Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 02:15 PM JST

PDB ID	:	6JC9
Title	:	Crystal structure of aminotransferase CrmG from Actinoalloteichus sp. WH1-2216-6 in complex with amino donor L-Gln
Authors	:	Xu, J.; Liu, J.
Deposited on	:	2019-01-28
Resolution	:	2.35 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:

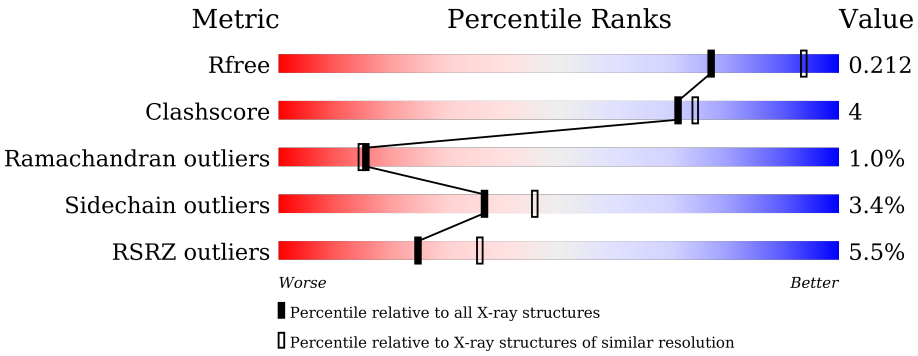
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	523	5% 85% 11%
1	B	523	6% 86% 11%
1	C	523	5% 88% 9%
1	D	523	6% 86% 10%

2 Entry composition

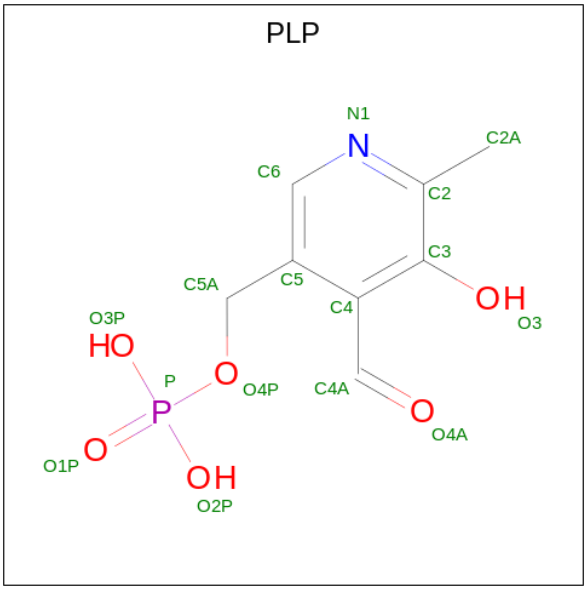
There are 6 unique types of molecules in this entry. The entry contains 16297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CrmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3958	2476	716	755	11			
1	B	512	Total	C	N	O	S	0	0	0
			3958	2476	716	755	11			
1	C	512	Total	C	N	O	S	0	0	0
			3958	2476	716	755	11			
1	D	508	Total	C	N	O	S	0	0	0
			3930	2460	711	748	11			

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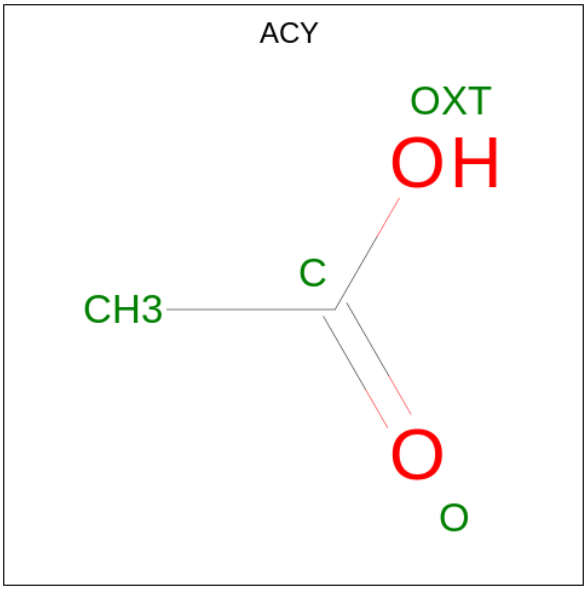
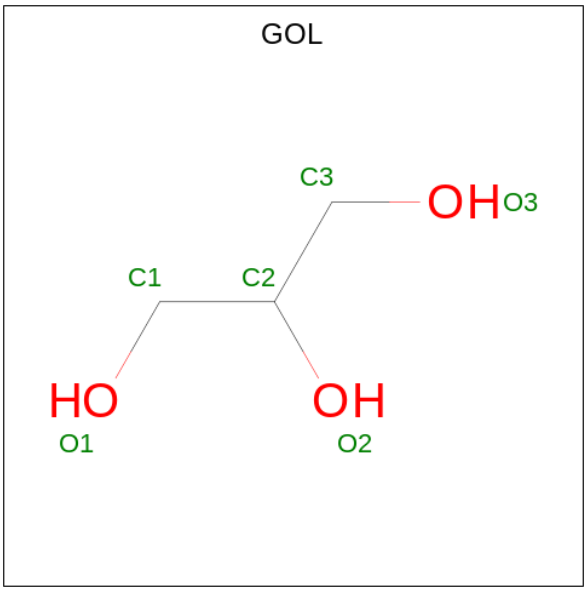
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



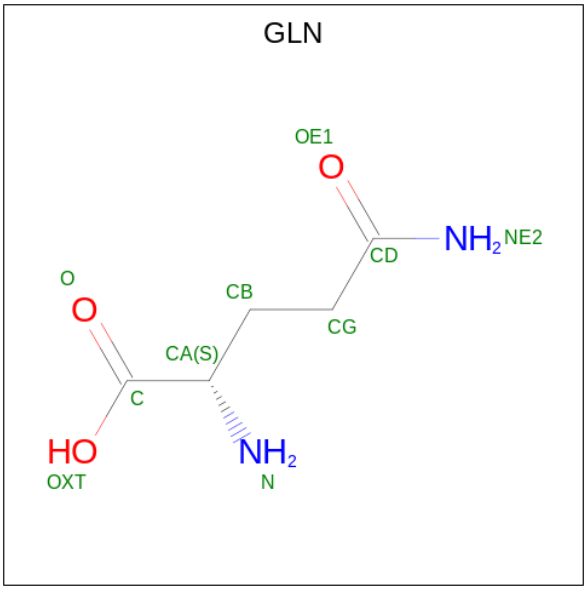
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	10	5	2	3	0	0

- Molecule 6 is water.

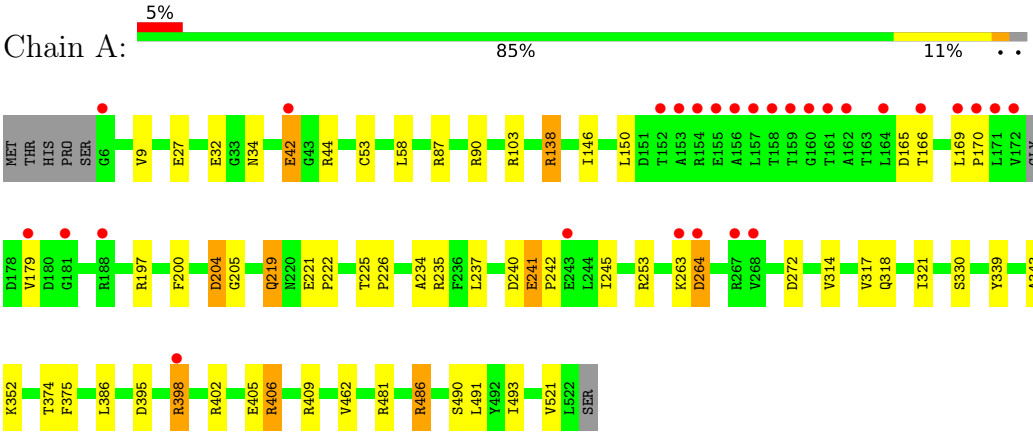
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	101	Total O 101 101	0	0
6	B	97	Total O 97 97	0	0
6	C	103	Total O 103 103	0	0
6	D	112	Total O 112 112	0	0

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.

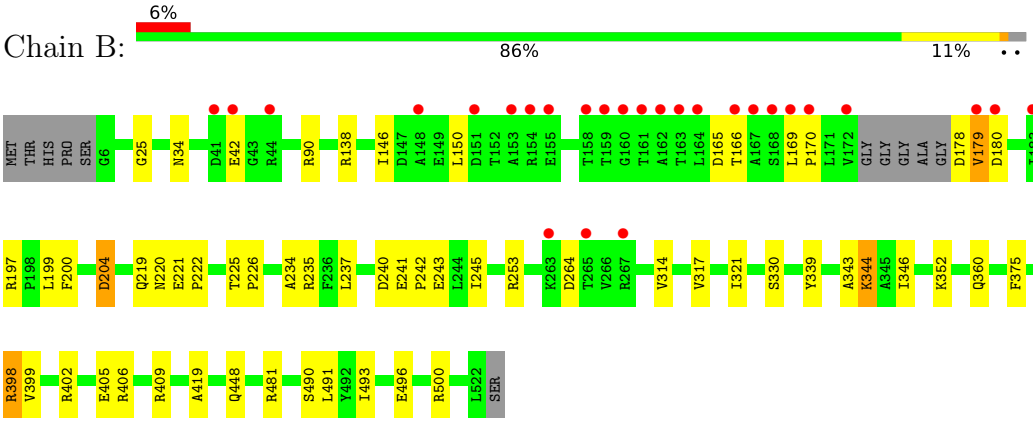
- Molecule 1: CrmG

Chain A:



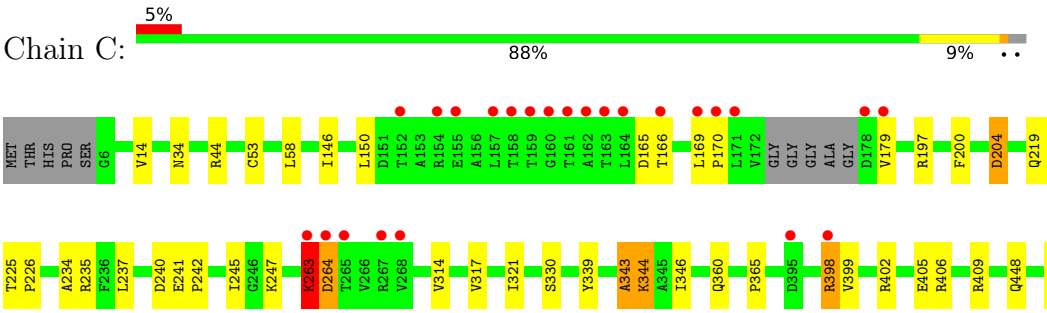
- Molecule 1: CrmG

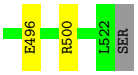
Chain B:



- Molecule 1: CrmG

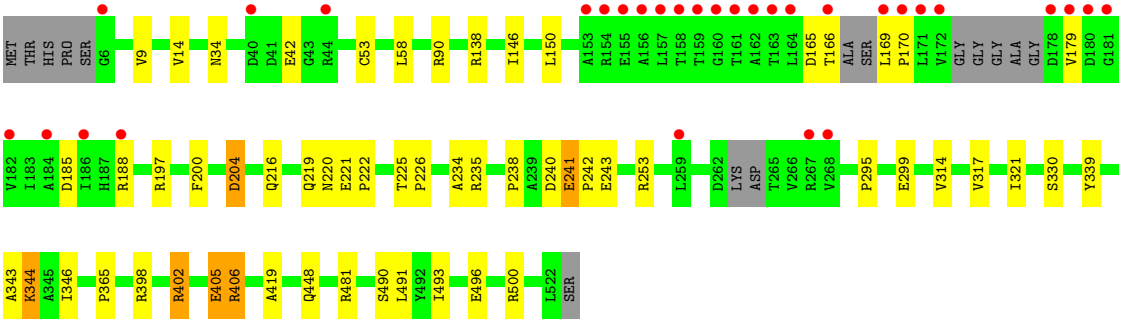
Chain C:





• Molecule 1: CrmG

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.04Å 83.88Å 88.41Å 106.48° 109.17° 94.98°	Depositor
Resolution (Å)	50.59 – 2.35 50.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.59-2.35) 91.2 (50.58-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.207 0.180 , 0.212	Depositor DCC
R_{free} test set	3992 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.117 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16297	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, ACY, 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	0.71	1/4025 (0.0%)	0.86	3/5453 (0.1%)
1	B	0.71	0/4025	0.86	6/5453 (0.1%)
1	C	0.71	0/4025	0.85	4/5453 (0.1%)
1	D	0.71	0/3995	0.85	4/5410 (0.1%)
All	All	0.71	1/16070 (0.0%)	0.86	17/21769 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	27	GLU	CD-OE1	-5.70	1.19	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	406	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	B	481	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	406	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	406	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	A	339	TYR	CB-CG-CD1	6.33	124.80	121.00
1	B	339	TYR	CB-CG-CD1	6.31	124.78	121.00
1	D	406	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	C	339	TYR	CB-CG-CD1	6.27	124.76	121.00
1	C	406	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	D	339	TYR	CB-CG-CD1	6.14	124.69	121.00
1	B	481	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	406	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	D	406	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	C	406	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	339	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	D	339	TYR	CB-CG-CD2	-5.13	117.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	TYR	CB-CG-CD2	-5.06	117.96	121.00

There are no chirality outliers.

There are no planarity outliers.

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	3958	0	3934	34	0
1	B	3958	0	3934	29	0
1	C	3958	0	3934	24	0
1	D	3930	0	3905	33	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	6	0	0
3	B	4	0	3	0	0
4	C	6	0	8	0	0
5	C	10	0	7	0	0
6	A	101	0	0	1	0
6	B	97	0	0	3	0
6	C	103	0	0	1	0
6	D	112	0	0	5	0
All	All	16297	0	15749	112	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 (112) 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:205:GLY:H	1:A:219:GLN:HE21	1.24	0.84
1:C:240:ASP:O	1:C:242:PRO:HD3	1.80	0.81
1:A:240:ASP:O	1:A:242:PRO:HD3	1.81	0.81
1:B:240:ASP:O	1:B:242:PRO:HD3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ASP:O	1:D:242:PRO:HD3	1.82	0.79
1:B:390:GLU:OE2	6:B:701:HOH:O	2.04	0.75
1:D:481:ARG:HD3	6:D:706:HOH:O	1.88	0.72
1:A:344:LYS:O	6:A:701:HOH:O	2.11	0.67
1:B:496:GLU:OE1	1:B:500:ARG:NH2	2.28	0.66
1:D:405:GLU:OE2	1:D:406:ARG:HD2	1.96	0.65
1:D:496:GLU:OE1	1:D:500:ARG:NH2	2.29	0.64
1:D:405:GLU:OE2	1:D:406:ARG:CD	2.47	0.62
1:D:90:ARG:HD2	6:D:743:HOH:O	2.00	0.62
1:C:34:ASN:ND2	1:C:490:SER:OG	2.34	0.60
1:A:169:LEU:N	1:A:170:PRO:HD2	2.17	0.60
1:A:34:ASN:ND2	1:A:490:SER:OG	2.34	0.59
1:A:314:VAL:HG11	1:A:330:SER:HB3	1.85	0.59
1:D:169:LEU:N	1:D:170:PRO:HD2	2.17	0.59
1:D:419:ALA:O	6:D:702:HOH:O	2.17	0.59
1:C:169:LEU:N	1:C:170:PRO:HD2	2.17	0.59
1:B:169:LEU:N	1:B:170:PRO:HD2	2.17	0.58
1:A:205:GLY:N	1:A:219:GLN:HE21	1.99	0.58
1:A:204:ASP:HA	1:A:219:GLN:NE2	2.20	0.57
1:D:34:ASN:ND2	1:D:490:SER:OG	2.37	0.57
1:B:34:ASN:ND2	1:B:490:SER:OG	2.36	0.57
1:C:402:ARG:HD2	1:C:491:LEU:HD13	1.87	0.57
1:B:314:VAL:HG11	1:B:330:SER:HB3	1.88	0.55
1:C:314:VAL:HG11	1:C:330:SER:HB3	1.87	0.55
1:A:318:GLN:OE1	1:A:486:ARG:NH1	2.39	0.54
1:B:138:ARG:NE	6:B:704:HOH:O	2.36	0.54
1:D:314:VAL:HG11	1:D:330:SER:HB3	1.88	0.54
1:A:402:ARG:HD2	1:A:491:LEU:HD13	1.90	0.53
1:B:146:ILE:O	1:B:150:LEU:HG	2.09	0.53
1:C:146:ILE:O	1:C:150:LEU:HG	2.09	0.53
1:D:146:ILE:O	1:D:150:LEU:HG	2.09	0.53
1:D:216:GLN:NE2	6:D:701:HOH:O	2.16	0.52
1:A:146:ILE:O	1:A:150:LEU:HG	2.09	0.52
1:D:343:ALA:O	1:D:346:ILE:HG22	2.10	0.52
1:A:9:VAL:O	1:B:360:GLN:NE2	2.42	0.51
1:A:90:ARG:HD3	1:A:386:LEU:HD12	1.93	0.51
1:A:42:GLU:HG3	1:A:44:ARG:HH11	1.76	0.50
1:A:343:ALA:O	1:A:346:ILE:HG22	2.11	0.50
1:B:419:ALA:O	6:B:702:HOH:O	2.20	0.49
1:C:343:ALA:O	1:C:346:ILE:HG22	2.13	0.49
1:D:138:ARG:HG2	1:D:138:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HH21	1:A:138:ARG:HG2	1.78	0.49
1:C:344:LYS:O	6:C:701:HOH:O	2.19	0.49
1:B:343:ALA:O	1:B:346:ILE:HG22	2.12	0.49
1:A:225:THR:N	1:A:226:PRO:CD	2.77	0.48
1:D:225:THR:N	1:D:226:PRO:CD	2.77	0.48
1:D:405:GLU:OE2	1:D:406:ARG:HD3	2.14	0.47
1:D:200:PHE:O	1:D:234:ALA:HA	2.16	0.46
1:B:225:THR:N	1:B:226:PRO:CD	2.78	0.46
1:C:225:THR:N	1:C:226:PRO:CD	2.79	0.46
1:B:179:VAL:HG13	1:B:180:ASP:H	1.81	0.45
1:B:398:ARG:HG3	1:B:399:VAL:N	2.31	0.45
1:B:264:ASP:OD1	1:B:264:ASP:N	2.44	0.45
1:B:200:PHE:O	1:B:234:ALA:HA	2.17	0.45
1:D:238:PRO:HB2	1:D:241:GLU:HG2	1.99	0.44
1:C:165:ASP:OD1	1:C:166:THR:N	2.51	0.44
1:C:398:ARG:HG3	1:C:399:VAL:N	2.32	0.44
1:A:200:PHE:O	1:A:234:ALA:HA	2.16	0.44
1:B:204:ASP:HA	1:B:219:GLN:OE1	2.19	0.43
1:C:200:PHE:O	1:C:234:ALA:HA	2.18	0.43
1:A:395:ASP:OD2	1:A:398:ARG:HD2	2.19	0.43
1:A:138:ARG:HH21	1:A:138:ARG:CG	2.31	0.43
1:A:165:ASP:OD1	1:A:166:THR:N	2.51	0.43
1:A:352:LYS:HD3	1:B:375:PHE:HB3	2.00	0.43
1:B:90:ARG:HD3	1:B:386:LEU:HD12	2.00	0.43
1:B:317:VAL:HG13	1:B:343:ALA:HB3	2.01	0.43
1:C:14:VAL:HG21	1:D:365:PRO:CB	2.48	0.43
1:A:375:PHE:HB3	1:B:352:LYS:HD3	2.01	0.43
1:D:185:ASP:OD1	1:D:188:ARG:NH2	2.52	0.43
1:B:165:ASP:OD1	1:B:166:THR:N	2.52	0.42
1:A:395:ASP:O	1:A:398:ARG:NH1	2.50	0.42
1:C:491:LEU:C	1:C:491:LEU:HD12	2.39	0.42
1:D:165:ASP:OD1	1:D:166:THR:N	2.52	0.42
1:D:402:ARG:HH21	1:D:402:ARG:CG	2.32	0.42
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.84	0.42
1:C:365:PRO:CB	1:D:14:VAL:HG21	2.49	0.42
1:B:402:ARG:CD	1:B:491:LEU:HD13	2.50	0.42
1:C:317:VAL:HG13	1:C:343:ALA:HB3	2.02	0.42
1:D:221:GLU:N	1:D:222:PRO:HD2	2.35	0.42
1:C:237:LEU:HB3	1:C:245:ILE:HG12	2.02	0.42
1:A:317:VAL:HG13	1:A:343:ALA:HB3	2.02	0.42
1:A:405:GLU:OE2	1:A:406:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:NH1	1:B:25:GLY:O	2.53	0.41
1:D:491:LEU:HD12	1:D:491:LEU:C	2.41	0.41
1:B:237:LEU:HB3	1:B:245:ILE:HG12	2.02	0.41
1:D:344:LYS:O	6:D:703:HOH:O	2.22	0.41
1:C:496:GLU:OE1	1:C:500:ARG:NH1	2.47	0.41
1:A:53:CYS:HB3	1:A:58:LEU:HB2	2.03	0.41
1:A:204:ASP:HA	1:A:219:GLN:HE22	1.85	0.41
1:B:221:GLU:N	1:B:222:PRO:HD2	2.35	0.41
1:D:295:PRO:O	1:D:299:GLU:HG2	2.20	0.41
1:A:221:GLU:N	1:A:222:PRO:HD2	2.35	0.41
1:B:491:LEU:HD12	1:B:491:LEU:C	2.41	0.41
1:C:204:ASP:HA	1:C:219:GLN:OE1	2.20	0.41
1:C:221:GLU:N	1:C:222:PRO:HD2	2.36	0.41
1:D:53:CYS:HB3	1:D:58:LEU:HB2	2.02	0.41
1:D:317:VAL:HG13	1:D:343:ALA:HB3	2.03	0.41
1:A:237:LEU:HB3	1:A:245:ILE:HG12	2.03	0.41
1:A:374:THR:HG21	1:B:344:LYS:HD3	2.02	0.41
1:C:360:GLN:NE2	1:D:9:VAL:O	2.49	0.41
1:A:462:VAL:HG11	1:A:521:VAL:HG22	2.03	0.41
1:C:263:LYS:H	1:C:263:LYS:HD2	1.86	0.40
1:D:165:ASP:OD1	1:D:165:ASP:C	2.60	0.40
1:D:204:ASP:HA	1:D:219:GLN:OE1	2.21	0.40
1:A:491:LEU:HD12	1:A:491:LEU:C	2.42	0.40
1:D:138:ARG:HH21	1:D:138:ARG:CG	2.34	0.40
1:C:165:ASP:OD1	1:C:165:ASP:C	2.59	0.40
1:C:53:CYS:HB3	1:C:58:LEU: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	508/523 (97%)	490 (96%)	13 (3%)	5 (1%)	15 15
1	B	508/523 (97%)	492 (97%)	12 (2%)	4 (1%)	19 20
1	C	508/523 (97%)	491 (97%)	10 (2%)	7 (1%)	11 9
1	D	500/523 (96%)	486 (97%)	10 (2%)	4 (1%)	19 20
All	All	2024/2092 (97%)	1959 (97%)	45 (2%)	20 (1%)	15 15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LYS
1	C	263	LYS
1	A	179	VAL
1	A	264	ASP
1	B	179	VAL
1	C	179	VAL
1	C	264	ASP
1	D	179	VAL
1	B	344	LYS
1	A	344	LYS
1	B	220	ASN
1	B	241	GLU
1	C	220	ASN
1	C	241	GLU
1	C	344	LYS
1	A	241	GLU
1	C	343	ALA
1	D	220	ASN
1	D	344	LYS
1	D	241	GLU

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	416/422 (99%)	398 (96%)	18 (4%)	29 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	416/422 (99%)	403 (97%)	13 (3%)	40	48
1	C	416/422 (99%)	403 (97%)	13 (3%)	40	48
1	D	413/422 (98%)	401 (97%)	12 (3%)	42	52
All	All	1661/1688 (98%)	1605 (97%)	56 (3%)	37	46

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	42	GLU
1	A	103	ARG
1	A	138	ARG
1	A	197	ARG
1	A	204	ASP
1	A	219	GLN
1	A	235	ARG
1	A	241	GLU
1	A	253	ARG
1	A	264	ASP
1	A	272	ASP
1	A	321	ILE
1	A	398	ARG
1	A	409	ARG
1	A	481	ARG
1	A	486	ARG
1	A	493	ILE
1	B	42	GLU
1	B	178	ASP
1	B	197	ARG
1	B	204	ASP
1	B	235	ARG
1	B	243	GLU
1	B	253	ARG
1	B	321	ILE
1	B	398	ARG
1	B	405	GLU
1	B	409	ARG
1	B	448	GLN
1	B	493	ILE
1	C	44	ARG
1	C	197	ARG

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Mol	Chain	Res	Type
1	C	204	ASP
1	C	235	ARG
1	C	247	LYS
1	C	263	LYS
1	C	264	ASP
1	C	321	ILE
1	C	398	ARG
1	C	405	GLU
1	C	409	ARG
1	C	448	GLN
1	C	493	ILE
1	D	42	GLU
1	D	197	ARG
1	D	204	ASP
1	D	235	ARG
1	D	243	GLU
1	D	253	ARG
1	D	321	ILE
1	D	398	ARG
1	D	402	ARG
1	D	405	GLU
1	D	448	GLN
1	D	493	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	88	GLN
1	A	219	GLN
1	B	34	ASN
1	C	34	ASN
1	D	34	ASN
1	D	88	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACY	B	602	-	3,3,3	1.20	0	3,3,3	0.59	0
4	GOL	C	602	-	5,5,5	0.12	0	5,5,5	0.45	0
2	PLP	C	601	1	15,15,16	0.83	0	20,22,23	1.52	2 (10%)
2	PLP	D	601	1	15,15,16	0.74	0	20,22,23	1.22	1 (5%)
2	PLP	A	601	1	15,15,16	0.80	1 (6%)	20,22,23	1.61	2 (10%)
5	GLN	C	603	-	8,9,9	0.56	0	10,11,11	1.41	2 (20%)
2	PLP	B	601	1	15,15,16	0.68	0	20,22,23	1.03	1 (5%)

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	GOL	C	602	-	-	2/4/4/4	-
2	PLP	C	601	1	-	0/6/6/8	0/1/1/1
2	PLP	D	601	1	-	0/6/6/8	0/1/1/1
2	PLP	A	601	1	-	0/6/6/8	0/1/1/1
5	GLN	C	603	-	-	3/9/9/9	-
2	PLP	B	601	1	-	0/6/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	PLP	C4A-C4	-2.15	1.47	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	PLP	C4A-C4-C5	5.54	126.64	120.94
2	C	601	PLP	C4A-C4-C5	4.49	125.56	120.94
2	D	601	PLP	C4A-C4-C5	3.42	124.46	120.94
2	B	601	PLP	C4A-C4-C5	2.97	124.00	120.94
5	C	603	GLN	OXT-C-O	-2.82	117.69	124.09
5	C	603	GLN	OXT-C-CA	2.74	122.70	113.38
2	A	601	PLP	C4A-C4-C3	-2.28	116.64	120.50
2	C	601	PLP	O4P-C5A-C5	2.17	113.49	109.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	602	GOL	C1-C2-C3-O3
5	C	603	GLN	CA-CB-CG-CD
4	C	602	GOL	O2-C2-C3-O3
5	C	603	GLN	O-C-CA-CB
5	C	603	GLN	OXT-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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	512/523 (97%)	-0.04	28 (5%)	25	36	17, 32, 69, 83	0
1	B	512/523 (97%)	0.08	29 (5%)	23	34	17, 32, 71, 99	0
1	C	512/523 (97%)	-0.05	24 (4%)	31	44	19, 32, 68, 91	0
1	D	508/523 (97%)	0.15	31 (6%)	21	31	17, 31, 75, 99	0
All	All	2044/2092 (97%)	0.03	112 (5%)	25	36	17, 32, 70, 99	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	159	THR	6.2
1	A	161	THR	5.9
1	D	164	LEU	5.5
1	C	159	THR	5.5
1	D	181	GLY	5.0
1	A	159	THR	4.9
1	B	179	VAL	4.8
1	C	154	ARG	4.7
1	B	170	PRO	4.6
1	A	169	LEU	4.6
1	D	158	THR	4.5
1	D	157	LEU	4.5
1	C	161	THR	4.4
1	A	160	GLY	4.4
1	B	160	GLY	4.3
1	D	172	VAL	4.3
1	D	179	VAL	4.3
1	A	179	VAL	4.3
1	B	172	VAL	4.2
1	B	263	LYS	4.2
1	C	179	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	182	VAL	4.0
1	C	155	GLU	4.0
1	B	44	ARG	4.0
1	A	157	LEU	4.0
1	B	154	ARG	3.9
1	D	170	PRO	3.9
1	C	170	PRO	3.8
1	B	166	THR	3.8
1	C	166	THR	3.8
1	D	161	THR	3.8
1	D	163	THR	3.8
1	D	154	ARG	3.8
1	A	170	PRO	3.7
1	A	263	LYS	3.7
1	D	171	LEU	3.6
1	D	186	ILE	3.6
1	D	169	LEU	3.6
1	B	155	GLU	3.5
1	B	161	THR	3.4
1	C	160	GLY	3.4
1	D	180	ASP	3.4
1	C	162	ALA	3.4
1	C	158	THR	3.3
1	A	166	THR	3.3
1	D	153	ALA	3.3
1	D	155	GLU	3.3
1	A	158	THR	3.3
1	B	169	LEU	3.3
1	B	42	GLU	3.2
1	B	180	ASP	3.2
1	A	162	ALA	3.1
1	D	268	VAL	3.0
1	B	168	SER	3.0
1	A	155	GLU	3.0
1	C	263	LYS	3.0
1	A	164	LEU	3.0
1	B	151	ASP	3.0
1	C	264	ASP	3.0
1	B	159	THR	3.0
1	C	164	LEU	2.9
1	B	162	ALA	2.9
1	B	163	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	164	LEU	2.9
1	A	172	VAL	2.8
1	C	268	VAL	2.8
1	C	267	ARG	2.7
1	A	264	ASP	2.7
1	A	154	ARG	2.7
1	A	268	VAL	2.7
1	B	41	ASP	2.7
1	C	157	LEU	2.7
1	D	160	GLY	2.7
1	C	169	LEU	2.6
1	C	398	ARG	2.6
1	C	265	THR	2.6
1	B	167	ALA	2.6
1	D	184	ALA	2.6
1	D	156	ALA	2.5
1	B	183	ILE	2.5
1	B	265	THR	2.5
1	D	44	ARG	2.5
1	A	153	ALA	2.5
1	A	6	GLY	2.5
1	A	156	ALA	2.5
1	C	152	THR	2.5
1	D	166	THR	2.5
1	C	171	LEU	2.4
1	D	162	ALA	2.4
1	D	188	ARG	2.4
1	B	184	ALA	2.4
1	C	395	ASP	2.4
1	A	267	ARG	2.4
1	A	188	ARG	2.4
1	B	188	ARG	2.4
1	A	243	GLU	2.3
1	C	163	THR	2.3
1	A	398	ARG	2.3
1	B	267	ARG	2.3
1	A	171	LEU	2.2
1	A	42	GLU	2.2
1	C	178	ASP	2.2
1	D	6	GLY	2.2
1	A	181	GLY	2.2
1	B	158	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	40	ASP	2.1
1	A	152	THR	2.1
1	D	259	LEU	2.1
1	B	148	ALA	2.1
1	D	178	ASP	2.1
1	D	267	ARG	2.1
1	B	153	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no 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
5	GLN	C	603	10/10	0.68	0.27	64,68,77,80	0
3	ACY	B	602	4/4	0.89	0.24	40,43,45,47	0
4	GOL	C	602	6/6	0.92	0.18	38,49,50,52	0
2	PLP	A	601	15/16	0.97	0.15	26,28,33,33	0
2	PLP	C	601	15/16	0.97	0.16	27,31,32,32	0
2	PLP	D	601	15/16	0.97	0.14	26,31,35,37	0
2	PLP	B	601	15/16	0.98	0.15	24,33,35,41	0

6.5 Other polymers (i)

There are no such residues in this entry.