HD22	1:A:308:PRO:HD2	1.72	0.54
1:B:24:ILE:HG23	1:B:47:ILE:HG22	1.90	0.54
1:B:208:HIS:O	1:B:235:VAL:HG23	2.07	0.54
1:B:400:VAL:HG21	1:B:407:THR:HG22	1.89	0.54
1:A:429:ALA:HA	1:A:432:PHE:CE1	2.43	0.53
1:B:374:LYS:N	1:B:375:PRO:CA	2.65	0.53
1:B:23:ILE:N	1:B:46:ASN:HD22	2.03	0.53
1:B:288:ASN:HD21	1:B:325:GLY:HA3	1.73	0.53
1:B:352:ALA:O	1:B:356:GLU:HG3	2.08	0.53
1:B:459:ARG:O	1:B:462:PHE:HB3	2.09	0.53
1:A:117:TYR:HB2	1:A:127:TYR:HE1	1.73	0.53
1:B:241:ILE:HD12	1:B:246:GLY:O	2.08	0.53
1:B:456:VAL:HA	1:B:459:ARG:HE	1.72	0.53
1:A:23:ILE:N	1:A:46:ASN:HD22	2.03	0.53
1:B:401:LEU:HD12	3:B:1008:FBP:O2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:VAL:HA	1:B:224:ILE:HD12	1.91	0.53
1:B:300:MET:O	1:B:301:LEU:HG	2.08	0.53
1:A:288:ASN:HD21	1:A:325:GLY:HA3	1.73	0.53
1:A:400:VAL:HG21	1:A:407:THR:HG22	1.91	0.53
1:A:419:PRO:HG2	1:A:472:ILE:HG23	1.91	0.53
1:A:230:GLU:H	1:A:230:GLU:CD	2.13	0.52
1:A:269:ILE:HD13	1:B:309:ARG:NH2	2.24	0.52
1:A:221:VAL:HA	1:A:224:ILE:HD12	1.91	0.52
1:A:98:ASP:O	1:A:100:ASP:N	2.42	0.52
1:A:24:ILE:HG23	1:A:47:ILE:HG22	1.91	0.52
1:A:352:ALA:O	1:A:356:GLU:HG3	2.09	0.52
1:B:108:GLU:HA	1:B:166:LYS:HA	1.90	0.52
1:B:240:LYS:HG2	1:B:261:MET:HB3	1.91	0.52
1:A:295:ILE:HG23	1:A:328:CYS:HB2	1.91	0.52
1:B:373:PRO:CB	1:B:376:THR:H	2.22	0.52
1:A:336:ALA:O	1:A:337:LYS:HB3	2.09	0.52
1:B:424:THR:HG21	1:B:430:ALA:HB2	1.90	0.52
1:A:459:ARG:O	1:A:462:PHE:HB3	2.09	0.52
1:A:46:ASN:O	1:A:79:LEU:HD22	2.09	0.52
1:A:265:GLY:HA3	1:A:298:THR:HG21	1.91	0.52
1:A:360:ALA:HB1	1:A:363:PRO:HG2	1.92	0.52
1:A:374:LYS:N	1:A:375:PRO:CA	2.66	0.52
1:B:336:ALA:O	1:B:337:LYS:HB3	2.10	0.52
1:A:108:GLU:HA	1:A:166:LYS:HA	1.91	0.51
1:A:424:THR:HG21	1:A:430:ALA:HB2	1.92	0.51
1:B:360:ALA:HB1	1:B:363:PRO:HG2	1.91	0.51
1:B:370:ASN:C	1:B:372:THR:H	2.13	0.51
1:B:405:GLY:O	1:B:408:PRO:HG2	2.11	0.51
1:A:333:GLY:HA2	1:A:336:ALA:HB3	1.91	0.51
1:A:370:ASN:C	1:A:372:THR:H	2.13	0.51
1:B:393:GLN:HB3	1:B:478:THR:HG21	1.93	0.51
1:A:349:ALA:O	1:A:353:VAL:HG23	2.10	0.51
1:B:419:PRO:HG2	1:B:472:ILE:HG23	1.91	0.51
1:B:46:ASN:O	1:B:79:LEU:HD22	2.10	0.51
1:A:208:HIS:O	1:A:235:VAL:HG23	2.11	0.51
1:B:88:PRO:HD2	1:B:214:PHE:HB2	1.92	0.51
1:A:34:PRO:HD3	1:A:66:ASN:CB	2.40	0.51
1:A:52:PHE:HD2	1:A:198:ASP:OD2	1.94	0.51
1:A:100:ASP:C	1:A:102:PRO:HD3	2.31	0.51
1:A:240:LYS:HG2	1:A:261:MET:HB3	1.93	0.51
1:A:241:ILE:HD12	1:A:246:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HD22	1:B:304:MET:HG3	1.93	0.50
1:A:192:SER:O	1:A:196:LYS:HD3	2.10	0.50
1:B:23:ILE:O	1:B:23:ILE:HG22	2.11	0.50
1:B:420:ILE:N	1:B:420:ILE:HD12	2.27	0.50
1:A:300:MET:O	1:A:301:LEU:HG	2.11	0.50
1:A:24:ILE:HG12	1:A:47:ILE:HB	1.93	0.50
1:A:56:SER:O	1:A:59:TYR:HB2	2.12	0.50
1:B:192:SER:O	1:B:196:LYS:HD3	2.11	0.50
1:B:356:GLU:HA	1:B:359:ILE:HG13	1.94	0.50
1:B:19:ARG:HD2	1:B:21:THR:O	2.11	0.50
1:B:265:GLY:CA	1:B:298:THR:HG21	2.42	0.50
1:A:130:TYR:O	1:A:133:ILE:HG22	2.12	0.50
1:A:301:LEU:HD23	1:A:314:GLU:HB3	1.94	0.50
1:B:123:ASP:C	1:B:125:ILE:H	2.15	0.50
1:B:41:ARG:HH21	1:B:79:LEU:HB2	1.77	0.50
1:A:356:GLU:HA	1:A:359:ILE:HG13	1.94	0.50
1:B:349:ALA:O	1:B:353:VAL:HG23	2.12	0.50
1:A:121:CYS:HA	1:A:125:ILE:HG23	1.94	0.50
1:B:105:PRO:O	1:B:106:ASN:HB2	2.12	0.50
1:B:265:GLY:HA3	1:B:298:THR:HG21	1.93	0.49
1:A:242:GLU:CG	1:A:263:ALA:HB1	2.33	0.49
1:A:272:PRO:HB2	1:A:275:GLU:HG3	1.93	0.49
1:A:301:LEU:HD22	1:A:310:PRO:HB3	1.94	0.49
1:A:400:VAL:O	1:A:422:LEU:HA	2.13	0.49
1:A:484:GLY:HA3	1:A:492:SER:H	1.77	0.49
1:B:130:TYR:O	1:B:133:ILE:HG22	2.11	0.49
1:B:429:ALA:HA	1:B:432:PHE:CE1	2.47	0.49
1:A:393:GLN:HB3	1:A:478:THR:HG21	1.93	0.49
1:A:282:LYS:HG3	1:B:10:LEU:HB2	1.94	0.49
1:B:230:GLU:H	1:B:230:GLU:CD	2.14	0.49
1:B:400:VAL:O	1:B:422:LEU:HA	2.11	0.49
1:B:41:ARG:HA	1:B:45:LEU:HB3	1.94	0.49
1:A:115:ASP:N	1:A:127:TYR:CE2	2.81	0.49
1:B:329:VAL:O	1:B:329:VAL:HG23	2.12	0.49
1:B:191:LEU:HD12	1:B:223:THR:HG22	1.95	0.49
1:B:301:LEU:HD22	1:B:310:PRO:HB3	1.94	0.49
1:A:265:GLY:CA	1:A:298:THR:HG21	2.42	0.49
1:B:56:SER:O	1:B:59:TYR:HB2	2.12	0.49
1:A:329:VAL:O	1:A:329:VAL:HG23	2.13	0.49
1:B:102:PRO:HB2	1:B:173:ILE:HG23	1.94	0.49
1:A:451:ASP:OD2	1:A:454:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:SER:HB2	1:B:496:GLN:HB3	1.94	0.49
1:A:86:LYS:O	1:A:87:GLY:O	2.31	0.49
1:B:301:LEU:HD23	1:B:314:GLU:CG	2.41	0.49
1:B:47:ILE:HG13	1:B:80:ALA:HB3	1.95	0.49
1:B:25:GLY:HA3	1:B:45:LEU:HD11	1.94	0.49
1:A:115:ASP:HA	1:A:118:ALA:HB2	1.95	0.48
1:A:156:GLU:HG2	1:A:164:LYS:HE2	1.95	0.48
1:A:192:SER:H	1:A:195:ASP:HB2	1.77	0.48
1:A:263:ALA:HB1	2:A:1005:PGA:O1	2.14	0.48
1:A:413:LYS:O	1:A:415:ARG:N	2.46	0.48
1:B:30:LYS:HD2	1:B:337:LYS:HA	1.95	0.48
1:B:378:THR:O	1:B:382:VAL:HG12	2.13	0.48
1:A:215:ILE:HD12	1:A:220:ASP:HB3	1.96	0.48
1:A:421:ILE:HD11	1:A:472:ILE:HG21	1.95	0.48
1:A:264:ARG:HB3	1:B:312:ARG:HG3	1.95	0.48
1:B:333:GLY:HA2	1:B:336:ALA:HB3	1.95	0.48
1:A:256:VAL:HG23	1:A:257:THR:N	2.28	0.48
1:A:401:LEU:HD21	1:A:460:ILE:HG13	1.95	0.48
1:A:41:ARG:HA	1:A:45:LEU:HB3	1.96	0.48
1:B:20:ARG:HB3	1:B:438:GLY:HA2	1.94	0.48
1:B:424:THR:CG2	1:B:430:ALA:HB2	2.43	0.48
1:B:451:ASP:OD2	1:B:454:ASP:HB2	2.12	0.48
1:B:484:GLY:HA3	1:B:492:SER:H	1.77	0.48
1:A:235:VAL:O	1:A:235:VAL:HG13	2.13	0.48
1:A:373:PRO:CB	1:A:376:THR:H	2.27	0.48
1:B:301:LEU:HD23	1:B:314:GLU:HB3	1.94	0.48
1:B:421:ILE:HD11	1:B:472:ILE:HG21	1.95	0.48
1:A:393:GLN:O	1:A:394:LYS:HB2	2.14	0.48
1:A:409:ARG:HG3	1:A:436:TYR:CZ	2.48	0.48
1:A:117:TYR:N	1:A:117:TYR:CD1	2.81	0.48
1:A:92:THR:HA	1:A:127:TYR:O	2.13	0.48
1:A:239:VAL:O	1:A:261:MET:N	2.47	0.48
1:A:420:ILE:HD12	1:A:420:ILE:N	2.29	0.48
1:A:175:SER:O	1:A:177:LYS:HE2	2.14	0.48
1:B:425:ARG:NH2	1:B:446:LYS:O	2.47	0.48
1:B:52:PHE:HD2	1:B:198:ASP:OD2	1.95	0.48
1:B:102:PRO:HB2	1:B:173:ILE:CG2	2.43	0.48
1:B:115:ASP:HA	1:B:118:ALA:HB2	1.95	0.48
1:A:108:GLU:HG2	1:A:108:GLU:H	1.52	0.48
1:A:232:GLY:C	1:A:235:VAL:HG12	2.35	0.48
1:B:114:ASP:C	1:B:116:LYS:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LYS:O	1:B:415:ARG:N	2.47	0.48
1:B:24:ILE:HG12	1:B:47:ILE:HB	1.94	0.48
1:A:25:GLY:HA3	1:A:45:LEU:HD11	1.95	0.47
1:A:301:LEU:HD23	1:A:314:GLU:CG	2.40	0.47
1:A:424:THR:CG2	1:A:430:ALA:HB2	2.44	0.47
1:B:49:ARG:HD2	1:B:84:ASP:HB2	1.95	0.47
1:A:105:PRO:O	1:A:106:ASN:HB2	2.13	0.47
1:A:416:PRO:HG2	1:A:420:ILE:HD11	1.97	0.47
1:A:474:LYS:HB2	1:A:477:ASP:OD1	2.14	0.47
1:A:47:ILE:HG13	1:A:80:ALA:HB3	1.96	0.47
1:A:100:ASP:HB3	1:A:102:PRO:HD3	1.96	0.47
1:A:123:ASP:C	1:A:125:ILE:H	2.18	0.47
1:A:281:LYS:HE2	1:B:323:LEU:HD13	1.97	0.47
1:B:117:TYR:CD1	1:B:117:TYR:N	2.82	0.47
1:B:121:CYS:HA	1:B:125:ILE:HG23	1.96	0.47
1:B:192:SER:H	1:B:195:ASP:HB2	1.79	0.47
1:B:56:SER:H	1:B:59:TYR:HD2	1.59	0.47
1:A:244:GLN:C	1:A:247:VAL:HG23	2.35	0.47
1:B:86:LYS:O	1:B:87:GLY:O	2.32	0.47
1:A:20:ARG:HB3	1:A:438:GLY:HA2	1.96	0.47
1:A:41:ARG:HH21	1:A:79:LEU:HB2	1.79	0.47
1:B:235:VAL:HG13	1:B:235:VAL:O	2.14	0.47
1:B:359:ILE:HG22	1:B:360:ALA:N	2.30	0.47
1:A:301:LEU:HD13	1:A:304:MET:SD	2.55	0.47
1:A:480:VAL:HA	1:A:496:GLN:O	2.15	0.47
1:B:250:PHE:O	1:B:250:PHE:CG	2.68	0.47
1:B:272:PRO:HB2	1:B:275:GLU:HG3	1.97	0.47
1:A:192:SER:N	1:A:195:ASP:HB2	2.30	0.47
1:B:192:SER:N	1:B:195:ASP:HB2	2.30	0.47
1:A:481:SER:HB2	1:A:496:GLN:HB3	1.97	0.46
1:B:141:ARG:HD2	1:B:184:THR:HG23	1.97	0.46
1:B:156:GLU:HG2	1:B:164:LYS:HE2	1.96	0.46
1:A:19:ARG:HD2	1:A:21:THR:O	2.14	0.46
1:A:359:ILE:HG22	1:A:360:ALA:N	2.30	0.46
1:B:115:ASP:N	1:B:127:TYR:CE2	2.80	0.46
1:B:175:SER:O	1:B:177:LYS:HE2	2.15	0.46
1:B:456:VAL:CG2	1:B:457:GLU:N	2.78	0.46
1:B:480:VAL:HA	1:B:496:GLN:O	2.16	0.46
1:A:114:ASP:C	1:A:116:LYS:H	2.19	0.46
1:A:250:PHE:O	1:A:254:LEU:HB2	2.15	0.46
1:B:380:GLU:CA	1:B:410:LEU:HD23	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD12	1:B:316:SER:HA	1.96	0.46
1:B:474:LYS:HB2	1:B:477:ASP:OD1	2.15	0.46
1:A:470:PHE:HB3	1:A:472:ILE:HG13	1.97	0.46
1:A:136:VAL:HG13	1:A:137:ILE:N	2.30	0.46
1:A:409:ARG:O	1:A:412:SER:N	2.49	0.46
1:B:200:ARG:O	1:B:204:LYS:HB2	2.16	0.46
1:B:41:ARG:HE	1:B:79:LEU:CB	2.27	0.46
1:B:401:LEU:HD21	1:B:460:ILE:HG13	1.98	0.46
1:B:92:THR:HA	1:B:127:TYR:O	2.14	0.46
1:A:425:ARG:NH2	1:A:446:LYS:O	2.46	0.46
1:B:232:GLY:C	1:B:235:VAL:HG12	2.36	0.46
1:B:470:PHE:HB3	1:B:472:ILE:HG13	1.98	0.46
1:A:30:LYS:HD2	1:A:337:LYS:HA	1.96	0.46
1:A:49:ARG:HD2	1:A:84:ASP:HB2	1.97	0.46
1:B:491:HIS:HA	3:B:1008:FBP:O4	2.15	0.46
1:B:24:ILE:CD1	1:B:295:ILE:HD13	2.45	0.46
1:B:136:VAL:HG13	1:B:137:ILE:N	2.31	0.46
1:A:264:ARG:HD2	1:A:280:GLN:NE2	2.31	0.46
1:B:401:LEU:HD22	1:B:459:ARG:HB3	1.98	0.46
1:A:297:ALA:CB	1:A:330:MET:HG2	2.47	0.45
1:A:159:ASP:HA	1:A:162:THR:HB	1.98	0.45
1:A:353:VAL:HG12	1:A:357:GLN:OE1	2.16	0.45
1:B:244:GLN:HG3	1:B:248:ASN:HD21	1.79	0.45
1:B:393:GLN:O	1:B:394:LYS:HB2	2.16	0.45
1:A:362:LEU:HB3	1:A:363:PRO:HD3	1.98	0.45
1:B:413:LYS:C	1:B:415:ARG:N	2.70	0.45
1:B:416:PRO:HG2	1:B:420:ILE:HD11	1.97	0.45
1:B:451:ASP:C	1:B:453:THR:N	2.68	0.45
1:A:244:GLN:HG3	1:A:248:ASN:HD21	1.78	0.45
1:A:380:GLU:CA	1:A:410:LEU:HD23	2.47	0.45
1:B:191:LEU:HD11	1:B:224:ILE:HA	1.98	0.45
1:A:141:ARG:HD2	1:A:184:THR:HG23	1.98	0.45
1:B:102:PRO:O	1:B:104:PRO:HD3	2.17	0.45
1:B:264:ARG:HD2	1:B:280:GLN:NE2	2.31	0.45
1:B:49:ARG:HG2	1:B:211:PHE:CE2	2.52	0.45
1:B:256:VAL:HG23	1:B:257:THR:N	2.32	0.45
1:B:293:PRO:HG3	1:B:436:TYR:HE1	1.81	0.45
1:B:416:PRO:C	1:B:418:CYS:H	2.20	0.45
1:B:49:ARG:HH11	1:B:84:ASP:CG	2.19	0.45
1:A:200:ARG:O	1:A:204:LYS:HB2	2.16	0.45
1:B:239:VAL:O	1:B:261:MET:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLU:CD	1:B:193:GLU:H	2.21	0.45
1:B:74:TYR:HA	1:B:75:PRO:HD2	1.71	0.45
1:B:250:PHE:O	1:B:254:LEU:HB2	2.17	0.45
1:B:362:LEU:HB3	1:B:363:PRO:HD3	1.99	0.45
1:A:242:GLU:HG3	1:A:263:ALA:HB3	1.91	0.44
1:A:56:SER:H	1:A:59:TYR:HD2	1.60	0.44
1:B:409:ARG:O	1:B:412:SER:N	2.49	0.44
1:A:138:SER:H	1:A:141:ARG:HG3	1.82	0.44
1:A:24:ILE:CD1	1:A:295:ILE:HD13	2.47	0.44
1:A:456:VAL:CG2	1:A:457:GLU:N	2.80	0.44
1:B:24:ILE:HD11	1:B:295:ILE:HD13	1.99	0.44
1:A:191:LEU:HD11	1:A:224:ILE:HA	1.99	0.44
1:A:312:ARG:NH1	1:B:268:GLY:HA3	2.32	0.44
1:B:40:LEU:HD12	1:B:342:ILE:HG22	1.99	0.44
1:B:77:ARG:NH2	1:B:442:PHE:CE1	2.85	0.44
1:B:460:ILE:O	1:B:464:ILE:HG13	2.18	0.44
1:B:242:GLU:CG	1:B:263:ALA:HB1	2.33	0.44
1:B:356:GLU:H	1:B:356:GLU:HG3	1.63	0.44
1:A:128:VAL:HG12	1:A:179:VAL:HG21	2.00	0.44
1:A:416:PRO:C	1:A:418:CYS:H	2.21	0.44
1:A:77:ARG:NH2	1:A:442:PHE:CE1	2.86	0.44
1:B:114:ASP:OD1	1:B:116:LYS:HB2	2.18	0.44
1:B:239:VAL:HG23	1:B:260:VAL:HA	2.00	0.44
1:A:362:LEU:HB3	1:A:363:PRO:CD	2.48	0.44
1:A:412:SER:O	1:A:415:ARG:HG3	2.18	0.44
1:B:138:SER:H	1:B:141:ARG:HG3	1.82	0.44
1:B:49:ARG:HG2	1:B:211:PHE:HE2	1.83	0.44
1:A:133:ILE:HA	1:A:136:VAL:HG12	2.00	0.43
1:A:144:TYR:HA	1:A:150:LEU:O	2.18	0.43
1:A:413:LYS:C	1:A:415:ARG:N	2.69	0.43
1:A:49:ARG:HH11	1:A:84:ASP:CG	2.21	0.43
1:B:133:ILE:O	1:B:137:ILE:HG22	2.18	0.43
1:B:234:ASP:OD1	1:B:428:ARG:NH1	2.51	0.43
1:B:353:VAL:HG12	1:B:357:GLN:OE1	2.18	0.43
1:A:286:LYS:HG2	1:B:8:THR:HG23	2.00	0.43
1:B:115:ASP:N	1:B:127:TYR:OH	2.51	0.43
1:A:456:VAL:CG1	1:A:459:ARG:HH21	2.24	0.43
1:A:193:GLU:CD	1:A:193:GLU:H	2.22	0.43
1:A:239:VAL:HG23	1:A:260:VAL:HA	2.00	0.43
1:A:40:LEU:HD12	1:A:342:ILE:HG22	1.99	0.43
1:A:49:ARG:HG2	1:A:211:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:O	1:A:253:ILE:HD11	2.19	0.43
1:B:242:GLU:HG2	1:B:266:ASP:HB2	2.01	0.43
1:B:273:ALA:O	1:B:276:VAL:HG12	2.19	0.43
1:B:467:ALA:CB	1:B:473:LEU:HD12	2.47	0.43
1:A:133:ILE:O	1:A:137:ILE:HG22	2.18	0.43
1:A:228:LEU:HG	1:A:235:VAL:CG1	2.48	0.43
1:B:114:ASP:OD2	1:B:116:LYS:HB2	2.19	0.43
1:B:363:PRO:O	1:B:366:ASP:HB2	2.18	0.43
1:A:217:THR:O	1:A:220:ASP:HB2	2.19	0.43
1:A:301:LEU:HD22	1:A:304:MET:HG3	2.01	0.43
1:A:90:ILE:HB	1:A:179:VAL:HB	2.01	0.43
1:A:34:PRO:O	1:A:38:VAL:N	2.51	0.43
1:B:243:ASN:HB2	1:B:244:GLN:H	1.72	0.43
1:B:301:LEU:HD13	1:B:304:MET:SD	2.59	0.43
1:B:432:PHE:C	1:B:432:PHE:CD1	2.92	0.43
1:A:191:LEU:HD12	1:A:223:THR:HG22	2.01	0.43
1:A:366:ASP:O	1:A:369:ARG:HG3	2.19	0.43
1:B:215:ILE:HD12	1:B:220:ASP:HB3	2.01	0.43
1:B:297:ALA:CB	1:B:330:MET:HG2	2.48	0.43
1:B:456:VAL:CG1	1:B:459:ARG:HH21	2.26	0.43
1:B:460:ILE:HD11	1:B:483:GLN:NE2	2.31	0.43
1:A:387:VAL:HG11	1:A:414:TYR:O	2.19	0.42
1:A:451:ASP:C	1:A:453:THR:N	2.69	0.42
1:A:401:LEU:HD22	1:A:459:ARG:HB3	2.00	0.42
1:B:23:ILE:H	1:B:46:ASN:ND2	2.07	0.42
1:A:250:PHE:CG	1:A:250:PHE:O	2.71	0.42
1:A:433:SER:HB3	1:A:439:VAL:HG11	2.01	0.42
1:A:273:ALA:O	1:A:276:VAL:HG12	2.20	0.42
1:A:363:PRO:O	1:A:366:ASP:HB2	2.19	0.42
1:A:432:PHE:CD1	1:A:432:PHE:C	2.92	0.42
1:B:81:ILE:N	1:B:208:HIS:ND1	2.58	0.42
1:A:293:PRO:HG3	1:A:436:TYR:HE1	1.85	0.42
1:B:380:GLU:HA	1:B:410:LEU:HD23	2.01	0.42
1:B:387:VAL:HG11	1:B:414:TYR:O	2.19	0.42
1:B:303:SER:HB3	1:B:314:GLU:OE1	2.20	0.42
1:A:115:ASP:N	1:A:127:TYR:OH	2.52	0.42
1:A:216:ARG:C	1:A:253:ILE:HD11	2.40	0.42
1:A:257:THR:OG1	1:A:258:ASP:N	2.53	0.42
1:A:304:MET:HA	1:A:307:ASN:O	2.20	0.42
1:A:378:THR:O	1:A:382:VAL:HG12	2.20	0.42
1:A:365:TYR:CD1	1:A:414:TYR:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HE	1:A:79:LEU:CB	2.28	0.42
1:A:460:ILE:O	1:A:464:ILE:HG13	2.19	0.42
1:B:41:ARG:HE	1:B:79:LEU:CG	2.32	0.42
1:A:422:LEU:HG	1:A:422:LEU:O	2.18	0.42
1:B:114:ASP:O	1:B:116:LYS:N	2.52	0.42
1:B:244:GLN:C	1:B:247:VAL:HG23	2.39	0.42
1:A:23:ILE:HG22	1:A:23:ILE:O	2.19	0.42
1:B:295:ILE:HG23	1:B:328:CYS:CB	2.50	0.42
1:A:24:ILE:HD11	1:A:295:ILE:HD13	2.02	0.42
1:A:467:ALA:CB	1:A:473:LEU:HD12	2.49	0.42
1:B:107:HIS:ND1	1:B:108:GLU:O	2.47	0.42
1:A:309:ARG:HH21	1:B:269:ILE:HD13	1.82	0.42
1:B:464:ILE:O	1:B:468:LYS:HG3	2.19	0.42
1:A:117:TYR:CD2	1:A:125:ILE:HD13	2.54	0.42
1:A:380:GLU:HA	1:A:410:LEU:HD23	2.02	0.42
1:A:456:VAL:O	1:A:460:ILE:HD12	2.20	0.42
1:B:194:LYS:O	1:B:198:ASP:OD1	2.38	0.41
1:A:83:LEU:HB3	1:A:210:VAL:HG22	2.02	0.41
1:A:486:LYS:H	1:A:490:GLY:HA2	1.84	0.41
1:B:241:ILE:HG23	1:B:246:GLY:O	2.20	0.41
1:B:90:ILE:HB	1:B:179:VAL:HB	2.01	0.41
1:A:486:LYS:HB2	1:A:490:GLY:HA2	2.01	0.41
1:B:159:ASP:HA	1:B:162:THR:OG1	2.20	0.41
1:B:222:LEU:O	1:B:225:ARG:HB3	2.20	0.41
1:A:114:ASP:O	1:A:116:LYS:N	2.53	0.41
1:B:110:ILE:HG23	1:B:125:ILE:HG13	2.02	0.41
1:B:144:TYR:HA	1:B:150:LEU:O	2.20	0.41
1:B:216:ARG:O	1:B:253:ILE:HD11	2.21	0.41
1:B:31:THR:HA	1:B:36:THR:HG21	2.03	0.41
1:B:218:ALA:O	1:B:221:VAL:HG23	2.20	0.41
1:B:305:THR:HG23	1:B:306:TYR:CD2	2.55	0.41
1:B:433:SER:HB3	1:B:439:VAL:HG11	2.01	0.41
1:A:106:ASN:HD21	1:A:166:LYS:NZ	2.17	0.41
1:A:88:PRO:HB2	1:A:188:LEU:HB3	2.03	0.41
1:B:128:VAL:HG12	1:B:179:VAL:HG21	2.01	0.41
1:A:323:LEU:HD13	1:B:281:LYS:HE2	2.02	0.41
1:B:486:LYS:HB2	1:B:490:GLY:HA2	2.02	0.41
1:A:110:ILE:HG23	1:A:125:ILE:HG13	2.01	0.41
1:B:216:ARG:C	1:B:253:ILE:HD11	2.41	0.41
1:A:225:ARG:NH2	1:A:258:ASP:OD2	2.44	0.41
1:A:264:ARG:O	1:A:267:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LYS:O	1:B:125:ILE:HB	2.20	0.41
1:B:373:PRO:CB	1:B:376:THR:N	2.79	0.41
1:B:422:LEU:O	1:B:422:LEU:HG	2.21	0.41
1:A:106:ASN:O	1:A:106:ASN:ND2	2.54	0.41
1:B:117:TYR:CD2	1:B:125:ILE:HD13	2.56	0.41
1:B:124:LYS:H	1:B:124:LYS:HG2	1.70	0.41
1:B:217:THR:O	1:B:220:ASP:HB2	2.21	0.41
1:B:362:LEU:HB3	1:B:363:PRO:CD	2.51	0.41
1:B:365:TYR:CD1	1:B:414:TYR:HB3	2.56	0.41
1:B:56:SER:O	1:B:59:TYR:N	2.54	0.41
1:B:412:SER:O	1:B:415:ARG:HG3	2.21	0.41
1:A:124:LYS:O	1:A:125:ILE:HB	2.21	0.40
1:A:390:VAL:O	1:A:394:LYS:N	2.54	0.40
1:A:426:CYS:HA	1:A:427:PRO:HD3	1.94	0.40
1:A:401:LEU:HD12	3:A:1007:FBP:O2	2.21	0.40
1:B:133:ILE:HA	1:B:136:VAL:HG12	2.02	0.40
1:B:466:LYS:O	1:B:469:GLU:HB2	2.21	0.40
1:A:47:ILE:HD11	1:A:434:HIS:HB2	2.03	0.40
1:B:108:GLU:HG2	1:B:108:GLU:H	1.51	0.40
1:B:241:ILE:HG23	1:B:246:GLY:C	2.42	0.40
1:A:114:ASP:OD1	1:A:116:LYS:HB2	2.22	0.40
1:A:116:LYS:HB3	1:A:116:LYS:NZ	2.36	0.40
1:A:305:THR:HG23	1:A:306:TYR:CD2	2.56	0.40
1:A:41:ARG:HE	1:A:79:LEU:CG	2.35	0.40
1:A:479:TYR:CE1	1:A:498:SER:HB3	2.56	0.40
1:A:477:ASP:O	1:A:499:THR:HG23	2.21	0.40
1:A:49:ARG:HG2	1:A:211:PHE:HE2	1.85	0.40
1:B:19:ARG:HG3	1:B:352:ALA:HB3	2.03	0.40
1:B:486:LYS:H	1:B:490:GLY:HA2	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/500 (97%)	398 (82%)	56 (12%)	32 (7%)	1	6
1	B	481/500 (96%)	394 (82%)	57 (12%)	30 (6%)	1	8
All	All	967/1000 (97%)	792 (82%)	113 (12%)	62 (6%)	1	7

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	99	VAL
1	A	106	ASN
1	A	170	ALA
1	A	337	LYS
1	A	373	PRO
1	A	374	LYS
1	A	449	VAL
1	A	475	LYS
1	A	485	PHE
1	B	78	PRO
1	B	106	ASN
1	B	170	ALA
1	B	337	LYS
1	B	373	PRO
1	B	374	LYS
1	B	449	VAL
1	B	475	LYS
1	B	485	PHE
1	A	87	GLY
1	A	123	ASP
1	A	130	TYR
1	A	232	GLY
1	A	233	LYS
1	A	415	ARG
1	A	487	ALA
1	A	492	SER
1	A	493	ASN
1	B	87	GLY
1	B	123	ASP
1	B	130	TYR
1	B	154	VAL
1	B	232	GLY
1	B	233	LYS
1	B	415	ARG

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Mol	Chain	Res	Type
1	B	487	ALA
1	B	492	SER
1	B	493	ASN
1	A	124	LYS
1	A	154	VAL
1	A	341	PRO
1	A	414	TYR
1	B	124	LYS
1	B	341	PRO
1	B	414	TYR
1	A	115	ASP
1	A	146	ASP
1	B	115	ASP
1	B	146	ASP
1	B	257	THR
1	A	257	THR
1	B	301	LEU
1	A	301	LEU
1	A	105	PRO
1	B	105	PRO
1	A	44	GLY
1	A	125	ILE
1	A	265	GLY
1	B	44	GLY
1	B	125	ILE
1	B	265	GLY
1	A	75	PRO

### 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	417/423 (99%)	307 (74%)	110 (26%)	0	2
1	B	414/423 (98%)	305 (74%)	109 (26%)	0	2
All	All	831/846 (98%)	612 (74%)	219 (26%)	0	2

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	LEU
1	A	6	ARG
1	A	9	SER
1	A	21	THR
1	A	22	SER
1	A	30	LYS
1	A	31	THR
1	A	37	LEU
1	A	42	LYS
1	A	45	LEU
1	A	49	ARG
1	A	50	MET
1	A	53	SER
1	A	56	SER
1	A	61	LYS
1	A	69	LYS
1	A	70	SER
1	A	73	LEU
1	A	86	LYS
1	A	96	THR
1	A	97	ASN
1	A	108	GLU
1	A	112	THR
1	A	114	ASP
1	A	116	LYS
1	A	119	LYS
1	A	123	ASP
1	A	124	LYS
1	A	126	MET
1	A	128	VAL
1	A	130	TYR
1	A	134	THR
1	A	135	LYS
1	A	138	SER
1	A	150	LEU
1	A	151	SER
1	A	153	GLN
1	A	156	GLU
1	A	158	VAL
1	A	162	THR
1	A	164	LYS

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Mol	Chain	Res	Type
1	A	176	HIS
1	A	181	LEU
1	A	184	THR
1	A	194	LYS
1	A	196	LYS
1	A	204	LYS
1	A	210	VAL
1	A	213	SER
1	A	219	ASN
1	A	221	VAL
1	A	228	LEU
1	A	233	LYS
1	A	234	ASP
1	A	240	LYS
1	A	242	GLU
1	A	243	ASN
1	A	247	VAL
1	A	249	ASN
1	A	252	GLU
1	A	254	LEU
1	A	261	MET
1	A	270	GLU
1	A	276	VAL
1	A	277	LEU
1	A	282	LYS
1	A	303	SER
1	A	307	ASN
1	A	312	ARG
1	A	314	GLU
1	A	315	VAL
1	A	316	SER
1	A	327	ASP
1	A	330	MET
1	A	337	LYS
1	A	339	ASN
1	A	356	GLU
1	A	357	GLN
1	A	369	ARG
1	A	374	LYS
1	A	376	THR
1	A	377	SER
1	A	379	THR

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Mol	Chain	Res	Type
1	A	385	SER
1	A	398	ILE
1	A	400	VAL
1	A	401	LEU
1	A	402	SER
1	A	403	THR
1	A	404	SER
1	A	413	LYS
1	A	422	LEU
1	A	425	ARG
1	A	431	ARG
1	A	432	PHE
1	A	433	SER
1	A	445	GLU
1	A	450	SER
1	A	451	ASP
1	A	459	ARG
1	A	461	ASN
1	A	465	GLU
1	A	474	LYS
1	A	486	LYS
1	A	491	HIS
1	A	492	SER
1	A	495	LEU
1	A	496	GLN
1	A	498	SER
1	B	3	ARG
1	B	4	LEU
1	B	6	ARG
1	B	9	SER
1	B	21	THR
1	B	22	SER
1	B	30	LYS
1	B	31	THR
1	B	37	LEU
1	B	42	LYS
1	B	45	LEU
1	B	49	ARG
1	B	50	MET
1	B	53	SER
1	B	56	SER
1	B	61	LYS

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Mol	Chain	Res	Type
1	B	69	LYS
1	B	70	SER
1	B	73	LEU
1	B	86	LYS
1	B	96	THR
1	B	97	ASN
1	B	108	GLU
1	B	112	THR
1	B	114	ASP
1	B	116	LYS
1	B	119	LYS
1	B	123	ASP
1	B	124	LYS
1	B	126	MET
1	B	128	VAL
1	B	130	TYR
1	B	134	THR
1	B	135	LYS
1	B	138	SER
1	B	150	LEU
1	B	151	SER
1	B	153	GLN
1	B	156	GLU
1	B	158	VAL
1	B	162	THR
1	B	164	LYS
1	B	176	HIS
1	B	181	LEU
1	B	184	THR
1	B	194	LYS
1	B	196	LYS
1	B	204	LYS
1	B	210	VAL
1	B	213	SER
1	B	219	ASN
1	B	221	VAL
1	B	228	LEU
1	B	233	LYS
1	B	234	ASP
1	B	240	LYS
1	B	242	GLU
1	B	243	ASN

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Mol	Chain	Res	Type
1	B	247	VAL
1	B	249	ASN
1	B	252	GLU
1	B	254	LEU
1	B	261	MET
1	B	270	GLU
1	B	276	VAL
1	B	277	LEU
1	B	282	LYS
1	B	303	SER
1	B	307	ASN
1	B	312	ARG
1	B	314	GLU
1	B	315	VAL
1	B	316	SER
1	B	327	ASP
1	B	330	MET
1	B	337	LYS
1	B	339	ASN
1	B	356	GLU
1	B	357	GLN
1	B	369	ARG
1	B	374	LYS
1	B	376	THR
1	B	377	SER
1	B	379	THR
1	B	385	SER
1	B	398	ILE
1	B	400	VAL
1	B	401	LEU
1	B	402	SER
1	B	403	THR
1	B	404	SER
1	B	413	LYS
1	B	422	LEU
1	B	425	ARG
1	B	431	ARG
1	B	432	PHE
1	B	445	GLU
1	B	450	SER
1	B	451	ASP
1	B	459	ARG

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Mol	Chain	Res	Type
1	B	461	ASN
1	B	465	GLU
1	B	474	LYS
1	B	486	LYS
1	B	491	HIS
1	B	492	SER
1	B	495	LEU
1	B	496	GLN
1	B	498	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	106	ASN
1	A	248	ASN
1	A	280	GLN
1	A	288	ASN
1	A	307	ASN
1	A	320	ASN
1	A	364	ASN
1	A	393	GLN
1	A	434	HIS
1	A	483	GLN
1	B	46	ASN
1	B	106	ASN
1	B	248	ASN
1	B	280	GLN
1	B	288	ASN
1	B	307	ASN
1	B	320	ASN
1	B	364	ASN
1	B	393	GLN
1	B	434	HIS
1	B	483	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	FBP	B	1008	-	18,20,20	1.08	1 (5%)	23,32,32	0.83	0
3	FBP	A	1007	-	18,20,20	1.04	0	23,32,32	0.68	0
2	PGA	A	1005	5,4	5,8,8	2.50	3 (60%)	6,11,11	3.73	3 (50%)
2	PGA	B	1006	5,4	5,8,8	2.44	2 (40%)	6,11,11	3.56	4 (66%)

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	FBP	B	1008	-	-	1/13/32/32	0/1/1/1
3	FBP	A	1007	-	-	2/13/32/32	0/1/1/1
2	PGA	A	1005	5,4	-	0/4/6/6	-
2	PGA	B	1006	5,4	-	1/4/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1006	PGA	P-O3P	4.16	1.70	1.54
2	A	1005	PGA	P-O3P	4.05	1.70	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1006	PGA	P-O2P	2.56	1.58	1.50
2	A	1005	PGA	P-O2P	2.47	1.58	1.50
3	B	1008	FBP	O5-C2	2.34	1.46	1.43
2	A	1005	PGA	O1P-C2	-2.01	1.37	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	PGA	O1P-P-O2P	7.74	128.19	106.47
2	B	1006	PGA	O1P-P-O2P	7.30	126.95	106.47
2	B	1006	PGA	O3P-P-O1P	3.09	114.94	106.73
2	A	1005	PGA	O3P-P-O1P	2.97	114.64	106.73
2	A	1005	PGA	O4P-P-O1P	-2.41	100.32	106.73
2	B	1006	PGA	O4P-P-O1P	-2.11	101.13	106.73
2	B	1006	PGA	O4P-P-O3P	-2.01	99.95	107.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1007	FBP	O5-C5-C6-O6
3	A	1007	FBP	C4-C5-C6-O6
3	B	1008	FBP	C4-C5-C6-O6
2	B	1006	PGA	C2-O1P-P-O3P

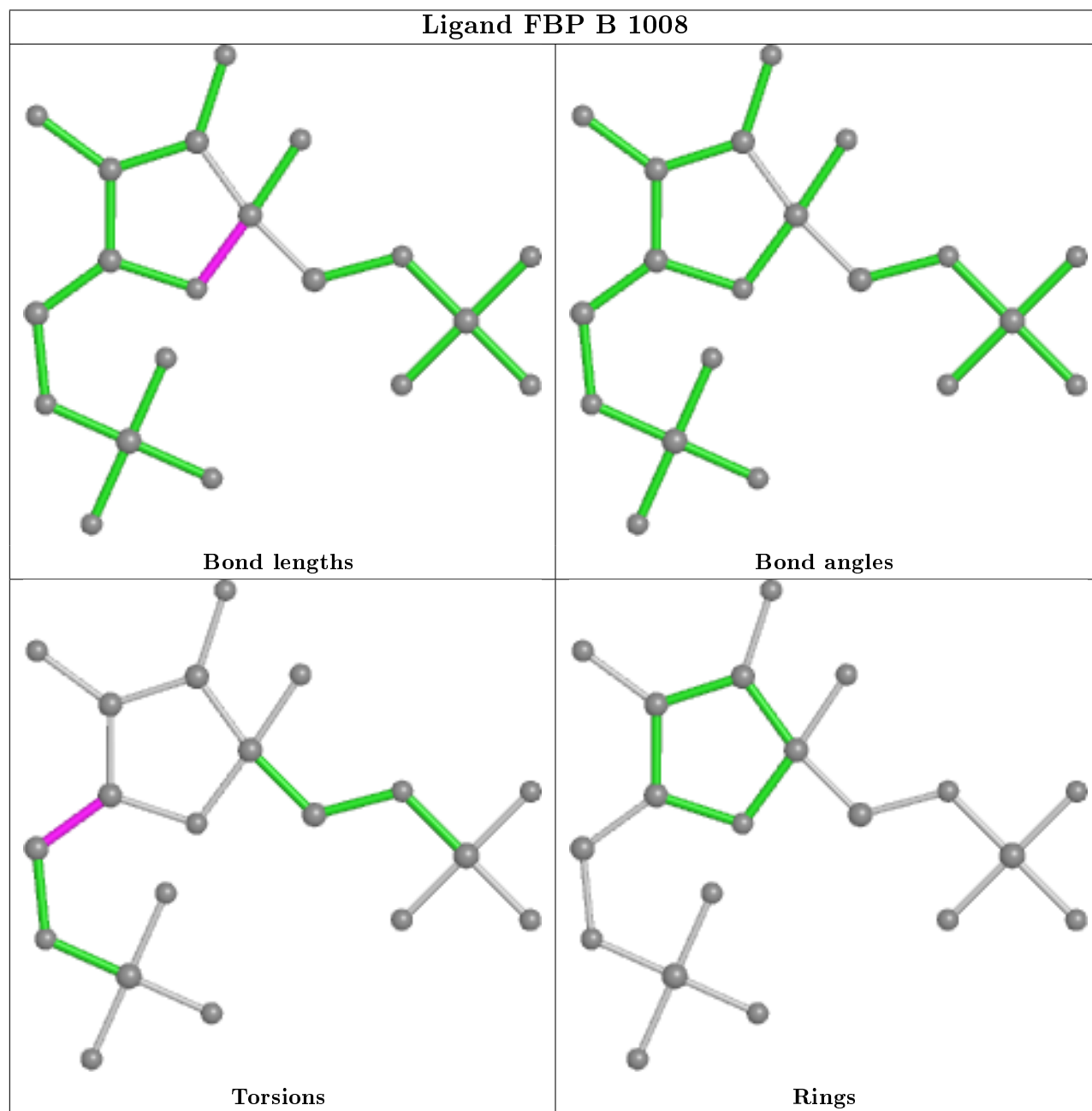
There are no ring outliers.

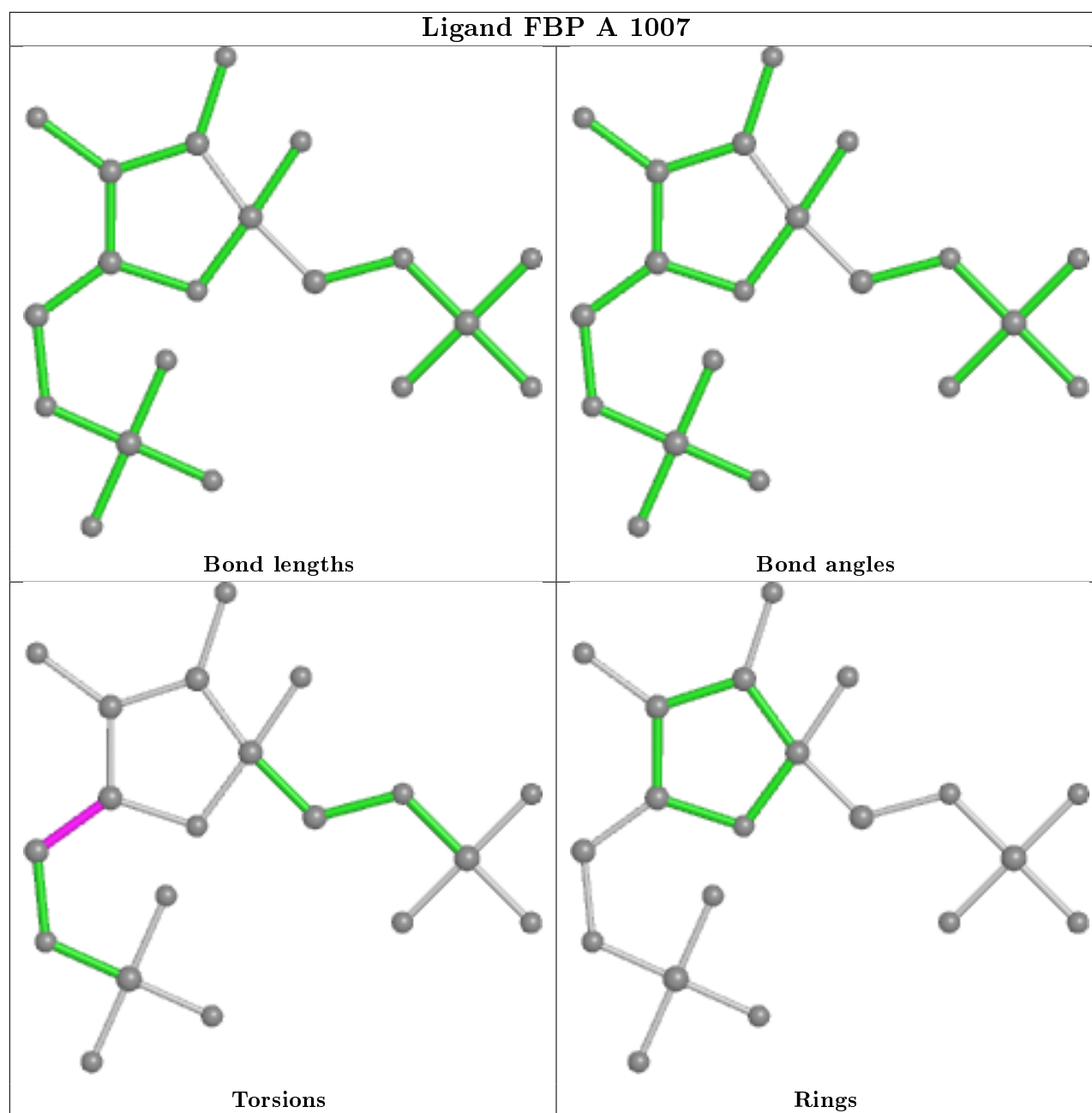
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1008	FBP	2	0
3	A	1007	FBP	3	0
2	A	1005	PGA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.