



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KTA
Title : HUMAN BRANCHED CHAIN AMINO ACID AMINOTRANSFERASE :
THREE DIMENSIONAL STRUCTURE OF THE ENZYME IN ITS PYRI-
DOXAMINE PHOSPHATE FORM.
Authors : Yennawar, N.H.; Conway, M.E.; Yennawar, H.P.; Farber, G.K.; Hutson, S.M.
Deposited on : 2002-01-15
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

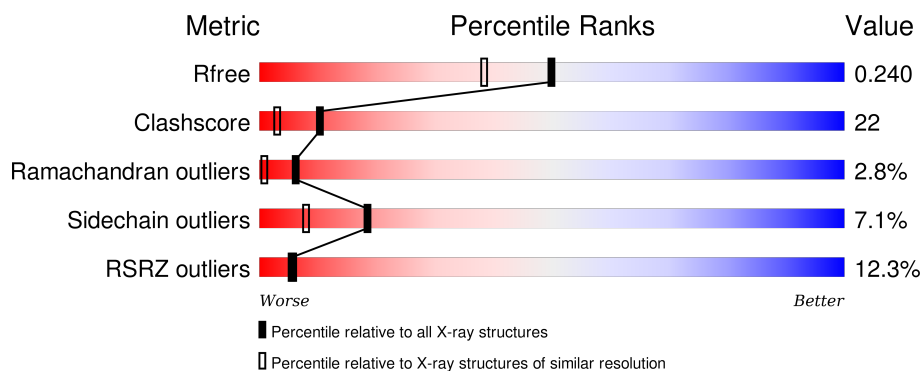
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	365	<div> <div>13%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	B	365	<div> <div>12%</div> <div>66%</div> <div>29%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KIV	B	3001	-	-	-	X
4	ACY	A	1003	-	-	-	X
4	ACY	A	1007	-	-	-	X
4	ACY	B	1005	-	-	-	X
5	GOL	B	2001	-	-	X	-

2 Entry composition [i](#)

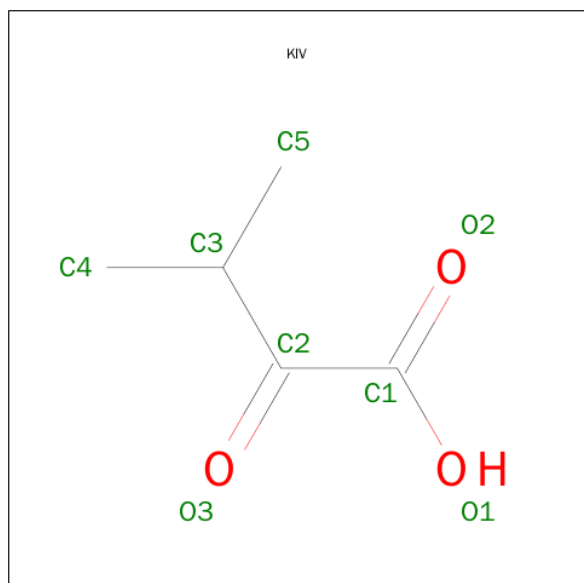
There are 6 unique types of molecules in this entry. The entry contains 6137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE, MITOCHONDRIAL.

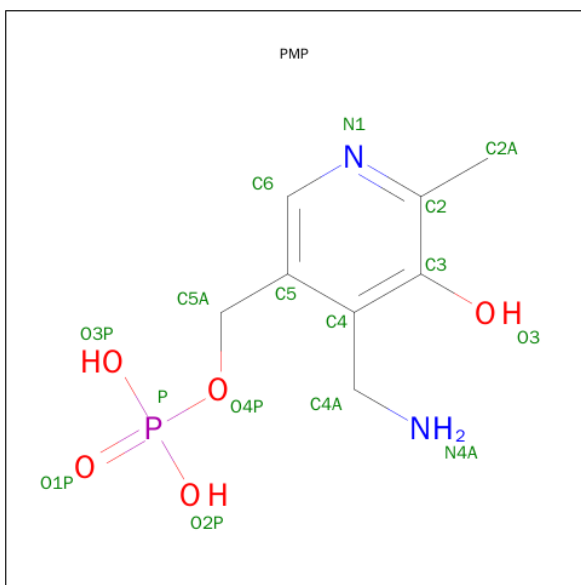
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			
1	B	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			

- Molecule 2 is 3-METHYL-2-OXOBUTANOIC ACID (three-letter code: KIV) (formula: $C_5H_8O_3$).



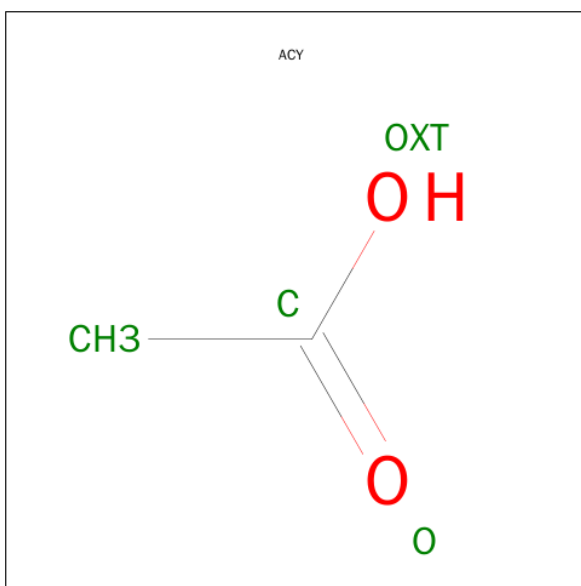
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			8	5	3		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total	O	0	0
			126	126		
6	B	117	Total	O	0	0
			117	117		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.45Å 105.31Å 107.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.96-1.90) 98.2 (19.96-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.287 0.244 , 0.240	Depositor DCC
R_{free} test set	3143 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.2	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 62232 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6137	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ACY, PMP, KIV

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	0.82	2/2987 (0.1%)	0.93	3/4053 (0.1%)
1	B	0.78	1/2987 (0.0%)	0.93	10/4053 (0.2%)
All	All	0.80	3/5974 (0.1%)	0.93	13/8106 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	CYS	CB-SG	-7.15	1.70	1.82
1	B	668	CYS	CB-SG	-5.98	1.72	1.81
1	A	247	TRP	CB-CG	5.34	1.59	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLY	C-N-CD	-9.91	98.80	120.60
1	B	585	ASP	N-CA-C	-8.63	87.69	111.00
1	B	804	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	529	VAL	N-CA-C	-6.94	92.25	111.00
1	B	527	PRO	N-CA-C	6.28	128.42	112.10
1	A	102	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	804	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	692	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	528	LEU	N-CA-C	5.53	125.92	111.00
1	B	506	LYS	N-CA-C	5.45	125.72	111.00
1	A	92	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	B	505	PHE	CB-CA-C	5.25	120.90	110.40
1	B	692	ARG	CG-CD-NE	-5.05	101.20	111.80

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	2910	0	2940	138	0
1	B	2910	0	2937	121	0
2	B	8	0	7	3	0
3	A	16	0	10	1	0
3	B	16	0	10	1	0
4	A	12	0	9	1	0
4	B	16	0	12	2	0
5	B	6	0	8	5	0
6	A	126	0	0	9	0
6	B	117	0	0	5	0
All	All	6137	0	5933	255	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 22.

All (255) 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:351:GLU:HG2	1:A:356:ILE:HD11	1.21	1.16
1:B:851:GLU:HG2	1:B:856:ILE:HD11	1.21	1.15
1:B:552:ARG:HE	1:B:554:GLN:NE2	1.48	1.10
1:A:179:VAL:HG11	1:A:346:GLN:HE22	1.08	1.10
1:B:552:ARG:NE	1:B:554:GLN:HE21	1.62	0.97
1:A:10:LEU:HD12	1:A:50:GLN:OE1	1.63	0.95
1:B:700:ASN:H	1:B:700:ASN:HD22	1.12	0.94
1:A:200:ASN:H	1:A:200:ASN:HD22	1.12	0.94
1:A:351:GLU:CG	1:A:356:ILE:HD11	1.99	0.93
1:B:851:GLU:CG	1:B:856:ILE:HD11	1.98	0.93
1:A:179:VAL:CG1	1:A:346:GLN:HE22	1.81	0.92
1:B:552:ARG:HE	1:B:554:GLN:HE21	0.92	0.92
1:B:859:HIS:HE2	5:B:2001:GOL:H11	1.32	0.92
1:B:816:GLN:HE22	1:B:853:GLN:HE22	1.17	0.91
1:B:584:LYS:O	1:B:585:ASP:HB3	1.73	0.88
1:A:179:VAL:HG11	1:A:346:GLN:NE2	1.90	0.87
1:A:6:LYS:O	1:A:8:ALA:N	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD23	1:A:52:ARG:HH11	1.40	0.86
1:B:582:LYS:HE3	1:B:632:VAL:HB	1.59	0.84
1:A:316:GLN:HE22	1:A:353:GLN:HE22	1.21	0.84
1:A:12:LEU:HD11	1:A:14:MET:SD	2.16	0.84
1:B:851:GLU:HG2	1:B:856:ILE:CD1	2.09	0.80
1:A:40:MET:HE1	6:A:1020:HOH:O	1.83	0.79
1:B:526:GLU:N	1:B:527:PRO:HD2	1.98	0.79
1:B:584:LYS:O	1:B:585:ASP:CB	2.32	0.78
1:A:326:LYS:O	1:A:327:ASP:HB2	1.85	0.77
1:B:515:THR:HG23	1:B:518:PRO:HG3	1.68	0.76
1:B:859:HIS:NE2	5:B:2001:GOL:H11	2.00	0.74
1:A:9:ASP:O	1:A:11:GLN:N	2.20	0.74
1:B:859:HIS:HE2	5:B:2001:GOL:C1	2.02	0.73
1:A:71:SER:H	1:B:573:GLN:HE22	1.36	0.72
1:A:351:GLU:HG2	1:A:356:ILE:CD1	2.11	0.72
1:B:585:ASP:OD2	1:B:587:GLN:HG3	1.89	0.72
2:B:3001:KIV:O2	2:B:3001:KIV:HC52	1.87	0.72
1:A:6:LYS:C	1:A:8:ALA:H	1.93	0.71
1:B:637:GLY:O	1:B:672:ALA:HA	1.91	0.70
1:A:191:ILE:HD12	1:B:695:VAL:O	1.91	0.70
1:B:512:LEU:HD11	1:B:514:MET:SD	2.32	0.70
1:B:716:GLU:OE1	1:B:719:LYS:HE3	1.92	0.69
1:A:249:HIS:CD2	1:A:250:GLU:H	2.10	0.69
1:B:512:LEU:HD21	1:B:514:MET:SD	2.33	0.69
1:B:510:LEU:HB2	1:B:550:GLN:HB2	1.73	0.68
1:B:509:ASP:O	1:B:511:GLN:N	2.24	0.68
1:B:815:CYS:SG	1:B:818:CYS:HB2	2.33	0.67
1:B:716:GLU:HA	1:B:719:LYS:HG3	1.76	0.67
1:B:552:ARG:NE	1:B:554:GLN:NE2	2.27	0.67
1:A:86:GLN:O	1:A:86:GLN:HG3	1.94	0.67
1:A:365:VAL:HG23	1:A:365:VAL:OXT	1.94	0.67
1:B:650:GLU:HG3	1:B:659:ARG:H	1.60	0.67
1:A:66:SER:HB2	1:A:72:LEU:HD12	1.77	0.66
1:B:700:ASN:ND2	4:B:1005:ACY:OXT	2.27	0.66
1:A:176:GLY:O	1:A:178:SER:N	2.27	0.66
1:B:566:SER:HB2	1:B:572:LEU:HD12	1.75	0.66
1:B:585:ASP:CG	1:B:587:GLN:HE21	1.99	0.66
1:B:719:LYS:NZ	1:B:719:LYS:HB2	2.11	0.65
1:B:838:GLY:O	6:B:239:HOH:O	2.13	0.65
1:A:150:GLU:HG2	1:A:159:ARG:H	1.61	0.65
1:A:150:GLU:OE1	1:A:151:PRO:HD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:THR:CG2	1:B:518:PRO:HG3	2.27	0.64
1:B:700:ASN:N	1:B:700:ASN:HD22	1.88	0.64
1:A:24:PRO:C	1:A:26:GLU:H	2.01	0.64
1:A:261:LEU:HD13	4:A:1003:ACY:H3	1.79	0.63
1:A:302:GLU:HG2	1:A:304:ARG:HD3	1.80	0.63
1:B:865:VAL:OXT	1:B:865:VAL:HG23	1.97	0.63
1:B:843:LEU:HD12	4:B:1002:ACY:H2	1.80	0.63
1:B:826:LYS:O	1:B:827:ASP:HB2	1.99	0.62
1:A:302:GLU:HB3	1:A:304:ARG:HD3	1.79	0.62
1:B:678:SER:O	1:B:679:VAL:HG23	2.00	0.62
1:B:700:ASN:ND2	1:B:700:ASN:H	1.92	0.61
1:B:572:LEU:HD13	1:B:658:PRO:HG3	1.81	0.60
1:B:861:TRP:CZ2	5:B:2001:GOL:H32	2.36	0.60
1:A:249:HIS:CG	1:A:250:GLU:H	2.19	0.60
1:A:10:LEU:CD2	1:A:52:ARG:HH11	2.10	0.60
1:B:816:GLN:NE2	1:B:853:GLN:HE22	1.96	0.59
1:A:7:ALA:C	1:A:9:ASP:H	2.06	0.59
1:B:504:SER:HB3	1:B:548:TRP:HD1	1.67	0.59
1:A:10:LEU:HB2	1:A:50:GLN:HB2	1.85	0.59
1:A:200:ASN:H	1:A:200:ASN:ND2	1.92	0.59
1:B:816:GLN:HE22	1:B:853:GLN:NE2	1.96	0.59
1:A:73:GLN:HE22	1:B:571:SER:H	1.50	0.58
1:A:25:GLY:C	1:A:27:PRO:HD3	2.23	0.58
1:A:275:LEU:O	1:A:279:GLN:HB2	2.03	0.58
1:A:8:ALA:HA	6:A:1009:HOH:O	2.03	0.58
1:A:85:ASP:OD1	1:A:87:GLN:HB2	2.03	0.57
1:A:326:LYS:HG2	6:A:1016:HOH:O	2.03	0.57
1:A:150:GLU:HG3	1:A:158:PRO:HA	1.85	0.57
1:A:10:LEU:HD23	1:A:52:ARG:NH1	2.17	0.57
1:B:692:ARG:HB2	1:B:727:TRP:CE3	2.40	0.57
1:A:315:CYS:SG	1:A:318:CYS:HB2	2.45	0.57
1:A:122:ARG:NH2	1:A:126:GLU:OE2	2.38	0.56
1:A:300:LEU:C	1:A:301:GLU:OE2	2.43	0.56
1:B:503:SER:O	1:B:504:SER:HB2	2.05	0.56
1:A:72:LEU:HD13	1:A:158:PRO:HG3	1.88	0.55
1:A:119:GLU:OE1	1:A:122:ARG:NH1	2.39	0.55
1:A:184:LEU:HD22	1:A:238:VAL:CG2	2.36	0.55
1:A:2:SER:H	1:A:6:LYS:HZ1	1.54	0.55
1:A:184:LEU:HD22	1:A:238:VAL:HG23	1.89	0.55
1:B:670:VAL:HG12	1:B:671:GLY:O	2.06	0.55
1:B:619:GLU:OE1	1:B:622:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LYS:NZ	1:A:351:GLU:OE2	2.33	0.54
1:B:544:ASN:OD1	1:B:546:LYS:N	2.31	0.54
1:B:585:ASP:OD1	1:B:587:GLN:NE2	2.28	0.54
1:A:351:GLU:HA	1:A:356:ILE:HG12	1.90	0.54
1:A:82:LYS:HE2	1:A:132:VAL:O	2.08	0.53
1:A:21:LYS:O	1:A:22:PRO:C	2.45	0.53
1:B:655:VAL:HG23	2:B:3001:KIV:HC43	1.90	0.53
1:A:239:GLY:C	6:A:1130:HOH:O	2.46	0.53
1:B:522:PRO:HB3	1:B:527:PRO:CB	2.39	0.53
1:B:804:ARG:NH2	6:B:129:HOH:O	2.42	0.53
1:B:719:LYS:NZ	1:B:719:LYS:CB	2.71	0.53
1:B:588:VAL:O	1:B:865:VAL:HA	2.08	0.53
1:A:316:GLN:HE22	1:A:353:GLN:NE2	2.00	0.52
1:A:296:LEU:HD22	1:A:300:LEU:HG	1.91	0.52
1:A:24:PRO:O	1:A:26:GLU:N	2.43	0.52
1:B:719:LYS:HZ2	1:B:719:LYS:HB2	1.75	0.52
2:B:3001:KIV:O2	2:B:3001:KIV:C5	2.57	0.51
1:B:687:ASP:HB3	1:B:690:PHE:CD1	2.45	0.51
1:B:586:GLN:O	1:B:629:LYS:HE3	2.10	0.51
1:A:10:LEU:HB2	1:A:50:GLN:CB	2.41	0.51
1:B:573:GLN:HE21	1:B:704:GLY:HA3	1.75	0.51
1:A:84:LYS:C	1:A:86:GLN:H	2.13	0.51
1:B:601:LEU:O	1:B:605:MET:HG2	2.12	0.50
1:A:187:ASP:HB3	1:A:190:PHE:CE1	2.47	0.50
1:A:338:GLY:O	1:A:340:GLU:N	2.44	0.50
1:B:851:GLU:HA	1:B:856:ILE:HG12	1.92	0.50
1:A:75:PHE:CE2	1:A:202:LYS:HE3	2.46	0.49
1:A:45:ASP:OD2	1:A:46:LYS:HG3	2.12	0.49
1:A:71:SER:H	1:B:573:GLN:NE2	2.07	0.49
1:A:192:ARG:HB2	1:A:227:TRP:CE3	2.47	0.49
1:B:781:TRP:CH2	1:B:844:ARG:HG2	2.47	0.49
1:B:509:ASP:HB2	1:B:551:PRO:O	2.13	0.49
1:A:42:GLU:HG2	1:A:162:LEU:CD1	2.42	0.49
1:B:684:LEU:HD22	1:B:738:VAL:CG2	2.42	0.49
1:B:833:PRO:O	1:B:836:GLU:HG2	2.12	0.49
1:A:281:TRP:CH2	1:A:344:ARG:HG2	2.48	0.49
1:B:702:LYS:NZ	3:B:900:PMP:N4A	2.61	0.49
1:B:633:PRO:HB2	1:B:638:THR:OG1	2.13	0.49
1:B:624:LEU:HG	1:B:667:LEU:HD11	1.94	0.49
1:A:179:VAL:CG1	1:A:346:GLN:NE2	2.63	0.48
1:B:644:PRO:HA	1:B:665:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:CB	1:A:356:ILE:HD11	2.42	0.48
1:B:684:LEU:HD22	1:B:738:VAL:HG23	1.95	0.48
1:B:540:MET:HG3	1:B:662:LEU:HD11	1.93	0.48
1:B:588:VAL:O	1:B:865:VAL:N	2.43	0.48
1:A:365:VAL:CG2	1:A:365:VAL:OXT	2.61	0.48
1:A:40:MET:CE	6:A:1020:HOH:O	2.53	0.48
1:A:10:LEU:C	1:A:11:GLN:O	2.51	0.48
1:B:802:GLU:HB2	1:B:804:ARG:HD3	1.96	0.48
1:B:812:GLY:O	1:B:816:GLN:HA	2.14	0.47
1:A:300:LEU:O	1:A:301:GLU:OE2	2.32	0.47
1:A:321:HIS:HD2	6:A:1127:HOH:O	1.97	0.47
1:A:316:GLN:NE2	1:A:353:GLN:HE22	2.01	0.47
1:B:572:LEU:HD13	1:B:658:PRO:CG	2.43	0.47
1:A:298:ARG:O	1:A:302:GLU:HB2	2.14	0.47
1:A:5:PHE:HB2	1:A:51:PRO:HG3	1.95	0.47
1:A:200:ASN:N	1:A:200:ASN:HD22	1.89	0.47
1:A:82:LYS:HE3	1:A:134:ASP:HB3	1.95	0.47
1:B:572:LEU:CD1	1:B:658:PRO:HG3	2.43	0.47
1:A:12:LEU:HD21	1:A:14:MET:SD	2.55	0.47
1:B:716:GLU:CD	1:B:719:LYS:HE3	2.35	0.47
1:A:124:LEU:HG	1:A:167:LEU:HD11	1.97	0.46
1:B:527:PRO:HB2	1:B:528:LEU:H	1.41	0.46
1:A:88:VAL:O	1:A:365:VAL:N	2.47	0.46
1:A:73:GLN:HE21	1:A:204:GLY:HA3	1.81	0.46
1:A:137:GLY:O	1:A:172:ALA:HA	2.16	0.46
1:A:88:VAL:O	1:A:365:VAL:HA	2.15	0.46
1:A:335:MET:HA	1:A:339:PRO:HD3	1.97	0.46
1:B:716:GLU:OE1	1:B:719:LYS:CE	2.63	0.46
1:B:663:LEU:HD23	1:B:664:PHE:N	2.30	0.46
1:B:815:CYS:SG	1:B:818:CYS:CB	3.02	0.46
1:A:10:LEU:CD1	1:A:50:GLN:OE1	2.49	0.45
1:A:2:SER:H	1:A:6:LYS:NZ	2.14	0.45
1:A:122:ARG:CG	1:A:365:VAL:OXT	2.64	0.45
1:B:673:TYR:CE2	1:B:815:CYS:HB2	2.51	0.45
1:B:510:LEU:HG	1:B:550:GLN:OE1	2.16	0.45
1:B:521:LYS:O	1:B:522:PRO:C	2.54	0.45
1:A:73:GLN:NE2	1:B:571:SER:H	2.15	0.45
1:B:851:GLU:CB	1:B:856:ILE:HD11	2.44	0.45
1:B:543:TRP:HB2	1:B:548:TRP:CE3	2.51	0.45
1:B:692:ARG:HB2	1:B:727:TRP:CD2	2.52	0.45
1:A:85:ASP:OD2	1:A:89:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LYS:HB3	1:B:520:LYS:NZ	2.32	0.45
1:A:159:ARG:HH11	1:A:159:ARG:CG	2.30	0.45
1:A:24:PRO:C	1:A:26:GLU:N	2.69	0.45
1:A:10:LEU:HD13	1:A:50:GLN:HB2	1.99	0.45
1:A:10:LEU:O	1:A:11:GLN:O	2.35	0.44
1:A:312:GLY:O	1:A:316:GLN:HA	2.17	0.44
1:A:249:HIS:CE1	1:A:289:ARG:NH1	2.86	0.44
1:A:150:GLU:CG	1:A:159:ARG:H	2.29	0.44
1:A:144:PRO:HA	1:A:165:VAL:HG22	1.99	0.44
1:A:122:ARG:HG3	1:A:365:VAL:OXT	2.17	0.44
1:B:542:GLU:HG2	1:B:662:LEU:CD1	2.47	0.44
1:B:583:GLY:O	1:B:584:LYS:C	2.55	0.44
1:A:198:VAL:HG23	1:A:206:ASN:HD21	1.83	0.44
1:A:43:TRP:HB2	1:A:48:TRP:CE3	2.53	0.44
1:A:101:LEU:O	1:A:105:MET:HG2	2.18	0.44
1:A:302:GLU:CG	1:A:304:ARG:HD3	2.48	0.43
1:B:585:ASP:CG	1:B:587:GLN:HG3	2.39	0.43
1:B:526:GLU:HB2	1:B:527:PRO:CD	2.48	0.43
1:A:249:HIS:CG	1:A:250:GLU:N	2.85	0.43
1:B:687:ASP:HA	1:B:688:PRO:HD3	1.86	0.43
1:B:716:GLU:CA	1:B:719:LYS:HG3	2.47	0.43
1:A:84:LYS:C	1:A:86:GLN:N	2.72	0.43
1:A:159:ARG:HH11	1:A:159:ARG:CB	2.32	0.43
1:B:522:PRO:HB3	1:B:527:PRO:HB2	2.01	0.43
1:B:859:HIS:CE1	5:B:2001:GOL:H11	2.53	0.43
1:B:521:LYS:HE3	1:B:631:TRP:CE2	2.54	0.42
1:A:302:GLU:CB	1:A:304:ARG:HD3	2.47	0.42
1:B:575:PHE:CE2	1:B:702:LYS:HE3	2.53	0.42
1:A:109:LEU:HB3	1:A:110:PRO:HD2	2.00	0.42
1:B:574:LEU:HD12	1:B:574:LEU:C	2.39	0.42
1:A:326:LYS:HA	6:A:1016:HOH:O	2.17	0.42
1:A:311:SER:HA	1:A:316:GLN:O	2.19	0.42
1:B:509:ASP:HB3	1:B:551:PRO:HD2	2.01	0.42
1:A:179:VAL:O	1:A:179:VAL:HG23	2.19	0.42
1:B:572:LEU:HA	1:B:572:LEU:HD23	1.87	0.42
1:A:24:PRO:O	1:A:26:GLU:HG2	2.20	0.42
1:A:9:ASP:C	1:A:11:GLN:N	2.73	0.42
1:A:202:LYS:NZ	3:A:400:PMP:N4A	2.68	0.42
1:A:74:LEU:CD2	1:A:104:ALA:HA	2.50	0.42
1:B:609:LEU:HB3	1:B:610:PRO:HD2	2.02	0.42
1:A:226:LEU:HD13	1:A:243:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ARG:HH12	1:A:123:ARG:HD3	1.84	0.41
1:A:187:ASP:HA	1:A:188:PRO:HD3	1.92	0.41
1:A:174:PHE:HA	1:A:175:PRO:HD2	1.79	0.41
1:A:7:ALA:C	1:A:9:ASP:N	2.72	0.41
1:B:816:GLN:NE2	6:B:198:HOH:O	2.53	0.41
1:A:72:LEU:CD1	1:A:158:PRO:HG3	2.49	0.41
1:A:351:GLU:CA	1:A:356:ILE:HG12	2.50	0.41
1:B:851:GLU:CA	1:B:856:ILE:HG12	2.51	0.41
1:B:509:ASP:CB	1:B:551:PRO:HD2	2.50	0.41
1:A:344:ARG:HD2	6:A:1086:HOH:O	2.20	0.41
1:B:622:ARG:CG	1:B:865:VAL:OXT	2.68	0.41
1:A:25:GLY:O	1:A:27:PRO:HD3	2.20	0.41
1:A:63:PRO:CG	1:B:557:GLN:O	2.69	0.41
1:A:251:ASP:OD2	1:A:251:ASP:N	2.49	0.41
1:A:289:ARG:HG2	1:A:290:THR:N	2.35	0.41
1:B:510:LEU:HB2	1:B:550:GLN:CB	2.48	0.41
1:A:82:LYS:NZ	1:A:86:GLN:NE2	2.68	0.41
1:A:72:LEU:HD13	1:A:158:PRO:CG	2.50	0.41
1:B:595:LEU:HD12	1:B:769:VAL:HG13	2.03	0.41
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.82	0.41
1:A:242:ASN:O	1:A:310:GLY:HA2	2.21	0.41
1:A:159:ARG:NH1	1:A:159:ARG:CG	2.84	0.40
1:B:698:VAL:HG23	1:B:706:ASN:HD21	1.86	0.40
1:B:811:SER:HA	1:B:816:GLN:O	2.22	0.40
1:A:8:ALA:CA	6:A:1009:HOH:O	2.66	0.40
1:A:338:GLY:HA2	1:A:339:PRO:HD2	1.57	0.40
1:A:168:CYS:HA	1:A:169:PRO:HD3	1.96	0.40
1:A:12:LEU:HG	1:A:14:MET:HG2	2.04	0.40
1:B:517:LYS:N	1:B:518:PRO:HD3	2.36	0.40
1:B:659:ARG:CG	1:B:659:ARG:HH11	2.34	0.40
1:B:687:ASP:HB3	1:B:690:PHE:CE1	2.57	0.40
1:B:686:ALA:HA	6:B:44:HOH:O	2.21	0.40
1:B:715:GLN:NE2	6:B:134:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	363/365 (100%)	333 (92%)	18 (5%)	12 (3%)	5	0
1	B	363/365 (100%)	337 (93%)	18 (5%)	8 (2%)	8	1
All	All	726/730 (100%)	670 (92%)	36 (5%)	20 (3%)	6	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ALA
1	A	10	LEU
1	A	177	GLY
1	A	339	PRO
1	B	505	PHE
1	B	510	LEU
1	B	527	PRO
1	B	585	ASP
1	A	11	GLN
1	B	528	LEU
1	A	9	ASP
1	A	25	GLY
1	A	27	PRO
1	A	175	PRO
1	B	586	GLN
1	A	249	HIS
1	A	174	PHE
1	A	338	GLY
1	B	679	VAL
1	B	833	PRO

5.3.2 Protein sidechains [i](#)

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	316/316 (100%)	297 (94%)	19 (6%)	24	12
1	B	316/316 (100%)	290 (92%)	26 (8%)	14	5
All	All	632/632 (100%)	587 (93%)	45 (7%)	18	8

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	10	LEU
1	A	12	LEU
1	A	40	MET
1	A	84	LYS
1	A	122	ARG
1	A	150	GLU
1	A	151	PRO
1	A	159	ARG
1	A	174	PHE
1	A	180	THR
1	A	200	ASN
1	A	218	LEU
1	A	247	TRP
1	A	275	LEU
1	A	279	GLN
1	A	296	LEU
1	A	301	GLU
1	A	302	GLU
1	B	502	SER
1	B	505	PHE
1	B	510	LEU
1	B	517	LYS
1	B	520	LYS
1	B	528	LEU
1	B	540	MET
1	B	545	ASP
1	B	552	ARG
1	B	584	LYS
1	B	585	ASP
1	B	622	ARG

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Mol	Chain	Res	Type
1	B	626	GLU
1	B	650	GLU
1	B	651	PRO
1	B	659	ARG
1	B	680	THR
1	B	700	ASN
1	B	718	LEU
1	B	719	LYS
1	B	732	ASP
1	B	747	TRP
1	B	760	PRO
1	B	775	LEU
1	B	779	GLN
1	B	796	LEU

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	54	GLN
1	A	73	GLN
1	A	200	ASN
1	A	206	ASN
1	A	215	GLN
1	A	224	GLN
1	A	234	GLN
1	A	242	ASN
1	A	249	HIS
1	A	316	GLN
1	A	346	GLN
1	B	554	GLN
1	B	573	GLN
1	B	587	GLN
1	B	700	ASN
1	B	706	ASN
1	B	715	GLN
1	B	724	GLN
1	B	734	GLN
1	B	742	ASN
1	B	779	GLN
1	B	816	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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$
4	ACY	A	1003	-	1,3,3	0.64	0	0,3,3	0.00	-
4	ACY	A	1006	-	1,3,3	3.41	1 (100%)	0,3,3	0.00	-
4	ACY	A	1007	-	1,3,3	3.06	1 (100%)	0,3,3	0.00	-
3	PMP	A	400	-	16,16,16	1.30	2 (12%)	20,23,23	1.52	5 (25%)
4	ACY	B	1001	-	1,3,3	4.18	1 (100%)	0,3,3	0.00	-
4	ACY	B	1002	-	1,3,3	4.91	1 (100%)	0,3,3	0.00	-
4	ACY	B	1004	-	1,3,3	3.69	1 (100%)	0,3,3	0.00	-
4	ACY	B	1005	-	1,3,3	3.72	1 (100%)	0,3,3	0.00	-
5	GOL	B	2001	-	5,5,5	0.83	0	5,5,5	0.42	0
2	KIV	B	3001	-	4,7,7	2.83	1 (25%)	4,9,9	1.18	1 (25%)
3	PMP	B	900	-	16,16,16	1.27	1 (6%)	20,23,23	1.39	4 (20%)

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
4	ACY	A	1003	-	-	0/0/0/0	0/0/0/0
4	ACY	A	1006	-	-	0/0/0/0	0/0/0/0
4	ACY	A	1007	-	-	0/0/0/0	0/0/0/0
3	PMP	A	400	-	-	0/8/8/8	0/1/1/1
4	ACY	B	1001	-	-	0/0/0/0	0/0/0/0
4	ACY	B	1002	-	-	0/0/0/0	0/0/0/0
4	ACY	B	1004	-	-	0/0/0/0	0/0/0/0
4	ACY	B	1005	-	-	0/0/0/0	0/0/0/0
5	GOL	B	2001	-	-	0/4/4/4	0/0/0/0
2	KIV	B	3001	-	-	0/4/8/8	0/0/0/0
3	PMP	B	900	-	-	0/8/8/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	PMP	P-O3P	-2.24	1.46	1.54
3	A	400	PMP	C2-N1	2.46	1.39	1.34
4	A	1007	ACY	CH3-C	3.06	1.53	1.48
3	B	900	PMP	C6-N1	3.35	1.41	1.34
4	A	1006	ACY	CH3-C	3.41	1.53	1.48
4	B	1004	ACY	CH3-C	3.69	1.53	1.48
4	B	1005	ACY	CH3-C	3.72	1.54	1.48
4	B	1001	ACY	CH3-C	4.18	1.54	1.48
4	B	1002	ACY	CH3-C	4.91	1.55	1.48
2	B	3001	KIV	C3-C2	5.34	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	900	PMP	C5-C6-N1	-2.49	119.53	123.86
3	A	400	PMP	C5-C6-N1	-2.29	119.88	123.86
3	B	900	PMP	O4P-P-O1P	2.02	112.28	107.14
3	A	400	PMP	O4P-C5A-C5	2.10	112.46	108.99
3	A	400	PMP	C2A-C2-C3	2.16	123.64	121.04
2	B	3001	KIV	O3-C2-C3	2.22	122.71	117.64
3	B	900	PMP	C6-C5-C4	2.22	119.75	118.09
3	A	400	PMP	O3P-P-O1P	2.30	117.99	110.58
3	B	900	PMP	O3P-P-O1P	2.45	118.47	110.58
3	A	400	PMP	C6-C5-C4	3.47	120.68	118.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	ACY	1	0
3	A	400	PMP	1	0
4	B	1002	ACY	1	0
4	B	1005	ACY	1	0
5	B	2001	GOL	5	0
2	B	3001	KIV	3	0
3	B	900	PMP	1	0

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	365/365 (100%)	0.94	46 (12%) 5 5	19, 34, 51, 60	0
1	B	365/365 (100%)	0.91	44 (12%) 6 6	21, 37, 54, 62	0
All	All	730/730 (100%)	0.93	90 (12%) 5 6	19, 36, 53, 62	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	SER	11.5
1	B	502	SER	10.3
1	A	174	PHE	10.2
1	B	501	ALA	9.2
1	A	24	PRO	9.0
1	B	510	LEU	8.9
1	B	503	SER	8.6
1	A	177	GLY	8.5
1	B	525	GLY	8.0
1	A	2	SER	7.7
1	A	172	ALA	7.7
1	A	25	GLY	7.6
1	A	175	PRO	7.6
1	A	1	ALA	7.4
1	B	676	GLY	6.7
1	A	176	GLY	6.3
1	B	677	GLY	6.1
1	A	173	TYR	6.1
1	B	527	PRO	6.0
1	B	526	GLU	5.9
1	A	27	PRO	5.7
1	B	523	GLY	5.4
1	A	26	GLU	5.4
1	A	3	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	675	PRO	5.1
1	A	358	ALA	4.9
1	A	23	GLY	4.9
1	A	338	GLY	4.9
1	B	528	LEU	4.7
1	B	520	LYS	4.6
1	B	524	PRO	4.6
1	A	357	ARG	4.2
1	B	674	PHE	4.2
1	A	11	GLN	4.2
1	A	179	VAL	4.0
1	B	511	GLN	4.0
1	A	10	LEU	3.9
1	B	673	TYR	3.8
1	A	84	LYS	3.8
1	B	522	PRO	3.7
1	B	583	GLY	3.7
1	A	45	ASP	3.7
1	B	678	SER	3.7
1	B	584	LYS	3.7
1	B	546	LYS	3.6
1	A	28	LEU	3.5
1	A	356	ILE	3.5
1	B	518	PRO	3.3
1	A	326	LYS	3.1
1	B	515	THR	3.0
1	A	8	ALA	3.0
1	A	365	VAL	3.0
1	A	252	GLY	3.0
1	B	865	VAL	2.9
1	B	512	LEU	2.9
1	A	245	VAL	2.9
1	A	7	ALA	2.7
1	B	815	CYS	2.7
1	A	85	ASP	2.6
1	A	91	PHE	2.6
1	B	519	HIS	2.6
1	B	547	GLY	2.5
1	B	552	ARG	2.5
1	B	516	GLN	2.5
1	A	301	GLU	2.5
1	B	530	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	517	LYS	2.4
1	A	83	GLY	2.4
1	A	308	VAL	2.4
1	A	167	LEU	2.3
1	B	627	VAL	2.3
1	A	327	ASP	2.3
1	B	553	ILE	2.3
1	A	20	LYS	2.3
1	A	39	LEU	2.2
1	A	159	ARG	2.2
1	A	140	LEU	2.2
1	A	168	CYS	2.2
1	B	647	ILE	2.2
1	B	624	LEU	2.1
1	A	29	VAL	2.1
1	A	246	TYR	2.1
1	A	136	ALA	2.1
1	B	663	LEU	2.1
1	B	545	ASP	2.1
1	B	860	GLU	2.0
1	B	536	ASP	2.0
1	B	665	VAL	2.0
1	B	745	VAL	2.0
1	B	508	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ACY	A	1007	4/4	0.86	0.28	15.37	39,42,43,45	0
4	ACY	B	1005	4/4	0.89	0.26	7.72	47,47,47,48	0
2	KIV	B	3001	8/8	0.69	0.31	7.34	42,43,44,46	8
4	ACY	A	1003	4/4	0.80	0.20	3.89	42,44,44,46	0
5	GOL	B	2001	6/6	0.86	0.21	0.94	47,48,49,49	0
3	PMP	B	900	16/16	0.94	0.13	0.31	28,35,37,38	0
3	PMP	A	400	16/16	0.97	0.10	-1.16	21,24,27,28	0
4	ACY	B	1002	4/4	0.52	0.40	-	49,51,52,52	0
4	ACY	A	1006	4/4	0.76	0.20	-	40,41,44,45	0
4	ACY	B	1001	4/4	0.49	0.28	-	51,52,52,53	0
4	ACY	B	1004	4/4	0.81	0.29	-	46,47,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.