Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 11:23 PM EDT

PDB ID	:	2NMP
Title	:	Crystal structure of human Cystathionine gamma lyase
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Deposited on	:	2006-10-23
Resolution	:	2.60 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:

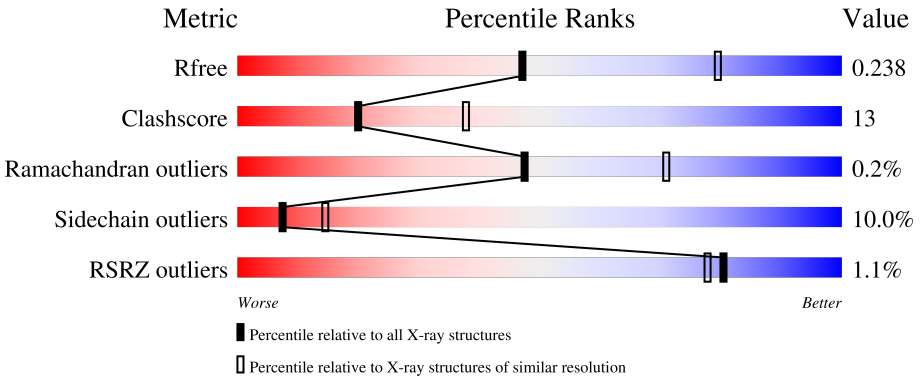
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	403	70% 19% • 7%
1	B	403	2% 68% 20% 5% 7%
1	C	403	% 71% 23% • •

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
1	D	403	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	D	500	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12048 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.

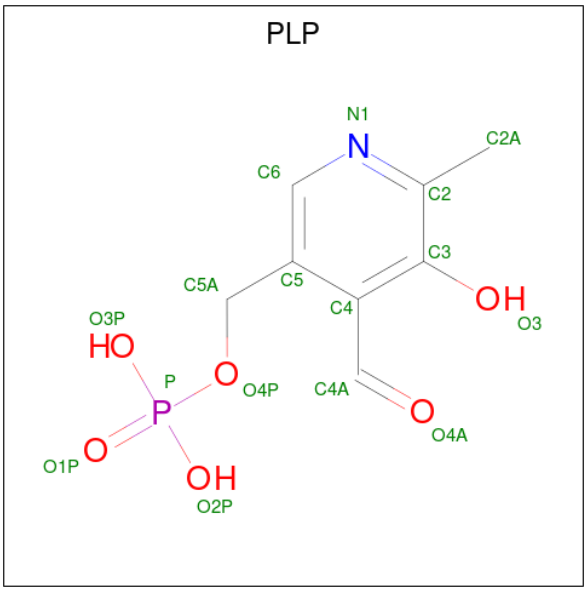
- Molecule 1 is a protein called Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2914	1860	497	538	19			
1	B	376	Total	C	N	O	S	0	0	0
			2906	1856	494	538	18			
1	C	390	Total	C	N	O	S	0	0	0
			3015	1922	515	559	19			
1	D	390	Total	C	N	O	S	0	0	0
			3011	1917	515	560	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P32929
B	0	SER	-	expression tag	UNP P32929
C	0	SER	-	expression tag	UNP P32929
D	0	SER	-	expression tag	UNP P32929

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 3 is water.

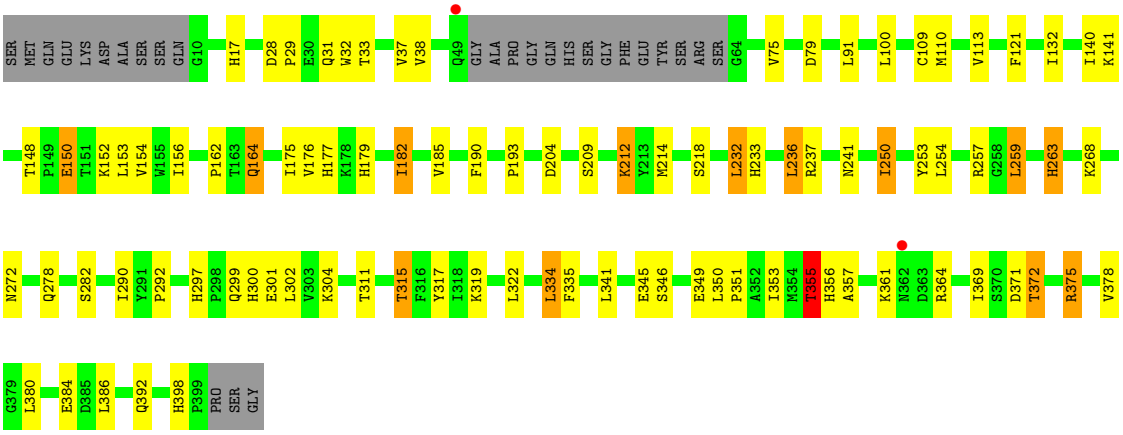
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	42	Total O 42 42	0	0
3	B	28	Total O 28 28	0	0
3	C	42	Total O 42 42	0	0
3	D	45	Total O 45 45	0	0

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.

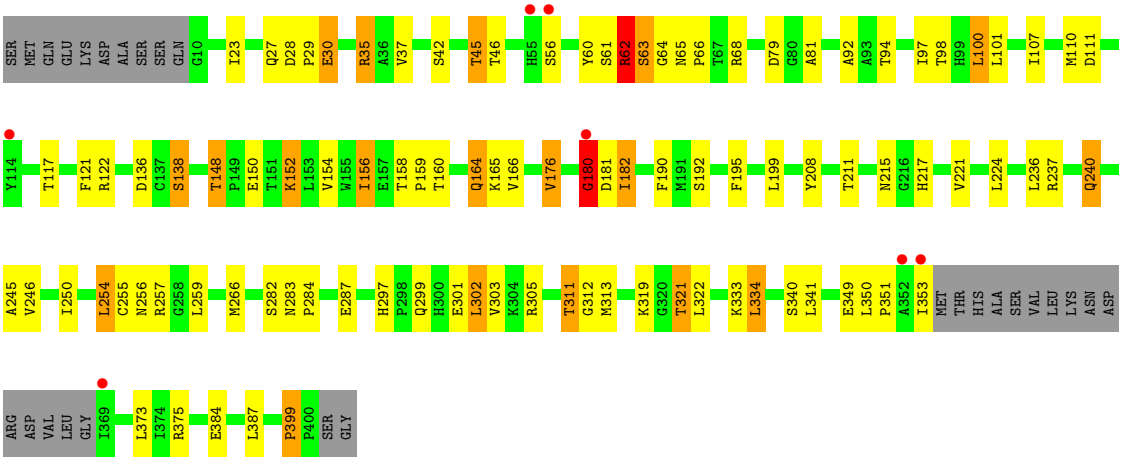
• Molecule 1: Cystathionine gamma-lyase

Chain A:



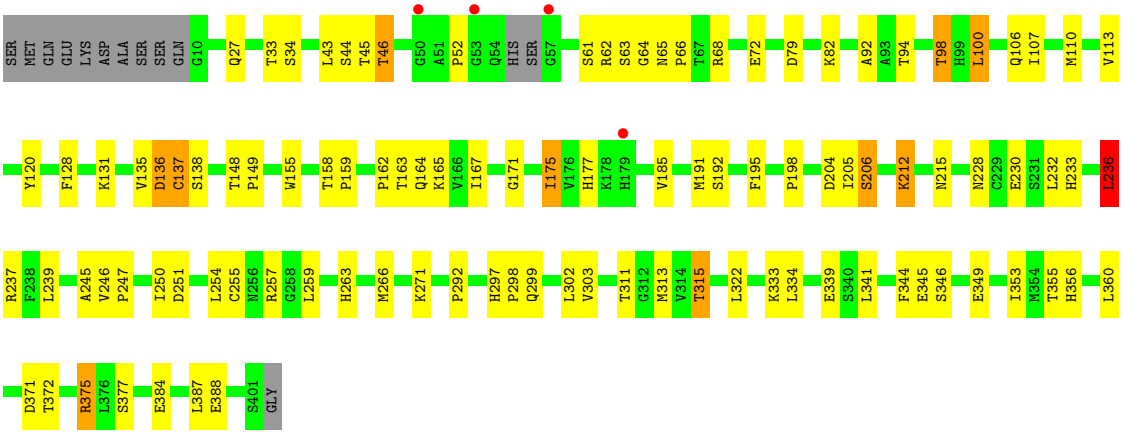
• Molecule 1: Cystathionine gamma-lyase

Chain B:



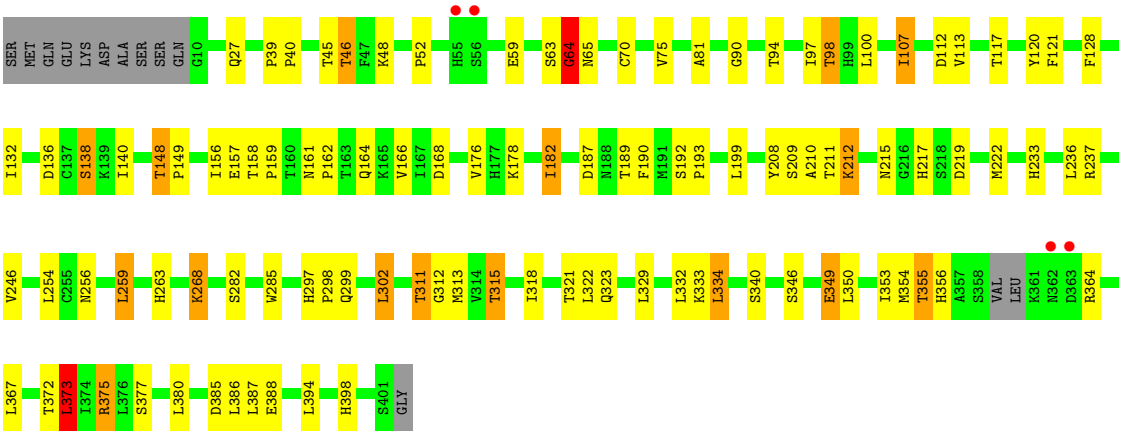
• Molecule 1: Cystathionine gamma-lyase

Chain C:



• Molecule 1: Cystathionine gamma-lyase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.78Å 107.57Å 153.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.60) 100.0 (19.93-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.245 0.172 , 0.238	Depositor DCC
R_{free} test set	2718 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12048	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.70	1/2978 (0.0%)	0.75	0/4041
1	B	0.69	1/2973 (0.0%)	0.78	6/4035 (0.1%)
1	C	0.70	1/3083 (0.0%)	0.78	2/4183 (0.0%)
1	D	0.72	1/3079 (0.0%)	0.80	2/4177 (0.0%)
All	All	0.70	4/12113 (0.0%)	0.78	10/16436 (0.1%)

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	A	0	1
1	B	0	3
1	C	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	GLU	CG-CD	7.11	1.62	1.51
1	D	70	CYS	CB-SG	-6.13	1.71	1.82
1	B	384	GLU	CG-CD	5.89	1.60	1.51
1	C	388	GLU	CG-CD	5.83	1.60	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	399	PRO	C-N-CD	-7.49	104.12	120.60
1	B	181	ASP	N-CA-C	-6.38	93.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	180	GLY	N-CA-C	-6.21	97.59	113.10
1	B	399	PRO	C-N-CA	5.64	145.71	122.00
1	B	254	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	236	LEU	CA-CB-CG	5.57	128.10	115.30
1	D	373	LEU	CA-CB-CG	5.43	127.79	115.30
1	D	64	GLY	N-CA-C	5.41	126.64	113.10
1	B	254	LEU	CB-CG-CD1	5.34	120.08	111.00
1	C	100	LEU	CA-CB-CG	5.24	127.34	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	HIS	Peptide
1	B	180	GLY	Peptide
1	B	399	PRO	Peptide
1	B	62	ARG	Peptide
1	C	136	ASP	Peptide

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	2914	0	2921	67	0
1	B	2906	0	2895	80	0
1	C	3015	0	3009	84	0
1	D	3011	0	2996	90	0
2	A	15	0	6	2	0
2	C	15	0	6	2	0
2	D	15	0	6	7	0
3	A	42	0	0	2	0
3	B	28	0	0	2	0
3	C	42	0	0	0	0
3	D	45	0	0	1	0
All	All	12048	0	11839	296	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 13.

All (296) 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:212:LYS:HZ2	2:A:500:PLP:C4A	1.51	1.18
1:A:355:THR:HG23	1:A:356:HIS:CD2	1.79	1.18
1:D:176:VAL:HG13	1:D:182:ILE:CD1	1.76	1.14
1:D:375:ARG:HH11	1:D:375:ARG:HG2	1.14	1.12
1:A:176:VAL:CG1	1:A:182:ILE:HD12	1.78	1.11
1:A:176:VAL:HG13	1:A:182:ILE:HD12	1.32	1.10
1:C:375:ARG:HG2	1:C:375:ARG:HH11	0.99	1.09
1:A:375:ARG:HG2	1:A:375:ARG:HH11	1.16	1.09
1:C:212:LYS:HZ2	2:C:500:PLP:C4A	1.59	1.08
1:A:355:THR:HG23	1:A:356:HIS:HD2	0.90	1.06
1:B:63:SER:H	1:B:64:GLY:HA2	1.21	1.05
1:B:60:TYR:O	1:B:63:SER:HB2	1.62	0.99
1:A:355:THR:CG2	1:A:356:HIS:HD2	1.76	0.98
1:B:148:THR:HG22	1:B:150:GLU:H	1.31	0.95
1:A:212:LYS:HZ1	2:A:500:PLP:C4A	1.75	0.93
1:B:215:ASN:HD21	1:C:257:ARG:HH22	1.17	0.93
1:D:349:GLU:OE2	1:D:355:THR:HB	1.69	0.92
1:C:212:LYS:HZ1	2:C:500:PLP:C4A	1.74	0.92
1:A:176:VAL:CG1	1:A:182:ILE:CD1	2.49	0.90
1:C:355:THR:HG23	1:C:356:HIS:ND1	1.86	0.89
1:B:257:ARG:HH22	1:C:215:ASN:HD21	1.14	0.89
1:C:98:THR:HG21	1:C:120:TYR:HE2	1.38	0.88
1:C:375:ARG:HG2	1:C:375:ARG:NH1	1.80	0.88
1:B:375:ARG:HH11	1:B:375:ARG:HG2	1.36	0.87
1:B:63:SER:H	1:B:64:GLY:CA	1.85	0.87
1:B:215:ASN:O	1:B:217:HIS:HD2	1.58	0.87
1:D:148:THR:HG22	1:D:149:PRO:HD2	1.56	0.84
1:A:349:GLU:OE2	1:A:355:THR:HB	1.78	0.83
1:A:176:VAL:HG11	1:A:182:ILE:CD1	2.06	0.83
1:B:63:SER:N	1:B:64:GLY:HA2	1.95	0.80
1:D:282:SER:HB2	3:D:517:HOH:O	1.82	0.80
1:D:375:ARG:HG2	1:D:375:ARG:NH1	1.92	0.80
1:C:339:GLU:O	1:D:46:THR:HG21	1.83	0.79
1:B:176:VAL:HG13	1:B:182:ILE:HG12	1.65	0.79
1:D:176:VAL:HG13	1:D:182:ILE:HD12	1.63	0.78
1:D:176:VAL:HG13	1:D:182:ILE:HD13	1.66	0.78
1:D:97:ILE:O	1:D:100:LEU:HB2	1.83	0.77
1:A:148:THR:HG22	1:A:150:GLU:H	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD12	1:A:386:LEU:HD23	1.67	0.76
1:C:164:GLN:HE21	1:C:315:THR:CG2	1.97	0.76
1:D:176:VAL:CG1	1:D:182:ILE:CD1	2.61	0.76
1:C:162:PRO:O	1:C:315:THR:HG21	1.85	0.76
1:D:94:THR:O	1:D:98:THR:HG23	1.85	0.76
1:B:97:ILE:O	1:B:100:LEU:HB2	1.86	0.76
1:A:154:VAL:HG23	1:A:182:ILE:HD11	1.69	0.75
1:C:171:GLY:O	1:C:175:ILE:HG23	1.87	0.75
1:C:110:MET:SD	1:C:137:CYS:HB3	2.28	0.74
1:A:349:GLU:OE1	1:A:355:THR:HG21	1.88	0.74
1:B:62:ARG:HG2	1:B:62:ARG:HH11	1.53	0.74
1:D:27:GLN:HE22	1:D:256:ASN:ND2	1.86	0.73
1:A:375:ARG:HG2	1:A:375:ARG:NH1	1.94	0.73
1:C:353:ILE:HD11	1:D:52:PRO:HB2	1.69	0.72
1:D:212:LYS:HZ2	2:D:500:PLP:C4A	2.03	0.71
1:B:136:ASP:OD2	1:B:138:SER:HB2	1.91	0.70
1:A:349:GLU:OE1	1:A:355:THR:CG2	2.40	0.69
1:C:311:THR:HG23	1:C:313:MET:H	1.57	0.69
1:D:212:LYS:HZ1	2:D:500:PLP:C4A	2.03	0.69
1:A:334:LEU:CD1	1:A:386:LEU:HD23	2.22	0.69
1:A:350:LEU:HD23	1:A:353:ILE:HD12	1.76	0.68
1:C:375:ARG:HH11	1:C:375:ARG:CG	1.90	0.67
1:A:190:PHE:O	1:A:311:THR:HG21	1.93	0.67
1:A:257:ARG:HH22	1:D:215:ASN:HD21	1.39	0.67
1:C:98:THR:HG21	1:C:120:TYR:CE2	2.27	0.67
1:C:68:ARG:HH11	1:C:246:VAL:CG2	2.06	0.67
1:B:110:MET:HG3	1:B:156:ILE:HA	1.75	0.67
1:B:237:ARG:HH11	1:B:240:GLN:HE22	1.41	0.66
1:C:135:VAL:O	1:C:137:CYS:HB2	1.95	0.66
1:B:311:THR:HG23	1:B:312:GLY:N	2.11	0.65
1:C:212:LYS:HD2	1:C:212:LYS:N	2.11	0.65
1:C:233:HIS:HE1	1:C:237:ARG:HH11	1.45	0.65
1:D:215:ASN:O	1:D:217:HIS:HD2	1.79	0.65
1:A:357:ALA:HA	1:A:364:ARG:HH21	1.61	0.64
1:D:297:HIS:HD2	1:D:299:GLN:H	1.46	0.64
1:B:60:TYR:O	1:B:63:SER:CB	2.43	0.64
1:B:94:THR:O	1:B:98:THR:HG23	1.97	0.64
2:D:500:PLP:C4A	2:D:500:PLP:O4P	2.46	0.64
1:C:344:PHE:HD2	1:C:345:GLU:HG3	1.61	0.64
1:A:297:HIS:HD2	1:A:299:GLN:H	1.44	0.63
1:B:311:THR:CG2	1:B:313:MET:H	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ASP:OD1	1:D:138:SER:HB3	1.99	0.63
1:C:45:THR:HA	1:C:61:SER:HB2	1.81	0.62
1:D:176:VAL:CG1	1:D:182:ILE:HD13	2.29	0.62
1:C:164:GLN:HE21	1:C:315:THR:HG22	1.64	0.62
1:A:91:LEU:HD12	1:B:62:ARG:CZ	2.30	0.62
1:B:81:ALA:HB2	1:B:199:LEU:CD1	2.29	0.61
1:D:321:THR:CG2	1:D:322:LEU:N	2.64	0.61
1:A:398:HIS:HE1	3:A:536:HOH:O	1.83	0.61
1:B:98:THR:HG21	1:B:121:PHE:HE1	1.65	0.61
1:C:52:PRO:HB2	1:D:353:ILE:HD11	1.82	0.61
1:C:68:ARG:HH11	1:C:246:VAL:HG21	1.63	0.61
1:C:246:VAL:HG23	1:C:247:PRO:HD2	1.83	0.60
1:C:212:LYS:HG3	1:C:341:LEU:HG	1.82	0.60
1:B:375:ARG:HG2	1:B:375:ARG:NH1	2.08	0.60
1:A:162:PRO:O	1:A:315:THR:HG21	2.01	0.60
1:B:148:THR:HG22	1:B:150:GLU:N	2.11	0.60
1:B:180:GLY:O	1:B:182:ILE:HG23	2.02	0.60
1:D:27:GLN:HE22	1:D:256:ASN:HD21	1.49	0.60
1:B:311:THR:HG23	1:B:313:MET:H	1.67	0.59
1:D:107:ILE:CD1	1:D:132:ILE:HG23	2.32	0.59
1:C:46:THR:HG21	1:D:340:SER:H	1.67	0.59
1:C:52:PRO:HB3	1:D:354:MET:HE2	1.83	0.59
1:A:193:PRO:HD3	1:A:214:MET:SD	2.42	0.59
1:A:364:ARG:HB3	1:A:369:ILE:HB	1.85	0.59
1:B:62:ARG:HH11	1:B:62:ARG:CG	2.16	0.59
1:B:154:VAL:HG23	1:B:182:ILE:CD1	2.32	0.59
1:C:297:HIS:HD2	1:C:299:GLN:H	1.50	0.58
1:D:350:LEU:H	1:D:354:MET:HE1	1.68	0.57
1:C:68:ARG:NH1	1:C:246:VAL:HG21	2.19	0.57
1:D:107:ILE:HD12	1:D:132:ILE:HD12	1.85	0.57
1:D:321:THR:HG22	1:D:323:GLN:H	1.70	0.57
1:B:176:VAL:HG13	1:B:182:ILE:CG1	2.34	0.56
1:D:321:THR:HG22	1:D:322:LEU:N	2.21	0.56
1:D:176:VAL:HG13	1:D:182:ILE:HD11	1.82	0.56
1:B:237:ARG:HH11	1:B:240:GLN:NE2	2.04	0.55
1:C:164:GLN:HE21	1:C:315:THR:HG23	1.68	0.55
3:A:509:HOH:O	1:D:217:HIS:HE1	1.90	0.55
1:B:257:ARG:NH2	1:C:215:ASN:HD21	1.93	0.55
1:C:163:THR:HG22	1:C:165:LYS:HG3	1.89	0.55
1:A:153:LEU:HD11	1:A:185:VAL:HG23	1.87	0.55
1:D:63:SER:N	1:D:64:GLY:HA3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:OG1	1:B:221:VAL:HA	2.07	0.55
1:B:321:THR:HG22	1:B:322:LEU:H	1.71	0.55
1:C:98:THR:CG2	1:C:120:TYR:HE2	2.16	0.55
1:B:215:ASN:O	1:B:217:HIS:CD2	2.49	0.54
1:C:344:PHE:CD2	1:C:345:GLU:HG3	2.42	0.54
1:C:63:SER:N	1:C:64:GLY:HA2	2.22	0.54
1:D:162:PRO:O	1:D:315:THR:HG21	2.08	0.54
1:C:191:MET:HE3	1:C:195:PHE:HB3	1.88	0.54
1:C:43:LEU:HD21	1:C:250:ILE:HG12	1.90	0.54
1:D:297:HIS:CD2	1:D:299:GLN:H	2.25	0.54
1:A:218:SER:O	1:B:45:THR:HB	2.08	0.53
1:A:100:LEU:HD21	1:A:236:LEU:HD13	1.89	0.53
1:C:155:TRP:CZ3	1:C:185:VAL:HG11	2.43	0.53
1:C:292:PRO:HB3	1:C:303:VAL:HG21	1.91	0.53
1:A:91:LEU:HD12	1:B:62:ARG:NE	2.25	0.52
1:A:322:LEU:HB2	1:A:371:ASP:HB3	1.92	0.52
1:C:322:LEU:HB2	1:C:371:ASP:HB3	1.90	0.52
1:D:233:HIS:HE1	1:D:237:ARG:HH11	1.58	0.52
1:D:373:LEU:C	1:D:373:LEU:HD12	2.31	0.51
1:D:329:LEU:HA	1:D:332:LEU:HD12	1.92	0.51
1:C:72:GLU:OE1	1:C:237:ARG:NH2	2.38	0.51
1:A:164:GLN:HG2	1:A:292:PRO:HD3	1.93	0.51
1:A:212:LYS:HG3	1:A:341:LEU:HG	1.92	0.51
1:B:158:THR:HA	1:B:159:PRO:C	2.30	0.51
1:D:311:THR:HG23	1:D:312:GLY:N	2.26	0.51
1:A:297:HIS:CD2	1:A:299:GLN:H	2.26	0.50
1:C:92:ALA:HB1	1:C:245:ALA:HB1	1.93	0.50
1:B:301:GLU:O	1:B:305:ARG:HG3	2.11	0.50
1:C:263:HIS:H	1:C:263:HIS:CD2	2.28	0.50
1:D:148:THR:CG2	1:D:149:PRO:HD2	2.36	0.50
1:A:263:HIS:H	1:A:263:HIS:CD2	2.30	0.50
1:C:353:ILE:HD11	1:D:52:PRO:CB	2.39	0.50
1:D:187:ASP:OD2	2:D:500:PLP:N1	2.45	0.50
1:C:68:ARG:NH1	1:C:246:VAL:CG2	2.73	0.50
1:A:109:CYS:SG	1:A:113:VAL:HG11	2.52	0.49
1:B:92:ALA:HB1	1:B:245:ALA:HB1	1.93	0.49
1:B:160:THR:O	1:B:164:GLN:HA	2.13	0.49
1:B:215:ASN:HD22	1:B:255:CYS:HA	1.76	0.49
1:A:140:ILE:HD12	1:A:140:ILE:H	1.77	0.49
1:B:28:ASP:OD1	1:B:30:GLU:HB2	2.12	0.49
1:B:65:ASN:ND2	3:B:405:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:HIS:HE1	1:A:204:ASP:OD2	1.96	0.49
1:D:107:ILE:HD13	1:D:107:ILE:O	2.13	0.49
1:B:154:VAL:HG23	1:B:182:ILE:HD11	1.94	0.48
1:C:136:ASP:HA	1:C:137:CYS:HB2	1.95	0.48
1:D:81:ALA:HB2	1:D:199:LEU:CD1	2.43	0.48
1:A:232:LEU:HD12	1:A:236:LEU:HD22	1.95	0.48
1:C:185:VAL:HG22	1:C:205:ILE:HB	1.95	0.48
1:C:106:GLN:HG2	1:C:107:ILE:N	2.28	0.48
1:D:268:LYS:HB3	1:D:380:LEU:HD22	1.95	0.48
1:A:317:TYR:HD2	1:A:372:THR:HG22	1.77	0.48
1:C:68:ARG:HH11	1:C:246:VAL:HG23	1.79	0.48
1:B:299:GLN:O	1:B:303:VAL:HG23	2.14	0.48
1:B:257:ARG:HH22	1:C:215:ASN:ND2	1.97	0.47
1:D:90:GLY:HA3	2:D:500:PLP:H5A2	1.96	0.47
1:A:351:PRO:HA	1:A:355:THR:HG22	1.96	0.47
1:B:166:VAL:HG12	1:B:302:LEU:HD13	1.96	0.47
1:C:215:ASN:HD22	1:C:255:CYS:HA	1.78	0.47
1:B:311:THR:CG2	1:B:312:GLY:N	2.77	0.47
1:D:373:LEU:C	1:D:373:LEU:CD1	2.82	0.47
1:B:65:ASN:ND2	1:B:68:ARG:H	2.12	0.47
1:C:346:SER:HA	1:C:377:SER:O	2.15	0.47
1:C:195:PHE:CE1	1:C:266:MET:HB3	2.50	0.46
1:B:45:THR:HA	1:B:61:SER:HB2	1.96	0.46
1:D:157:GLU:HG3	1:D:187:ASP:HB3	1.97	0.46
1:D:318:ILE:O	1:D:372:THR:HG23	2.16	0.46
1:A:375:ARG:HH11	1:A:375:ARG:CG	2.05	0.46
1:D:121:PHE:O	1:D:132:ILE:HG13	2.15	0.46
1:C:65:ASN:ND2	1:C:68:ARG:H	2.13	0.46
1:C:297:HIS:CD2	1:C:299:GLN:H	2.31	0.46
1:D:349:GLU:CD	1:D:355:THR:HB	2.33	0.46
1:A:257:ARG:NH2	1:D:215:ASN:HD21	2.12	0.46
1:B:29:PRO:O	1:B:35:ARG:HA	2.16	0.46
1:A:176:VAL:HG11	1:A:182:ILE:HD13	1.92	0.46
1:A:233:HIS:HE1	1:A:237:ARG:HH11	1.63	0.46
1:D:112:ASP:HB2	1:D:367:LEU:HD22	1.98	0.46
1:B:190:PHE:HE2	1:B:341:LEU:HD21	1.81	0.45
1:B:23:ILE:CG2	1:C:345:GLU:HG2	2.47	0.45
1:B:190:PHE:CE2	1:B:341:LEU:HD11	2.51	0.45
1:C:65:ASN:HB2	1:C:66:PRO:CD	2.46	0.45
1:C:158:THR:HA	1:C:159:PRO:C	2.35	0.45
1:D:233:HIS:HE1	1:D:237:ARG:NH1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PRO:HG2	1:D:48:LYS:HD2	1.99	0.45
1:D:148:THR:HG22	1:D:149:PRO:CD	2.39	0.45
1:A:153:LEU:HD11	1:A:185:VAL:CG2	2.46	0.45
1:A:268:LYS:HB3	1:A:380:LEU:HD22	1.99	0.45
1:B:79:ASP:OD1	1:B:208:TYR:OH	2.34	0.45
1:D:297:HIS:HD2	1:D:299:GLN:N	2.12	0.45
1:A:28:ASP:HA	1:A:29:PRO:HD3	1.79	0.45
1:D:346:SER:HA	1:D:377:SER:O	2.17	0.45
1:D:375:ARG:NH1	1:D:375:ARG:CG	2.70	0.45
1:A:154:VAL:CG2	1:A:182:ILE:HD11	2.43	0.44
1:A:263:HIS:CD2	1:A:263:HIS:N	2.85	0.44
1:B:340:SER:O	1:B:341:LEU:HB3	2.18	0.44
1:A:154:VAL:HG23	1:A:182:ILE:CD1	2.44	0.44
1:B:287:GLU:HG2	1:B:319:LYS:HG2	1.98	0.44
1:C:232:LEU:O	1:C:236:LEU:HB2	2.18	0.44
1:D:209:SER:HB2	2:D:500:PLP:C5	2.47	0.44
1:B:215:ASN:HD21	1:C:257:ARG:NH2	1.99	0.44
1:D:161:ASN:HB2	1:D:190:PHE:CZ	2.53	0.44
1:A:121:PHE:HB3	1:A:132:ILE:HG21	1.99	0.44
1:C:138:SER:HA	1:C:167:ILE:HG13	2.00	0.44
1:A:75:VAL:HG22	1:A:259:LEU:HD21	2.00	0.43
1:C:82:LYS:H	1:C:228:ASN:ND2	2.16	0.43
1:A:38:VAL:HB	1:C:44:SER:HB3	2.00	0.43
1:B:27:GLN:HE22	1:B:256:ASN:HD21	1.66	0.43
1:B:62:ARG:CG	1:B:62:ARG:NH1	2.79	0.43
1:C:82:LYS:H	1:C:228:ASN:HD22	1.66	0.43
1:C:128:PHE:HB3	1:D:128:PHE:HB3	2.00	0.43
1:C:177:HIS:HE1	1:C:204:ASP:OD2	2.01	0.43
1:D:75:VAL:HG22	1:D:259:LEU:HD21	2.01	0.43
1:D:298:PRO:HB2	1:D:299:GLN:NE2	2.34	0.43
1:B:283:ASN:HA	1:B:284:PRO:HD3	1.84	0.43
1:D:182:ILE:HD13	1:D:182:ILE:C	2.38	0.43
1:C:339:GLU:C	1:D:46:THR:HG21	2.37	0.43
1:A:164:GLN:HB3	1:A:290:ILE:HG22	2.00	0.43
1:B:65:ASN:HB2	1:B:66:PRO:HD2	2.00	0.43
1:D:285:TRP:CD1	1:D:394:LEU:HB3	2.53	0.43
1:C:43:LEU:HB3	1:D:219:ASP:HB2	2.01	0.43
1:C:94:THR:O	1:C:98:THR:HG22	2.18	0.43
1:C:62:ARG:HG3	1:C:246:VAL:HG11	2.01	0.43
1:C:136:ASP:CA	1:C:137:CYS:HB2	2.49	0.43
1:A:28:ASP:O	1:A:31:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ASP:OD2	1:B:138:SER:CB	2.64	0.43
1:C:198:PRO:HG2	1:C:206:SER:HB2	2.01	0.43
1:D:98:THR:HG21	1:D:120:TYR:HE2	1.83	0.43
1:C:43:LEU:HD23	1:C:43:LEU:HA	1.78	0.42
1:D:158:THR:HA	1:D:159:PRO:C	2.39	0.42
1:D:398:HIS:O	1:D:398:HIS:CD2	2.72	0.42
1:A:272:ASN:HB3	1:A:378:VAL:HG11	2.01	0.42
1:B:148:THR:CG2	1:B:150:GLU:H	2.16	0.42
1:B:297:HIS:CD2	1:B:299:GLN:H	2.37	0.42
1:B:350:LEU:HD12	1:B:373:LEU:O	2.18	0.42
1:D:140:ILE:HD11	1:D:168:ASP:HB3	2.01	0.42
1:D:318:ILE:O	1:D:372:THR:CG2	2.68	0.42
1:A:350:LEU:CD2	1:A:353:ILE:HD12	2.47	0.42
1:B:349:GLU:O	1:B:351:PRO:HD3	2.18	0.42
1:D:189:THR:HB	2:D:500:PLP:H2A2	2.02	0.42
1:B:311:THR:HG22	1:B:313:MET:H	1.84	0.42
1:C:136:ASP:O	1:C:136:ASP:CG	2.56	0.42
1:C:239:LEU:HD23	1:C:239:LEU:HA	1.68	0.42
1:C:246:VAL:CG2	1:C:247:PRO:HD2	2.48	0.42
1:B:208:TYR:HB2	1:B:224:LEU:HB2	2.00	0.42
1:C:110:MET:HE2	1:C:167:ILE:HD11	2.02	0.42
1:D:311:THR:CG2	1:D:313:MET:H	2.33	0.42
1:B:79:ASP:OD2	1:B:208:TYR:HE1	2.03	0.42
1:A:250:ILE:HG21	1:B:250:ILE:HD12	2.02	0.41
1:D:268:LYS:HA	1:D:268:LYS:HD3	1.88	0.41
1:D:355:THR:CG2	1:D:356:HIS:ND1	2.84	0.41
1:D:166:VAL:HG12	1:D:302:LEU:HD13	2.03	0.41
1:D:334:LEU:HD13	1:D:386:LEU:HD23	2.01	0.41
1:B:98:THR:HG21	1:B:121:PHE:CE1	2.50	0.41
1:A:17:HIS:HD2	1:D:385:ASP:OD2	2.03	0.41
1:A:335:PHE:CD2	1:A:346:SER:HB3	2.55	0.41
1:B:81:ALA:HB2	1:B:199:LEU:HD11	2.01	0.41
1:D:321:THR:CG2	1:D:322:LEU:H	2.33	0.41
1:D:350:LEU:HB3	1:D:354:MET:HE3	2.02	0.41
1:A:300:HIS:NE2	1:A:304:LYS:HE2	2.35	0.41
1:B:42:SER:HB3	3:B:405:HOH:O	2.20	0.41
1:B:195:PHE:CE1	1:B:266:MET:HB3	2.55	0.41
1:C:297:HIS:HA	1:C:298:PRO:HD3	1.89	0.41
1:D:39:PRO:HA	1:D:40:PRO:HD3	1.98	0.41
1:D:193:PRO:HD3	1:D:208:TYR:CE2	2.55	0.41
1:A:361:LYS:HA	1:A:364:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HD22	1:B:334:LEU:HA	1.81	0.41
1:C:215:ASN:ND2	1:C:255:CYS:HA	2.36	0.41
1:A:253:TYR:OH	1:D:219:ASP:OD1	2.29	0.40
1:D:94:THR:O	1:D:98:THR:CG2	2.64	0.40
1:D:263:HIS:CD2	1:D:263:HIS:H	2.39	0.40
1:C:148:THR:CG2	1:C:149:PRO:HD2	2.52	0.40
1:C:46:THR:CG2	1:D:340:SER:H	2.34	0.40
1:D:210:ALA:HB3	1:D:222:MET:HB3	2.03	0.40
1:B:98:THR:C	1:B:100:LEU:H	2.24	0.40
1:B:101:LEU:HD22	1:B:152:LYS:HB3	2.02	0.40
1:A:349:GLU:CD	1:A:355:THR:HB	2.40	0.40
1:B:138:SER:OG	1:B:165:LYS:HD2	2.22	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	372/403 (92%)	357 (96%)	14 (4%)	1 (0%)	41 64
1	B	372/403 (92%)	350 (94%)	22 (6%)	0	100 100
1	C	386/403 (96%)	363 (94%)	23 (6%)	0	100 100
1	D	386/403 (96%)	363 (94%)	21 (5%)	2 (0%)	29 52
All	All	1516/1612 (94%)	1433 (94%)	80 (5%)	3 (0%)	47 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	THR
1	A	355	THR
1	D	64	GLY

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	321/342 (94%)	288 (90%)	33 (10%)	7	13
1	B	318/342 (93%)	284 (89%)	34 (11%)	6	12
1	C	331/342 (97%)	301 (91%)	30 (9%)	9	18
1	D	330/342 (96%)	297 (90%)	33 (10%)	7	14
All	All	1300/1368 (95%)	1170 (90%)	130 (10%)	7	14

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TRP
1	A	33	THR
1	A	37	VAL
1	A	79	ASP
1	A	110	MET
1	A	141	LYS
1	A	150	GLU
1	A	152	LYS
1	A	156	ILE
1	A	164	GLN
1	A	175	ILE
1	A	182	ILE
1	A	209	SER
1	A	212	LYS
1	A	232	LEU
1	A	236	LEU
1	A	241	ASN
1	A	250	ILE
1	A	254	LEU
1	A	259	LEU
1	A	263	HIS
1	A	278	GLN
1	A	282	SER
1	A	301	GLU

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Mol	Chain	Res	Type
1	A	302	LEU
1	A	315	THR
1	A	319	LYS
1	A	334	LEU
1	A	345	GLU
1	A	355	THR
1	A	372	THR
1	A	375	ARG
1	A	392	GLN
1	B	30	GLU
1	B	35	ARG
1	B	37	VAL
1	B	45	THR
1	B	46	THR
1	B	56	SER
1	B	62	ARG
1	B	63	SER
1	B	100	LEU
1	B	107	ILE
1	B	111	ASP
1	B	117	THR
1	B	122	ARG
1	B	138	SER
1	B	148	THR
1	B	152	LYS
1	B	156	ILE
1	B	164	GLN
1	B	176	VAL
1	B	182	ILE
1	B	192	SER
1	B	236	LEU
1	B	240	GLN
1	B	246	VAL
1	B	254	LEU
1	B	259	LEU
1	B	282	SER
1	B	302	LEU
1	B	311	THR
1	B	321	THR
1	B	333	LYS
1	B	334	LEU
1	B	353	ILE

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Mol	Chain	Res	Type
1	B	387	LEU
1	C	27	GLN
1	C	33	THR
1	C	34	SER
1	C	46	THR
1	C	79	ASP
1	C	98	THR
1	C	100	LEU
1	C	113	VAL
1	C	131	LYS
1	C	137	CYS
1	C	175	ILE
1	C	192	SER
1	C	206	SER
1	C	212	LYS
1	C	230	GLU
1	C	236	LEU
1	C	251	ASP
1	C	254	LEU
1	C	259	LEU
1	C	271	LYS
1	C	302	LEU
1	C	315	THR
1	C	333	LYS
1	C	334	LEU
1	C	349	GLU
1	C	360	LEU
1	C	372	THR
1	C	375	ARG
1	C	384	GLU
1	C	387	LEU
1	D	45	THR
1	D	46	THR
1	D	59	GLU
1	D	65	ASN
1	D	98	THR
1	D	107	ILE
1	D	113	VAL
1	D	117	THR
1	D	138	SER
1	D	148	THR
1	D	156	ILE

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Mol	Chain	Res	Type
1	D	164	GLN
1	D	178	LYS
1	D	182	ILE
1	D	192	SER
1	D	212	LYS
1	D	236	LEU
1	D	246	VAL
1	D	254	LEU
1	D	259	LEU
1	D	268	LYS
1	D	302	LEU
1	D	311	THR
1	D	315	THR
1	D	333	LYS
1	D	334	LEU
1	D	349	GLU
1	D	355	THR
1	D	364	ARG
1	D	373	LEU
1	D	375	ARG
1	D	387	LEU
1	D	388	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	17	HIS
1	A	21	GLN
1	A	27	GLN
1	A	177	HIS
1	A	233	HIS
1	A	240	GLN
1	A	256	ASN
1	A	263	HIS
1	A	297	HIS
1	A	323	GLN
1	A	356	HIS
1	A	392	GLN
1	A	398	HIS
1	B	16	GLN
1	B	17	HIS

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Mol	Chain	Res	Type
1	B	54	GLN
1	B	65	ASN
1	B	106	GLN
1	B	215	ASN
1	B	217	HIS
1	B	233	HIS
1	B	240	GLN
1	B	256	ASN
1	B	263	HIS
1	B	297	HIS
1	B	323	GLN
1	C	17	HIS
1	C	27	GLN
1	C	65	ASN
1	C	164	GLN
1	C	177	HIS
1	C	215	ASN
1	C	228	ASN
1	C	233	HIS
1	C	240	GLN
1	C	241	ASN
1	C	256	ASN
1	C	263	HIS
1	C	297	HIS
1	D	14	HIS
1	D	17	HIS
1	D	65	ASN
1	D	106	GLN
1	D	215	ASN
1	D	217	HIS
1	D	233	HIS
1	D	256	ASN
1	D	263	HIS
1	D	297	HIS
1	D	323	GLN
1	D	398	HIS

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
2	PLP	D	500	1	15,15,16	1.21	2 (13%)	20,22,23	1.42	3 (15%)
2	PLP	C	500	1	15,15,16	1.20	1 (6%)	20,22,23	1.40	2 (10%)
2	PLP	A	500	1	15,15,16	1.56	2 (13%)	20,22,23	1.23	2 (10%)

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	PLP	D	500	1	-	2/6/6/8	0/1/1/1
2	PLP	C	500	1	-	0/6/6/8	0/1/1/1
2	PLP	A	500	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLP	C2A-C2	4.23	1.57	1.50
2	A	500	PLP	P-O2P	2.52	1.64	1.54
2	D	500	PLP	C2A-C2	2.41	1.54	1.50
2	C	500	PLP	P-O3P	2.38	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PLP	P-O3P	2.29	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	PLP	O4P-P-O1P	3.38	115.96	106.47
2	D	500	PLP	O2P-P-O4P	-2.95	98.88	106.73
2	C	500	PLP	C4A-C4-C5	-2.53	118.33	120.94
2	C	500	PLP	C6-C5-C4	-2.52	116.18	118.16
2	A	500	PLP	C2A-C2-N1	2.46	122.48	117.67
2	A	500	PLP	C2A-C2-C3	-2.27	118.09	120.89
2	D	500	PLP	C6-N1-C2	2.08	123.02	119.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	PLP	C4-C5-C5A-O4P
2	D	500	PLP	C6-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	PLP	7	0
2	C	500	PLP	2	0
2	A	500	PLP	2	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, 95^{th} 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	376/403 (93%)	-0.65	2 (0%)	91	89	15, 23, 37, 54	0
1	B	376/403 (93%)	-0.58	7 (1%)	66	62	12, 23, 38, 44	0
1	C	390/403 (96%)	-0.67	4 (1%)	82	80	13, 23, 36, 48	0
1	D	390/403 (96%)	-0.68	4 (1%)	82	80	12, 23, 37, 51	0
All	All	1532/1612 (95%)	-0.65	17 (1%)	80	78	12, 23, 37, 54	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	369	ILE	4.5
1	A	49	GLN	3.6
1	D	55	HIS	3.5
1	D	56	SER	3.4
1	B	352	ALA	3.4
1	B	56	SER	3.1
1	C	179	HIS	3.0
1	D	363	ASP	3.0
1	C	53	GLY	3.0
1	B	55	HIS	2.9
1	D	362	ASN	2.8
1	B	114	TYR	2.6
1	A	362	ASN	2.4
1	C	57	GLY	2.4
1	B	353	ILE	2.4
1	B	180	GLY	2.2
1	C	50	GLY	2.1

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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	PLP	A	500	15/16	0.96	0.14	25,27,29,29	0
2	PLP	D	500	15/16	0.96	0.17	37,43,44,44	0
2	PLP	C	500	15/16	0.98	0.12	19,23,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.