



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:36 PM UTC

PDB ID : 1KTA / pdb_00001kta
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

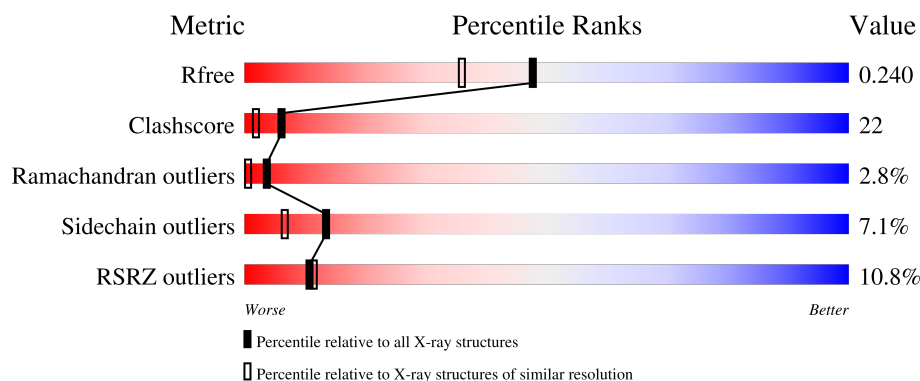
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	10% 60% 32% 7%
1	B	365	11% 63% 29% 5%

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
5	GOL	B	2001	-	-	X	-

2 Entry composition [i](#)

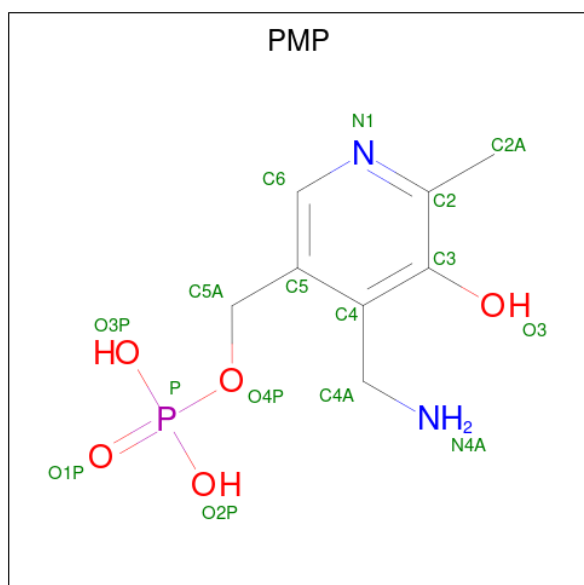
There are 6 unique types of molecules in this entry. The entry contains 6137 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

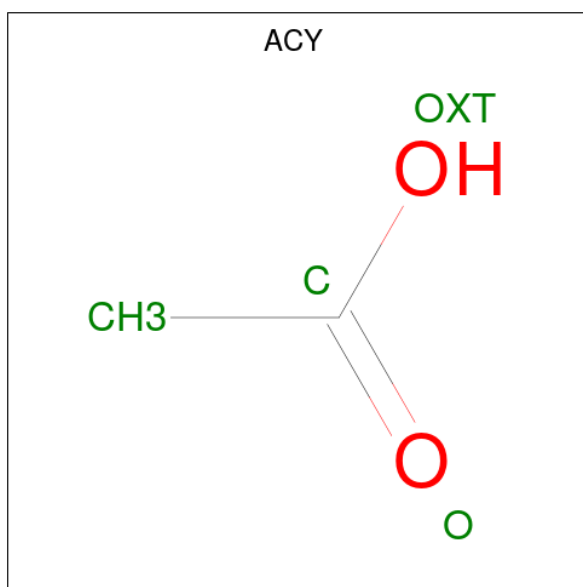
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			
1	B	365	Total	C	N	O	S	0	0	0
			2910	1875	507	510	18			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



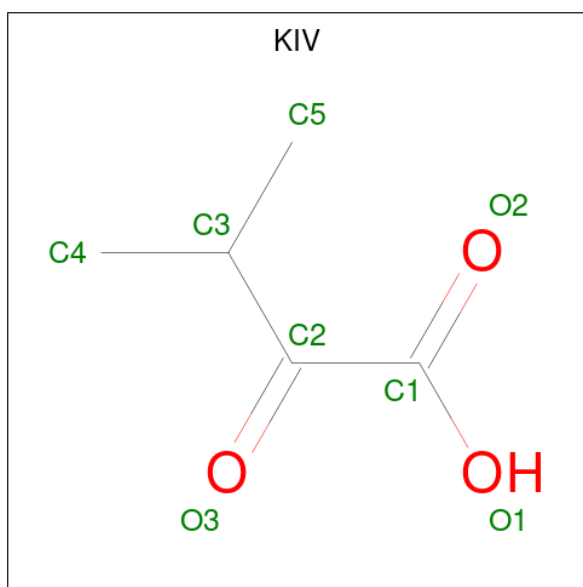
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



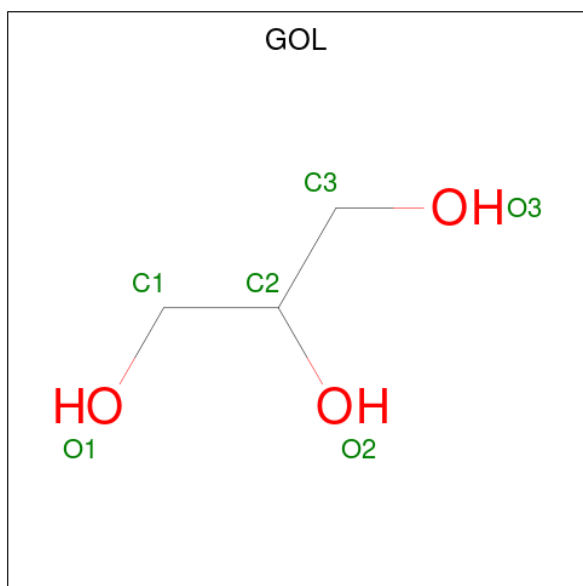
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 3-METHYL-2-OXOBUTANOIC ACID (CCD ID: KIV) (formula: C₅H₈O₃).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

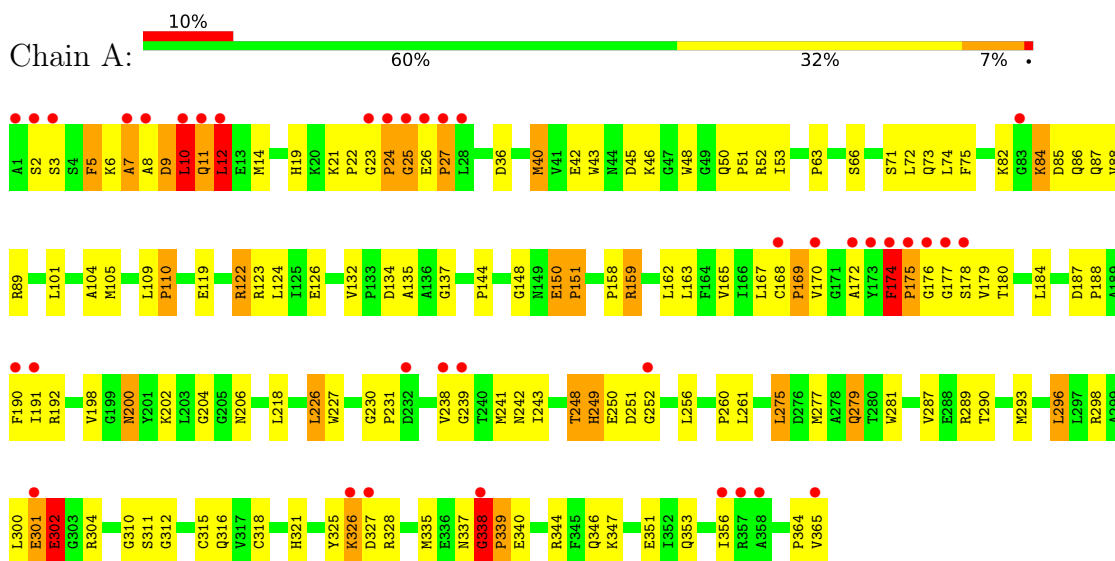
- Molecule 6 is water.

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

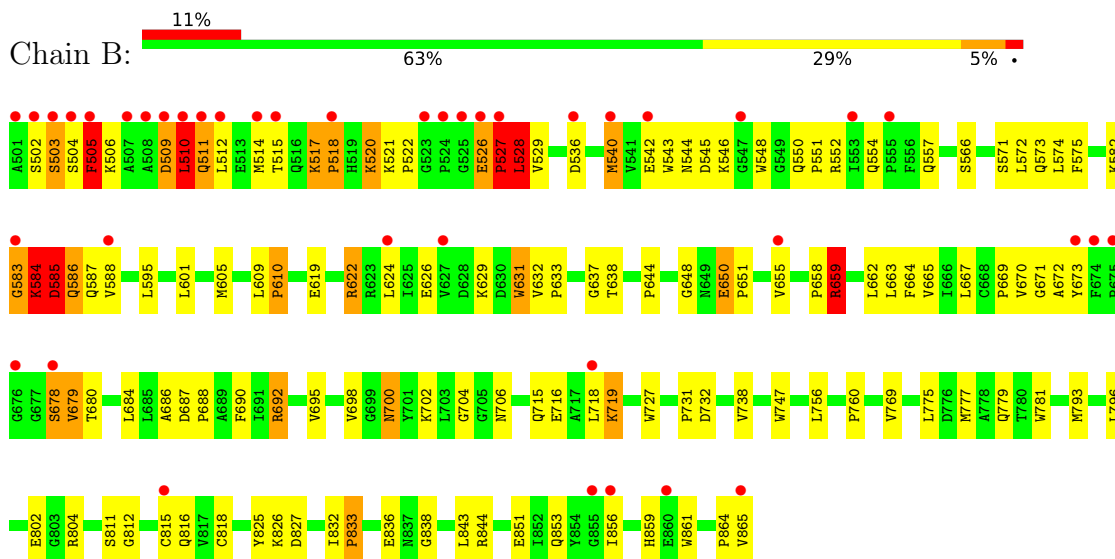
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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) 98.4 (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	3153 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, GOL, 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	0.99	2/2987 (0.1%)	1.27	27/4053 (0.7%)
1	B	0.92	1/2987 (0.0%)	1.27	25/4053 (0.6%)
All	All	0.96	3/5974 (0.1%)	1.27	52/8106 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	MET	SD-CE	-7.70	1.60	1.79
1	A	277	MET	SD-CE	-7.61	1.60	1.79
1	B	777	MET	SD-CE	-5.94	1.64	1.79

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	GLY	CA-C-N	12.93	136.00	119.84
1	A	338	GLY	C-N-CA	12.93	136.00	119.84
1	B	585	ASP	N-CA-C	-10.85	87.69	110.80
1	B	526	GLU	CA-C-N	10.78	133.32	119.84
1	B	526	GLU	C-N-CA	10.78	133.32	119.84
1	B	506	LYS	N-CA-C	10.73	125.72	109.41
1	B	529	VAL	N-CA-C	-10.68	92.25	109.12
1	A	302	GLU	N-CA-C	-10.28	98.19	113.61
1	A	148	GLY	N-CA-C	-8.25	101.44	112.82
1	B	527	PRO	N-CA-C	7.74	128.42	112.47
1	A	174	PHE	CA-C-N	7.52	129.24	119.84
1	A	174	PHE	C-N-CA	7.52	129.24	119.84
1	A	364	PRO	N-CA-C	7.48	122.55	111.03
1	A	337	ASN	N-CA-C	-7.37	104.25	112.57
1	B	503	SER	N-CA-C	7.36	121.47	109.85
1	B	864	PRO	N-CA-C	7.35	122.35	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	528	LEU	N-CA-C	7.10	125.92	110.80
1	A	231	PRO	N-CA-C	-6.83	104.63	113.57
1	A	36	ASP	N-CA-C	6.67	119.55	111.82
1	B	648	GLY	N-CA-C	-6.48	103.88	112.82
1	A	338	GLY	C-N-CD	-6.39	98.80	125.00
1	B	756	LEU	N-CA-C	-6.37	98.13	108.52
1	B	536	ASP	N-CA-C	6.31	119.14	111.82
1	A	110	PRO	N-CA-C	6.10	120.42	111.03
1	B	731	PRO	N-CA-C	-6.09	106.25	113.86
1	B	692	ARG	N-CA-C	5.82	118.58	111.82
1	B	583	GLY	N-CA-C	-5.81	101.82	110.71
1	A	326	LYS	CB-CA-C	-5.78	104.42	111.82
1	A	226	LEU	N-CA-C	-5.77	98.34	108.20
1	A	135	ALA	N-CA-C	-5.67	103.04	110.53
1	A	287	VAL	N-CA-C	5.67	117.99	108.81
1	A	53	ILE	N-CA-C	-5.59	99.69	107.80
1	B	610	PRO	N-CA-C	5.54	119.56	111.03
1	B	631	TRP	N-CA-C	-5.42	106.17	112.89
1	B	659	ARG	N-CA-C	-5.41	105.90	112.88
1	B	669	PRO	N-CA-C	-5.39	102.11	111.32
1	B	832	ILE	CA-C-N	5.33	126.50	119.84
1	B	832	ILE	C-N-CA	5.33	126.50	119.84
1	B	505	PHE	CB-CA-C	5.26	120.90	110.42
1	B	678	SER	N-CA-C	-5.23	99.65	110.80
1	A	5	PHE	N-CA-C	-5.22	103.63	110.53
1	B	584	LYS	N-CA-C	-5.20	103.08	110.35
1	A	248	THR	N-CA-C	-5.18	100.28	108.73
1	A	170	VAL	N-CA-C	5.14	116.12	108.46
1	A	23	GLY	CA-C-N	5.10	125.39	119.47
1	A	23	GLY	C-N-CA	5.10	125.39	119.47
1	A	12	LEU	N-CA-C	-5.07	101.43	109.59
1	B	509	ASP	N-CA-C	5.06	117.81	109.72
1	A	230	GLY	CA-C-N	5.03	124.53	119.19
1	A	230	GLY	C-N-CA	5.03	124.53	119.19
1	A	169	PRO	N-CA-C	-5.03	103.29	111.19
1	A	19	HIS	N-CA-C	-5.03	103.77	110.55

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	145	0
1	B	2910	0	2937	125	0
2	A	16	0	10	1	0
2	B	16	0	10	1	0
3	A	12	0	9	1	0
3	B	16	0	12	2	0
4	B	8	0	7	3	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	266	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 (266) 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:12:LEU:HD11	1:A:14:MET:SD	2.16	0.84
1:A:316:GLN:HE22	1:A:353:GLN:HE22	1.21	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:A:6:LYS:C	1:A:8:ALA:H	1.93	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
4:B:3001:KIV:HC52	4:B:3001:KIV:O2	1.87	0.72
1:B:585:ASP:CG	1:B:587:GLN:HE21	1.99	0.70
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:A:24:PRO:C	1:A:26:GLU:H	2.01	0.68
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: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	3: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:A:86:GLN:O	1:A:86:GLN:HG3	1.94	0.66
1:A:365:VAL:HG23	1:A:365:VAL:OXT	1.94	0.65
1:B:719:LYS:HB2	1:B:719:LYS:HZ2	1.59	0.65
1:B:719:LYS:HB2	1:B:719:LYS:NZ	2.11	0.65
1:B:838:GLY:O	6:B:239:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:700:ASN:HD22	1:B:700:ASN:N	1.88	0.64
1:A:7:ALA:C	1:A:9:ASP:H	2.06	0.64
1:A:261:LEU:HD13	3:A:1003:ACY:H3	1.79	0.63
1:A:302:GLU:HG2	1:A:304:ARG:HD3	1.80	0.63
1:A:25:GLY:C	1:A:27:PRO:HD3	2.23	0.63
1:B:865:VAL:HG23	1:B:865:VAL:OXT	1.97	0.63
1:B:843:LEU:HD12	3: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:A:300:LEU:C	1:A:301:GLU:OE2	2.43	0.61
1:B:700:ASN:H	1:B:700:ASN:ND2	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: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: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: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:21:LYS:O	1:A:22:PRO:C	2.45	0.58
1:A:239:GLY:C	6:A:1130:HOH:O	2.46	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:B:503:SER:O	1:B:504:SER:HB2	2.05	0.56
1:A:84:LYS:C	1:A:86:GLN:H	2.13	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:184:LEU:HD22	1:A:238:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:655:VAL:HG23	4:B:3001:KIV:HC43	1.90	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:10:LEU:C	1:A:11:GLN:O	2.51	0.52
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:716:GLU:CD	1:B:719:LYS:HE3	2.35	0.51
1:B:586:GLN:O	1:B:629:LYS:HE3	2.10	0.51
1:B:687:ASP:HB3	1:B:690:PHE:CD1	2.45	0.51
4:B:3001:KIV:O2	4:B:3001:KIV:C5	2.57	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:200:ASN:H	1:A:200:ASN:ND2	1.92	0.50
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:B:521:LYS:O	1:B:522:PRO:C	2.54	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:A:42:GLU:HG2	1:A:162:LEU:CD1	2.42	0.49
1:B:509:ASP:HB2	1:B:551:PRO:O	2.13	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:633:PRO:HB2	1:B:638:THR:OG1	2.13	0.49
1:B:702:LYS:NZ	2:B:900:PMP:N4A	2.61	0.49
1:B:624:LEU:HG	1:B:667:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:HE2	1:A:325:TYR:CG	2.48	0.49
1:A:179:VAL:CG1	1:A:346:GLN:NE2	2.63	0.48
1:B:583:GLY:O	1:B:584:LYS:C	2.55	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:540:MET:HG3	1:B:662:LEU:HD11	1.93	0.48
1:B:684:LEU:HD22	1:B:738:VAL:HG23	1.95	0.48
1:B:588:VAL:O	1:B:865:VAL:N	2.43	0.48
1:A:84:LYS:C	1:A:86:GLN:N	2.72	0.48
1:B:585:ASP:CG	1:B:587:GLN:HG3	2.39	0.48
1:A:365:VAL:OXT	1:A:365:VAL:CG2	2.61	0.48
1:A:40:MET:CE	6:A:1020:HOH:O	2.53	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:B:793:MET:HE2	1:B:825:TYR:CG	2.48	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:B:574:LEU:HD12	1:B:574:LEU:C	2.39	0.47
1:A:5:PHE:HB2	1:A:51:PRO:HG3	1.95	0.47
1:A:298:ARG:O	1:A:302:GLU:HB2	2.14	0.47
1:B:509:ASP:C	1:B:511:GLN:H	2.20	0.47
1:A:82:LYS:HE3	1:A:134:ASP:HB3	1.95	0.47
1:A:200:ASN:HD22	1:A:200:ASN:N	1.89	0.47
1:A:9:ASP:C	1:A:11:GLN:N	2.73	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:A:124:LEU:HG	1:A:167:LEU:HD11	1.97	0.46
1:A:88:VAL:O	1:A:365:VAL:N	2.47	0.46
1:B:527:PRO:HB2	1:B:528:LEU:H	1.41	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:A:7:ALA:C	1:A:9:ASP:N	2.72	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:2:SER:H	1:A:6:LYS:NZ	2.14	0.45
1:A:10:LEU:CD1	1:A:50:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2:SER:H	1:A:6:LYS:HZ1	1.63	0.45
1:A:73:GLN:NE2	1:B:571:SER:H	2.15	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:B:851:GLU:CB	1:B:856:ILE:HD11	2.44	0.45
1:A:85:ASP:OD2	1:A:89:ARG:NH2	2.50	0.45
1:B:520:LYS:NZ	1:B:520:LYS:HB3	2.32	0.45
1:A:159:ARG:HH11	1:A:159:ARG:CG	2.30	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:144:PRO:HA	1:A:165:VAL:HG22	1.99	0.44
1:A:150:GLU:CG	1:A:159:ARG:H	2.29	0.44
1:A:122:ARG:HG3	1:A:365:VAL:OXT	2.17	0.44
1:A:260:PRO:HD3	1:A:289:ARG:C	2.43	0.44
1:B:542:GLU:HG2	1:B:662:LEU:CD1	2.47	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:A:249:HIS:CG	1:A:250:GLU:N	2.85	0.43
1:B:526:GLU:HB2	1:B:527:PRO:CD	2.48	0.43
1:B:687:ASP:HA	1:B:688:PRO:HD3	1.86	0.43
1:B:663:LEU:HD23	1:B:663:LEU:C	2.44	0.43
1:B:716:GLU:CA	1:B:719:LYS:HG3	2.47	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:A:326:LYS:C	1:A:328:ARG:H	2.26	0.43
1:A:163:LEU:HD23	1:A:163:LEU:C	2.43	0.43
1:B:859:HIS:CE1	5:B:2001:GOL:H11	2.53	0.43
1:A:302:GLU:CB	1:A:304:ARG:HD3	2.47	0.42
1:A:326:LYS:C	1:A:328:ARG:N	2.76	0.42
1:B:521:LYS:HE3	1:B:631:TRP:CE2	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ASP:HB3	1:B:551:PRO:HD2	2.01	0.42
1:A:6:LYS:C	1:A:8:ALA:N	2.60	0.42
1:B:747:TRP:CD1	1:B:747:TRP:C	2.97	0.42
1:A:24:PRO:O	1:A:26:GLU:HG2	2.20	0.42
1:A:179:VAL:HG23	1:A:179:VAL:O	2.19	0.42
1:B:572:LEU:HD23	1:B:572:LEU:HA	1.87	0.42
1:A:74:LEU:CD2	1:A:104:ALA:HA	2.50	0.42
1:A:202:LYS:NZ	2:A:400:PMP:N4A	2.68	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:174:PHE:HA	1:A:175:PRO:HD2	1.79	0.41
1:A:187:ASP:HA	1:A:188:PRO:HD3	1.92	0.41
1:A:72:LEU:CD1	1:A:158:PRO:HG3	2.49	0.41
1:B:816:GLN:NE2	6:B:198:HOH:O	2.53	0.41
1:A:344:ARG:HD2	6:A:1086:HOH:O	2.20	0.41
1:A:351:GLU:CA	1:A:356:ILE:HG12	2.50	0.41
1:B:509:ASP:CB	1:B:551:PRO:HD2	2.50	0.41
1:B:851:GLU:CA	1:B:856:ILE:HG12	2.51	0.41
1:A:25:GLY:O	1:A:27:PRO:HD3	2.20	0.41
1:B:622:ARG:CG	1:B:865:VAL:OXT	2.68	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:72:LEU:HD13	1:A:158:PRO:CG	2.50	0.41
1:A:82:LYS:NZ	1:A:86:GLN:NE2	2.68	0.41
1:A:248:THR:HG22	1:A:252:GLY:C	2.46	0.41
1:A:256:LEU:HA	1:A:256:LEU:HD12	1.82	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:B:595:LEU:HD12	1:B:769:VAL:HG13	2.03	0.41
1:A:242:ASN:O	1:A:310:GLY:HA2	2.21	0.41
1:A:24:PRO:C	1:A:26:GLU:N	2.69	0.40
1:A:159:ARG:CG	1:A:159:ARG:NH1	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:168:CYS:HA	1:A:169:PRO:HD3	1.96	0.40
1:A:338:GLY:HA2	1:A:339:PRO:HD2	1.57	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:HH11	1:B:659:ARG:CG	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:ALA:HA	6:B:44:HOH:O	2.21	0.40
1:B:687:ASP:HB3	1:B:690:PHE:CE1	2.57	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%)	3	0
1	B	363/365 (100%)	337 (93%)	18 (5%)	8 (2%)	5	1
All	All	726/730 (100%)	670 (92%)	36 (5%)	20 (3%)	4	0

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

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Mol	Chain	Res	Type
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%)	17	9
1	B	316/316 (100%)	290 (92%)	26 (8%)	10	5
All	All	632/632 (100%)	587 (93%)	45 (7%)	13	7

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	24	PRO
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	275	LEU
1	A	279	GLN
1	A	296	LEU
1	A	301	GLU

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Mol	Chain	Res	Type
1	A	302	GLU
1	B	502	SER
1	B	505	PHE
1	B	510	LEU
1	B	511	GLN
1	B	517	LYS
1	B	518	PRO
1	B	520	LYS
1	B	528	LEU
1	B	540	MET
1	B	545	ASP
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	760	PRO
1	B	775	LEU
1	B	779	GLN
1	B	796	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	57	GLN
1	A	73	GLN
1	A	200	ASN
1	A	206	ASN
1	A	224	GLN
1	A	234	GLN
1	A	249	HIS
1	A	316	GLN
1	A	346	GLN
1	B	554	GLN

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Mol	Chain	Res	Type
1	B	557	GLN
1	B	573	GLN
1	B	700	ASN
1	B	706	ASN
1	B	715	GLN
1	B	724	GLN
1	B	779	GLN
1	B	816	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	ACY	A	1003	-	3,3,3	1.83	1 (33%)	3,3,3	1.48	0
3	ACY	B	1004	-	3,3,3	1.78	1 (33%)	3,3,3	1.50	1 (33%)
3	ACY	A	1006	-	3,3,3	1.54	1 (33%)	3,3,3	1.56	1 (33%)
3	ACY	A	1007	-	3,3,3	1.84	1 (33%)	3,3,3	1.71	1 (33%)
5	GOL	B	2001	-	5,5,5	0.79	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PMP	B	900	-	16,16,16	1.35	1 (6%)	22,23,23	1.40	4 (18%)
3	ACY	B	1001	-	3,3,3	1.74	1 (33%)	3,3,3	1.64	1 (33%)
3	ACY	B	1002	-	3,3,3	1.55	1 (33%)	3,3,3	1.59	1 (33%)
2	PMP	A	400	-	16,16,16	1.42	4 (25%)	22,23,23	1.50	4 (18%)
4	KIV	B	3001	-	7,7,7	2.03	2 (28%)	8,9,9	1.25	1 (12%)
3	ACY	B	1005	-	3,3,3	1.63	1 (33%)	3,3,3	1.33	0

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	PMP	B	900	-	-	0/8/8/8	0/1/1/1
2	PMP	A	400	-	-	0/8/8/8	0/1/1/1
5	GOL	B	2001	-	-	0/4/4/4	-
4	KIV	B	3001	-	-	2/7/8/8	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3001	KIV	C3-C2	4.37	1.58	1.51
2	B	900	PMP	C6-N1	3.55	1.41	1.34
3	A	1003	ACY	O-C	3.15	1.36	1.22
2	A	400	PMP	C2-N1	3.06	1.39	1.33
3	A	1007	ACY	O-C	3.02	1.35	1.22
3	B	1004	ACY	O-C	2.82	1.34	1.22
3	B	1001	ACY	O-C	2.67	1.33	1.22
4	B	3001	KIV	O1-C1	-2.61	1.23	1.30
3	A	1006	ACY	O-C	2.41	1.32	1.22
3	B	1005	ACY	O-C	2.33	1.32	1.22
2	A	400	PMP	P-O3P	-2.19	1.46	1.54
3	B	1002	ACY	O-C	2.11	1.31	1.22
2	A	400	PMP	C6-N1	2.06	1.38	1.34
2	A	400	PMP	C2A-C2	2.03	1.53	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PMP	C6-C5-C4	3.46	120.68	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	PMP	C5-C6-N1	-2.64	119.53	123.83
2	A	400	PMP	C2A-C2-C3	2.43	123.64	120.80
2	A	400	PMP	C5-C6-N1	-2.43	119.88	123.83
3	A	1007	ACY	O-C-CH3	-2.29	113.15	122.53
2	B	900	PMP	O2P-P-O4P	-2.25	100.81	106.67
3	B	1001	ACY	O-C-CH3	-2.24	113.33	122.53
2	B	900	PMP	C6-C5-C4	2.23	119.75	118.06
3	B	1002	ACY	O-C-CH3	-2.18	113.58	122.53
2	B	900	PMP	O4P-P-O1P	2.16	112.28	106.44
2	A	400	PMP	O2P-P-O4P	-2.11	101.16	106.67
3	A	1006	ACY	O-C-CH3	-2.07	114.03	122.53
4	B	3001	KIV	O1-C1-O2	-2.03	119.06	123.90
3	B	1004	ACY	O-C-CH3	-2.01	114.28	122.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3001	KIV	C1-C2-C3-C5
4	B	3001	KIV	O3-C2-C3-C5

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	ACY	1	0
5	B	2001	GOL	5	0
2	B	900	PMP	1	0
3	B	1002	ACY	1	0
2	A	400	PMP	1	0
4	B	3001	KIV	3	0
3	B	1005	ACY	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%)	0.71	38 (10%)	11 12	19, 34, 51, 60	0
1	B	365/365 (100%)	0.79	41 (11%)	10 10	21, 37, 54, 62	0
All	All	730/730 (100%)	0.75	79 (10%)	11 11	19, 36, 53, 62	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	SER	6.2
1	A	338	GLY	5.9
1	A	8	ALA	5.8
1	A	24	PRO	5.2
1	B	503	SER	5.0
1	B	512	LEU	4.7
1	A	25	GLY	4.6
1	A	174	PHE	4.5
1	A	177	GLY	4.4
1	A	10	LEU	4.3
1	A	175	PRO	4.3
1	B	508	ALA	4.1
1	A	172	ALA	4.0
1	B	502	SER	4.0
1	B	523	GLY	4.0
1	A	2	SER	4.0
1	A	27	PRO	3.9
1	A	11	GLN	3.8
1	B	527	PRO	3.7
1	B	627	VAL	3.6
1	A	357	ARG	3.6
1	B	525	GLY	3.5
1	B	510	LEU	3.5
1	A	173	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	518	PRO	3.4
1	A	238	VAL	3.4
1	A	176	GLY	3.3
1	A	358	ALA	3.3
1	B	865	VAL	3.3
1	B	504	SER	3.3
1	A	365	VAL	3.2
1	B	501	ALA	3.1
1	A	7	ALA	3.1
1	B	547	GLY	3.1
1	B	815	CYS	3.0
1	B	583	GLY	3.0
1	A	1	ALA	2.9
1	A	252	GLY	2.9
1	B	509	ASP	2.9
1	B	553	ILE	2.8
1	B	536	ASP	2.8
1	A	23	GLY	2.7
1	A	26	GLU	2.7
1	B	507	ALA	2.7
1	B	673	TYR	2.7
1	B	860	GLU	2.7
1	A	28	LEU	2.7
1	B	540	MET	2.6
1	A	170	VAL	2.6
1	A	326	LYS	2.6
1	B	511	GLN	2.6
1	A	3	SER	2.6
1	B	674	PHE	2.5
1	B	655	VAL	2.5
1	B	515	THR	2.5
1	A	301	GLU	2.5
1	B	624	LEU	2.5
1	A	239	GLY	2.4
1	B	675	PRO	2.4
1	B	505	PHE	2.4
1	A	327	ASP	2.3
1	B	856	ILE	2.3
1	B	588	VAL	2.3
1	B	526	GLU	2.3
1	A	83	GLY	2.3
1	B	524	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	232	ASP	2.3
1	B	678	SER	2.2
1	B	542	GLU	2.2
1	B	676	GLY	2.2
1	A	12	LEU	2.2
1	B	718	LEU	2.2
1	A	168	CYS	2.2
1	A	190	PHE	2.1
1	A	356	ILE	2.1
1	B	514	MET	2.1
1	A	191	ILE	2.1
1	B	855	GLY	2.1
1	B	555	PRO	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACY	B	1001	4/4	0.57	0.16	51,52,52,53	0
4	KIV	B	3001	8/8	0.62	0.20	42,43,44,46	8
3	ACY	B	1004	4/4	0.72	0.18	46,47,48,48	0
3	ACY	B	1002	4/4	0.72	0.15	49,51,52,52	0
3	ACY	B	1005	4/4	0.76	0.16	47,47,47,48	0
3	ACY	A	1003	4/4	0.77	0.15	42,44,44,46	0
3	ACY	A	1006	4/4	0.85	0.11	40,41,44,45	0
5	GOL	B	2001	6/6	0.85	0.10	47,48,49,49	0
3	ACY	A	1007	4/4	0.87	0.11	39,42,43,45	0
2	PMP	B	900	16/16	0.93	0.10	28,35,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PMP	A	400	16/16	0.97	0.07	21,24,27,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.