



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 12:11 am BST

PDB ID : 2BHS / pdb_00002bhs
Title : Crystal Structure of Cysteine Synthase B
Authors : Claus, M.T.; Zocher, G.E.; Maier, T.H.P.; Schulz, G.E.
Deposited on : 2005-01-18
Resolution : 2.67 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

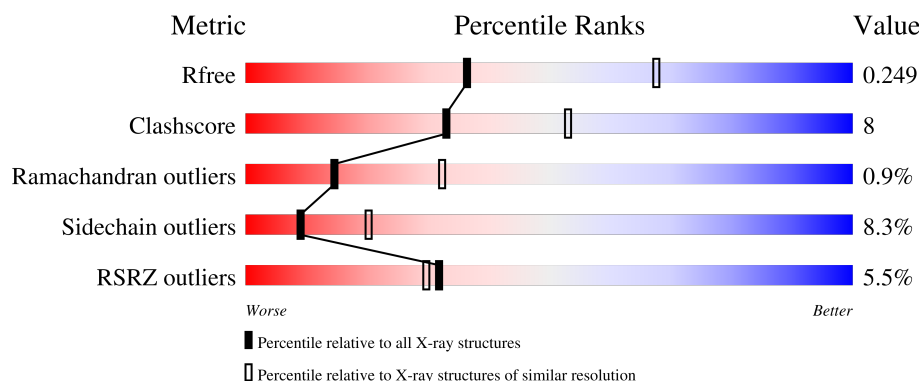
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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	303	 3% 77% 17% . . .
1	B	303	 7% 77% 17% . .
1	C	303	 3% 78% 17% . .
1	D	303	 9% 74% 19% . .

2 Entry composition [i](#)

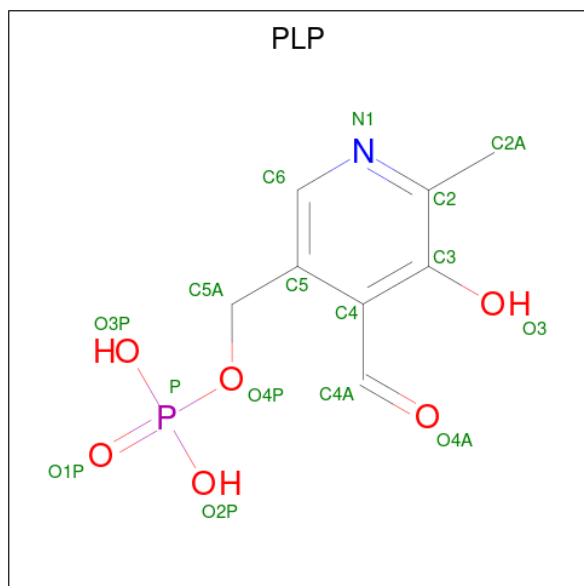
There are 3 unique types of molecules in this entry. The entry contains 9128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYSTEINE SYNTHASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2203	1368	395	426	14			
1	B	291	Total	C	N	O	S	0	0	0
			2199	1366	394	425	14			
1	C	291	Total	C	N	O	S	0	0	0
			2199	1366	394	425	14			
1	D	291	Total	C	N	O	S	0	0	0
			2199	1366	394	425	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

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

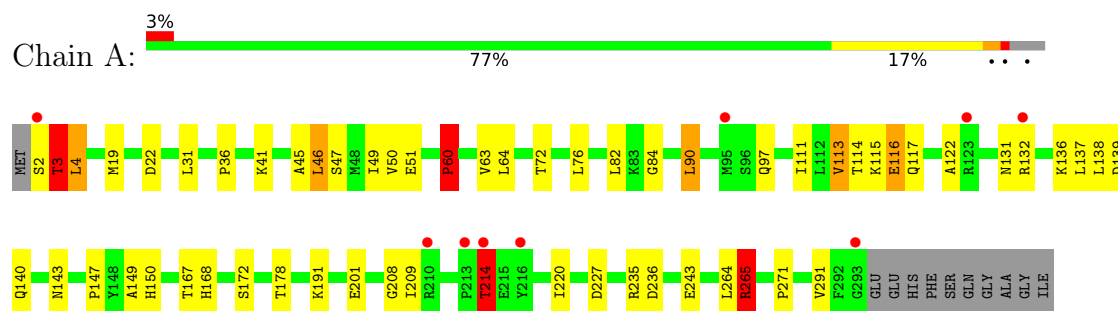
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	85	Total	O	0	0
			85	85		
3	C	54	Total	O	0	0
			54	54		
3	D	57	Total	O	0	0
			57	57		

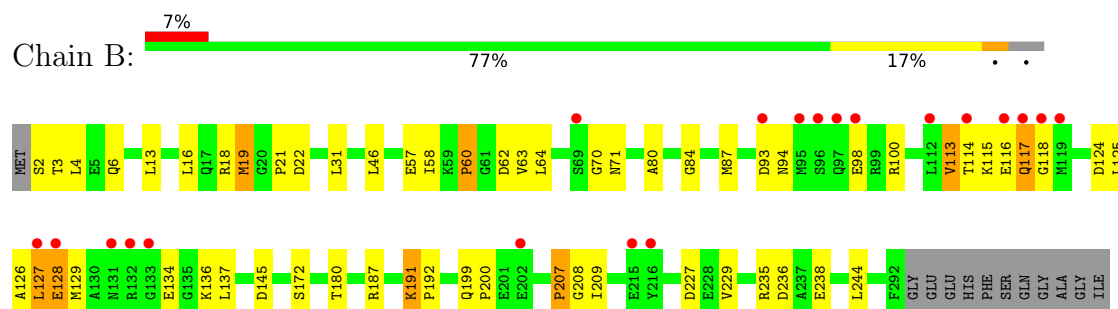
3 Residue-property plots [i](#)

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.

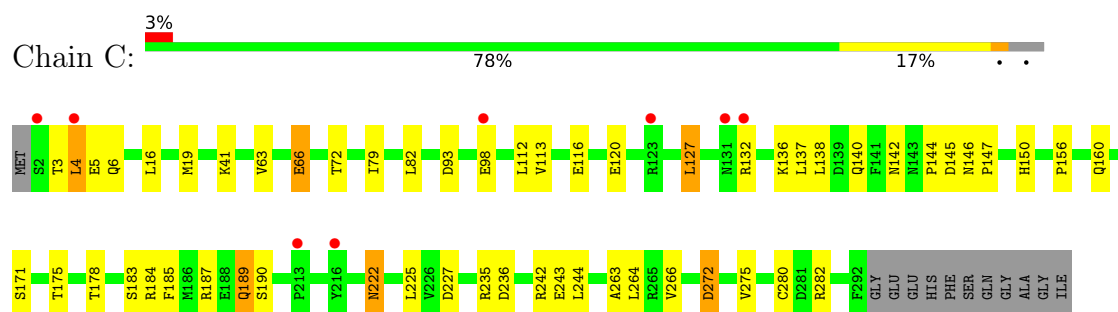
• Molecule 1: CYSTEINE SYNTHASE B



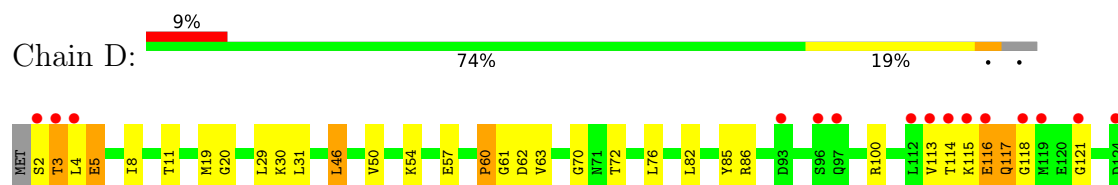
• Molecule 1: CYSTEINE SYNTHASE B

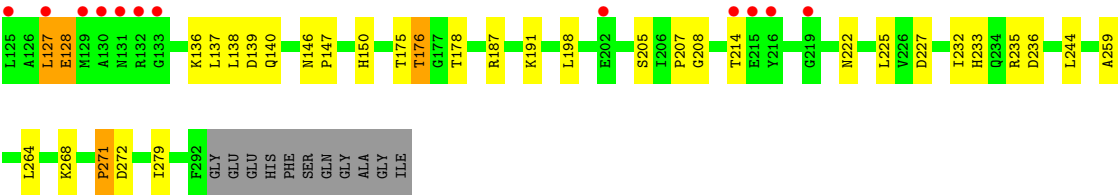


• Molecule 1: CYSTEINE SYNTHASE B



• Molecule 1: CYSTEINE SYNTHASE B





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	195.58Å 195.58Å 235.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 2.67 19.88 – 2.67	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-2.67) 99.6 (19.88-2.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.67Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.222 , 0.253 0.225 , 0.249	Depositor DCC
R_{free} test set	2263 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9128	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2071e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.57	0/2237	0.85	7/3024 (0.2%)
1	B	0.59	1/2233 (0.0%)	0.83	5/3019 (0.2%)
1	C	0.56	0/2233	0.81	4/3019 (0.1%)
1	D	0.60	0/2233	0.83	5/3019 (0.2%)
All	All	0.58	1/8936 (0.0%)	0.83	21/12081 (0.2%)

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	B	0	1
1	D	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	MET	SD-CE	-5.23	1.48	1.77

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	227	ASP	CB-CG-OD2	8.56	126.01	118.30
1	A	3	THR	N-CA-C	-7.87	89.76	111.00
1	C	227	ASP	CB-CG-OD2	7.58	125.12	118.30
1	B	227	ASP	CB-CG-OD2	7.06	124.65	118.30
1	D	127	LEU	N-CA-C	6.27	127.92	111.00
1	A	227	ASP	CB-CG-OD2	5.96	123.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	145	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	265	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	62	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	62	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	236	ASP	CB-CG-OD2	5.59	123.33	118.30
1	C	236	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	214	THR	N-CA-C	5.40	125.59	111.00
1	C	272	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	124	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	145	ASP	CB-CG-OD2	5.26	123.03	118.30
1	D	139	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	139	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	22	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	236	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	128	GLU	Peptide
1	D	2	SER	Peptide
1	D	20	GLY	Peptide

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	2203	0	2206	37	0
1	B	2199	0	2203	37	0
1	C	2199	0	2203	30	0
1	D	2199	0	2203	36	0
2	A	15	0	6	1	0
2	B	15	0	6	2	0
2	C	15	0	6	1	0
2	D	15	0	6	1	0
3	A	72	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	85	0	0	13	0
3	C	54	0	0	7	0
3	D	57	0	0	6	0
All	All	9128	0	8839	137	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 8.

All (137) 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:B:3:THR:HG22	1:B:6:GLN:HE21	1.21	1.03
1:D:127:LEU:HD22	1:D:127:LEU:O	1.76	0.84
1:A:114:THR:HB	1:A:116:GLU:OE2	1.82	0.79
1:D:175:THR:O	1:D:176:THR:HB	1.82	0.79
1:B:3:THR:HG22	1:B:6:GLN:NE2	2.02	0.73
1:C:5:GLU:HG3	1:C:82:LEU:HD21	1.73	0.69
1:D:85:TYR:HB3	3:D:2022:HOH:O	1.95	0.66
1:C:275:VAL:HG11	3:C:2045:HOH:O	1.95	0.66
1:D:128:GLU:OE1	3:D:2030:HOH:O	2.15	0.65
1:A:265:ARG:HG2	1:A:265:ARG:HH11	1.64	0.62
1:C:41:LYS:HE2	1:C:72:THR:OG1	2.00	0.61
1:D:3:THR:O	1:D:4:LEU:C	2.38	0.61
1:B:238:GLU:HA	3:B:2065:HOH:O	2.01	0.61
1:A:147:PRO:HG3	1:A:220:ILE:HG23	1.83	0.61
1:B:129:MET:O	1:B:134:GLU:HB3	2.00	0.61
1:C:127:LEU:C	3:C:2026:HOH:O	2.39	0.61
1:A:2:SER:HB2	1:B:13:LEU:O	2.01	0.61
1:A:113:VAL:HG13	1:A:117:GLN:HG3	1.83	0.60
1:B:128:GLU:OE2	1:B:128:GLU:HA	2.01	0.60
1:A:3:THR:O	1:A:4:LEU:C	2.39	0.59
1:D:4:LEU:HD12	1:D:4:LEU:N	2.17	0.58
1:D:127:LEU:HD23	1:D:137:LEU:HD22	1.86	0.58
1:B:70:GLY:N	3:B:2025:HOH:O	2.37	0.57
1:C:275:VAL:HG21	3:C:2045:HOH:O	2.05	0.56
1:D:72:THR:HG21	1:D:140:GLN:OE1	2.05	0.56
1:C:266:VAL:HB	3:C:2045:HOH:O	2.04	0.56
1:A:60:PRO:O	1:A:84:GLY:O	2.23	0.55
1:C:93:ASP:HB3	1:C:112:LEU:HD13	1.89	0.55
1:A:291:VAL:HB	3:A:2067:HOH:O	2.07	0.55
1:C:140:GLN:HG3	1:C:175:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD22	1:A:138:LEU:HD13	1.90	0.54
1:D:222:ASN:HB3	1:D:225:LEU:HD12	1.89	0.54
1:A:2:SER:CB	1:B:13:LEU:O	2.56	0.53
1:B:80:ALA:HB2	1:B:87:MET:HG2	1.91	0.53
1:B:16:LEU:HD13	1:B:19:MET:HB2	1.91	0.52
1:D:175:THR:O	1:D:176:THR:CB	2.55	0.52
1:A:114:THR:CB	1:A:116:GLU:OE2	2.55	0.52
1:A:150:HIS:CD2	1:A:178:THR:HA	2.44	0.52
1:A:41:LYS:HE2	1:A:72:THR:OG1	2.09	0.52
1:A:114:THR:OG1	1:A:117:GLN:HG2	2.10	0.51
1:D:19:MET:HE3	1:D:244:LEU:HA	1.92	0.51
1:C:222:ASN:HB3	1:C:225:LEU:HD12	1.95	0.49
1:D:3:THR:HG21	3:D:2001:HOH:O	2.13	0.49
1:A:82:LEU:O	1:B:18:ARG:NH2	2.45	0.49
1:C:66:GLU:HG2	1:C:138:LEU:HB2	1.94	0.49
1:A:45:ALA:O	1:A:49:ILE:HG12	2.13	0.48
1:C:146:ASN:HB3	1:C:147:PRO:HD3	1.94	0.48
1:D:233:HIS:HB3	1:D:236:ASP:OD2	2.14	0.48
1:C:263:ALA:O	3:C:2045:HOH:O	2.20	0.47
1:D:232:ILE:HG12	3:D:2043:HOH:O	2.13	0.47
1:B:116:GLU:HG3	3:B:2036:HOH:O	2.13	0.47
1:C:142:ASN:O	1:C:144:PRO:HD3	2.15	0.47
1:B:208:GLY:N	3:B:2057:HOH:O	2.28	0.47
1:C:242:ARG:HD2	3:C:2040:HOH:O	2.14	0.47
1:D:117:GLN:O	1:D:121:GLY:HA3	2.15	0.47
1:D:127:LEU:O	1:D:127:LEU:CD2	2.57	0.47
1:A:167:THR:OG1	1:A:168:HIS:HD2	1.99	0.46
1:C:160:GLN:OE1	1:C:160:GLN:C	2.54	0.46
1:D:70:GLY:N	3:D:2019:HOH:O	2.47	0.46
1:A:220:ILE:HG21	3:A:2042:HOH:O	2.15	0.46
1:D:5:GLU:HA	1:D:8:ILE:HD12	1.97	0.46
1:D:57:GLU:OE1	1:D:136:LYS:NZ	2.37	0.46
1:A:19:MET:HE2	1:A:243:GLU:HG2	1.98	0.46
1:B:71:ASN:ND2	2:B:320:PLP:H2A1	2.31	0.46
1:B:180:THR:HG22	3:B:2059:HOH:O	2.16	0.46
1:D:4:LEU:HD12	1:D:4:LEU:H	1.81	0.46
1:B:200:PRO:HD3	1:B:209:ILE:HD12	1.98	0.45
1:C:4:LEU:O	1:C:4:LEU:HG	2.15	0.45
1:B:60:PRO:O	1:B:84:GLY:O	2.34	0.45
1:B:180:THR:CB	3:B:2048:HOH:O	2.64	0.45
1:A:4:LEU:HD23	1:A:4:LEU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLN:HG3	3:C:2033:HOH:O	2.16	0.45
1:D:29:LEU:HD13	1:D:279:ILE:HD11	1.99	0.45
1:B:93:ASP:HB2	3:B:2030:HOH:O	2.17	0.45
1:C:19:MET:HE3	1:C:244:LEU:HA	1.99	0.45
1:A:136:LYS:HD3	1:A:137:LEU:O	2.17	0.45
1:D:150:HIS:CG	1:D:178:THR:HA	2.52	0.45
1:D:208:GLY:HA3	2:D:320:PLP:C2	2.46	0.45
1:D:86:ARG:N	3:D:2022:HOH:O	2.50	0.44
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.29	0.44
1:C:136:LYS:HD3	1:C:137:LEU:O	2.17	0.44
1:D:4:LEU:N	1:D:4:LEU:CD1	2.80	0.44
1:C:136:LYS:CD	1:C:137:LEU:O	2.66	0.44
1:B:115:LYS:HG3	3:B:2036:HOH:O	2.16	0.44
1:B:126:ALA:O	3:B:2039:HOH:O	2.21	0.44
1:D:46:LEU:HD22	1:D:50:VAL:CG2	2.48	0.44
1:A:220:ILE:HB	3:A:2042:HOH:O	2.18	0.44
1:D:116:GLU:O	1:D:117:GLN:CG	2.66	0.43
1:C:127:LEU:HD13	1:C:127:LEU:O	2.17	0.43
1:B:114:THR:CB	3:B:2035:HOH:O	2.67	0.43
1:C:280:CYS:HG	2:C:320:PLP:C6	2.31	0.43
1:B:229:VAL:HG12	3:B:2062:HOH:O	2.17	0.43
1:C:222:ASN:C	1:C:222:ASN:HD22	2.22	0.43
1:D:11:THR:OG1	1:D:30:LYS:HE3	2.18	0.43
1:C:183:SER:O	1:C:184:ARG:C	2.57	0.43
1:D:198:LEU:CD1	1:D:259:ALA:HA	2.48	0.43
1:C:3:THR:H	1:C:6:GLN:HE21	1.66	0.43
1:D:60:PRO:O	1:D:61:GLY:C	2.57	0.43
1:A:72:THR:HG21	1:A:140:GLN:OE1	2.19	0.42
1:B:113:VAL:HG13	1:B:114:THR:N	2.34	0.42
1:A:172:SER:HB3	1:A:209:ILE:HG21	2.01	0.42
1:D:46:LEU:HD22	1:D:50:VAL:HG23	2.01	0.42
1:B:127:LEU:HD23	1:B:137:LEU:HD22	2.02	0.42
1:A:76:LEU:CD2	1:A:138:LEU:HD13	2.49	0.42
1:B:71:ASN:HD22	2:B:320:PLP:H2A1	1.85	0.42
1:C:140:GLN:HG3	1:C:175:THR:CG2	2.50	0.42
1:B:64:LEU:HB2	1:B:87:MET:SD	2.60	0.42
1:D:4:LEU:H	1:D:4:LEU:CD1	2.32	0.42
1:A:208:GLY:HA3	2:A:320:PLP:C2	2.50	0.42
1:A:143:ASN:C	1:A:220:ILE:HD11	2.40	0.42
1:B:180:THR:HB	3:B:2048:HOH:O	2.19	0.42
1:A:4:LEU:HD22	1:A:36:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:HB2	3:A:2034:HOH:O	2.20	0.41
1:A:90:LEU:HD22	1:A:111:ILE:HB	2.02	0.41
1:B:114:THR:OG1	1:B:117:GLN:CG	2.68	0.41
1:D:146:ASN:HB3	1:D:147:PRO:CD	2.51	0.41
1:A:47:SER:CB	1:A:149:ALA:HB2	2.51	0.41
1:A:150:HIS:CG	1:A:178:THR:HA	2.56	0.41
1:B:19:MET:HE3	1:B:244:LEU:HA	2.02	0.41
1:B:172:SER:HB3	1:B:209:ILE:HG21	2.02	0.41
1:C:156:PRO:HG3	1:C:185:PHE:CE2	2.56	0.41
1:B:125:LEU:HG	1:B:129:MET:CE	2.51	0.41
1:B:21:PRO:O	1:B:22:ASP:HB3	2.21	0.41
1:B:191:LYS:HB2	1:B:192:PRO:HD2	2.02	0.41
1:C:150:HIS:CD2	1:C:178:THR:HA	2.56	0.41
1:A:46:LEU:HD22	1:A:50:VAL:HG23	2.02	0.41
1:A:49:ILE:HD12	1:A:64:LEU:HD13	2.02	0.41
1:B:116:GLU:O	1:B:117:GLN:CG	2.69	0.41
1:B:199:GLN:HG2	3:B:2062:HOH:O	2.21	0.41
1:A:131:ASN:HA	3:A:2036:HOH:O	2.21	0.41
1:B:58:ILE:HG23	1:B:136:LYS:HG3	2.02	0.41
1:C:3:THR:H	1:C:6:GLN:NE2	2.18	0.40
1:C:19:MET:HE1	1:C:243:GLU:C	2.40	0.40
1:D:4:LEU:HB2	1:D:82:LEU:HD22	2.02	0.40
1:D:198:LEU:HD12	1:D:259:ALA:HA	2.03	0.40
1:A:47:SER:HB2	1:A:149:ALA:HB2	2.04	0.40
1:D:76:LEU:HD22	1:D:138:LEU:HD13	2.03	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	290/303 (96%)	271 (93%)	15 (5%)	4 (1%)	9 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	289/303 (95%)	276 (96%)	10 (4%)	3 (1%)	13	29
1	C	289/303 (95%)	272 (94%)	16 (6%)	1 (0%)	37	59
1	D	289/303 (95%)	260 (90%)	27 (9%)	2 (1%)	19	38
All	All	1157/1212 (96%)	1079 (93%)	68 (6%)	10 (1%)	14	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	LYS
1	A	214	THR
1	B	118	GLY
1	C	4	LEU
1	B	207	PRO
1	A	60	PRO
1	B	60	PRO
1	D	118	GLY
1	D	271	PRO
1	A	271	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	232/240 (97%)	214 (92%)	18 (8%)	10	23
1	B	232/240 (97%)	216 (93%)	16 (7%)	13	28
1	C	232/240 (97%)	213 (92%)	19 (8%)	9	21
1	D	232/240 (97%)	208 (90%)	24 (10%)	6	13
All	All	928/960 (97%)	851 (92%)	77 (8%)	9	20

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR

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Mol	Chain	Res	Type
1	A	4	LEU
1	A	31	LEU
1	A	46	LEU
1	A	51	GLU
1	A	60	PRO
1	A	63	VAL
1	A	90	LEU
1	A	97	GLN
1	A	113	VAL
1	A	116	GLU
1	A	132	ARG
1	A	191	LYS
1	A	201	GLU
1	A	214	THR
1	A	235	ARG
1	A	264	LEU
1	A	265	ARG
1	B	2	SER
1	B	4	LEU
1	B	31	LEU
1	B	46	LEU
1	B	57	GLU
1	B	63	VAL
1	B	94	ASN
1	B	98	GLU
1	B	100	ARG
1	B	113	VAL
1	B	117	GLN
1	B	127	LEU
1	B	187	ARG
1	B	191	LYS
1	B	207	PRO
1	B	235	ARG
1	C	16	LEU
1	C	63	VAL
1	C	66	GLU
1	C	79	ILE
1	C	98	GLU
1	C	113	VAL
1	C	116	GLU
1	C	120	GLU
1	C	127	LEU

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Mol	Chain	Res	Type
1	C	132	ARG
1	C	171	SER
1	C	187	ARG
1	C	189	GLN
1	C	190	SER
1	C	222	ASN
1	C	235	ARG
1	C	264	LEU
1	C	272	ASP
1	C	282	ARG
1	D	3	THR
1	D	5	GLU
1	D	31	LEU
1	D	46	LEU
1	D	54	LYS
1	D	60	PRO
1	D	63	VAL
1	D	100	ARG
1	D	113	VAL
1	D	114	THR
1	D	115	LYS
1	D	116	GLU
1	D	117	GLN
1	D	128	GLU
1	D	176	THR
1	D	187	ARG
1	D	191	LYS
1	D	205	SER
1	D	207	PRO
1	D	214	THR
1	D	235	ARG
1	D	264	LEU
1	D	268	LYS
1	D	271	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	168	HIS
1	B	6	GLN
1	B	94	ASN

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Mol	Chain	Res	Type
1	B	117	GLN
1	B	131	ASN
1	C	6	GLN
1	C	131	ASN
1	C	222	ASN
1	D	97	GLN
1	D	117	GLN
1	D	239	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](#)

4 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	C	320	1	15,15,16	3.01	4 (26%)	20,22,23	1.60	4 (20%)
2	PLP	B	320	1	15,15,16	2.78	3 (20%)	20,22,23	1.61	4 (20%)
2	PLP	A	320	1	15,15,16	3.06	3 (20%)	20,22,23	1.51	3 (15%)
2	PLP	D	320	1	15,15,16	2.91	3 (20%)	20,22,23	1.56	3 (15%)

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	C	320	1	-	0/6/6/8	0/1/1/1
2	PLP	B	320	1	-	0/6/6/8	0/1/1/1
2	PLP	A	320	1	-	3/6/6/8	0/1/1/1
2	PLP	D	320	1	-	4/6/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	320	PLP	C5-C4	7.92	1.49	1.40
2	C	320	PLP	C5-C4	7.85	1.49	1.40
2	B	320	PLP	C5-C4	7.44	1.48	1.40
2	D	320	PLP	C5-C4	7.30	1.48	1.40
2	A	320	PLP	C3-C2	7.18	1.48	1.40
2	C	320	PLP	C3-C2	7.15	1.48	1.40
2	D	320	PLP	C3-C2	6.87	1.47	1.40
2	B	320	PLP	C3-C2	6.18	1.47	1.40
2	A	320	PLP	C3-C4	4.24	1.48	1.40
2	D	320	PLP	C3-C4	4.08	1.48	1.40
2	C	320	PLP	C3-C4	3.69	1.47	1.40
2	B	320	PLP	C3-C4	3.34	1.47	1.40
2	C	320	PLP	O3-C3	-2.03	1.32	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	320	PLP	O4P-C5A-C5	4.02	117.02	109.35
2	C	320	PLP	O4P-C5A-C5	3.74	116.48	109.35
2	B	320	PLP	O4P-C5A-C5	3.21	115.47	109.35
2	A	320	PLP	O4P-C5A-C5	3.09	115.25	109.35
2	D	320	PLP	C6-N1-C2	3.06	124.83	119.17
2	B	320	PLP	C6-N1-C2	2.81	124.37	119.17
2	B	320	PLP	C4A-C4-C5	2.70	123.72	120.94
2	A	320	PLP	O3P-P-O2P	2.63	117.67	107.64
2	A	320	PLP	C6-N1-C2	2.59	123.97	119.17
2	C	320	PLP	C6-N1-C2	2.56	123.91	119.17
2	C	320	PLP	O3-C3-C2	2.24	122.38	117.49
2	C	320	PLP	O3P-P-O2P	2.20	116.05	107.64
2	B	320	PLP	O3P-P-O2P	2.16	115.88	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	320	PLP	O2P-P-O4P	-2.01	101.37	106.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	320	PLP	C4-C5-C5A-O4P
2	A	320	PLP	C6-C5-C5A-O4P
2	D	320	PLP	C4-C5-C5A-O4P
2	D	320	PLP	C6-C5-C5A-O4P
2	D	320	PLP	C5A-O4P-P-O1P
2	D	320	PLP	C5A-O4P-P-O3P
2	A	320	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	320	PLP	1	0
2	B	320	PLP	2	0
2	A	320	PLP	1	0
2	D	320	PLP	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	292/303 (96%)	-0.03	9 (3%) 51 50	42, 61, 88, 103	0
1	B	291/303 (96%)	0.01	20 (6%) 24 22	41, 59, 95, 103	0
1	C	291/303 (96%)	0.01	8 (2%) 56 55	44, 61, 86, 99	0
1	D	291/303 (96%)	0.28	27 (9%) 16 15	44, 64, 96, 105	0
All	All	1165/1212 (96%)	0.07	64 (5%) 32 30	41, 61, 93, 105	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	GLY	4.6
1	B	128	GLU	4.3
1	C	2	SER	4.1
1	D	119	MET	4.0
1	D	130	ALA	3.7
1	D	127	LEU	3.7
1	D	132	ARG	3.6
1	B	116	GLU	3.6
1	D	131	ASN	3.5
1	A	216	TYR	3.5
1	B	133	GLY	3.5
1	D	202	GLU	3.4
1	D	112	LEU	3.3
1	A	210	ARG	3.3
1	B	98	GLU	3.3
1	D	214	THR	3.3
1	B	131	ASN	3.3
1	D	4	LEU	3.2
1	D	216	TYR	3.2
1	D	215	GLU	3.2
1	B	132	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	95	MET	3.2
1	D	96	SER	3.1
1	D	114	THR	3.1
1	D	116	GLU	3.0
1	C	98	GLU	2.9
1	B	69	SER	2.8
1	C	216	TYR	2.8
1	D	115	LYS	2.8
1	A	2	SER	2.7
1	B	215	GLU	2.7
1	B	112	LEU	2.7
1	B	118	GLY	2.7
1	D	129	MET	2.7
1	D	93	ASP	2.6
1	B	119	MET	2.6
1	D	124	ASP	2.6
1	D	121	GLY	2.6
1	B	202	GLU	2.6
1	B	216	TYR	2.5
1	B	93	ASP	2.5
1	B	117	GLN	2.5
1	C	123	ARG	2.5
1	B	114	THR	2.5
1	D	125	LEU	2.4
1	D	97	GLN	2.4
1	C	131	ASN	2.4
1	A	123	ARG	2.3
1	C	132	ARG	2.3
1	C	213	PRO	2.3
1	D	118	GLY	2.3
1	D	3	THR	2.3
1	D	113	VAL	2.3
1	A	95	MET	2.3
1	D	2	SER	2.3
1	A	132	ARG	2.3
1	A	213	PRO	2.3
1	A	214	THR	2.2
1	B	97	GLN	2.2
1	C	4	LEU	2.1
1	D	219	GLY	2.1
1	D	133	GLY	2.0
1	B	127	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	96	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 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(\AA^2)	Q<0.9
2	PLP	A	320	15/16	0.98	0.05	43,49,49,50	0
2	PLP	B	320	15/16	0.98	0.06	45,50,51,53	0
2	PLP	C	320	15/16	0.98	0.07	45,51,53,53	0
2	PLP	D	320	15/16	0.98	0.06	47,56,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.