



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:55 AM GMT

PDB ID : 3COG
Title : Crystal structure of human cystathionase (Cystathionine gamma lyase) in complex with DL-propargylglycine
Authors : Collins, R.; Karlberg, T.; Lehtio, L.; Arrowsmith, C.H.; Berglund, H.; Dahlgren, L.G.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, I.; Kallas, A.; Kotenyova, T.; Moche, M.; Nilsson, M.E.; Nordlund, P.; Nyman, T.; Olesen, K.; Persson, C.; Schuler, H.; Svensson, L.; Thorsell, A.G.; Tresaugues, L.; Van den Berg, S.; Sagermark, J.; Busam, R.D.; Welin, M.; Weigelt, J.; Wikstrom, M.; Structural Genomics Consortium (SGC)
Deposited on : 2008-03-28
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

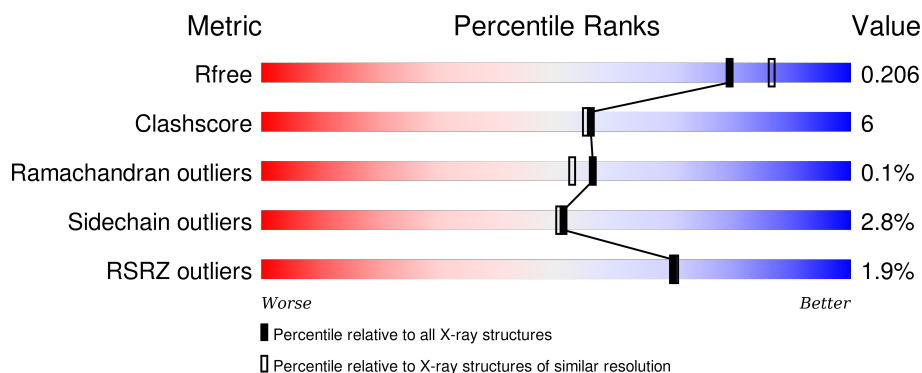
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	403	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>
1	B	403	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>7%</div> </div> </div>
1	C	403	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	403	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>••</div> </div> </div>

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	NO3	A	608	-	X	-	-
2	NO3	C	606	-	X	-	-
2	NO3	D	607	-	X	-	X
3	PLP	A	500	-	-	-	X
4	2AG	A	501	-	-	-	X
4	2AG	D	501	-	-	-	X
5	GOL	D	604	-	-	-	X
5	GOL	D	605	-	-	X	X
6	PEG	A	609	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13153 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.

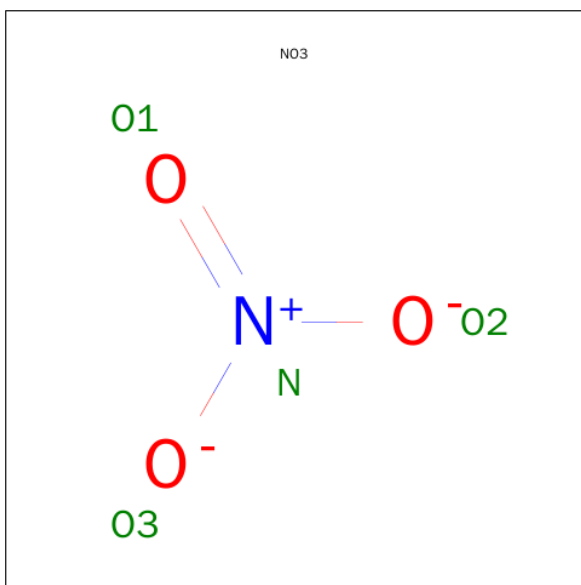
- Molecule 1 is a protein called Cystathionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	1	0
			2922	1866	497	540	19			
1	B	373	Total	C	N	O	S	0	1	0
			2891	1845	492	536	18			
1	C	390	Total	C	N	O	S	0	1	0
			3024	1930	515	560	19			
1	D	392	Total	C	N	O	S	0	2	0
			3038	1938	519	562	19			

There are 4 discrepancies between the modelled and reference sequences:

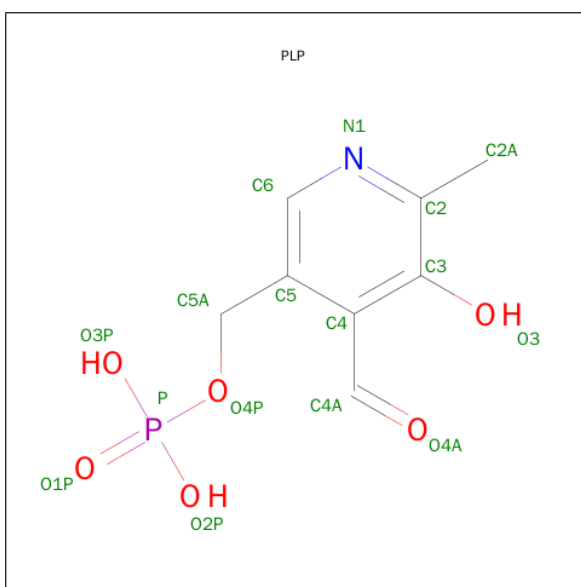
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P32929
B	-1	SER	-	EXPRESSION TAG	UNP P32929
C	-1	SER	-	EXPRESSION TAG	UNP P32929
D	-1	SER	-	EXPRESSION TAG	UNP P32929

- Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



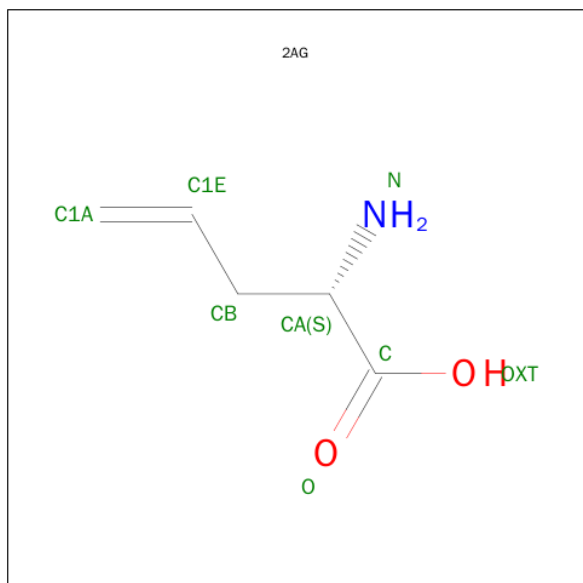
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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

- Molecule 4 is (2S)-2-AMINOPENT-4-ENOIC ACID (three-letter code: 2AG) (formula: $C_5H_9NO_2$).



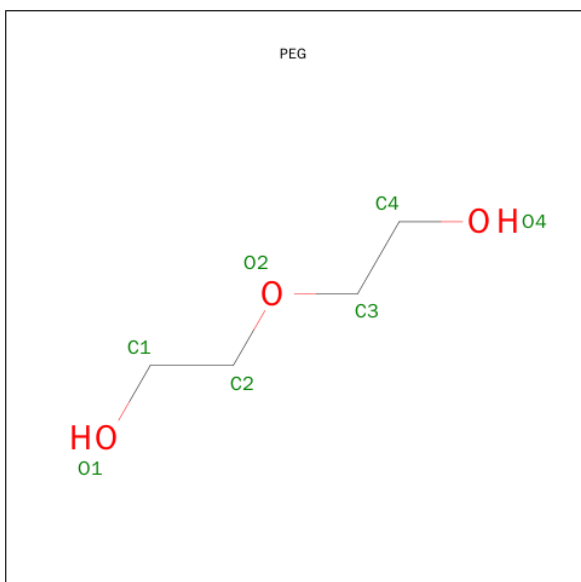
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	5	1	2		
4	C	1	Total	C	N	O	0	0
			8	5	1	2		
4	D	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

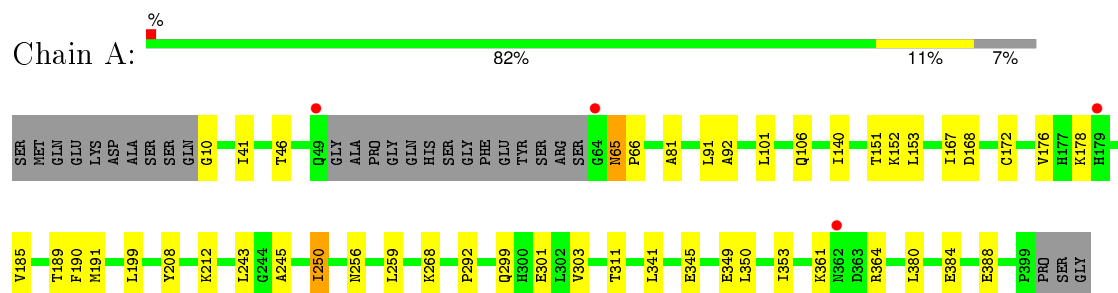
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	273	Total	O	0	0
			273	273		
7	B	240	Total	O	0	0
			240	240		
7	C	320	Total	O	0	0
			320	320		
7	D	327	Total	O	0	0
			327	327		

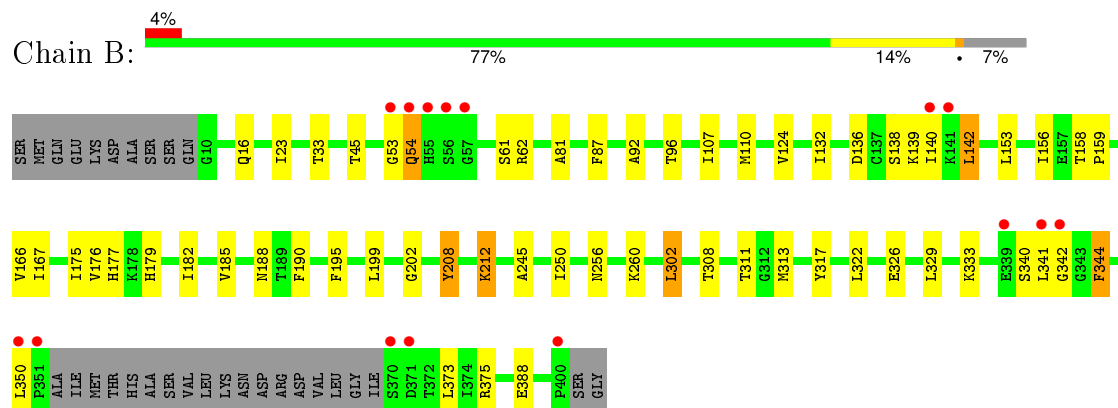
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

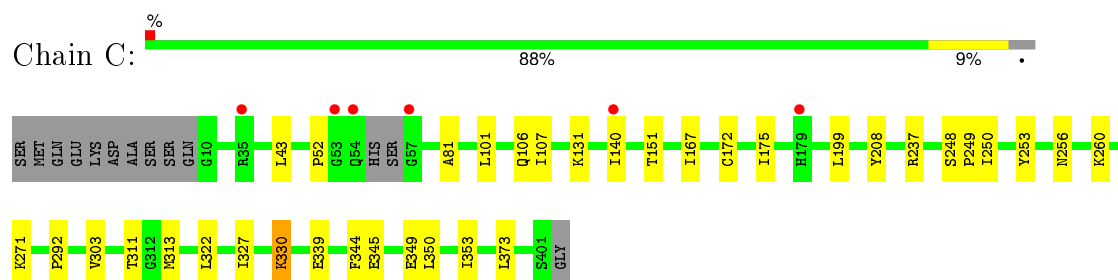
- Molecule 1: Cystathionine gamma-lyase



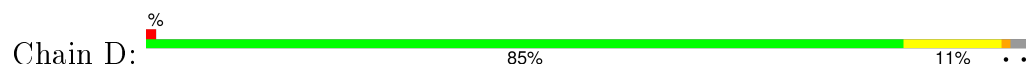
- Molecule 1: Cystathionine gamma-lyase

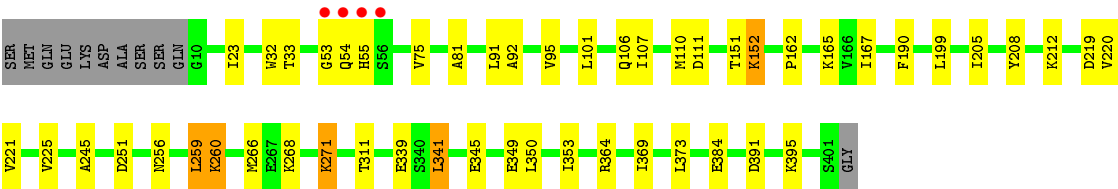


- Molecule 1: Cystathionine gamma-lyase



- Molecule 1: Cystathionine gamma-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.35Å 107.22Å 153.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.00 19.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.91-2.00) 93.0 (19.91-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.158 , 0.204 0.164 , 0.206	Depositor DCC
R_{free} test set	5460 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.2	EDS
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 109200 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13153	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PEG, 2AG, PLP, NO3, GOL

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	0.61	0/2987	0.66	2/4055 (0.0%)
1	B	0.58	0/2961	0.67	0/4018
1	C	0.64	1/3096 (0.0%)	0.70	2/4201 (0.0%)
1	D	0.61	0/3114	0.69	1/4227 (0.0%)
All	All	0.61	1/12158 (0.0%)	0.68	5/16501 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	CYS	CB-SG	-5.65	1.72	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	C	237	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	D	271	LYS	CD-CE-NZ	6.40	126.42	111.70
1	A	364	ARG	NE-CZ-NH2	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	TYR	Peptide
1	B	208	TYR	Peptide
1	C	208	TYR	Peptide
1	D	208	TYR	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	2922	0	2915	32	0
1	B	2891	0	2876	69	0
1	C	3024	0	3015	24	0
1	D	3038	0	3032	35	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	15	0	7	1	0
3	C	15	0	6	0	0
3	D	15	0	7	0	0
4	A	8	0	7	0	0
4	C	8	0	7	1	0
4	D	8	0	7	1	0
5	A	6	0	8	1	0
5	C	6	0	8	1	0
5	D	18	0	24	10	0
6	A	7	0	10	3	0
7	A	273	0	0	2	0
7	B	240	0	0	4	0
7	C	320	0	0	0	0
7	D	327	0	0	2	0
All	All	13153	0	11929	148	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 6.

All (148) 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:341:LEU:HD23	1:B:342:GLY:N	1.75	1.02
1:D:190:PHE:O	1:D:311:THR:HG21	1.70	0.91
1:B:313:MET:CE	1:B:341:LEU:HD11	2.01	0.90
1:A:10:GLY:N	7:A:845:HOH:O	2.05	0.88
1:B:313:MET:HE2	1:B:341:LEU:HD11	1.56	0.87
1:A:350:LEU:HD23	1:A:353:ILE:HD12	1.56	0.84
1:B:54[A]:GLN:HE21	1:B:54[A]:GLN:H	1.22	0.83
1:B:33:THR:HG23	1:D:33:THR:HG23	1.61	0.82
1:B:190:PHE:CE2	1:B:341:LEU:HD13	2.16	0.81
1:B:341:LEU:HD23	1:B:342:GLY:CA	2.11	0.81
1:B:329:LEU:HD11	1:B:350:LEU:HB2	1.64	0.79
1:A:388:GLU:HG2	7:A:687:HOH:O	1.85	0.76
1:C:52:PRO:HB2	1:D:353[A]:ILE:HD11	1.70	0.74
1:B:175:ILE:HD12	7:B:591:HOH:O	1.87	0.73
1:A:299:GLN:HA	6:A:609:PEG:H32	1.71	0.73
1:B:139:LYS:HB2	1:B:142:LEU:HD12	1.72	0.72
1:B:140:ILE:HD12	1:B:140:ILE:H	1.55	0.71
1:A:106:GLN:NE2	1:A:151:THR:OG1	2.23	0.71
1:D:220:VAL:HA	5:D:605:GOL:H2	1.72	0.70
1:B:190:PHE:CE2	1:B:341:LEU:HD22	2.27	0.70
1:B:190:PHE:HE2	1:B:341:LEU:HD13	1.55	0.69
1:A:250:ILE:O	1:A:250:ILE:HD13	1.93	0.69
1:C:350:LEU:HD23	1:C:353:ILE:HD12	1.73	0.69
1:A:190:PHE:O	1:A:311:THR:HG21	1.92	0.68
1:C:311:THR:HG23	1:C:313:MET:H	1.61	0.66
1:B:190:PHE:HE2	1:B:341:LEU:HD22	1.62	0.64
1:B:322:LEU:C	1:B:322:LEU:HD13	2.19	0.62
1:A:101:LEU:O	5:A:603:GOL:H2	2.00	0.61
1:B:175:ILE:CD1	7:B:591:HOH:O	2.47	0.61
1:D:266:MET:CE	1:D:311:THR:HG22	2.31	0.61
1:A:250:ILE:HD12	1:B:250:ILE:HD12	1.82	0.61
1:B:322:LEU:HD11	1:B:326:GLU:CD	2.24	0.58
1:B:166:VAL:HG12	1:B:302:LEU:HD13	1.84	0.58
1:B:167:ILE:N	1:B:167:ILE:HD12	2.19	0.57
1:C:43:LEU:HD22	5:D:605:GOL:H31	1.86	0.57
1:B:190:PHE:HE2	1:B:341:LEU:CD1	2.17	0.57
1:B:190:PHE:CE2	1:B:341:LEU:CD1	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:MET:SD	1:B:341:LEU:HD21	2.46	0.56
1:B:322:LEU:O	1:B:322:LEU:HD13	2.06	0.56
1:A:167:ILE:HD12	1:A:167:ILE:N	2.22	0.56
1:B:350:LEU:HD12	1:B:373:LEU:O	2.07	0.55
1:D:75:VAL:HG22	1:D:259:LEU:HD21	1.89	0.55
1:C:292:PRO:HB3	1:C:303:VAL:HG21	1.88	0.54
1:B:333:LYS:NZ	7:B:565:HOH:O	2.41	0.54
1:C:248:SER:OG	1:C:250:ILE:HG22	2.08	0.54
1:C:101:LEU:O	5:C:602:GOL:H2	2.08	0.53
1:B:322:LEU:HD11	1:B:326:GLU:OE2	2.08	0.53
1:C:249:PRO:HD2	5:D:605:GOL:C3	2.38	0.53
1:C:52:PRO:HB2	1:D:353[A]:ILE:CD1	2.37	0.53
1:D:271:LYS:HD3	7:D:831:HOH:O	2.07	0.53
1:D:219:ASP:O	5:D:605:GOL:H2	2.09	0.52
1:D:110:MET:HE2	1:D:167:ILE:HD11	1.91	0.52
1:A:250:ILE:C	1:A:250:ILE:HD13	2.29	0.52
1:C:249:PRO:HD2	5:D:605:GOL:H31	1.92	0.51
1:D:212:LYS:HD2	1:D:341:LEU:HG	1.92	0.51
1:A:81:ALA:HB2	1:A:199:LEU:CD1	2.41	0.51
1:A:46:THR:HG23	1:B:340:SER:OG	2.10	0.51
1:A:301:GLU:HB2	6:A:609:PEG:H31	1.92	0.51
1:B:190:PHE:HE2	1:B:341:LEU:CD2	2.23	0.50
1:B:341:LEU:HD12	1:B:375:ARG:NH1	2.27	0.50
1:B:322:LEU:CD1	1:B:326:GLU:CD	2.80	0.50
1:B:313:MET:CE	1:B:341:LEU:CD1	2.83	0.49
1:A:250:ILE:HD12	1:B:250:ILE:CD1	2.41	0.49
1:B:87:PHE:CE2	1:B:96:THR:HG21	2.47	0.49
1:B:153:LEU:HD11	1:B:185:VAL:HG23	1.92	0.49
1:B:136:ASP:OD2	1:B:138:SER:OG	2.26	0.49
1:D:350:LEU:HD23	1:D:353[B]:ILE:HD12	1.93	0.49
1:B:23:ILE:HA	1:B:260:LYS:HD3	1.95	0.49
1:D:23:ILE:HA	1:D:260:LYS:HD3	1.94	0.49
1:B:167:ILE:CD1	1:B:167:ILE:N	2.76	0.49
1:A:41:ILE:HD13	1:A:250:ILE:HG12	1.93	0.48
1:C:327:ILE:HA	1:C:330:LYS:HE2	1.95	0.48
1:A:212:LYS:HD2	1:A:341:LEU:HG	1.95	0.48
1:B:140:ILE:HD11	7:B:524:HOH:O	2.13	0.48
1:A:140:ILE:HD11	1:A:168:ASP:HB3	1.94	0.48
1:B:176:VAL:HG13	1:B:182:ILE:CG2	2.44	0.48
1:D:339:GLU:OE2	4:D:501:2AG:N	2.47	0.47
1:B:190:PHE:CE2	1:B:341:LEU:CD2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ILE:HD12	1:B:132:ILE:CD1	2.45	0.47
1:D:81:ALA:HB2	1:D:199:LEU:CD1	2.45	0.47
1:D:251:ASP:OD1	5:D:605:GOL:O1	2.32	0.46
1:C:249:PRO:HD3	5:D:605:GOL:H12	1.97	0.46
1:A:81:ALA:HB2	1:A:199:LEU:HD12	1.98	0.46
1:B:329:LEU:CD1	1:B:350:LEU:HB2	2.38	0.46
1:D:268:LYS:HA	1:D:271:LYS:CE	2.46	0.46
1:C:106:GLN:OE1	1:C:151:THR:OG1	2.22	0.46
1:B:92:ALA:HB1	1:B:245:ALA:HB1	1.98	0.46
1:D:266:MET:HE1	1:D:311:THR:HG22	1.97	0.46
1:B:375:ARG:HG2	1:B:375:ARG:HH11	1.81	0.45
1:B:177:HIS:HE1	1:B:202:GLY:O	1.99	0.45
1:A:65:ASN:HD22	1:A:66:PRO:HD2	1.80	0.45
1:D:91:LEU:O	1:D:95:VAL:HG23	2.16	0.45
1:D:92:ALA:HB1	1:D:245:ALA:HB1	1.98	0.45
1:B:175:ILE:O	1:B:179:HIS:HD2	2.00	0.45
1:A:299:GLN:CA	6:A:609:PEG:H32	2.45	0.45
1:B:344:PHE:CZ	1:C:260:LYS:HD2	2.52	0.45
1:C:339:GLU:OE1	4:C:501:2AG:N	2.41	0.45
1:D:350:LEU:HD23	1:D:353[A]:ILE:HD11	1.99	0.45
1:D:268:LYS:HA	1:D:271:LYS:HE2	1.99	0.45
1:B:313:MET:HE1	1:B:341:LEU:HD11	1.94	0.45
1:D:106:GLN:HG2	1:D:107:ILE:N	2.32	0.44
1:A:153:LEU:HD11	1:A:185:VAL:HG23	2.00	0.44
1:C:167:ILE:N	1:C:167:ILE:HD12	2.33	0.44
1:D:165:LYS:HD2	7:D:853:HOH:O	2.17	0.44
1:C:373:LEU:C	1:C:373:LEU:HD23	2.39	0.44
1:D:101:LEU:HD22	1:D:152:LYS:HB3	1.99	0.43
1:C:140:ILE:HB	1:C:175:ILE:HD11	1.99	0.43
1:B:54[A]:GLN:NE2	1:B:54[A]:GLN:H	2.03	0.43
1:C:81:ALA:HB2	1:C:199:LEU:CD1	2.49	0.43
1:A:92:ALA:HB1	1:A:245:ALA:HB1	2.00	0.43
1:B:153:LEU:HD11	1:B:185:VAL:CG2	2.49	0.43
1:C:353:ILE:CG2	1:D:53:GLY:HA3	2.48	0.43
1:A:191:MET:HA	1:A:311:THR:HG21	1.99	0.43
1:A:353:ILE:CG2	1:B:53:GLY:HA3	2.49	0.43
1:C:106:GLN:HG2	1:C:107:ILE:N	2.33	0.43
1:D:111:ASP:OD2	1:D:165:LYS:NZ	2.51	0.43
1:B:81:ALA:HB2	1:B:199:LEU:CD1	2.49	0.43
1:B:313:MET:HE1	1:B:341:LEU:CD1	2.49	0.42
1:B:136:ASP:HB3	1:B:142:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:CB	1:B:142:LEU:HD12	2.45	0.42
1:C:140:ILE:HB	1:C:175:ILE:CD1	2.49	0.42
1:A:172:CYS:O	1:A:176:VAL:HG23	2.19	0.42
1:D:32:TRP:HB3	5:D:604:GOL:H31	2.01	0.42
1:B:341:LEU:CD2	1:B:342:GLY:N	2.64	0.42
1:B:136:ASP:OD2	1:B:136:ASP:C	2.57	0.42
1:D:364:ARG:HG2	1:D:369:ILE:HB	2.02	0.42
1:C:322:LEU:CD1	1:C:350:LEU:HD21	2.49	0.41
1:A:91:LEU:HD12	1:B:62:ARG:CZ	2.50	0.41
1:B:195:PHE:HA	1:B:308:THR:OG1	2.20	0.41
1:D:391:ASP:OD2	1:D:395:LYS:HE2	2.21	0.41
1:A:353:ILE:HG22	1:B:53:GLY:HA3	2.01	0.41
1:D:350:LEU:HD23	1:D:353[A]:ILE:CD1	2.50	0.41
1:B:317:TYR:CZ	1:B:373:LEU:HD12	2.56	0.41
1:A:243:LEU:HD21	1:B:124:VAL:HG11	2.03	0.41
1:B:110:MET:HG3	1:B:156:ILE:HG22	2.03	0.41
1:A:189:THR:HB	3:A:500:PLP:H2A2	2.02	0.41
1:A:268:LYS:HB3	1:A:380:LEU:HD22	2.02	0.41
1:C:249:PRO:CD	5:D:605:GOL:H12	2.51	0.41
1:B:188:ASN:HB3	1:B:208:TYR:CE2	2.57	0.40
1:D:205:ILE:HG23	1:D:225:VAL:HG13	2.03	0.40
1:B:158:THR:HA	1:B:159:PRO:C	2.41	0.40
1:A:292:PRO:HB3	1:A:303:VAL:HG21	2.04	0.40
1:B:190:PHE:O	1:B:311:THR:HG21	2.20	0.40
1:D:106:GLN:OE1	1:D:151:THR:OG1	2.32	0.40
1:D:221:VAL:H	5:D:605:GOL:C1	2.34	0.40
1:B:45:THR:HA	1:B:61:SER:HB2	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	373/403 (93%)	365 (98%)	8 (2%)	0	100	100
1	B	370/403 (92%)	361 (98%)	8 (2%)	1 (0%)	46	41
1	C	387/403 (96%)	378 (98%)	9 (2%)	0	100	100
1	D	392/403 (97%)	380 (97%)	11 (3%)	1 (0%)	46	41
All	All	1522/1612 (94%)	1484 (98%)	36 (2%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	LYS
1	D	55	HIS

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	321/342 (94%)	311 (97%)	10 (3%)	47	46
1	B	317/342 (93%)	308 (97%)	9 (3%)	51	50
1	C	332/342 (97%)	323 (97%)	9 (3%)	52	52
1	D	334/342 (98%)	323 (97%)	11 (3%)	45	43
All	All	1304/1368 (95%)	1265 (97%)	39 (3%)	51	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	152	LYS
1	A	178	LYS
1	A	250	ILE
1	A	256	ASN
1	A	259	LEU
1	A	345	GLU
1	A	349	GLU
1	A	361	LYS

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Mol	Chain	Res	Type
1	A	384	GLU
1	B	16	GLN
1	B	54[A]	GLN
1	B	54[B]	GLN
1	B	142	LEU
1	B	212	LYS
1	B	256	ASN
1	B	302	LEU
1	B	344	PHE
1	B	388	GLU
1	C	131	LYS
1	C	253[A]	TYR
1	C	253[B]	TYR
1	C	256	ASN
1	C	271	LYS
1	C	330	LYS
1	C	344	PHE
1	C	345	GLU
1	C	349	GLU
1	D	54	GLN
1	D	152	LYS
1	D	162	PRO
1	D	256	ASN
1	D	259	LEU
1	D	260	LYS
1	D	341	LEU
1	D	345	GLU
1	D	349	GLU
1	D	373	LEU
1	D	384	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	49	GLN
1	A	65	ASN
1	A	106	GLN
1	A	278	GLN
1	B	164	GLN
1	B	179	HIS
1	B	278	GLN

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Mol	Chain	Res	Type
1	C	241	ASN
1	D	16	GLN
1	D	362	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 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	PLP	A	500	1	15,15,16	1.23	2 (13%)	21,22,23	1.34	3 (14%)
4	2AG	A	501	1	4,7,7	1.11	0	2,8,8	0.68	0
5	GOL	A	603	-	5,5,5	0.33	0	5,5,5	0.37	0
2	NO3	A	608	-	3,3,3	3.01	3 (100%)	3,3,3	0.06	0
6	PEG	A	609	-	6,6,6	0.60	0	5,5,5	0.45	0
3	PLP	C	500	1	15,15,16	1.12	1 (6%)	21,22,23	1.23	1 (4%)
4	2AG	C	501	1	4,7,7	1.07	0	2,8,8	0.64	0
5	GOL	C	602	-	5,5,5	0.30	0	5,5,5	0.41	0
2	NO3	C	606	-	3,3,3	2.97	3 (100%)	3,3,3	0.45	0
3	PLP	D	500	1	15,15,16	1.06	1 (6%)	21,22,23	1.41	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2AG	D	501	1	4,7,7	1.21	0	2,8,8	0.26	0
5	GOL	D	601	-	5,5,5	0.42	0	5,5,5	0.38	0
5	GOL	D	604	-	5,5,5	0.48	0	5,5,5	0.85	0
5	GOL	D	605	-	5,5,5	0.48	0	5,5,5	0.77	0
2	NO3	D	607	-	3,3,3	2.83	3 (100%)	3,3,3	0.73	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
3	PLP	A	500	1	-	0/6/6/8	0/1/1/1
4	2AG	A	501	1	-	0/3/7/7	0/0/0/0
5	GOL	A	603	-	-	0/4/4/4	0/0/0/0
2	NO3	A	608	-	-	0/0/0/0	0/0/0/0
6	PEG	A	609	-	-	0/4/4/4	0/0/0/0
3	PLP	C	500	1	-	0/6/6/8	0/1/1/1
4	2AG	C	501	1	-	0/3/7/7	0/0/0/0
5	GOL	C	602	-	-	0/4/4/4	0/0/0/0
2	NO3	C	606	-	-	0/0/0/0	0/0/0/0
3	PLP	D	500	1	-	0/6/6/8	0/1/1/1
4	2AG	D	501	1	-	0/3/7/7	0/0/0/0
5	GOL	D	601	-	-	0/4/4/4	0/0/0/0
5	GOL	D	604	-	-	0/4/4/4	0/0/0/0
5	GOL	D	605	-	-	0/4/4/4	0/0/0/0
2	NO3	D	607	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	PLP	C6-N1	2.13	1.39	1.34
3	D	500	PLP	C6-N1	2.41	1.39	1.34
3	C	500	PLP	C6-N1	2.42	1.39	1.34
2	A	608	NO3	O2-N	2.49	1.38	1.25
2	C	606	NO3	O2-N	2.65	1.39	1.25
2	D	607	NO3	O3-N	2.67	1.39	1.25
2	A	608	NO3	O3-N	2.72	1.39	1.25
3	A	500	PLP	C2-N1	2.74	1.39	1.34
2	C	606	NO3	O3-N	2.76	1.39	1.25
2	D	607	NO3	O2-N	2.83	1.40	1.25
2	D	607	NO3	O1-N	2.98	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	606	NO3	O1-N	3.44	1.38	1.24
2	A	608	NO3	O1-N	3.69	1.39	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	PLP	C2A-C2-C3	-3.55	116.76	121.04
3	D	500	PLP	C4A-C4-C5	-2.91	117.85	120.88
3	A	500	PLP	C4A-C4-C3	-2.24	116.29	120.36
3	C	500	PLP	O4P-C5A-C5	2.44	113.03	108.99
3	A	500	PLP	C2A-C2-N1	2.53	123.55	117.95
3	D	500	PLP	O4P-C5A-C5	3.27	114.40	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	PLP	1	0
5	A	603	GOL	1	0
6	A	609	PEG	3	0
4	C	501	2AG	1	0
5	C	602	GOL	1	0
4	D	501	2AG	1	0
5	D	604	GOL	1	0
5	D	605	GOL	9	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	376/403 (93%)	-0.47	4 (1%) 82 83	8, 17, 31, 42	0
1	B	373/403 (92%)	-0.16	15 (4%) 42 44	9, 19, 37, 43	0
1	C	390/403 (96%)	-0.55	6 (1%) 76 77	7, 14, 26, 42	0
1	D	392/403 (97%)	-0.57	4 (1%) 84 84	8, 14, 25, 41	0
All	All	1531/1612 (94%)	-0.44	29 (1%) 70 70	7, 15, 31, 43	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	LEU	8.4
1	D	55	HIS	7.9
1	B	55	HIS	7.4
1	D	56	SER	5.0
1	A	49	GLN	4.9
1	B	56	SER	4.5
1	B	53	GLY	4.3
1	B	54[A]	GLN	3.8
1	A	179	HIS	3.7
1	A	64	GLY	3.6
1	B	342	GLY	3.5
1	B	351	PRO	3.5
1	C	53	GLY	3.0
1	B	57	GLY	3.0
1	C	57	GLY	3.0
1	C	179	HIS	2.8
1	D	54	GLN	2.8
1	B	339	GLU	2.7
1	B	371	ASP	2.6
1	D	53	GLY	2.6
1	C	54	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	140	ILE	2.4
1	A	362	ASN	2.3
1	B	350	LEU	2.2
1	B	140	ILE	2.1
1	B	141	LYS	2.1
1	C	35	ARG	2.0
1	B	400	PRO	2.0
1	B	370	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	D	605	6/6	0.92	0.27	15.58	30,34,34,34	0
5	GOL	D	604	6/6	0.89	0.22	9.18	17,23,24,26	0
6	PEG	A	609	7/7	0.56	0.31	6.85	38,39,40,41	0
3	PLP	A	500	15/16	0.95	0.15	5.08	18,21,23,24	0
4	2AG	A	501	8/8	0.86	0.17	3.85	31,33,34,34	0
2	NO3	D	607	4/4	0.98	0.11	2.17	18,19,19,22	0
4	2AG	D	501	8/8	0.91	0.13	2.09	18,23,25,25	0
3	PLP	D	500	15/16	0.98	0.10	1.77	12,15,18,18	0
2	NO3	C	606	4/4	0.97	0.09	0.86	13,13,14,17	0
4	2AG	C	501	8/8	0.97	0.10	0.77	20,22,23,23	0
3	PLP	C	500	15/16	0.98	0.08	0.67	11,12,14,15	0
5	GOL	C	602	6/6	0.96	0.11	0.60	28,29,30,30	0
2	NO3	A	608	4/4	0.98	0.09	0.29	22,22,23,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	603	6/6	0.92	0.10	-0.41	28,32,33,34	0
5	GOL	D	601	6/6	0.97	0.08	-0.61	25,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.