



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:40 PM GMT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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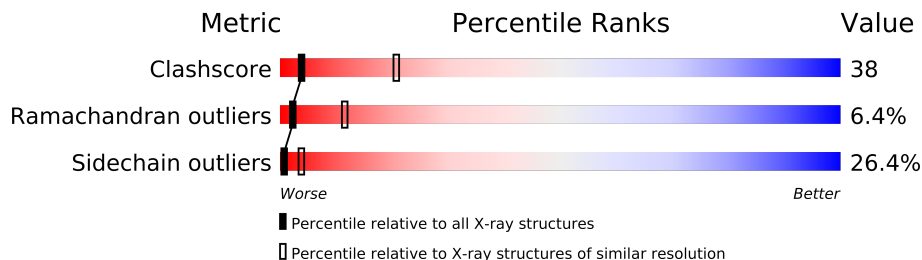
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PGA	A	1005	X	-

## 2 Entry composition

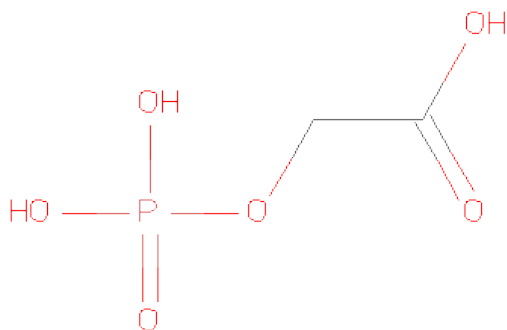
There are 5 unique types of molecules in this entry. The entry contains 7581 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

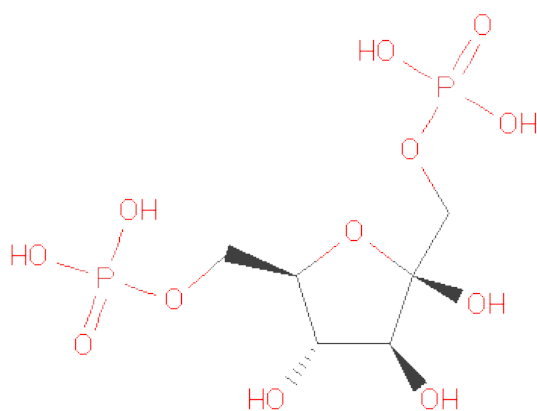
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3773	2380	650	726	17			
1	B	489	Total	C	N	O	S	0	0	0
			3746	2362	647	720	17			

- Molecule 2 is SUGAR (2-PHOSPHOGLYCOLIC ACID) (three-letter code: PGA) (formula: C<sub>2</sub>H<sub>5</sub>O<sub>6</sub>P).



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 SUGAR (FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



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		

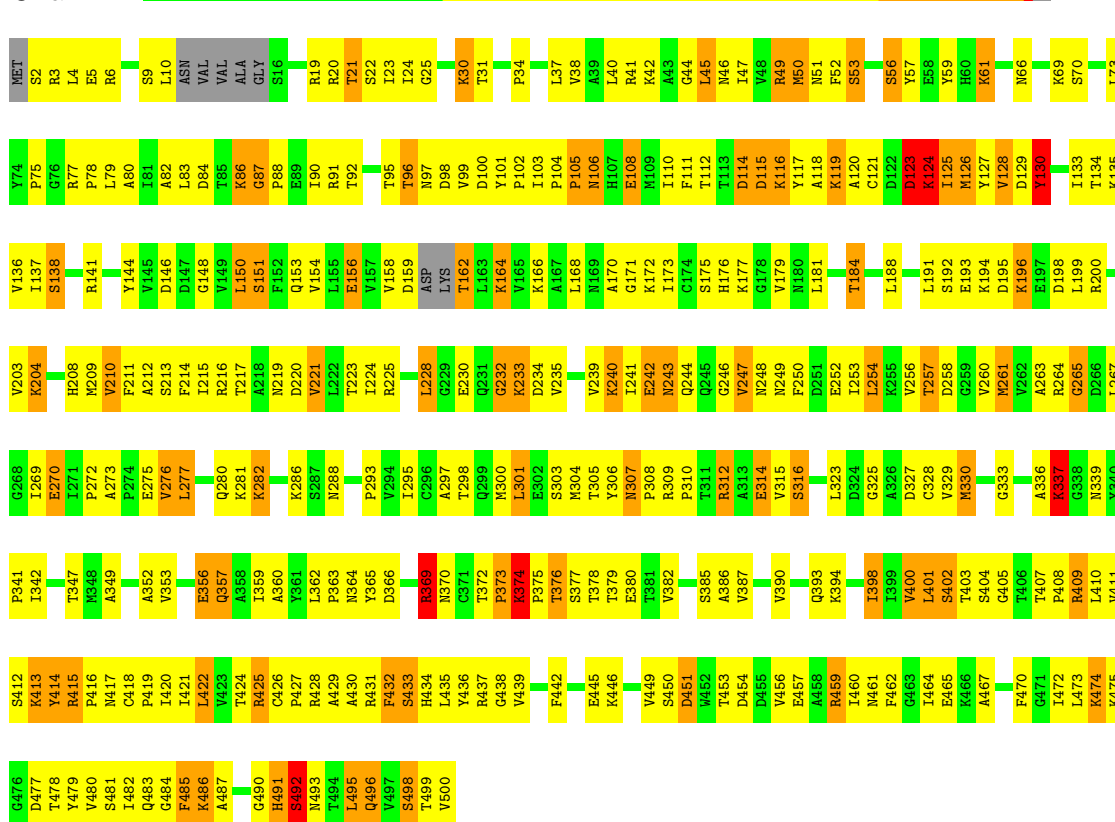
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

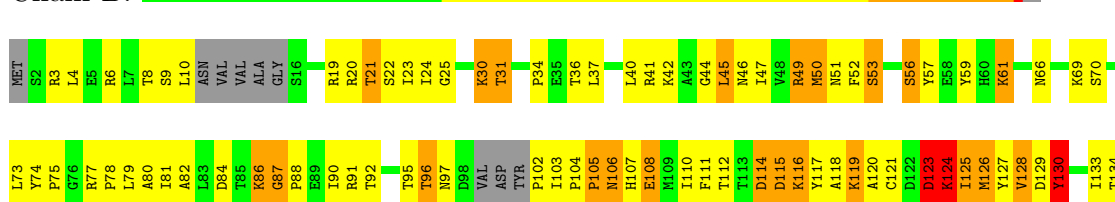
#### • Molecule 1: PYRUVATE KINASE

Chain A:



#### • Molecule 1: PYRUVATE KINASE

Chain B:





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.40Å 102.70Å 110.90Å 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

All (579) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:B:119:LYS:HE2	1:B:119:LYS:H	1.40	0.86
1:A:282:LYS:HE2	1:B:10:LEU:H	1.40	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(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:373:PRO:O	1:B:374:LYS:HB2	1.78	0.81
1:B:110:ILE:HD11	1:B:162:THR:HG22	1.62	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:B:144:TYR:HB3	1:B:148:GLY:HA2	1.65	0.79
1:A:456:VAL:HG12	1:A:459:ARG:HH21	1.46	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:374:LYS:H	1:B:375:PRO:CA	1.96	0.77
1:B:30:LYS:HE3	1:B:30:LYS:H	1.48	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:B:373:PRO:HB2	1:B:376:THR:N	2.03	0.74
1:A:91:ARG:H	1:A:129:ASP:HB2	1.52	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
1:A:90:ILE:HG23	1:A:130:TYR:H	1.55	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:295:ILE:HG12	1:A:328:CYS:HB2	1.73	0.69
1:A:102:PRO:O	1:A:173:ILE:HG22	1.93	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:B:373:PRO:HB2	1:B:376:THR:H	1.59	0.68
1:A:378:THR:HG21	1:A:486:LYS:HE2	1.75	0.68
1:B:246:GLY:O	1:B:250:PHE:HB2	1.94	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: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:90:ILE:HG23	1:B:130:TYR:H	1.58	0.67
1:B:432:PHE:O	1:B:435:LEU:HB2	1.95	0.67
1:B:295:ILE:HG12	1:B:328:CYS:HB2	1.76	0.67
1:B:19:ARG:HH12	1:B:46:ASN:HD21	1.42	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:398:ILE:HD11	1:B:482:ILE:CD1	2.23	0.66
1:B:263:ALA:O	1:B:267:LEU:HB2	1.95	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
1:A:360:ALA:O	1:A:364:ASN:HB2	1.96	0.66
1:B:130:TYR:HB3	1:B:133:ILE:HB	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:460:ILE:HD11	1:B:483:GLN:HE21	1.61	0.66
1:A:413:LYS:C	1:A:415:ARG:H	1.99	0.66
1:B:95:THR:HG23	1:B:175:SER:HB3	1.77	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:A:50:MET:HB2	1:A:82:ALA:O	1.96	0.65
1:A:96:THR:HA	1:A:120:ALA:HA	1.76	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:24:ILE:HD12	1:B:295:ILE:HG21	1.77	0.65
1:B:117:TYR:HB2	1:B:127:TYR:CE1	2.32	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:460:ILE:HD11	1:A:483:GLN:HE21	1.62	0.65
1:A:30:LYS:HE3	1:A:30:LYS:N	2.12	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:B:30:LYS:HE3	1:B:30:LYS:N	2.11	0.64
1:A:258:ASP:O	1:A:293:PRO:HD2	1.97	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:B:159:ASP:HA	1:B:162:THR:CB	2.28	0.62
1:A:484:GLY:O	1:A:485:PHE:HB2	2.00	0.62
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:215:ILE:HG13	1:B:239:VAL:HG12	1.85	0.58
1:A:103:ILE:HG12	1:A:172:LYS:HB3	1.85	0.58
1:B:212:ALA:O	1:B:240:LYS:HB2	2.04	0.58
1:A:53:SER:HA	1:A:86:LYS:HB2	1.84	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:B:103:ILE:HG12	1:B:172:LYS:HB3	1.86	0.57
1:A:228:LEU:HG	1:A:235:VAL:HG11	1.86	0.57
1:A:250:PHE:CE1	1:A:260:VAL:HG11	2.39	0.57
1:A:323:LEU:HD23	1:A:359:ILE:HG12	1.86	0.57
1:A:316:SER:HA	1:B:277:LEU:HD12	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:215:ILE:HD11	1:B:224:ILE:HD11	1.86	0.57
1:B:117:TYR:HB2	1:B:127:TYR:HE1	1.70	0.57
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:10:LEU:HB2	1:B:282:LYS:HG3	1.89	0.55
1:B:228:LEU:HG	1:B:235:VAL:HG11	1.89	0.55
1:B:366:ASP:O	1:B:369:ARG:HG3	2.07	0.55
1:A:88:PRO:HD2	1:A:214:PHE:HB2	1.88	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:B:102:PRO:O	1:B:173:ILE:HG22	2.07	0.54
1:A:456:VAL:HA	1:A:459:ARG:HE	1.71	0.54
1:A:405:GLY:O	1:A:408:PRO:HG2	2.08	0.54
1:A:307:ASN:HD22	1:A:308:PRO:HD2	1.72	0.54
1:A:20:ARG:HH12	1:A:417:ASN:HA	1.71	0.54
1:B:24:ILE:HG23	1:B:47:ILE:HG22	1.90	0.54
1:B:400:VAL:HG21	1:B:407:THR:HG22	1.89	0.54
1:B:208:HIS:O	1:B:235:VAL:HG23	2.07	0.54
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:A:429:ALA:HA	1:A:432:PHE:CE1	2.43	0.53
1:B:352:ALA:O	1:B:356:GLU:HG3	2.08	0.53
1:B:288:ASN:HD21	1:B:325:GLY:HA3	1.73	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: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: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
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:288:ASN:HD21	1:A:325:GLY:HA3	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:240:LYS:HG2	1:B:261:MET:HB3	1.91	0.52
1:B:108:GLU:HA	1:B:166:LYS:HA	1.90	0.52
1:B:373:PRO:CB	1:B:376:THR:H	2.22	0.52
1:A:295:ILE:HG23	1:A:328:CYS:HB2	1.91	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: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:360:ALA:HB1	1:A:363:PRO:HG2	1.92	0.52
1:A:265:GLY:HA3	1:A:298:THR:HG21	1.91	0.52
1:A:108:GLU:HA	1:A:166:LYS:HA	1.91	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:424:THR:HG21	1:A:430:ALA:HB2	1.92	0.51
1:A:333:GLY:HA2	1:A:336:ALA:HB3	1.91	0.51
1:B:393:GLN:HB3	1:B:478:THR:HG21	1.93	0.51
1:A:370:ASN:C	1:A:372:THR:H	2.13	0.51
1:B:46:ASN:O	1:B:79:LEU:HD22	2.10	0.51
1:B:419:PRO:HG2	1:B:472:ILE:HG23	1.91	0.51
1:A:349:ALA:O	1:A:353:VAL:HG23	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
1:B:301:LEU:HD22	1:B:304:MET:HG3	1.93	0.50
1:B:23:ILE:O	1:B:23:ILE:HG22	2.11	0.50
1:B:420:ILE:HD12	1:B:420:ILE:N	2.27	0.50
1:A:192:SER:O	1:A:196:LYS:HD3	2.10	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:356:GLU:HA	1:B:359:ILE:HG13	1.94	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: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: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:130:TYR:O	1:A:133:ILE:HG22	2.12	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:301:LEU:HD22	1:A:310:PRO:HB3	1.94	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:484:GLY:HA3	1:A:492:SER:H	1.77	0.49
1:A:400:VAL:O	1:A:422:LEU:HA	2.13	0.49
1:A:272:PRO:HB2	1:A:275:GLU:HG3	1.93	0.49
1:A:282:LYS:HG3	1:B:10:LEU:HB2	1.94	0.49
1:B:41:ARG:HA	1:B:45:LEU:HB3	1.94	0.49
1:B:400:VAL:O	1:B:422:LEU:HA	2.11	0.49
1:A:393:GLN:HB3	1:A:478:THR:HG21	1.93	0.49
1:B:230:GLU:H	1:B:230:GLU:CD	2.14	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:B:56:SER:O	1:B:59:TYR:HB2	2.12	0.49
1:A:265:GLY:CA	1:A:298:THR:HG21	2.42	0.49
1:B:102:PRO:HB2	1:B:173:ILE:HG23	1.94	0.49
1:A:329:VAL:O	1:A:329:VAL:HG23	2.13	0.49
1:A:451:ASP:OD2	1:A:454:ASP:HB2	2.12	0.49
1:B:481:SER:HB2	1:B:496:GLN:HB3	1.94	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:A:86:LYS:O	1:A:87:GLY:O	2.31	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:263:ALA:HB1	2:A:1005:PGA:O1	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:413:LYS:O	1:A:415:ARG:N	2.46	0.48
1:A:192:SER:H	1:A:195:ASP:HB2	1.77	0.48
1:A:156:GLU:HG2	1:A:164:LYS:HE2	1.95	0.48
1:A:215:ILE:HD12	1:A:220:ASP:HB3	1.96	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:421:ILE:HD11	1:A:472:ILE:HG21	1.95	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:A:256:VAL:HG23	1:A:257:THR:N	2.28	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: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: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:A:235:VAL:HG13	1:A:235:VAL:O	2.13	0.48
1:B:421:ILE:HD11	1:B:472:ILE:HG21	1.95	0.48
1:A:409:ARG:HG3	1:A:436:TYR:CZ	2.48	0.48
1:A:393:GLN:O	1:A:394:LYS:HB2	2.14	0.48
1:A:239:VAL:O	1:A:261:MET:N	2.47	0.48
1:A:117:TYR:CD1	1:A:117:TYR:N	2.81	0.48
1:A:92:THR:HA	1:A:127:TYR:O	2.13	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:52:PHE:HD2	1:B:198:ASP:OD2	1.95	0.48
1:B:425:ARG:NH2	1:B:446:LYS:O	2.47	0.48
1:B:115:ASP:HA	1:B:118:ALA:HB2	1.95	0.48
1:B:102:PRO:HB2	1:B:173:ILE:CG2	2.43	0.48
1:B:24:ILE:HG12	1:B:47:ILE:HB	1.94	0.48
1:B:413:LYS:O	1:B:415:ARG:N	2.47	0.48
1:A:232:GLY:C	1:A:235:VAL:HG12	2.35	0.48
1:A:108:GLU:H	1:A:108:GLU:HG2	1.52	0.48
1:B:114:ASP:C	1:B:116:LYS:H	2.17	0.48
1:A:301:LEU:HD23	1:A:314:GLU:CG	2.40	0.47
1:A:25:GLY:HA3	1:A:45:LEU:HD11	1.95	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:47:ILE:HG13	1:A:80:ALA:HB3	1.96	0.47
1:A:105:PRO:O	1:A:106:ASN:HB2	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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: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:A:281:LYS:HE2	1:B:323:LEU:HD13	1.97	0.47
1:B:56:SER:H	1:B:59:TYR:HD2	1.59	0.47
1:B:192:SER:H	1:B:195:ASP:HB2	1.79	0.47
1:B:359:ILE:HG22	1:B:360:ALA:N	2.30	0.47
1:A:41:ARG:HH21	1:A:79:LEU:HB2	1.79	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:B:235:VAL:HG13	1:B:235:VAL:O	2.14	0.47
1:A:20:ARG:HB3	1:A:438:GLY:HA2	1.96	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:B:141:ARG:HD2	1:B:184:THR:HG23	1.97	0.46
1:A:481:SER:HB2	1:A:496:GLN:HB3	1.97	0.46
1:B:156:GLU:HG2	1:B:164:LYS:HE2	1.96	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:A:19:ARG:HD2	1:A:21:THR:O	2.14	0.46
1:B:456:VAL:CG2	1:B:457:GLU:N	2.78	0.46
1:A:359:ILE:HG22	1:A:360:ALA:N	2.30	0.46
1:B:480:VAL:HA	1:B:496:GLN:O	2.16	0.46
1:A:250:PHE:O	1:A:254:LEU:HB2	2.15	0.46
1:A:114:ASP:C	1:A:116:LYS:H	2.19	0.46
1:B:380:GLU:CA	1:B:410:LEU:HD23	2.46	0.46
1:B:474:LYS:HB2	1:B:477:ASP:OD1	2.15	0.46
1:A:277:LEU:HD12	1:B:316:SER:HA	1.96	0.46
1:A:470:PHE:HB3	1:A:472:ILE:HG13	1.97	0.46
1:B:92:THR:HA	1:B:127:TYR:O	2.14	0.46
1:B:41:ARG:HE	1:B:79:LEU:CB	2.27	0.46
1:A:136:VAL:HG13	1:A:137:ILE:N	2.30	0.46
1:B:401:LEU:HD21	1:B:460:ILE:HG13	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:425:ARG:NH2	1:A:446:LYS:O	2.46	0.46
1:B:24:ILE:CD1	1:B:295:ILE:HD13	2.45	0.46
1:A:30:LYS:HD2	1:A:337:LYS:HA	1.96	0.46
1:B:491:HIS:HA	3:B:1008:FBP:O4	2.15	0.46
1:A:49:ARG:HD2	1:A:84:ASP:HB2	1.97	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: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:353:VAL:HG12	1:A:357:GLN:OE1	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:451:ASP:C	1:B:453:THR:N	2.68	0.45
1:B:416:PRO:HG2	1:B:420:ILE:HD11	1.97	0.45
1:B:191:LEU:HD11	1:B:224:ILE:HA	1.98	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:102:PRO:O	1:B:104:PRO:HD3	2.17	0.45
1:A:141:ARG:HD2	1:A:184:THR:HG23	1.98	0.45
1:B:264:ARG:HD2	1:B:280:GLN:NE2	2.31	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:HG2	1:B:211:PHE:CE2	2.52	0.45
1:B:49:ARG:HH11	1:B:84:ASP:CG	2.19	0.45
1:B:256:VAL:HG23	1:B:257:THR:N	2.32	0.45
1:B:239:VAL:O	1:B:261:MET:N	2.46	0.45
1:A:200:ARG:O	1:A:204:LYS:HB2	2.16	0.45
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:B:24:ILE:HD11	1:B:295:ILE:HD13	1.99	0.44
1:A:24:ILE:CD1	1:A:295:ILE:HD13	2.47	0.44
1:A:138:SER:H	1:A:141:ARG:HG3	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:456:VAL:CG2	1:A:457:GLU:N	2.80	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:460:ILE:O	1:B:464:ILE:HG13	2.18	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:242:GLU:CG	1:B:263:ALA:HB1	2.33	0.44
1:B:356:GLU:HG3	1:B:356:GLU:H	1.63	0.44
1:B:239:VAL:HG23	1:B:260:VAL:HA	2.00	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:B:114:ASP:OD1	1:B:116:LYS:HB2	2.18	0.44
1:A:77:ARG:NH2	1:A:442:PHE:CE1	2.86	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:B:133:ILE:O	1:B:137:ILE:HG22	2.18	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:B:353:VAL:HG12	1:B:357:GLN:OE1	2.18	0.43
1:A:49:ARG:HH11	1:A:84:ASP:CG	2.21	0.43
1:A:286:LYS:HG2	1:B:8:THR:HG23	2.00	0.43
1:B:234:ASP:OD1	1:B:428:ARG:NH1	2.51	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:239:VAL:HG23	1:A:260:VAL:HA	2.00	0.43
1:A:49:ARG:HG2	1:A:211:PHE:CE2	2.53	0.43
1:A:193:GLU:CD	1:A:193:GLU:H	2.22	0.43
1:A:40:LEU:HD12	1:A:342:ILE:HG22	1.99	0.43
1:B:242:GLU:HG2	1:B:266:ASP:HB2	2.01	0.43
1:B:467:ALA:CB	1:B:473:LEU:HD12	2.47	0.43
1:B:273:ALA:O	1:B:276:VAL:HG12	2.19	0.43
1:A:216:ARG:O	1:A:253:ILE:HD11	2.19	0.43
1:B:363:PRO:O	1:B:366:ASP:HB2	2.18	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: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:B:301:LEU:HD13	1:B:304:MET:SD	2.59	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:ILE:HB	1:A:179:VAL:HB	2.01	0.43
1:B:432:PHE:C	1:B:432:PHE:CD1	2.92	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:A:191:LEU:HD12	1:A:223:THR:HG22	2.01	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:366:ASP:O	1:A:369:ARG:HG3	2.19	0.43
1:B:23:ILE:H	1:B:46:ASN:ND2	2.07	0.42
1:A:401:LEU:HD22	1:A:459:ARG:HB3	2.00	0.42
1:A:451:ASP:C	1:A:453:THR:N	2.69	0.42
1:A:387:VAL:HG11	1:A:414:TYR:O	2.19	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:432:PHE:CD1	1:A:432:PHE:C	2.92	0.42
1:A:363:PRO:O	1:A:366:ASP:HB2	2.19	0.42
1:B:81:ILE:N	1:B:208:HIS:ND1	2.58	0.42
1:A:273:ALA:O	1:A:276:VAL:HG12	2.20	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:304:MET:HA	1:A:307:ASN:O	2.20	0.42
1:A:115:ASP:N	1:A:127:TYR:OH	2.52	0.42
1:B:41:ARG:HE	1:B:79:LEU:CG	2.32	0.42
1:A:460:ILE:O	1:A:464:ILE:HG13	2.19	0.42
1:A:41:ARG:HE	1:A:79:LEU:CB	2.28	0.42
1:A:378:THR:O	1:A:382:VAL:HG12	2.20	0.42
1:A:257:THR:OG1	1:A:258:ASP:N	2.53	0.42
1:A:216:ARG:C	1:A:253:ILE:HD11	2.40	0.42
1:A:365:TYR:CD1	1:A:414:TYR:HB3	2.55	0.42
1:B:244:GLN:C	1:B:247:VAL:HG23	2.39	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:295:ILE:HG23	1:B:328:CYS:CB	2.50	0.42
1:A:23:ILE:O	1:A:23:ILE:HG22	2.19	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:464:ILE:O	1:B:468:LYS:HG3	2.19	0.42
1:A:309:ARG:HH21	1:B:269:ILE:HD13	1.82	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:107:HIS:ND1	1:B:108:GLU:O	2.47	0.42
1:A:117:TYR:CD2	1:A:125:ILE:HD13	2.54	0.42
1:A:456:VAL:O	1:A:460:ILE:HD12	2.20	0.42
1:A:380:GLU:HA	1:A:410:LEU:HD23	2.02	0.42
1:B:194:LYS:O	1:B:198:ASP:OD1	2.38	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:H	1:A:490:GLY:HA2	1.84	0.41
1:A:83:LEU:HB3	1:A:210:VAL:HG22	2.02	0.41
1:B:159:ASP:HA	1:B:162:THR:OG1	2.20	0.41
1:A:486:LYS:HB2	1:A:490:GLY:HA2	2.01	0.41
1:B:222:LEU:O	1:B:225:ARG:HB3	2.20	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:A:114:ASP:O	1:A:116:LYS:N	2.53	0.41
1:B:31:THR:HA	1:B:36:THR:HG21	2.03	0.41
1:B:216:ARG:O	1:B:253:ILE:HD11	2.21	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:B:128:VAL:HG12	1:B:179:VAL:HG21	2.01	0.41
1:A:88:PRO:HB2	1:A:188:LEU:HB3	2.03	0.41
1:A:106:ASN:HD21	1:A:166:LYS:NZ	2.17	0.41
1:B:486:LYS:HB2	1:B:490:GLY:HA2	2.02	0.41
1:A:323:LEU:HD13	1:B:281:LYS:HE2	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:B:373:PRO:CB	1:B:376:THR:N	2.79	0.41
1:A:264:ARG:O	1:A:267:LEU:N	2.54	0.41
1:B:217:THR:O	1:B:220:ASP:HB2	2.21	0.41
1:B:124:LYS:O	1:B:125:ILE:HB	2.20	0.41
1:B:124:LYS:H	1:B:124:LYS:HG2	1.70	0.41
1:B:117:TYR:CD2	1:B:125:ILE:HD13	2.56	0.41
1:B:362:LEU:HB3	1:B:363:PRO:CD	2.51	0.41
1:B:56:SER:O	1:B:59:TYR:N	2.54	0.41
1:A:225:ARG:NH2	1:A:258:ASP:OD2	2.44	0.41
1:B:422:LEU:HG	1:B:422:LEU:O	2.21	0.41
1:A:106:ASN:O	1:A:106:ASN:ND2	2.54	0.41
1:B:365:TYR:CD1	1:B:414:TYR:HB3	2.56	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:426:CYS:HA	1:A:427:PRO:HD3	1.94	0.40
1:B:133:ILE:HA	1:B:136:VAL:HG12	2.02	0.40
1:A:401:LEU:HD12	3:A:1007:FBP:O2	2.21	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:B:19:ARG:HG3	1:B:352:ALA:HB3	2.03	0.40
1:A:41:ARG:HE	1:A:79:LEU:CG	2.35	0.40
1:B:486:LYS:H	1:B:490:GLY:HA2	1.85	0.40
1:A:477:ASP:O	1:A:499:THR:HG23	2.21	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:49:ARG:HG2	1:A:211:PHE:HE2	1.85	0.40
1:A:479:TYR:CE1	1:A:498:SER:HB3	2.56	0.40
1:A:305:THR:HG23	1:A:306:TYR:CD2	2.56	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%)	2	10
1	B	481/500 (96%)	394 (82%)	57 (12%)	30 (6%)	2	13
All	All	967/1000 (97%)	792 (82%)	113 (12%)	62 (6%)	2	11

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	1	4
1	B	414/423 (98%)	305 (74%)	109 (26%)	1	4
All	All	831/846 (98%)	612 (74%)	219 (26%)	1	4

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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$
2	PGA	A	1005	5,4	8,8,8	3.47	4 (50%)	11,11,11	3.25	7 (63%)
3	FBP	A	1007	-	20,20,20	1.05	0	32,32,32	0.87	1 (3%)
2	PGA	B	1006	5,4	8,8,8	2.74	3 (37%)	11,11,11	3.27	6 (54%)
3	FBP	B	1008	-	20,20,20	1.18	2 (10%)	32,32,32	0.98	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGA	A	1005	5,4	-	0/6/6/6	0/0/0/0
3	FBP	A	1007	-	-	0/13/32/32	0/1/1/1
2	PGA	B	1006	5,4	-	0/6/6/6	0/0/0/0
3	FBP	B	1008	-	-	0/13/32/32	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	O1P-C2	-8.20	1.37	1.43
2	B	1006	PGA	O1P-C2	-5.32	1.39	1.43
2	B	1006	PGA	P-O3P	4.42	1.70	1.54
2	A	1005	PGA	P-O3P	4.31	1.70	1.54
3	B	1008	FBP	C1-C2	2.39	1.55	1.52
3	B	1008	FBP	O5-C2	2.37	1.46	1.43
2	B	1006	PGA	P-O2P	2.27	1.58	1.51
2	A	1005	PGA	P-O2P	2.17	1.58	1.51
2	A	1005	PGA	P-O4P	-2.07	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	PGA	O1P-P-O2P	7.33	128.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	PGA	O1P-P-O2P	6.91	126.95	106.71
2	B	1006	PGA	O1P-C2-C1	4.58	117.94	110.54
2	A	1005	PGA	O1P-C2-C1	4.02	117.04	110.54
2	B	1006	PGA	P-O1P-C2	3.51	133.90	121.22
2	A	1005	PGA	P-O1P-C2	3.37	133.37	121.22
2	B	1006	PGA	O2-C1-O1	-3.25	115.02	123.30
2	B	1006	PGA	O3P-P-O1P	3.01	114.94	106.65
2	A	1005	PGA	O2-C1-O1	-2.94	115.83	123.30
2	A	1005	PGA	O3P-P-O1P	2.90	114.64	106.65
3	B	1008	FBP	O5-C2-C1	2.53	112.16	108.17
3	A	1007	FBP	C1-C2-C3	-2.46	111.05	115.80
2	A	1005	PGA	O4P-P-O2P	-2.30	102.92	110.44
2	A	1005	PGA	O4P-P-O1P	-2.29	100.32	106.65
3	B	1008	FBP	C1-C2-C3	-2.14	111.65	115.80
2	B	1006	PGA	O4P-P-O2P	-2.04	103.76	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.