



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:23 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 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/ValidationPDFNotes.html>

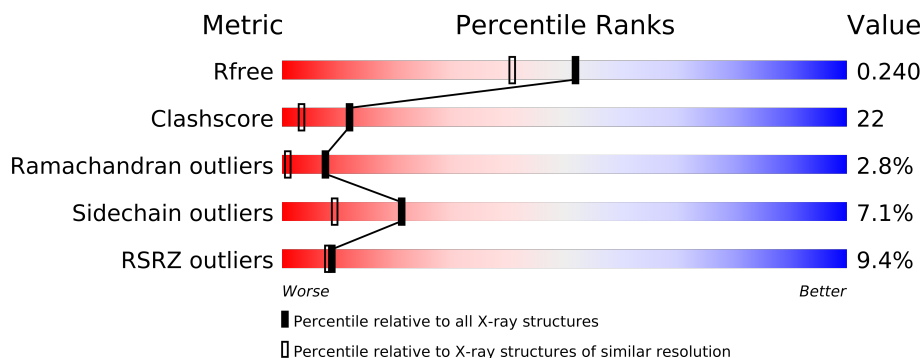
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
1	B	365	

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	KIV	B	3001	-	X
4	ACY	A	1003	-	X
4	ACY	A	1006	-	X
4	ACY	A	1007	-	X
4	ACY	B	1002	-	X
4	ACY	B	1004	-	X
4	ACY	B	1005	-	X

2 Entry composition i

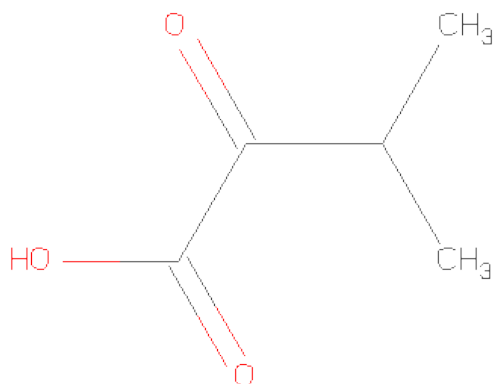
There are 6 unique types of molecules in this entry. The entry contains 6137 atoms, of which 0 are hydrogen and 0 are deuterium.

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 BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE, MITOCHONDRIAL.

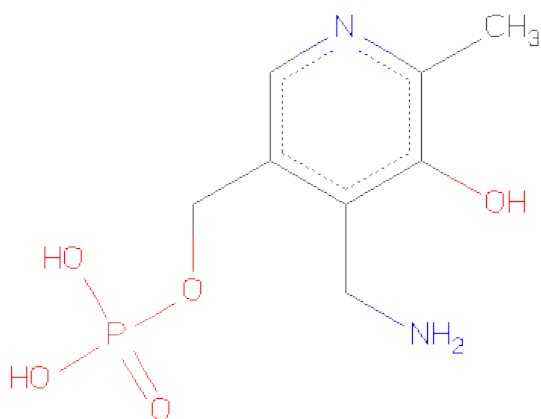
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			
1	B	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			

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



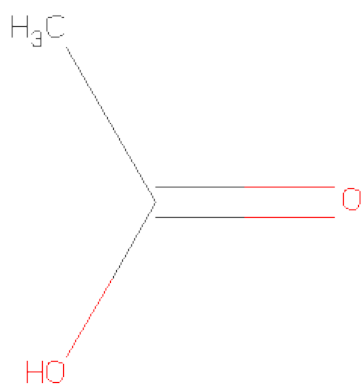
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			8	5	3		

- 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).



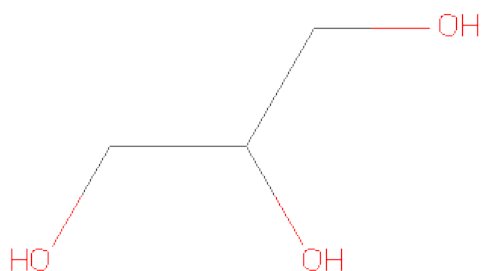
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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: $C_3H_8O_3$).



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

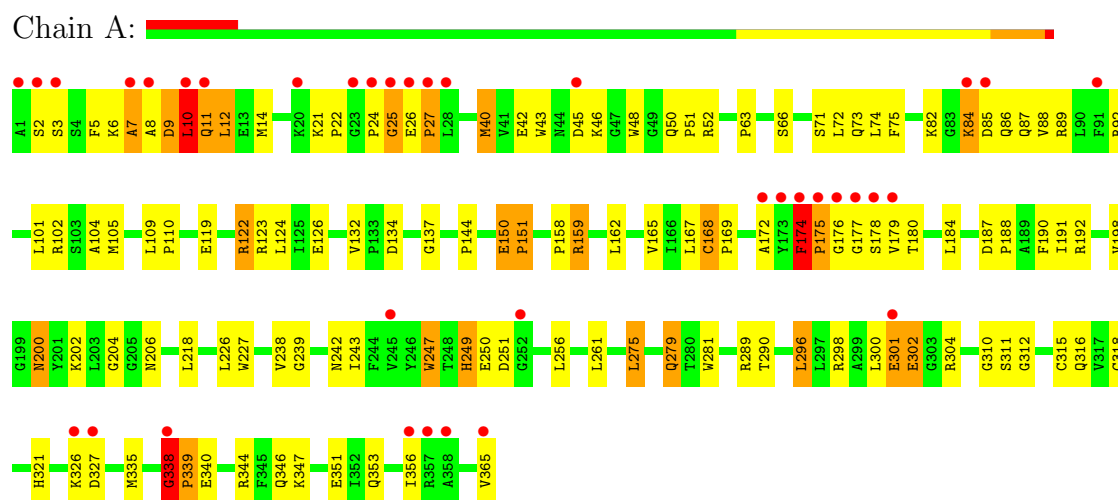
- Molecule 6 is water.

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

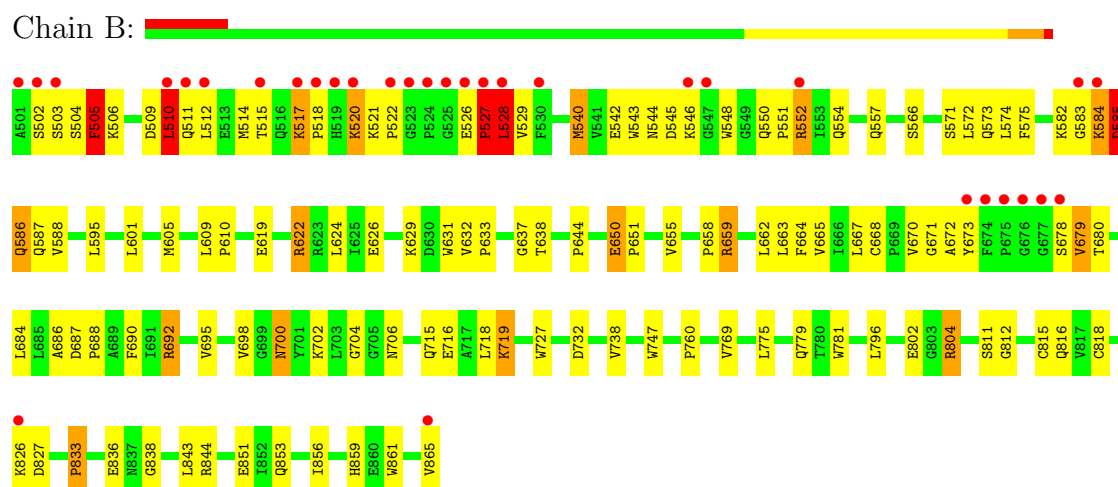
3 Residue-property plots

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.

- Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE, MITOCHONDRIAL



- Molecule 1: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE, MITOCHONDRIAL



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 , 42.3	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

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 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	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

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 22.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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
1:B:515:THR:CG2	1:B:518:PRO:HG3	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	363/365 (100%)	333 (92%)	18 (5%)	12 (3%)	6 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	363/365 (100%)	337 (93%)	18 (5%)	8 (2%)	10	2
All	All	726/730 (100%)	670 (92%)	36 (5%)	20 (3%)	8	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 ⓘ

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%)	27	13
1	B	316/316 (100%)	290 (92%)	26 (8%)	17	6
All	All	632/632 (100%)	587 (93%)	45 (7%)	21	9

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 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

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	-	3,3,3	1.48	1 (33%)	3,3,3	1.32	0
4	ACY	A	1006	-	3,3,3	1.26	0	3,3,3	1.40	0
4	ACY	A	1007	-	3,3,3	1.52	1 (33%)	3,3,3	1.53	1 (33%)
3	PMP	A	400	-	16,16,16	1.34	2 (12%)	23,23,23	1.42	4 (17%)
4	ACY	B	1001	-	3,3,3	1.44	1 (33%)	3,3,3	1.46	1 (33%)
4	ACY	B	1002	-	3,3,3	1.29	0	3,3,3	1.41	0
4	ACY	B	1004	-	3,3,3	1.46	1 (33%)	3,3,3	1.34	0
4	ACY	B	1005	-	3,3,3	1.33	0	3,3,3	1.18	0
5	GOL	B	2001	-	5,5,5	0.80	0	5,5,5	0.42	0
2	KIV	B	3001	-	7,7,7	2.21	2 (28%)	9,9,9	1.48	2 (22%)
3	PMP	B	900	-	16,16,16	1.25	1 (6%)	23,23,23	1.32	4 (17%)

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	-	-	0/8/8/8	0/0/0/0
3	PMP	B	900	-	-	0/8/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	KIV	C3-C2	5.18	1.58	1.51
3	B	900	PMP	C6-N1	3.20	1.41	1.34
3	A	400	PMP	C2-N1	2.92	1.39	1.33
4	A	1003	ACY	O-C	2.55	1.36	1.22
4	A	1007	ACY	O-C	2.45	1.35	1.22
4	B	1004	ACY	O-C	2.28	1.34	1.22
3	A	400	PMP	P-O3P	-2.20	1.46	1.54
4	B	1001	ACY	O-C	2.15	1.33	1.22
2	B	3001	KIV	O1-C1	-2.14	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	PMP	C6-C5-C4	3.40	120.68	118.10
2	B	3001	KIV	O1-C1-C2	2.49	119.38	114.14
3	B	900	PMP	O3P-P-O1P	2.45	118.47	110.44
3	B	900	PMP	C5-C6-N1	-2.40	119.53	123.86
3	A	400	PMP	O3P-P-O1P	2.31	117.99	110.44
3	A	400	PMP	C5-C6-N1	-2.21	119.88	123.86
3	B	900	PMP	C6-C5-C4	2.17	119.75	118.10
3	A	400	PMP	C2A-C2-C3	2.16	123.64	121.02
3	B	900	PMP	O2P-P-O4P	-2.12	100.81	106.65
2	B	3001	KIV	O3-C2-C3	2.10	122.71	117.97
4	A	1007	ACY	O-C-CH3	-2.04	113.15	122.06
4	B	1001	ACY	O-C-CH3	-2.00	113.33	122.06

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 ⓘ

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%)	0.75	36 (9%) 8 7	19, 34, 51, 60	0
1	B	365/365 (100%)	0.71	32 (8%) 10 9	21, 37, 54, 62	0
All	All	730/730 (100%)	0.73	68 (9%) 9 8	19, 36, 53, 62	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	SER	9.6
1	A	174	PHE	9.3
1	B	502	SER	8.9
1	A	24	PRO	8.4
1	A	1	ALA	8.2
1	B	501	ALA	8.0
1	B	503	SER	8.0
1	A	177	GLY	7.7
1	A	25	GLY	7.1
1	A	175	PRO	7.0
1	B	510	LEU	6.9
1	B	525	GLY	6.3
1	A	2	SER	6.2
1	A	172	ALA	5.8
1	A	173	TYR	5.8
1	B	676	GLY	5.7
1	A	176	GLY	5.7
1	B	526	GLU	5.2
1	B	677	GLY	5.0
1	A	26	GLU	4.8
1	A	27	PRO	4.8
1	B	527	PRO	4.7
1	B	523	GLY	4.5
1	B	675	PRO	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	338	GLY	4.3
1	B	520	LYS	4.2
1	A	23	GLY	4.2
1	B	524	PRO	4.1
1	A	358	ALA	4.1
1	B	528	LEU	4.0
1	A	3	SER	3.9
1	A	357	ARG	3.9
1	A	84	LYS	3.8
1	B	511	GLN	3.6
1	B	584	LYS	3.6
1	B	674	PHE	3.6
1	A	11	GLN	3.5
1	B	673	TYR	3.5
1	A	356	ILE	3.2
1	A	179	VAL	3.2
1	B	583	GLY	3.2
1	A	45	ASP	3.2
1	A	10	LEU	3.1
1	B	518	PRO	3.1
1	B	546	LYS	3.0
1	B	512	LEU	2.9
1	B	522	PRO	2.7
1	A	28	LEU	2.7
1	A	365	VAL	2.7
1	B	515	THR	2.7
1	B	678	SER	2.6
1	A	8	ALA	2.5
1	A	326	LYS	2.5
1	A	85	ASP	2.4
1	B	530	PHE	2.3
1	A	252	GLY	2.3
1	B	517	LYS	2.3
1	A	327	ASP	2.2
1	A	301	GLU	2.2
1	A	245	VAL	2.2
1	B	519	HIS	2.1
1	A	7	ALA	2.1
1	B	547	GLY	2.1
1	B	552	ARG	2.0
1	A	20	LYS	2.0
1	B	865	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	91	PHE	2.0
1	B	826	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ACY	B	1004	4/4	0.25	16.14	46,47,48,48	0
4	ACY	A	1007	4/4	0.27	10.60	39,42,43,45	0
4	ACY	B	1002	4/4	0.34	9.46	49,51,52,52	0
2	KIV	B	3001	8/8	0.32	7.71	42,43,44,46	8
4	ACY	B	1005	4/4	0.25	7.58	47,47,47,48	0
4	ACY	A	1006	4/4	0.19	4.88	40,41,44,45	0
4	ACY	A	1003	4/4	0.19	3.72	42,44,44,46	0
5	GOL	B	2001	6/6	0.21	1.04	47,48,49,49	0
3	PMP	B	900	16/16	0.13	0.54	28,35,37,38	0
3	PMP	A	400	16/16	0.09	-1.44	21,24,27,28	0
4	ACY	B	1001	4/4	0.23	-	51,52,52,53	0

6.5 Other polymers ⓘ

There are no such residues in this entry.