



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:13 AM UTC

PDB ID : 5YHV / pdb_00005yhv
Title : Crystal structure of an aminotransferase from Mycobacterium tuberculosis
Authors : Saroj, D.C.; Biswal, B.K.
Deposited on : 2017-09-30
Resolution : 2.70 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

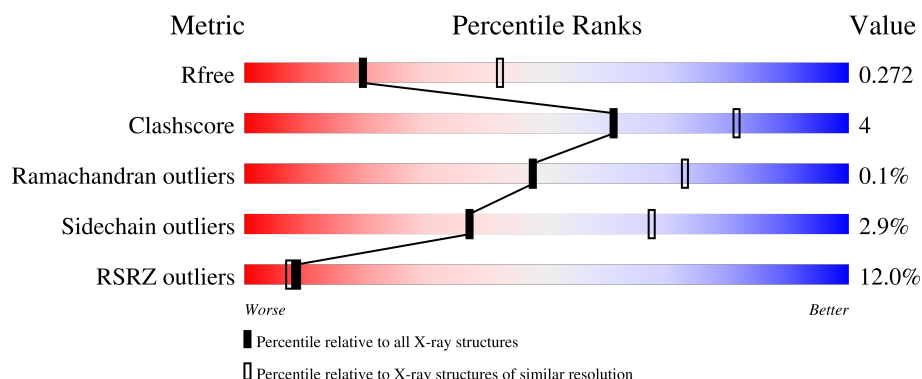
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	394	
1	B	394	
1	C	394	
1	D	394	

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
4	PLP	D	401	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11078 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 Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			2894	1837	499	545	13			
1	B	387	Total	C	N	O	S	0	0	0
			2826	1788	484	542	12			
1	C	384	Total	C	N	O	S	0	0	0
			2707	1708	467	520	12			
1	D	364	Total	C	N	O	S	0	0	0
			2342	1464	411	455	12			

There are 24 discrepancies between the modelled and reference sequences:

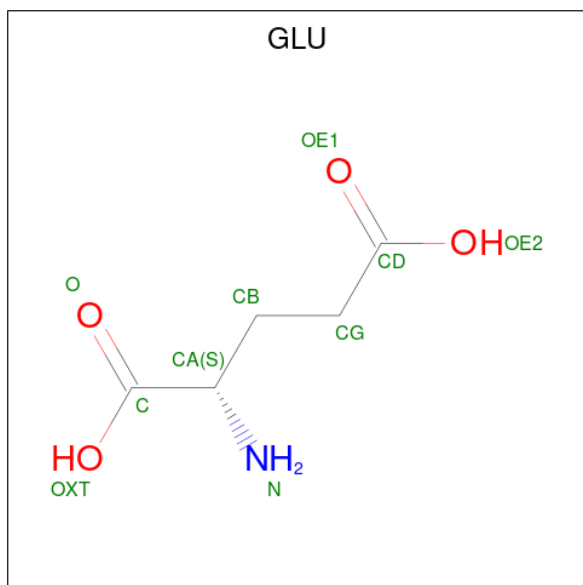
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P96847
A	-4	HIS	-	expression tag	UNP P96847
A	-3	HIS	-	expression tag	UNP P96847
A	-2	HIS	-	expression tag	UNP P96847
A	-1	HIS	-	expression tag	UNP P96847
A	0	HIS	-	expression tag	UNP P96847
B	-5	HIS	-	expression tag	UNP P96847
B	-4	HIS	-	expression tag	UNP P96847
B	-3	HIS	-	expression tag	UNP P96847
B	-2	HIS	-	expression tag	UNP P96847
B	-1	HIS	-	expression tag	UNP P96847
B	0	HIS	-	expression tag	UNP P96847
C	-5	HIS	-	expression tag	UNP P96847
C	-4	HIS	-	expression tag	UNP P96847
C	-3	HIS	-	expression tag	UNP P96847
C	-2	HIS	-	expression tag	UNP P96847
C	-1	HIS	-	expression tag	UNP P96847
C	0	HIS	-	expression tag	UNP P96847
D	-5	HIS	-	expression tag	UNP P96847
D	-4	HIS	-	expression tag	UNP P96847
D	-3	HIS	-	expression tag	UNP P96847

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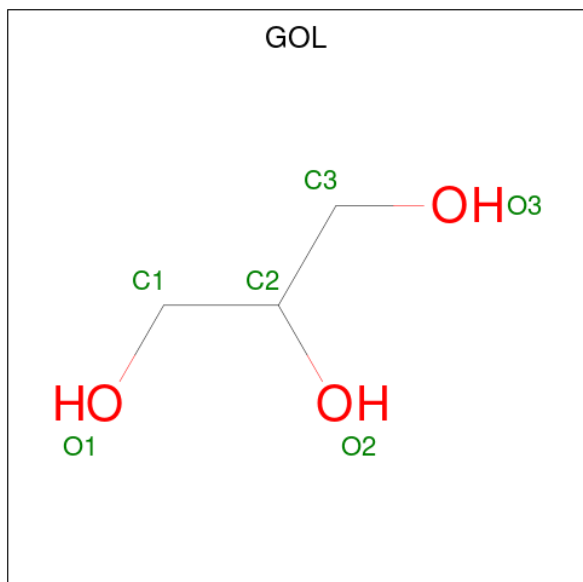
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	expression tag	UNP P96847
D	-1	HIS	-	expression tag	UNP P96847
D	0	HIS	-	expression tag	UNP P96847

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



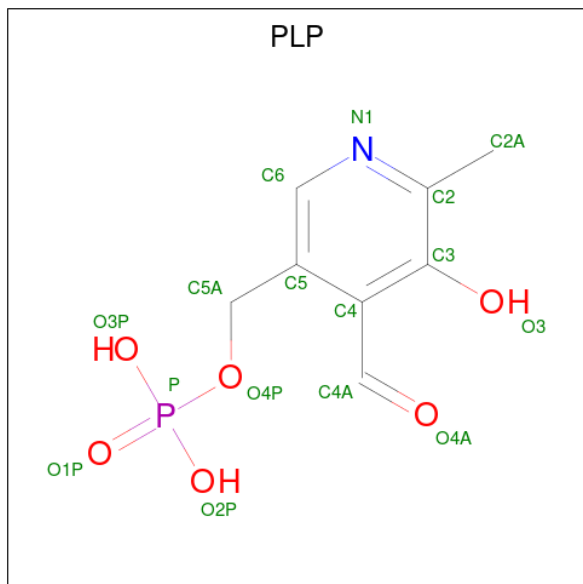
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



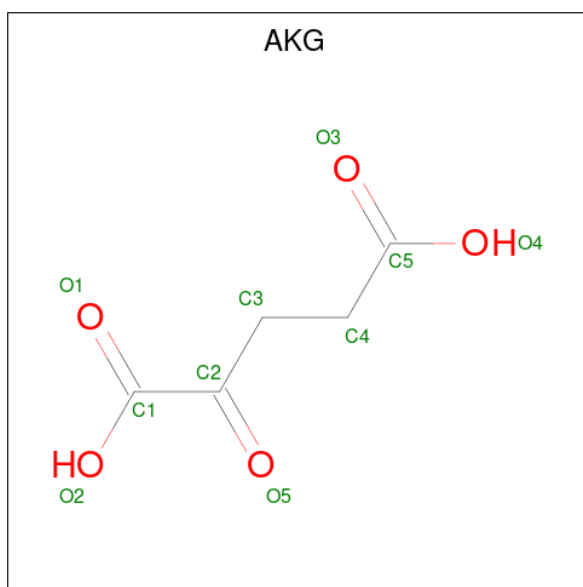
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
4	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	5	5		
5	C	1	Total	C	O	0	0
			10	5	5		

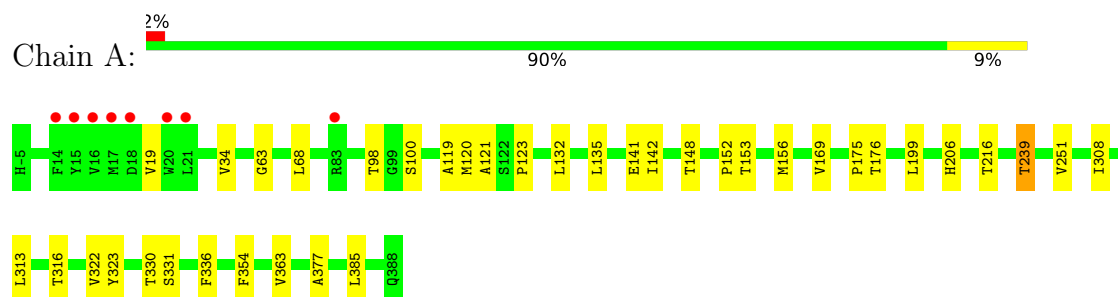
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total	O	0	0
			79	79		
6	B	73	Total	O	0	0
			73	73		
6	C	34	Total	O	0	0
			34	34		
6	D	15	Total	O	0	0
			15	15		

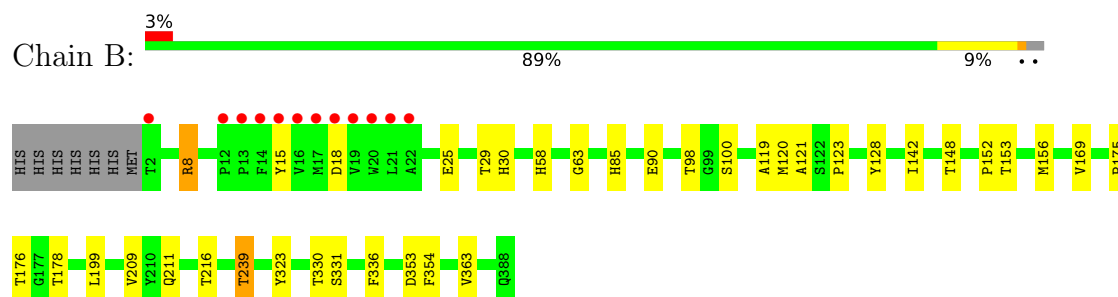
3 Residue-property plots [i](#)

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.

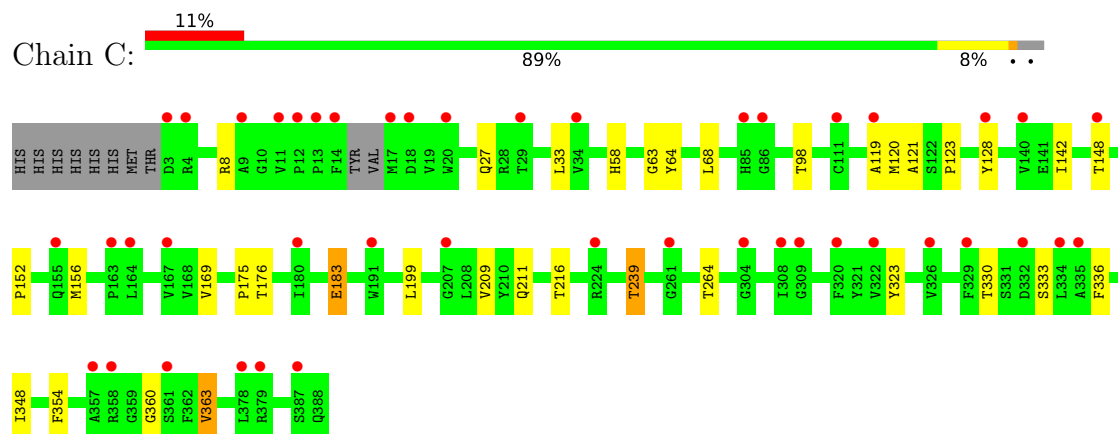
• Molecule 1: Aminotransferase



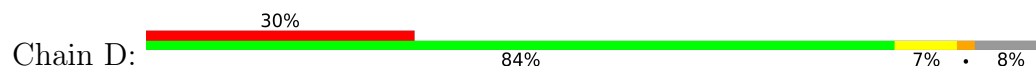
• Molecule 1: Aminotransferase

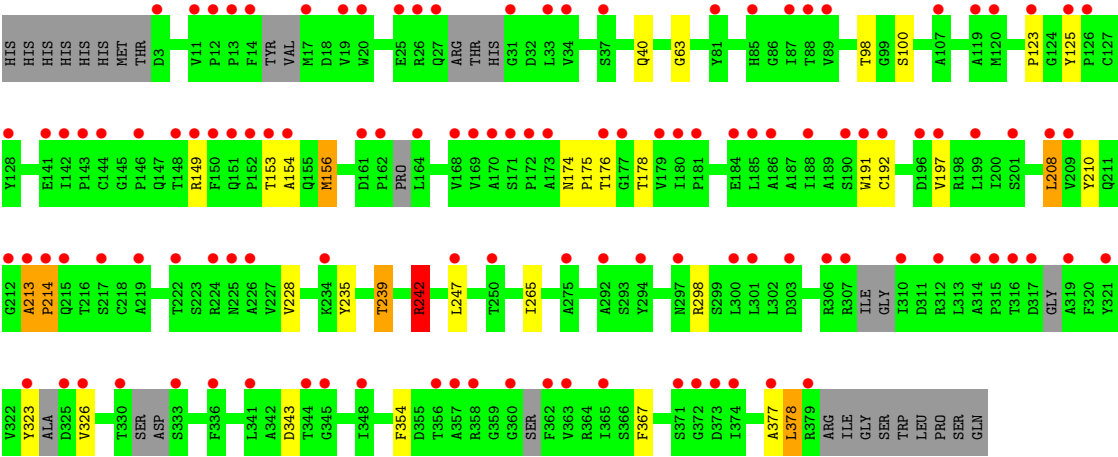


• Molecule 1: Aminotransferase



• Molecule 1: Aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.28Å 98.22Å 198.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.39 – 2.70 99.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (99.39-2.70) 99.3 (99.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.236 , 0.272 0.235 , 0.272	Depositor DCC
R_{free} test set	2563 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11078	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, GOL, PLP

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	0.54	0/2968	0.98	0/4070
1	B	0.54	0/2894	0.99	0/3964
1	C	0.54	0/2769	0.99	0/3797
1	D	0.61	0/2393	1.08	6/3264 (0.2%)
All	All	0.56	0/11024	1.01	6/15095 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	VAL	N-CA-C	9.62	122.00	109.58
1	D	214	PRO	CA-N-CD	-6.12	103.43	112.00
1	D	213	ALA	CA-C-N	5.85	127.15	119.84
1	D	213	ALA	C-N-CA	5.85	127.15	119.84
1	D	242	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	D	377	ALA	N-CA-C	5.05	117.17	111.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	149	ARG	Peptide
1	D	343	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	2894	0	2786	24	0
1	B	2826	0	2717	23	0
1	C	2707	0	2506	24	0
1	D	2342	0	1894	29	0
2	A	10	0	5	3	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	15	0	6	2	0
4	B	15	0	6	1	0
4	C	15	0	6	1	0
4	D	15	0	6	8	0
5	B	10	0	4	1	0
5	C	10	0	4	0	0
6	A	79	0	0	1	0
6	B	73	0	0	0	0
6	C	34	0	0	0	0
6	D	15	0	0	0	0
All	All	11078	0	9964	88	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 4.

All (88) 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:D:192:CYS:SG	1:D:197:VAL:O	1.95	1.23
1:D:100:SER:OG	4:D:401:PLP:H5A1	1.59	1.02
1:A:206:HIS:HB3	2:A:401:GLU:HA	1.41	1.00
1:D:100:SER:OG	4:D:401:PLP:C5A	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:SER:HG	4:D:401:PLP:H5A1	1.33	0.90
1:C:64:TYR:H	1:D:40:GLN:HE22	1.19	0.88
1:B:25:GLU:O	1:B:29:THR:HG22	1.86	0.75
1:B:100:SER:OG	4:B:401:PLP:H6	1.89	0.72
1:D:210:TYR:HH	1:D:367:PHE:HE2	1.39	0.66
1:A:316:THR:HG21	1:A:322:VAL:HG22	1.78	0.66
1:A:206:HIS:HB3	2:A:401:GLU:CA	2.24	0.66
1:A:120:MET:HE1	1:A:132:LEU:HD12	1.78	0.66
1:C:27:GLN:HG2	1:C:33:LEU:HB3	1.78	0.65
1:A:100:SER:OG	4:A:403:PLP:H5A2	1.98	0.64
1:D:100:SER:OG	4:D:401:PLP:H5A2	1.96	0.63
1:A:206:HIS:CB	2:A:401:GLU:HA	2.21	0.63
1:A:63:GLY:HA2	1:B:239:THR:HG23	1.81	0.63
1:C:64:TYR:N	1:D:40:GLN:HE22	1.96	0.61
1:C:183:GLU:H	1:C:183:GLU:CD	2.08	0.61
1:A:135:LEU:O	1:B:8:ARG:NH1	2.33	0.61
1:D:175:PRO:HG3	1:D:354:PHE:CG	2.36	0.59
1:C:120:MET:HE1	1:C:128:TYR:HB2	1.84	0.59
1:D:208:LEU:CD1	1:D:235:TYR:HD1	2.14	0.59
1:C:64:TYR:H	1:D:40:GLN:NE2	1.95	0.58
1:D:208:LEU:HD13	1:D:235:TYR:HD1	1.69	0.58
1:C:63:GLY:HA2	1:D:239:THR:HG23	1.85	0.58
1:D:210:TYR:OH	1:D:367:PHE:HE2	1.87	0.58
1:A:121:ALA:HB2	1:A:152:PRO:HD3	1.84	0.58
1:B:120:MET:HE1	1:B:128:TYR:HB2	1.85	0.57
1:B:29:THR:HG23	1:B:30:HIS:HD2	1.70	0.57
1:C:121:ALA:HB2	1:C:152:PRO:HD3	1.87	0.56
1:B:121:ALA:HB2	1:B:152:PRO:HD3	1.86	0.56
1:A:175:PRO:HG3	1:A:354:PHE:CG	2.40	0.56
1:B:175:PRO:HG3	1:B:354:PHE:CG	2.40	0.56
1:C:175:PRO:HG3	1:C:354:PHE:CG	2.40	0.56
1:D:154:ALA:HB1	1:D:191:TRP:CD1	2.41	0.56
1:A:239:THR:HG23	1:B:63:GLY:HA2	1.89	0.55
1:C:239:THR:HG23	1:D:63:GLY:HA2	1.88	0.55
4:C:403:PLP:H5A2	1:D:265:ILE:HD11	1.88	0.55
1:D:210:TYR:CD2	1:D:298:ARG:CD	2.91	0.54
1:D:174:ASN:CB	4:D:401:PLP:H2A1	2.39	0.53
1:A:148:THR:HG21	1:A:156:MET:HE2	1.92	0.52
1:C:264:THR:O	1:D:242:ARG:NH2	2.43	0.52
1:B:148:THR:HG21	1:B:156:MET:HE2	1.92	0.51
1:A:169:VAL:HG22	1:A:199:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG21	1:B:98:THR:HG21	1.92	0.50
1:D:153:THR:HG23	1:D:156:MET:H	1.76	0.50
1:C:148:THR:HG21	1:C:156:MET:HE2	1.93	0.50
1:B:169:VAL:HG22	1:B:199:LEU:HD11	1.94	0.49
1:C:169:VAL:HG22	1:C:199:LEU:HD11	1.94	0.49
1:B:29:THR:HG23	1:B:30:HIS:CD2	2.46	0.49
1:B:85:HIS:NE2	5:B:403:AKG:H32	2.28	0.49
1:C:330:THR:HG21	1:C:336:PHE:HB2	1.95	0.48
1:D:174:ASN:HB3	4:D:401:PLP:H2A1	1.96	0.48
1:B:330:THR:HG21	1:B:336:PHE:HB2	1.96	0.48
1:A:176:THR:HA	1:A:323:TYR:HB2	1.95	0.47
1:D:176:THR:HA	1:D:323:TYR:HB2	1.96	0.47
1:D:378:LEU:HD22	1:D:378:LEU:H	1.78	0.47
1:B:176:THR:HA	1:B:323:TYR:HB2	1.96	0.47
1:A:308:ILE:HG22	1:A:385:LEU:HD23	1.97	0.47
1:C:98:THR:HG21	1:D:98:THR:HG21	1.96	0.46
1:C:176:THR:HA	1:C:323:TYR:HB2	1.97	0.46
1:A:251:VAL:HG23	6:A:556:HOH:O	2.15	0.46
1:A:100:SER:OG	4:A:403:PLP:C5A	2.64	0.45
1:B:58:HIS:CD2	1:C:58:HIS:CE1	3.05	0.44
1:A:330:THR:HG21	1:A:336:PHE:HB2	1.98	0.44
1:B:120:MET:CE	1:B:128:TYR:HB2	2.48	0.43
1:A:123:PRO:HG3	1:A:323:TYR:CE2	2.54	0.42
1:B:209:VAL:HG11	1:B:216:THR:HG23	2.01	0.42
1:C:120:MET:CE	1:C:128:TYR:HB2	2.47	0.42
1:B:123:PRO:HG3	1:B:323:TYR:CE2	2.54	0.42
1:A:119:ALA:HB1	1:A:142:ILE:HD11	2.01	0.42
1:B:153:THR:H	1:B:156:MET:HE3	1.84	0.42
1:B:119:ALA:HB1	1:B:142:ILE:HD11	2.02	0.42
1:C:119:ALA:HB1	1:C:142:ILE:HD11	2.01	0.42
1:A:153:THR:H	1:A:156:MET:HE3	1.85	0.41
1:D:123:PRO:HG3	1:D:323:TYR:CE2	2.55	0.41
1:C:209:VAL:HG11	1:C:216:THR:HG23	2.01	0.41
1:C:333:SER:OG	1:C:360:GLY:C	2.64	0.41
1:D:125:TYR:HB2	4:D:401:PLP:H2A3	2.02	0.41
1:C:348:ILE:HG21	1:C:363:VAL:HG13	2.02	0.41
1:A:34:VAL:HG11	1:A:377:ALA:HB2	2.03	0.40
1:D:242:ARG:HH12	4:D:401:PLP:P	2.43	0.40
1:B:15:TYR:HB3	1:B:353:ASP:CG	2.47	0.40
1:C:333:SER:OG	1:C:360:GLY:O	2.38	0.40
1:A:153:THR:N	1:A:156:MET:HE3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:VAL:HB	1:D:247:LEU:HB2	2.03	0.40
1:C:123:PRO:HG3	1:C:323:TYR:CE2	2.57	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	392/394 (100%)	384 (98%)	8 (2%)	0	100	100
1	B	385/394 (98%)	378 (98%)	7 (2%)	0	100	100
1	C	380/394 (96%)	372 (98%)	8 (2%)	0	100	100
1	D	346/394 (88%)	334 (96%)	10 (3%)	2 (1%)	21	44
All	All	1503/1576 (95%)	1468 (98%)	33 (2%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	214	PRO
1	D	213	ALA

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	291/306 (95%)	283 (97%)	8 (3%)	39	69
1	B	286/306 (94%)	278 (97%)	8 (3%)	38	68
1	C	252/306 (82%)	246 (98%)	6 (2%)	43	72
1	D	178/306 (58%)	172 (97%)	6 (3%)	32	62
All	All	1007/1224 (82%)	979 (97%)	28 (3%)	37	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	68	LEU
1	A	141	GLU
1	A	216	THR
1	A	239	THR
1	A	313	LEU
1	A	331	SER
1	A	363	VAL
1	B	8	ARG
1	B	18	ASP
1	B	90	GLU
1	B	178	THR
1	B	211	GLN
1	B	239	THR
1	B	331	SER
1	B	363	VAL
1	C	8	ARG
1	C	68	LEU
1	C	183	GLU
1	C	211	GLN
1	C	239	THR
1	C	363	VAL
1	D	156	MET
1	D	178	THR
1	D	208	LEU
1	D	239	THR
1	D	242	ARG
1	D	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	130	ASN
1	A	225	ASN
1	A	262	ASN
1	A	388	GLN
1	B	30	HIS
1	B	130	ASN
1	B	155	GLN
1	B	262	ASN
1	C	58	HIS
1	C	130	ASN
1	C	215	GLN
1	C	225	ASN
1	C	262	ASN
1	C	297	ASN
1	D	40	GLN
1	D	130	ASN
1	D	262	ASN

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](#)

10 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	PLP	C	403	1	15,15,16	3.22	3 (20%)	21,22,23	1.63	5 (23%)
5	AKG	C	402	-	9,9,9	1.81	1 (11%)	11,11,11	1.69	3 (27%)
3	GOL	B	402	-	5,5,5	0.36	0	5,5,5	0.25	0
4	PLP	A	403	1	15,15,16	3.47	3 (20%)	21,22,23	2.57	9 (42%)
3	GOL	C	401	-	5,5,5	0.35	0	5,5,5	0.19	0
3	GOL	A	402	-	5,5,5	0.43	0	5,5,5	0.42	0
4	PLP	B	401	1	15,15,16	2.85	3 (20%)	21,22,23	2.04	8 (38%)
2	GLU	A	401	-	8,9,9	1.10	1 (12%)	8,11,11	1.17	1 (12%)
5	AKG	B	403	-	9,9,9	1.89	1 (11%)	11,11,11	1.34	2 (18%)
4	PLP	D	401	1	15,15,16	3.08	3 (20%)	21,22,23	1.68	5 (23%)

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	PLP	C	403	1	-	1/6/6/8	0/1/1/1
5	AKG	C	402	-	-	4/9/9/9	-
3	GOL	B	402	-	-	2/4/4/4	-
4	PLP	A	403	1	-	2/6/6/8	0/1/1/1
3	GOL	C	401	-	-	2/4/4/4	-
3	GOL	A	402	-	-	1/4/4/4	-
4	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	GLU	A	401	-	-	6/9/9/9	-
5	AKG	B	403	-	-	3/9/9/9	-
4	PLP	D	401	1	-	5/6/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	PLP	C3-C2	8.82	1.50	1.41
4	A	403	PLP	C5-C4	8.59	1.50	1.40
4	C	403	PLP	C3-C2	8.31	1.49	1.41
4	D	401	PLP	C3-C2	7.99	1.49	1.41
4	C	403	PLP	C5-C4	7.77	1.49	1.40
4	B	401	PLP	C3-C2	7.41	1.48	1.41
4	D	401	PLP	C5-C4	7.25	1.48	1.40
4	B	401	PLP	C5-C4	6.48	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	AKG	C2-C1	-4.78	1.46	1.53
4	A	403	PLP	C3-C4	4.63	1.48	1.40
5	C	402	AKG	C2-C1	-4.31	1.47	1.53
4	D	401	PLP	C3-C4	4.19	1.48	1.40
4	C	403	PLP	C3-C4	4.19	1.48	1.40
4	B	401	PLP	C3-C4	3.47	1.46	1.40
2	A	401	GLU	OXT-C	-2.25	1.23	1.30

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	PLP	O4P-C5A-C5	7.06	122.59	109.36
4	A	403	PLP	C5A-C5-C6	-5.26	110.79	119.36
4	B	401	PLP	C5A-C5-C4	-4.12	114.50	122.64
4	D	401	PLP	O4P-C5A-C5	3.98	116.81	109.36
4	B	401	PLP	C5A-C5-C6	3.66	125.33	119.36
4	A	403	PLP	C4A-C4-C5	3.48	124.53	120.94
5	C	402	AKG	C3-C2-C1	3.44	121.70	115.86
4	C	403	PLP	C6-C5-C4	3.35	120.84	118.10
4	D	401	PLP	C6-C5-C4	3.23	120.75	118.10
4	A	403	PLP	C5A-C5-C4	3.21	128.98	122.64
4	B	401	PLP	O4P-C5A-C5	3.20	115.35	109.36
4	C	403	PLP	C4A-C4-C5	3.01	124.04	120.94
4	C	403	PLP	O3P-P-O4P	-2.90	99.11	106.67
4	C	403	PLP	C3-C4-C5	-2.79	115.24	118.59
2	A	401	GLU	OXT-C-O	-2.64	118.08	124.08
4	A	403	PLP	C6-C5-C4	2.60	120.23	118.10
4	A	403	PLP	C3-C4-C5	-2.55	115.53	118.59
4	B	401	PLP	C6-C5-C4	2.54	120.17	118.10
5	C	402	AKG	O2-C1-C2	2.50	120.52	113.59
4	B	401	PLP	O3-C3-C2	2.47	122.70	117.58
4	B	401	PLP	O4P-P-O1P	-2.38	100.01	106.44
5	B	403	AKG	C3-C2-C1	2.38	119.90	115.86
4	C	403	PLP	O3-C3-C2	2.31	122.37	117.58
4	D	401	PLP	O3-C3-C2	2.22	122.19	117.58
4	A	403	PLP	O3-C3-C2	2.21	122.16	117.58
4	A	403	PLP	O4P-P-O1P	-2.19	100.51	106.44
5	C	402	AKG	O1-C1-C2	-2.19	119.08	121.81
4	B	401	PLP	C2A-C2-C3	-2.18	118.25	120.80
4	B	401	PLP	C2A-C2-N1	2.07	121.55	117.64
4	A	403	PLP	C2A-C2-C3	2.05	123.20	120.80
4	D	401	PLP	C4-C3-C2	-2.04	116.84	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	PLP	O4P-P-O1P	-2.03	100.95	106.44
5	B	403	AKG	O4-C5-C4	2.03	120.41	114.00

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GLU	C-CA-CB-CG
3	B	402	GOL	O1-C1-C2-O2
3	B	402	GOL	O1-C1-C2-C3
3	C	401	GOL	O1-C1-C2-C3
4	A	403	PLP	C4-C5-C5A-O4P
4	A	403	PLP	C6-C5-C5A-O4P
4	D	401	PLP	C4-C5-C5A-O4P
4	D	401	PLP	C6-C5-C5A-O4P
4	D	401	PLP	C5A-O4P-P-O2P
4	D	401	PLP	C5A-O4P-P-O3P
5	B	403	AKG	O1-C1-C2-O5
5	B	403	AKG	O1-C1-C2-C3
5	B	403	AKG	O2-C1-C2-C3
3	A	402	GOL	O1-C1-C2-C3
3	C	401	GOL	O1-C1-C2-O2
4	D	401	PLP	C5A-O4P-P-O1P
5	C	402	AKG	C1-C2-C3-C4
2	A	401	GLU	N-CA-CB-CG
2	A	401	GLU	CA-CB-CG-CD
5	C	402	AKG	O2-C1-C2-O5
4	C	403	PLP	C5A-O4P-P-O1P
2	A	401	GLU	OE2-CD-CG-CB
5	C	402	AKG	C3-C4-C5-O3
5	C	402	AKG	C3-C4-C5-O4
2	A	401	GLU	OE1-CD-CG-CB
2	A	401	GLU	OXT-C-CA-CB

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	PLP	1	0
4	A	403	PLP	2	0
4	B	401	PLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GLU	3	0
5	B	403	AKG	1	0
4	D	401	PLP	8	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	394/394 (100%)	0.19	8 (2%) 65 62	28, 43, 70, 97	0
1	B	387/394 (98%)	0.21	12 (3%) 51 48	29, 42, 72, 118	0
1	C	384/394 (97%)	0.82	44 (11%) 9 8	33, 63, 95, 116	0
1	D	364/394 (92%)	1.50	119 (32%) 1 1	36, 84, 112, 124	0
All	All	1529/1576 (97%)	0.66	183 (11%) 9 7	28, 49, 103, 124	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	5.5
1	B	14	PHE	5.5
1	D	317	ASP	5.3
1	B	13	PRO	4.9
1	B	20	TRP	4.7
1	C	14	PHE	4.6
1	D	379	ARG	4.4
1	D	209	VAL	4.3
1	A	20	TRP	4.1
1	D	27	GLN	4.1
1	D	31	GLY	4.1
1	D	360	GLY	4.1
1	D	168	VAL	4.0
1	C	119	ALA	3.9
1	D	180	ILE	3.8
1	D	321	TYR	3.8
1	D	348	ILE	3.8
1	A	14	PHE	3.8
1	D	148	THR	3.7
1	C	11	VAL	3.7
1	D	312	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	12	PRO	3.6
1	D	14	PHE	3.5
1	D	142	ILE	3.5
1	A	18	ASP	3.5
1	C	86	GLY	3.5
1	D	310	ILE	3.4
1	D	152	PRO	3.3
1	D	176	THR	3.3
1	D	315	PRO	3.3
1	D	316	THR	3.3
1	D	169	VAL	3.3
1	B	15	TYR	3.2
1	D	149	ARG	3.2
1	D	190	SER	3.2
1	D	333	SER	3.2
1	B	16	VAL	3.2
1	D	303	ASP	3.2
1	A	21	LEU	3.2
1	D	186	ALA	3.2
1	D	371	SER	3.1
1	D	162	PRO	3.1
1	D	120	MET	3.1
1	D	177	GLY	3.1
1	D	307	ARG	3.1
1	C	29	THR	3.1
1	D	344	THR	3.1
1	A	17	MET	3.1
1	D	119	ALA	3.0
1	D	201	SER	3.0
1	C	18	ASP	3.0
1	D	377	ALA	3.0
1	D	179	VAL	3.0
1	D	164	LEU	3.0
1	B	19	VAL	3.0
1	D	141	GLU	2.9
1	D	26	ARG	2.9
1	D	319	ALA	2.9
1	D	362	PHE	2.9
1	C	191	TRP	2.9
1	D	358	ARG	2.9
1	D	197	VAL	2.9
1	D	326	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	185	LEU	2.9
1	B	2	THR	2.9
1	D	37	SER	2.9
1	D	192	CYS	2.8
1	D	330	THR	2.8
1	D	17	MET	2.8
1	D	3	ASP	2.8
1	C	128	TYR	2.8
1	D	170	ALA	2.8
1	D	219	ALA	2.8
1	D	89	VAL	2.8
1	C	4	ARG	2.8
1	D	306	ARG	2.8
1	D	217	SER	2.8
1	D	234	LYS	2.8
1	C	304	GLY	2.8
1	D	33	LEU	2.8
1	D	314	ALA	2.8
1	C	34	VAL	2.7
1	D	356	THR	2.7
1	D	125	TYR	2.7
1	D	222	THR	2.7
1	D	143	PRO	2.7
1	D	214	PRO	2.7
1	C	140	VAL	2.7
1	D	173	ALA	2.7
1	D	172	PRO	2.7
1	D	188	ILE	2.7
1	D	161	ASP	2.7
1	D	372	GLY	2.6
1	C	329	PHE	2.6
1	D	213	ALA	2.6
1	C	17	MET	2.6
1	D	151	GLN	2.6
1	C	20	TRP	2.6
1	D	275	ALA	2.6
1	D	365	ILE	2.5
1	D	224	ARG	2.5
1	D	128	TYR	2.5
1	C	322	VAL	2.5
1	D	144	CYS	2.5
1	D	292	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	323	TYR	2.5
1	C	164	LEU	2.5
1	D	20	TRP	2.5
1	B	18	ASP	2.4
1	C	3	ASP	2.4
1	B	17	MET	2.4
1	D	363	VAL	2.4
1	D	226	ALA	2.4
1	D	212	GLY	2.4
1	A	15	TYR	2.4
1	D	19	VAL	2.4
1	C	9	ALA	2.4
1	D	199	LEU	2.4
1	D	191	TRP	2.4
1	D	13	PRO	2.4
1	D	150	PHE	2.4
1	D	336	PHE	2.4
1	D	196	ASP	2.4
1	D	325	ASP	2.4
1	D	146	PRO	2.4
1	D	357	ALA	2.4
1	B	21	LEU	2.3
1	D	250	THR	2.3
1	C	111	CYS	2.3
1	D	11	VAL	2.3
1	D	34	VAL	2.3
1	B	22	ALA	2.3
1	C	361	SER	2.3
1	D	215	GLN	2.3
1	D	345	GLY	2.3
1	C	334	LEU	2.3
1	C	378	LEU	2.3
1	D	341	LEU	2.3
1	D	247	LEU	2.3
1	D	374	ILE	2.3
1	D	153	THR	2.3
1	D	294	TYR	2.3
1	C	13	PRO	2.3
1	D	171	SER	2.3
1	C	155	GLN	2.3
1	D	87	ILE	2.2
1	C	224	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	225	ASN	2.2
1	D	297	ASN	2.2
1	D	181	PRO	2.2
1	C	261	GLY	2.2
1	D	300	LEU	2.2
1	C	180	ILE	2.2
1	C	379	ARG	2.2
1	C	163	PRO	2.2
1	C	387	SER	2.2
1	D	373	ASP	2.2
1	C	335	ALA	2.2
1	C	148	THR	2.2
1	D	301	LEU	2.2
1	B	12	PRO	2.1
1	C	308	ILE	2.1
1	C	326	VAL	2.1
1	C	332	ASP	2.1
1	C	320	PHE	2.1
1	C	85	HIS	2.1
1	C	167	VAL	2.1
1	D	184	GLU	2.1
1	D	123	PRO	2.1
1	D	81	TYR	2.1
1	C	357	ALA	2.1
1	C	358	ARG	2.1
1	D	154	ALA	2.1
1	C	12	PRO	2.1
1	D	107	ALA	2.0
1	D	88	THR	2.0
1	D	208	LEU	2.0
1	D	85	HIS	2.0
1	C	207	GLY	2.0
1	A	83	ARG	2.0
1	D	25	GLU	2.0
1	D	126	PRO	2.0
1	C	309	GLY	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 [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
5	AKG	B	403	10/10	0.70	0.18	70,72,73,74	0
3	GOL	C	401	6/6	0.76	0.18	61,63,65,66	0
2	GLU	A	401	10/10	0.83	0.19	60,64,71,72	0
3	GOL	B	402	6/6	0.85	0.16	63,65,65,66	0
5	AKG	C	402	10/10	0.85	0.15	67,73,78,81	0
3	GOL	A	402	6/6	0.89	0.13	51,56,58,58	0
4	PLP	D	401	15/16	0.89	0.14	59,76,79,82	0
4	PLP	C	403	15/16	0.92	0.12	50,59,63,65	0
4	PLP	B	401	15/16	0.93	0.13	43,54,57,58	1
4	PLP	A	403	15/16	0.95	0.11	40,50,55,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.