



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:27 AM GMT

PDB ID : 2D32
Title : Crystal Structure of Michaelis Complex of gamma-Glutamylcysteine Synthetase
Authors : Hibi, T.; Nakayama, M.; Nii, H.; Kurokawa, Y.; Katano, H.; Oda, J.
Deposited on : 2005-09-25
Resolution : 2.40 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

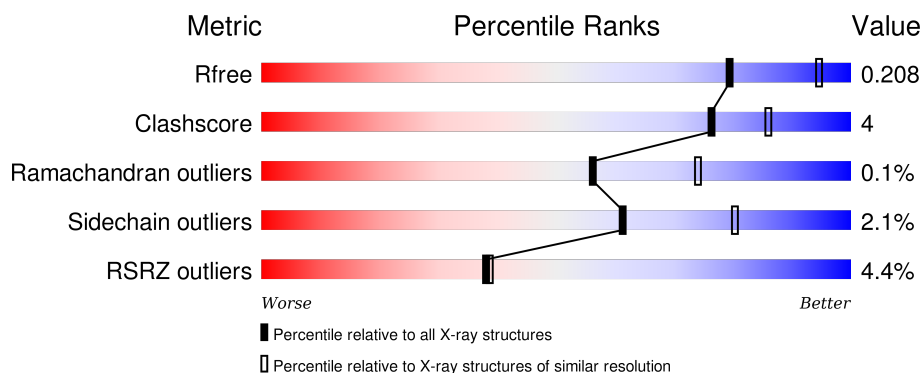
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	518	<div> <div>90%</div> <div>8%</div> <div>••</div> </div>
1	B	518	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>•</div> </div>
1	C	518	<div> <div>7%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	D	518	<div> <div>6%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16833 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 Glutamate–cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4030	2558	689	765	18			
1	B	499	Total	C	N	O	S	0	0	0
			3937	2507	670	742	18			
1	C	499	Total	C	N	O	S	0	0	0
			3906	2489	665	734	18			
1	D	504	Total	C	N	O	S	0	0	0
			3955	2517	678	742	18			

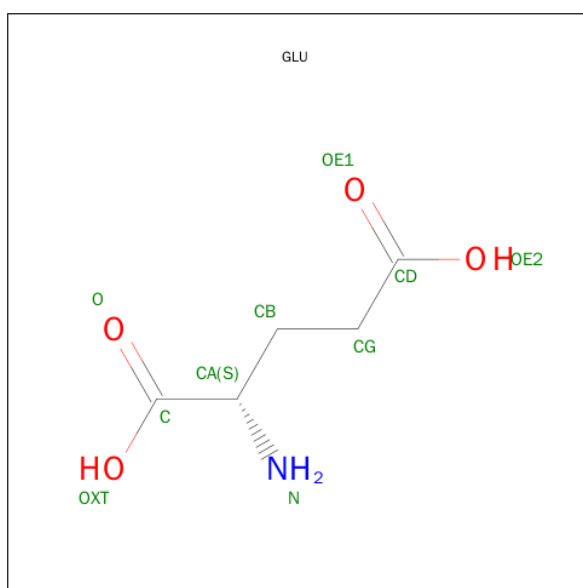
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	CYS	ENGINEERED	UNP P0A6W9
A	164	SER	CYS	ENGINEERED	UNP P0A6W9
A	205	SER	CYS	ENGINEERED	UNP P0A6W9
A	223	SER	CYS	ENGINEERED	UNP P0A6W9
B	106	SER	CYS	ENGINEERED	UNP P0A6W9
B	164	SER	CYS	ENGINEERED	UNP P0A6W9
B	205	SER	CYS	ENGINEERED	UNP P0A6W9
B	223	SER	CYS	ENGINEERED	UNP P0A6W9
C	106	SER	CYS	ENGINEERED	UNP P0A6W9
C	164	SER	CYS	ENGINEERED	UNP P0A6W9
C	205	SER	CYS	ENGINEERED	UNP P0A6W9
C	223	SER	CYS	ENGINEERED	UNP P0A6W9
D	106	SER	CYS	ENGINEERED	UNP P0A6W9
D	164	SER	CYS	ENGINEERED	UNP P0A6W9
D	205	SER	CYS	ENGINEERED	UNP P0A6W9
D	223	SER	CYS	ENGINEERED	UNP P0A6W9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

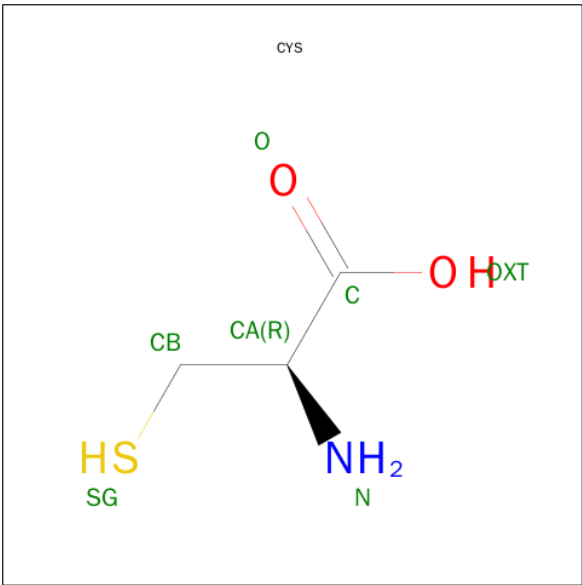
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total 3 Mg 3	0	0
2	A	4	Total 4 Mg 4	0	0
2	D	3	Total 3 Mg 3	0	0
2	C	3	Total 3 Mg 3	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



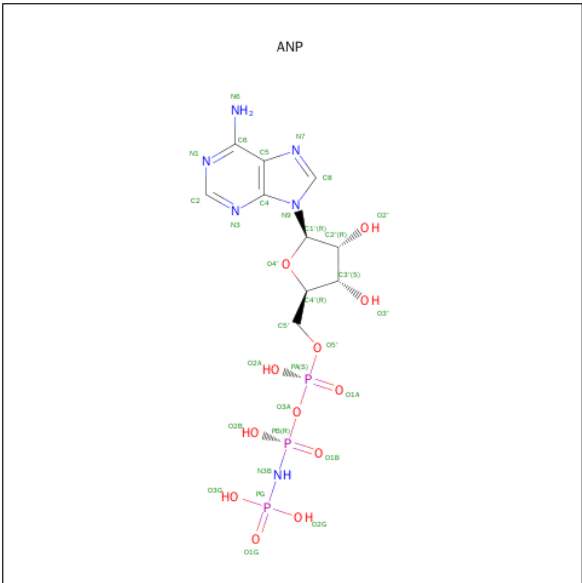
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 10 C 5 N 1 O 4	0	0
3	B	1	Total 10 C 5 N 1 O 4	0	0
3	C	1	Total 10 C 5 N 1 O 4	0	0
3	D	1	Total 10 C 5 N 1 O 4	0	0

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

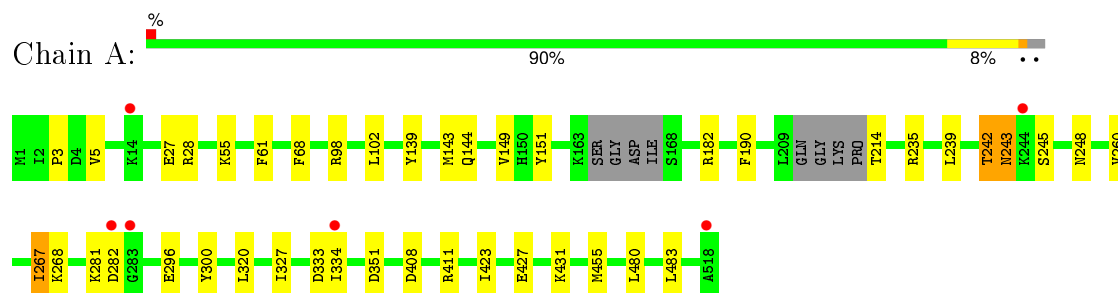
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	363	Total	O	0	0
			363	363		
6	B	163	Total	O	0	0
			163	163		
6	C	87	Total	O	0	0
			87	87		
6	D	187	Total	O	0	0
			187	187		

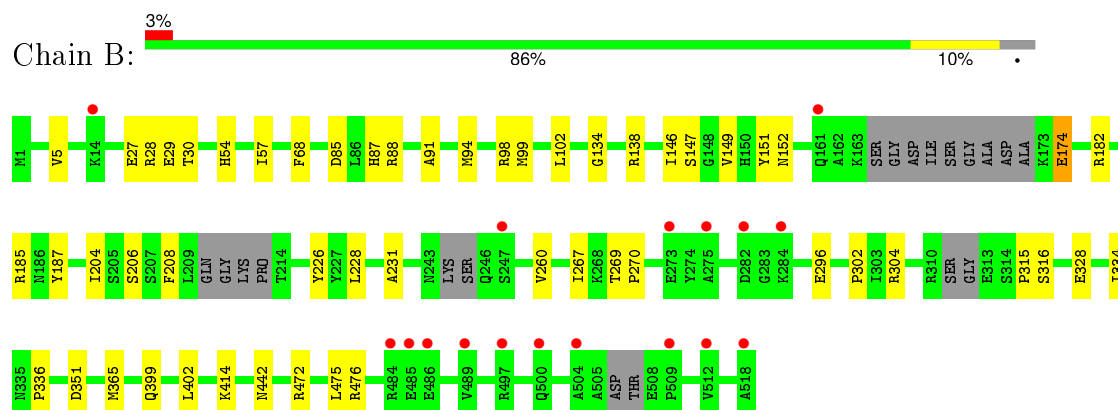
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

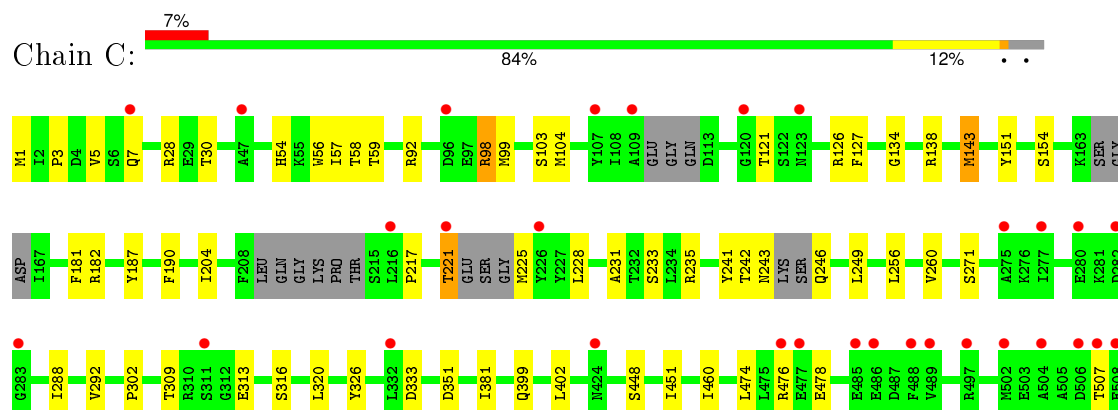
• Molecule 1: Glutamate–cysteine ligase

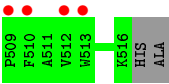


• Molecule 1: Glutamate–cysteine ligase

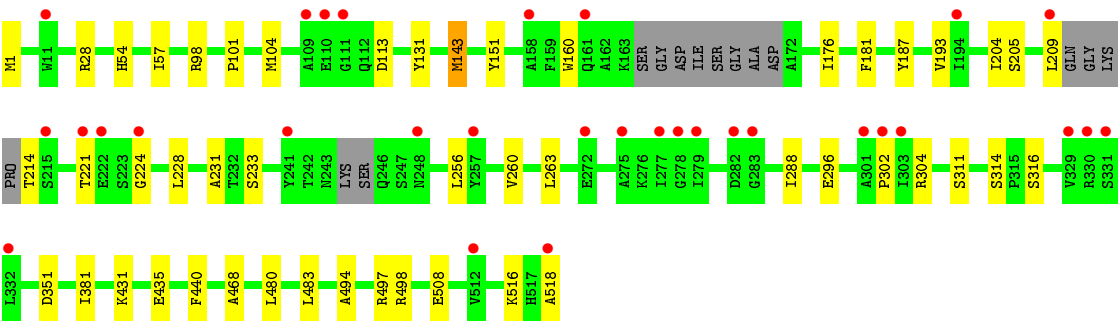
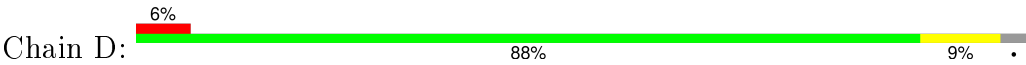


• Molecule 1: Glutamate–cysteine ligase





● Molecule 1: Glutamate–cysteine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	325.53Å 325.53Å 105.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.40 39.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.40) 100.0 (39.79-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.168 , 0.198 0.179 , 0.208	Depositor DCC
R_{free} test set	8122 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 162217 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16833	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: MG, ANP

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	0.78	0/4117	0.73	0/5572
1	B	0.61	0/4021	0.65	0/5443
1	C	0.58	0/3989	0.61	1/5403 (0.0%)
1	D	0.65	0/4041	0.67	0/5476
All	All	0.66	0/16168	0.67	1/21894 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333	ASP	CB-CG-OD1	5.75	123.47	118.30

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	4030	0	3944	26	0
1	B	3937	0	3835	32	0
1	C	3906	0	3785	40	0
1	D	3955	0	3845	23	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
3	C	10	0	5	0	0
3	D	10	0	5	0	0
4	A	7	0	4	0	0
4	B	7	0	4	0	0
4	C	7	0	4	0	0
4	D	7	0	4	0	0
5	A	31	0	13	0	0
5	B	31	0	13	0	0
5	C	31	0	13	0	0
5	D	31	0	13	0	0
6	A	363	0	0	1	0
6	B	163	0	0	1	0
6	C	87	0	0	1	0
6	D	187	0	0	1	0
All	All	16833	0	15497	120	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 (120) 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:139:TYR:HB3	1:A:242:THR:HB	1.52	0.90
1:C:54:HIS:HD2	1:C:56:TRP:H	1.30	0.80
1:A:143:MET:HG3	1:A:242:THR:HG23	1.70	0.73
1:D:508:GLU:CD	1:D:508:GLU:H	1.92	0.73
1:B:472:ARG:O	1:B:476:ARG:HG3	1.89	0.72
1:D:263:LEU:HD21	1:D:296:GLU:HG2	1.73	0.68
1:B:260:VAL:HG13	1:B:316:SER:HB2	1.77	0.66
1:C:121:THR:O	1:C:126:ARG:HD2	1.96	0.65
1:D:1:MET:HE3	6:D:4709:HOH:O	1.99	0.62
1:B:91:ALA:HA	1:B:94:MET:CE	2.30	0.61
1:D:314:SER:HB3	1:D:518:ALA:HA	1.85	0.58
1:C:54:HIS:CD2	1:C:57:ILE:H	2.22	0.58
1:D:260:VAL:HG13	1:D:316:SER:HB2	1.86	0.57
1:C:5:VAL:O	1:C:5:VAL:HG12	2.05	0.57
1:C:260:VAL:HG11	1:C:320:LEU:HG	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD13	1:A:455:MET:CE	2.37	0.55
1:B:94:MET:HE1	1:B:99:MET:HG3	1.89	0.55
1:B:152:ASN:OD1	1:B:328:GLU:HG3	2.07	0.54
1:D:104:MET:HE2	1:D:204:ILE:HG13	1.90	0.54
1:B:91:ALA:HA	1:B:94:MET:HE2	1.89	0.53
1:C:104:MET:HE1	1:C:235:ARG:HA	1.90	0.53
1:B:206:SER:HB3	1:B:226:TYR:HE1	1.74	0.53
1:D:494:ALA:O	1:D:498:ARG:HG3	2.07	0.53
1:D:187:TYR:HE1	1:D:302:PRO:HB2	1.74	0.53
1:C:181:PHE:CE2	1:C:256:LEU:HA	2.44	0.53
1:C:143:MET:HE3	1:C:241:TYR:HA	1.90	0.52
1:B:149:VAL:HG23	1:B:334:ILE:HD13	1.91	0.51
1:A:427:GLU:O	1:A:431:LYS:HG2	2.11	0.51
1:A:408:ASP:OD1	1:A:411:ARG:NH2	2.43	0.51
1:B:185:ARG:HB3	1:B:365:MET:CE	2.41	0.51
1:D:263:LEU:CD2	1:D:296:GLU:HG2	2.41	0.51
1:C:225:MET:SD	1:C:460:ILE:HG13	2.51	0.50
1:A:139:TYR:CB	1:A:242:THR:HB	2.33	0.50
1:D:431:LYS:HE3	1:D:435:GLU:OE2	2.12	0.50
1:A:139:TYR:HB3	1:A:242:THR:CB	2.32	0.49
1:D:228:LEU:HB2	1:D:231:ALA:HB2	1.94	0.49
1:A:214:THR:HG21	1:A:239:LEU:HD21	1.94	0.49
1:D:131:TYR:HB2	1:D:288:ILE:HD11	1.93	0.49
1:B:187:TYR:HE1	1:B:302:PRO:HB2	1.76	0.49
1:D:104:MET:CE	1:D:204:ILE:HG13	2.42	0.49
1:A:260:VAL:HG11	1:A:320:LEU:HG	1.93	0.49
1:C:151:TYR:OH	1:C:351:ASP:OD1	2.30	0.49
1:C:104:MET:SD	1:C:204:ILE:HG22	2.53	0.49
1:C:309:THR:HB	1:C:313:GLU:HB3	1.95	0.49
1:D:480:LEU:HB3	1:D:483:LEU:O	2.13	0.49
1:A:267:ILE:HD11	1:A:296:GLU:N	2.27	0.48
1:D:151:TYR:OH	1:D:351:ASP:OD1	2.32	0.48
1:B:228:LEU:HB2	1:B:231:ALA:HB2	1.95	0.48
1:A:5:VAL:HG12	1:A:5:VAL:O	2.13	0.48
1:B:91:ALA:HA	1:B:94:MET:HE3	1.94	0.48
1:A:245:SER:HB2	1:A:248:ASN:H	1.77	0.48
1:B:146:ILE:HD11	1:B:208:PHE:CE2	2.49	0.48
1:B:402:LEU:C	1:B:402:LEU:HD23	2.34	0.47
1:C:104:MET:HE3	1:C:235:ARG:HB2	1.96	0.47
1:B:267:ILE:HG22	1:B:267:ILE:O	2.14	0.47
1:B:134:GLY:O	1:B:138:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ASN:C	1:C:246:GLN:HB2	2.34	0.47
1:A:55:LYS:HE3	6:A:1757:HOH:O	2.13	0.47
1:A:151:TYR:OH	1:A:351:ASP:OD1	2.33	0.47
1:C:54:HIS:CD2	1:C:56:TRP:H	2.21	0.46
1:D:101:PRO:HD3	1:D:468:ALA:HB2	1.97	0.46
1:B:5:VAL:HG12	1:B:5:VAL:O	2.16	0.46
1:C:228:LEU:HB2	1:C:231:ALA:HB2	1.95	0.46
1:C:134:GLY:O	1:C:138:ARG:HG3	2.15	0.46
1:B:54:HIS:HB3	1:B:57:ILE:O	2.16	0.46
1:B:296:GLU:OE1	1:B:315:PRO:HD2	2.16	0.46
1:B:365:MET:HE2	6:B:2659:HOH:O	2.16	0.45
1:D:233:SER:O	1:D:381:ILE:HG23	2.17	0.45
1:B:174:GLU:OE1	1:B:174:GLU:HA	2.16	0.45
1:A:268:LYS:O	1:A:268:LYS:HG2	2.16	0.45
1:B:204:ILE:HG12	1:B:208:PHE:HB2	1.99	0.44
1:C:260:VAL:HG13	1:C:316:SER:HB2	1.98	0.44
1:A:61:PHE:CD2	1:A:144:GLN:HB2	2.53	0.44
1:D:193:VAL:HG23	1:D:440:PHE:HZ	1.82	0.44
1:C:249:LEU:HD21	1:C:292:VAL:HG11	1.99	0.44
1:C:1:MET:HE3	6:C:3599:HOH:O	2.17	0.44
1:C:181:PHE:HE2	1:C:256:LEU:HA	1.83	0.43
1:C:474:LEU:O	1:C:478:GLU:HG3	2.18	0.43
1:C:30:THR:OG1	1:C:99:MET:HB3	2.19	0.43
1:C:221:THR:CG2	1:C:225:MET:HB3	2.48	0.43
1:A:268:LYS:HE3	1:B:442:ASN:HA	1.99	0.43
1:B:151:TYR:OH	1:B:351:ASP:OD1	2.35	0.43
1:B:87:HIS:HB3	1:B:475:LEU:HD13	2.01	0.43
1:D:54:HIS:HB3	1:D:57:ILE:O	2.18	0.42
1:B:27:GLU:HA	1:B:68:PHE:O	2.18	0.42
1:C:104:MET:CE	1:C:235:ARG:HA	2.49	0.42
1:C:92:ARG:HG2	1:C:476:ARG:HG2	2.02	0.42
1:D:160:TRP:CD1	1:D:176:ILE:HG12	2.55	0.42
1:A:235:ARG:HD3	1:A:333:ASP:OD1	2.18	0.42
1:A:281:LYS:O	1:A:282:ASP:HB2	2.19	0.42
1:C:320:LEU:HD23	1:C:320:LEU:HA	1.92	0.42
1:D:143:MET:O	1:D:143:MET:HG2	2.18	0.42
1:C:187:TYR:HE1	1:C:302:PRO:HB2	1.84	0.42
1:B:29:GLU:HB2	1:B:147:SER:HB2	2.01	0.42
1:A:27:GLU:HA	1:A:68:PHE:O	2.20	0.42
1:C:143:MET:HE3	1:C:242:THR:H	1.85	0.41
1:B:296:GLU:OE2	1:B:316:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HB2	1:A:300:TYR:HB2	2.00	0.41
1:C:127:PHE:CZ	1:C:288:ILE:HD13	2.55	0.41
1:B:102:LEU:HD23	1:B:336:PRO:HB3	2.02	0.41
1:D:181:PHE:CE2	1:D:256:LEU:HA	2.55	0.41
1:A:3:PRO:HD3	1:A:190:PHE:CZ	2.55	0.41
1:B:269:THR:HA	1:B:270:PRO:HD3	1.96	0.41
1:C:58:THR:OG1	1:C:59:THR:N	2.54	0.41
1:C:233:SER:O	1:C:381:ILE:HG23	2.20	0.41
1:C:154:SER:HB3	1:C:326:TYR:HB3	2.03	0.41
1:B:30:THR:OG1	1:B:99:MET:HB3	2.20	0.41
1:C:143:MET:O	1:C:143:MET:HG2	2.21	0.41
1:C:241:TYR:O	1:C:242:THR:HG23	2.21	0.41
1:C:448:SER:HA	1:C:451:ILE:HG22	2.03	0.41
1:C:98:ARG:H	1:C:98:ARG:HD2	1.86	0.41
1:C:3:PRO:HD3	1:C:190:PHE:CZ	2.56	0.41
1:D:221:THR:O	1:D:224:GLY:N	2.52	0.41
1:C:402:LEU:C	1:C:402:LEU:HD23	2.42	0.41
1:A:480:LEU:HB3	1:A:483:LEU:O	2.21	0.40
1:C:54:HIS:HB3	1:C:57:ILE:O	2.22	0.40
1:A:214:THR:CG2	1:A:239:LEU:HD21	2.52	0.40
1:B:85:ASP:HA	1:B:88:ARG:HD2	2.02	0.40
1:A:149:VAL:HG23	1:A:334:ILE:HD13	2.03	0.40
1:A:102:LEU:HD13	1:A:455:MET:HE1	2.02	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	504/518 (97%)	491 (97%)	13 (3%)	0	100	100
1	B	487/518 (94%)	473 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	487/518 (94%)	471 (97%)	14 (3%)	2 (0%)	39	56
1	D	496/518 (96%)	484 (98%)	12 (2%)	0	100	100
All	All	1974/2072 (95%)	1919 (97%)	53 (3%)	2 (0%)	56	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	507	THR
1	C	217	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	422/434 (97%)	414 (98%)	8 (2%)	65	83
1	B	409/434 (94%)	402 (98%)	7 (2%)	68	85
1	C	400/434 (92%)	391 (98%)	9 (2%)	58	78
1	D	407/434 (94%)	396 (97%)	11 (3%)	52	73
All	All	1638/1736 (94%)	1603 (98%)	35 (2%)	61	80

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	98	ARG
1	A	182	ARG
1	A	242	THR
1	A	243	ASN
1	A	267	ILE
1	A	327	ILE
1	A	423	ILE
1	B	28	ARG
1	B	98	ARG

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Mol	Chain	Res	Type
1	B	174	GLU
1	B	182	ARG
1	B	304	ARG
1	B	399	GLN
1	B	414	LYS
1	C	7	GLN
1	C	28	ARG
1	C	98	ARG
1	C	103	SER
1	C	143	MET
1	C	182	ARG
1	C	221	THR
1	C	271	SER
1	C	399	GLN
1	D	28	ARG
1	D	98	ARG
1	D	113	ASP
1	D	143	MET
1	D	205	SER
1	D	209	LEU
1	D	214	THR
1	D	304	ARG
1	D	311	SER
1	D	497	ARG
1	D	516	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	500	GLN
1	A	517	HIS
1	B	34	ASN
1	B	123	ASN
1	C	54	HIS
1	C	378	ASN
1	C	399	GLN
1	D	118	GLN
1	D	297	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 ⓘ

Of 25 ligands modelled in this entry, 13 are monoatomic - leaving 12 for Mogul analysis.

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	GLU	A	1519	2	3,9,9	0.28	0	2,11,11	0.58	0
4	CYS	A	1520	-	3,6,6	1.17	1 (33%)	1,7,7	0.73	0
5	ANP	A	1521	2	27,33,33	2.68	7 (25%)	30,52,52	2.32	8 (26%)
3	GLU	B	2519	2	3,9,9	0.33	0	2,11,11	0.31	0
4	CYS	B	2520	-	3,6,6	0.51	0	1,7,7	1.16	0
5	ANP	B	2521	2	27,33,33	2.53	6 (22%)	30,52,52	1.89	6 (20%)
3	GLU	C	3519	2	3,9,9	0.37	0	2,11,11	0.34	0
4	CYS	C	3520	-	3,6,6	0.50	0	1,7,7	0.76	0
5	ANP	C	3521	2	27,33,33	2.44	6 (22%)	30,52,52	2.19	8 (26%)
3	GLU	D	4519	2	3,9,9	0.23	0	2,11,11	0.55	0
4	CYS	D	4520	-	3,6,6	1.14	0	1,7,7	1.01	0
5	ANP	D	4521	2	27,33,33	2.75	6 (22%)	30,52,52	2.15	6 (20%)

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	GLU	A	1519	2	-	0/3/9/9	0/0/0/0
4	CYS	A	1520	-	-	0/2/6/6	0/0/0/0
5	ANP	A	1521	2	-	0/12/38/38	0/3/3/3
3	GLU	B	2519	2	-	0/3/9/9	0/0/0/0
4	CYS	B	2520	-	-	0/2/6/6	0/0/0/0
5	ANP	B	2521	2	-	0/12/38/38	0/3/3/3
3	GLU	C	3519	2	-	0/3/9/9	0/0/0/0
4	CYS	C	3520	-	-	0/2/6/6	0/0/0/0
5	ANP	C	3521	2	-	0/12/38/38	0/3/3/3
3	GLU	D	4519	2	-	0/3/9/9	0/0/0/0
4	CYS	D	4520	-	-	0/2/6/6	0/0/0/0
5	ANP	D	4521	2	-	0/12/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1520	CYS	CB-CA	2.02	1.55	1.53
5	A	1521	ANP	O4'-C1'	2.11	1.43	1.41
5	C	3521	ANP	C5-C4	2.91	1.47	1.40
5	A	1521	ANP	C5-C4	3.06	1.47	1.40
5	D	4521	ANP	C5-C4	3.10	1.47	1.40
5	B	2521	ANP	C5-C4	3.31	1.48	1.40
5	A	1521	ANP	PB-O3A	3.34	1.63	1.59
5	B	2521	ANP	PB-O3A	3.36	1.63	1.59
5	B	2521	ANP	PB-N3B	4.33	1.74	1.63
5	A	1521	ANP	PG-N3B	4.38	1.74	1.63
5	D	4521	ANP	PB-N3B	4.47	1.75	1.63
5	D	4521	ANP	PG-N3B	4.55	1.75	1.63
5	D	4521	ANP	PB-O3A	4.59	1.64	1.59
5	C	3521	ANP	PG-N3B	4.60	1.75	1.63
5	C	3521	ANP	PB-N3B	4.65	1.75	1.63
5	B	2521	ANP	PG-N3B	4.70	1.75	1.63
5	C	3521	ANP	PB-O3A	4.72	1.65	1.59
5	A	1521	ANP	PB-N3B	4.88	1.76	1.63
5	C	3521	ANP	PB-O1B	5.79	1.52	1.46
5	C	3521	ANP	PG-O1G	6.30	1.53	1.46
5	D	4521	ANP	PB-O1B	6.60	1.53	1.46
5	B	2521	ANP	PB-O1B	6.84	1.54	1.46
5	A	1521	ANP	PB-O1B	6.87	1.54	1.46
5	B	2521	ANP	PG-O1G	7.00	1.54	1.46
5	A	1521	ANP	PG-O1G	8.23	1.55	1.46
5	D	4521	ANP	PG-O1G	8.82	1.56	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1521	ANP	N3-C2-N1	-9.20	121.85	128.89
5	D	4521	ANP	N3-C2-N1	-8.33	122.52	128.89
5	C	3521	ANP	N3-C2-N1	-8.19	122.62	128.89
5	B	2521	ANP	N3-C2-N1	-7.19	123.39	128.89
5	C	3521	ANP	C4-C5-N7	-3.35	106.40	109.48
5	B	2521	ANP	C4-C5-N7	-3.15	106.58	109.48
5	C	3521	ANP	O1B-PB-N3B	-2.98	107.32	111.90
5	B	2521	ANP	O1B-PB-N3B	-2.91	107.43	111.90
5	D	4521	ANP	C1'-N9-C4	-2.86	122.63	126.94
5	D	4521	ANP	O1B-PB-N3B	-2.82	107.57	111.90
5	D	4521	ANP	O1G-PG-N3B	-2.74	107.69	111.90
5	B	2521	ANP	O1G-PG-N3B	-2.71	107.74	111.90
5	C	3521	ANP	O1G-PG-N3B	-2.66	107.82	111.90
5	A	1521	ANP	C1'-N9-C4	-2.49	123.18	126.94
5	A	1521	ANP	C4-C5-N7	-2.45	107.22	109.48
5	D	4521	ANP	O2B-PB-O3A	-2.37	94.33	105.09
5	A	1521	ANP	O2B-PB-O3A	-2.31	94.62	105.09
5	C	3521	ANP	C1'-N9-C4	-2.12	123.74	126.94
5	C	3521	ANP	O5'-C5'-C4'	-2.08	101.46	109.12
5	A	1521	ANP	O1B-PB-N3B	-2.07	108.72	111.90
5	B	2521	ANP	PA-O3A-PB	-2.06	125.74	132.67
5	A	1521	ANP	C4'-O4'-C1'	2.13	112.06	109.72
5	C	3521	ANP	O3G-PG-O2G	2.41	114.71	107.58
5	A	1521	ANP	O3G-PG-O2G	2.57	115.19	107.58
5	B	2521	ANP	O2B-PB-O1B	3.29	116.87	110.00
5	C	3521	ANP	O2B-PB-O1B	3.46	117.22	110.00
5	A	1521	ANP	O2B-PB-O1B	4.22	118.80	110.00
5	D	4521	ANP	O2B-PB-O1B	4.29	118.95	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	510/518 (98%)	-0.26	6 (1%) 81 81	20, 33, 58, 85	0
1	B	499/518 (96%)	-0.10	17 (3%) 49 49	27, 46, 73, 100	0
1	C	499/518 (96%)	0.12	34 (6%) 20 20	35, 53, 85, 95	0
1	D	504/518 (97%)	0.01	31 (6%) 24 25	28, 44, 75, 94	0
All	All	2012/2072 (97%)	-0.06	88 (4%) 38 39	20, 45, 76, 100	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	ALA	6.3
1	D	111	GLY	5.4
1	C	109	ALA	4.9
1	D	278	GLY	4.4
1	D	109	ALA	3.9
1	B	512	VAL	3.9
1	C	107	TYR	3.8
1	D	209	LEU	3.8
1	B	500	GLN	3.8
1	D	110	GLU	3.7
1	C	226	TYR	3.7
1	C	504	ALA	3.5
1	D	161	GLN	3.5
1	C	283	GLY	3.4
1	D	257	TYR	3.4
1	D	301	ALA	3.3
1	D	518	ALA	3.3
1	C	512	VAL	3.3
1	D	221	THR	3.3
1	A	282	ASP	3.1
1	D	282	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	489	VAL	3.0
1	C	123	ASN	3.0
1	C	507	THR	3.0
1	B	275	ALA	3.0
1	D	272	GLU	3.0
1	C	509	PRO	2.9
1	D	283	GLY	2.9
1	D	215	SER	2.9
1	B	284	LYS	2.9
1	B	14	LYS	2.8
1	D	279	ILE	2.8
1	B	247	SER	2.8
1	D	303	ILE	2.8
1	C	277	ILE	2.7
1	C	216	LEU	2.7
1	D	194	ILE	2.7
1	D	331	SER	2.7
1	D	275	ALA	2.6
1	D	329	VAL	2.6
1	C	332	LEU	2.6
1	B	484	ARG	2.6
1	A	14	LYS	2.6
1	C	311	SER	2.6
1	C	497	ARG	2.6
1	C	477	GLU	2.6
1	D	224	GLY	2.6
1	B	509	PRO	2.5
1	D	222	GLU	2.5
1	D	277	ILE	2.4
1	D	158	ALA	2.4
1	C	489	VAL	2.4
1	B	282	ASP	2.4
1	C	508	GLU	2.4
1	D	248	ASN	2.4
1	B	497	ARG	2.4
1	B	486	GLU	2.4
1	C	47	ALA	2.3
1	C	502	MET	2.3
1	C	510	PHE	2.3
1	C	488	PHE	2.3
1	C	513	TRP	2.3
1	D	241	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	504	ALA	2.2
1	C	282	ASP	2.2
1	D	330	ARG	2.2
1	A	334	ILE	2.2
1	D	332	LEU	2.2
1	A	244	LYS	2.1
1	C	506	ASP	2.1
1	C	7	GLN	2.1
1	B	273	GLU	2.1
1	C	424	ASN	2.1
1	C	275	ALA	2.1
1	C	476	ARG	2.1
1	C	96	ASP	2.1
1	C	221	THR	2.1
1	D	512	VAL	2.1
1	C	120	GLY	2.1
1	A	518	ALA	2.1
1	D	302	PRO	2.1
1	D	11	TRP	2.1
1	A	283	GLY	2.1
1	B	485	GLU	2.0
1	B	161	GLN	2.0
1	C	280	GLU	2.0
1	C	485	GLU	2.0
1	C	486	GLU	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
4	CYS	D	4520	7/7	0.92	0.21	0.41	42,52,54,55	0
4	CYS	C	3520	7/7	0.92	0.14	0.07	58,59,60,60	0
3	GLU	A	1519	10/10	0.91	0.16	-0.32	44,46,49,50	0
3	GLU	C	3519	10/10	0.96	0.17	-0.40	56,57,59,59	0
4	CYS	B	2520	7/7	0.95	0.12	-0.43	50,53,54,54	0
3	GLU	D	4519	10/10	0.95	0.22	-0.58	36,38,39,39	0
5	ANP	B	2521	31/31	0.93	0.11	-0.81	39,44,64,65	0
5	ANP	C	3521	31/31	0.93	0.12	-0.84	37,52,72,72	0
5	ANP	D	4521	31/31	0.95	0.10	-1.07	30,38,62,63	0
4	CYS	A	1520	7/7	0.97	0.10	-1.16	31,36,39,40	0
3	GLU	B	2519	10/10	0.95	0.14	-1.45	45,48,49,51	0
5	ANP	A	1521	31/31	0.96	0.10	-1.58	25,34,58,58	0
2	MG	C	3523	1/1	0.98	0.15	-1.83	58,58,58,58	0
2	MG	A	1523	1/1	0.94	0.10	-	49,49,49,49	0
2	MG	A	1522	1/1	0.93	0.06	-	38,38,38,38	0
2	MG	B	2523	1/1	0.90	0.14	-	49,49,49,49	0
2	MG	A	1524	1/1	0.98	0.06	-	42,42,42,42	0
2	MG	B	2524	1/1	0.90	0.18	-	76,76,76,76	0
2	MG	B	2522	1/1	0.88	0.12	-	45,45,45,45	0
2	MG	D	4523	1/1	0.95	0.07	-	45,45,45,45	0
2	MG	D	4522	1/1	0.92	0.29	-	33,33,33,33	0
2	MG	C	3522	1/1	0.91	0.16	-	52,52,52,52	0
2	MG	A	1525	1/1	0.98	0.16	-	40,40,40,40	0
2	MG	D	4524	1/1	0.98	0.04	-	48,48,48,48	0
2	MG	C	3524	1/1	0.94	0.04	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.