Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 10:11 PM JST

PDB ID	:	6K1O
Title	:	Apo form of a putative cystathionine gamma-lyase
Authors	:	Chen, S.; Wang, Y.
Deposited on	:	2019-05-10
Resolution	:	2.03 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:

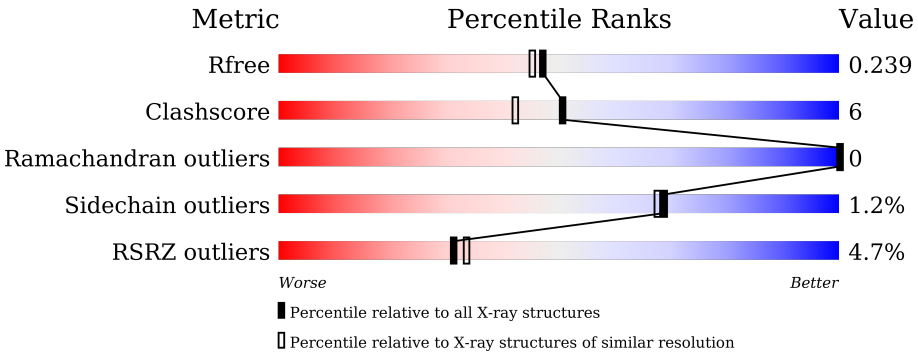
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.03 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	392	5% 84% 10% 6%
1	B	392	5% 84% 10% • 5%
1	C	392	4% 85% 9% 6%
1	D	392	4% 80% 14% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11458 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	368	Total	C	N	O	S	0	0	0
			2718	1730	465	508	15			
1	B	371	Total	C	N	O	S	0	0	0
			2732	1731	474	512	15			
1	C	369	Total	C	N	O	S	0	0	0
			2718	1728	466	509	15			
1	D	370	Total	C	N	O	S	0	0	0
			2715	1722	470	508	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B4SII9
A	0	SER	-	expression tag	UNP B4SII9
B	-1	GLY	-	expression tag	UNP B4SII9
B	0	SER	-	expression tag	UNP B4SII9
C	-1	GLY	-	expression tag	UNP B4SII9
C	0	SER	-	expression tag	UNP B4SII9
D	-1	GLY	-	expression tag	UNP B4SII9
D	0	SER	-	expression tag	UNP B4SII9

- Molecule 2 is water.

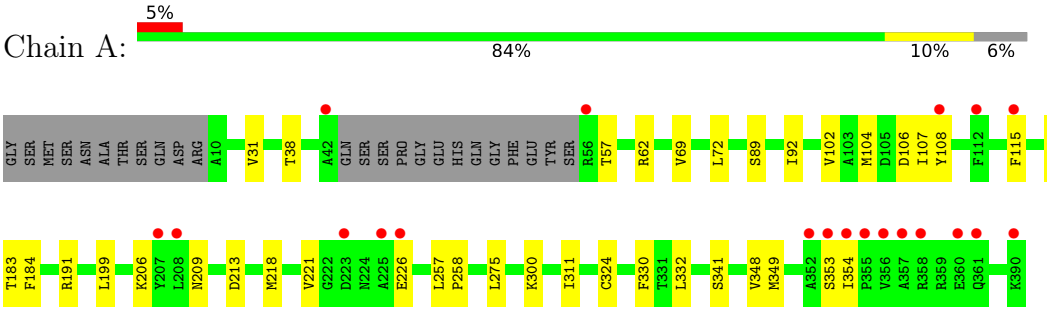
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		
2	B	160	Total	O	0	0
			160	160		
2	C	132	Total	O	0	0
			132	132		
2	D	150	Total	O	0	0
			150	150		

3 Residue-property plots (i)

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

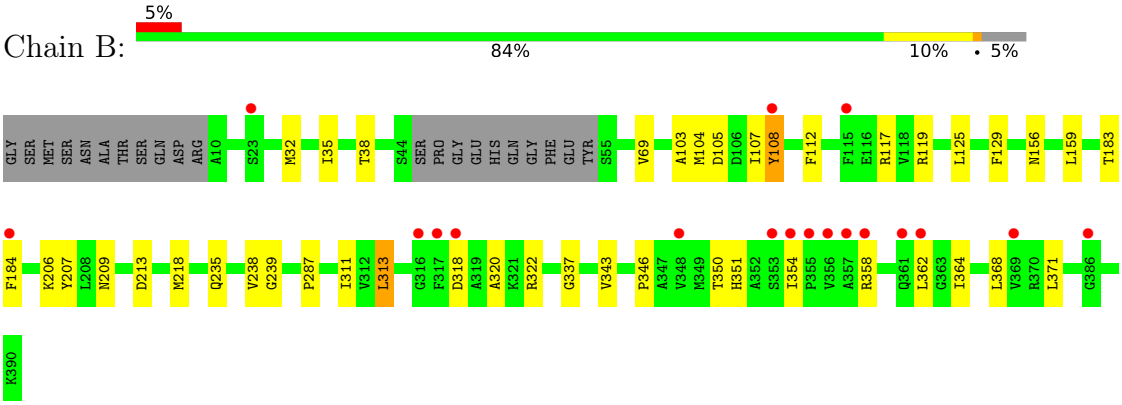
• Molecule 1: Cystathionine gamma-lyase

Chain A:



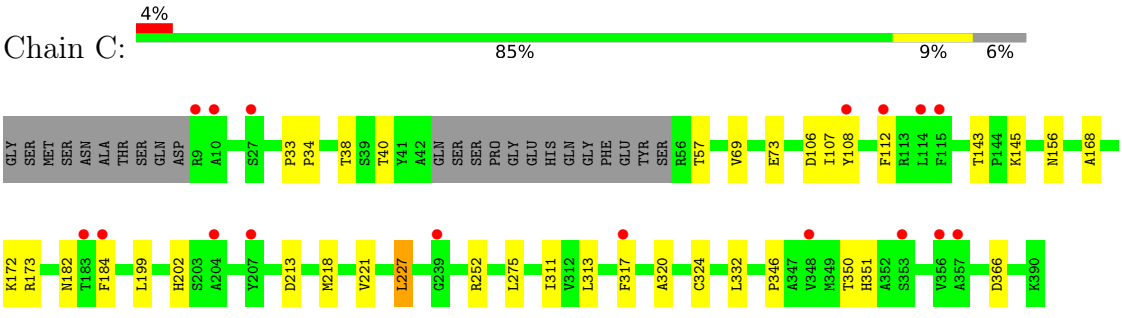
• Molecule 1: Cystathionine gamma-lyase

Chain B:



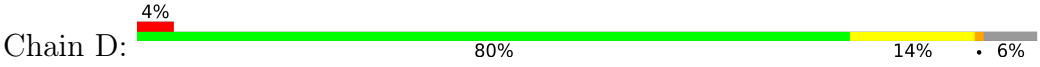
• Molecule 1: Cystathionine gamma-lyase

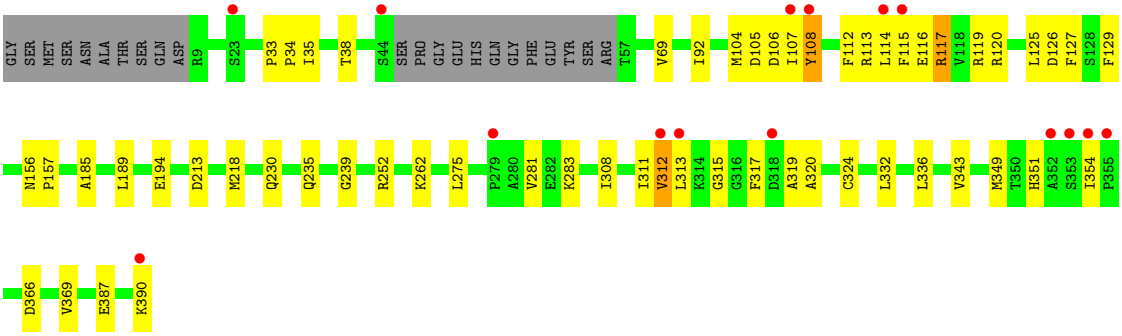
Chain C:



• Molecule 1: Cystathionine gamma-lyase

Chain D:




GLY SER MET SER ASN ALA THR SER GLN ASP R9 S23 P33 P34 I35 T38 S44 SER PRO GLY GLU HIS GLN GLY PHE GLU TYR SER ARG T57 V69 I92 M104 D105 D106 I107 Y108 F112 R113 L114 F115 E116 R117 V118 R119 R120 L125 D126 F127 S128 F129
N156 P157 A185 L189 E194 D213 M218 Q230 Q235 G239 R252 K262 L275 P279 A280 V281 E282 K283 I308 I311 V312 L313 K314 G315 G316 F317 D318 A319 A320 C324 L332 L336 V343 M349 T350 H351 A352 S353 I354 P355
D366 V369 E387 K390

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.75Å 154.30Å 159.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.42 – 2.03 33.42 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.42-2.03) 98.9 (33.42-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.189 , 0.242 0.191 , 0.239	Depositor DCC
R_{free} test set	1994 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11458	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 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.42	0/2771	0.59	0/3764
1	B	0.42	0/2783	0.58	0/3780
1	C	0.41	0/2770	0.58	0/3763
1	D	0.41	0/2766	0.60	0/3759
All	All	0.41	0/11090	0.59	0/15066

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2718	0	2720	26	0
1	B	2732	0	2736	36	0
1	C	2718	0	2717	25	0
1	D	2715	0	2714	47	0
2	A	133	0	0	0	0
2	B	160	0	0	0	0
2	C	132	0	0	4	0
2	D	150	0	0	1	0
All	All	11458	0	10887	124	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 (124) 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:D:283:LYS:HB3	1:D:312:VAL:CG2	1.77	1.14
1:D:351:HIS:O	1:D:354:ILE:HG22	1.49	1.11
1:B:313:LEU:HD11	1:B:320:ALA:CA	1.81	1.10
1:D:283:LYS:HB3	1:D:312:VAL:HG23	1.07	1.04
1:B:313:LEU:HD11	1:B:320:ALA:HA	1.52	0.90
1:B:313:LEU:HD11	1:B:320:ALA:CB	2.11	0.80
1:D:112:PHE:O	1:D:116:GLU:HB2	1.84	0.76
1:B:313:LEU:HD11	1:B:320:ALA:N	2.01	0.76
1:C:346:PRO:HA	1:C:350:THR:HG22	1.71	0.73
1:B:313:LEU:HD11	1:B:320:ALA:HB2	1.71	0.70
1:B:156:ASN:HB2	1:B:184:PHE:CZ	2.27	0.69
1:B:313:LEU:CD1	1:B:320:ALA:N	2.56	0.68
1:A:92:ILE:HD11	1:A:115:PHE:CE1	2.29	0.67
1:A:69:VAL:HG11	1:A:218:MET:HG2	1.79	0.65
1:D:116:GLU:OE2	1:D:120:ARG:HD2	1.97	0.65
1:D:108:TYR:HD2	1:D:354:ILE:HD11	1.62	0.64
1:D:311:ILE:HG12	1:D:369:VAL:HG23	1.78	0.64
1:A:199:LEU:HD23	1:A:221:VAL:HG22	1.80	0.62
1:D:107:ILE:O	1:D:107:ILE:HG13	1.97	0.62
1:D:283:LYS:CB	1:D:312:VAL:CG2	2.69	0.61
1:C:350:THR:HG23	1:C:351:HIS:ND1	2.15	0.61
1:A:107:ILE:HG13	1:A:107:ILE:O	1.99	0.61
1:D:108:TYR:HD2	1:D:354:ILE:CD1	2.14	0.60
1:D:108:TYR:CD2	1:D:354:ILE:HD11	2.37	0.60
1:D:106:ASP:O	1:D:108:TYR:N	2.33	0.60
1:D:115:PHE:O	1:D:127:PHE:CE2	2.54	0.60
1:B:358:ARG:O	1:B:362:LEU:HD12	2.01	0.60
1:C:313:LEU:HD12	1:C:320:ALA:HA	1.84	0.59
1:B:313:LEU:CD1	1:B:320:ALA:CA	2.70	0.58
1:D:332:LEU:HD12	1:D:343:VAL:HG13	1.84	0.58
1:D:313:LEU:HD12	1:D:320:ALA:HA	1.85	0.58
1:C:107:ILE:O	1:C:107:ILE:HG13	2.04	0.58
1:D:283:LYS:CB	1:D:312:VAL:HG23	2.04	0.57
1:D:283:LYS:HB3	1:D:312:VAL:HG21	1.82	0.56
1:A:348:VAL:HG23	1:A:349:MET:HG3	1.88	0.56
1:C:143:THR:HG22	1:C:145:LYS:H	1.70	0.55
1:B:354:ILE:HG22	1:B:358:ARG:HB3	1.89	0.54
1:B:183:THR:HG21	1:B:206:LYS:HD2	1.89	0.53
1:D:311:ILE:CG1	1:D:369:VAL:HG23	2.39	0.53
1:A:213:ASP:HA	1:B:38:THR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:HG11	1:C:218:MET:HG2	1.90	0.52
1:C:213:ASP:HA	1:D:38:THR:HA	1.92	0.52
1:C:317:PHE:HB2	1:C:366:ASP:HB3	1.92	0.52
1:A:57:THR:O	1:A:57:THR:HG23	2.09	0.52
1:B:313:LEU:CD1	1:B:320:ALA:HA	2.31	0.52
1:A:57:THR:HG23	1:A:62:ARG:HH22	1.76	0.51
1:A:108:TYR:HD2	1:A:354:ILE:HD12	1.75	0.51
1:D:108:TYR:CD2	1:D:354:ILE:CD1	2.93	0.51
1:A:92:ILE:HD11	1:A:115:PHE:HE1	1.73	0.51
1:A:156:ASN:HB2	1:A:184:PHE:CZ	2.45	0.51
1:A:324:CYS:HB3	1:A:332:LEU:HD13	1.94	0.50
1:D:119:ARG:HB3	1:D:125:LEU:HD12	1.93	0.50
1:B:108:TYR:HE2	1:B:358:ARG:NH1	2.10	0.50
1:C:38:THR:HA	1:D:213:ASP:HA	1.93	0.49
1:B:235:GLN:O	1:B:239:GLY:HA2	2.12	0.49
1:D:230:GLN:NE2	2:D:407:HOH:O	2.46	0.49
1:B:108:TYR:CD1	1:B:112:PHE:CB	2.96	0.48
1:A:38:THR:HA	1:B:213:ASP:HA	1.95	0.48
1:B:105:ASP:HA	1:B:129:PHE:HB3	1.94	0.48
1:C:156:ASN:HB2	1:C:184:PHE:CZ	2.49	0.47
1:B:108:TYR:HD1	1:B:112:PHE:CB	2.28	0.47
1:D:275:LEU:HD13	1:D:311:ILE:HG21	1.97	0.47
1:A:330:PHE:CD2	1:A:341:SER:HB3	2.50	0.46
1:B:108:TYR:HE2	1:B:358:ARG:HH11	1.63	0.46
1:D:235:GLN:O	1:D:239:GLY:HA2	2.15	0.46
1:A:106:ASP:O	1:A:108:TYR:N	2.43	0.46
1:D:114:LEU:O	1:D:114:LEU:HD23	2.16	0.46
1:D:105:ASP:HA	1:D:129:PHE:HB3	1.98	0.46
1:D:262:LYS:HB3	1:D:262:LYS:HE2	1.58	0.46
1:D:324:CYS:HB3	1:D:332:LEU:HD13	1.98	0.46
1:B:343:VAL:HG23	1:B:371:LEU:HD23	1.97	0.46
1:A:31:VAL:HG21	1:C:40:THR:HG23	1.98	0.46
1:D:120:ARG:NH2	1:D:126:ASP:OD1	2.47	0.46
1:C:73:GLU:OE1	1:C:202:HIS:NE2	2.47	0.45
1:D:114:LEU:HD23	1:D:114:LEU:C	2.36	0.45
1:A:108:TYR:CD2	1:A:354:ILE:HD12	2.51	0.45
1:A:183:THR:HG21	1:A:206:LYS:HD2	1.98	0.45
1:A:31:VAL:HG23	1:C:40:THR:O	2.17	0.45
1:B:313:LEU:H	1:B:313:LEU:HG	1.69	0.45
1:C:173:ARG:NH1	2:C:408:HOH:O	2.50	0.45
1:B:318:ASP:O	1:B:322:ARG:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:O	1:A:107:ILE:HG12	2.18	0.44
1:B:32:MET:HE2	2:C:409:HOH:O	2.18	0.44
1:D:387:GLU:HA	1:D:390:LYS:HE2	1.99	0.44
1:C:199:LEU:CD2	1:C:221:VAL:HG22	2.47	0.44
1:D:185:ALA:O	1:D:189:LEU:HB2	2.17	0.44
1:D:351:HIS:HB3	1:D:354:ILE:HG21	1.99	0.43
1:B:207:TYR:CE1	1:B:337:GLY:HA2	2.53	0.43
1:B:103:ALA:HB1	1:B:107:ILE:HD11	1.99	0.43
1:B:35:ILE:HB	1:D:35:ILE:HB	2.01	0.43
1:B:351:HIS:CD2	1:B:364:ILE:CD1	3.02	0.43
1:D:317:PHE:HB2	1:D:366:ASP:HB3	2.01	0.43
1:B:346:PRO:HA	1:B:350:THR:OG1	2.19	0.43
1:C:106:ASP:O	1:C:108:TYR:N	2.52	0.43
1:D:315:GLY:HA3	1:D:319:ALA:HB2	2.00	0.43
1:D:281:VAL:HG12	1:D:313:LEU:CD2	2.49	0.42
1:A:102:VAL:O	1:A:149:VAL:HA	2.18	0.42
1:B:104:MET:O	1:B:107:ILE:HG12	2.19	0.42
1:C:227:LEU:O	1:C:227:LEU:HD12	2.19	0.42
1:D:117:ARG:HA	1:D:117:ARG:HD3	1.38	0.42
1:A:72:LEU:O	1:A:191:ARG:NH1	2.52	0.42
1:A:89:SER:OG	1:B:238:VAL:HG13	2.19	0.42
1:A:275:LEU:HD13	1:A:311:ILE:HG21	2.01	0.42
1:B:209:ASN:OD1	1:C:252:ARG:NH2	2.52	0.42
1:A:209:ASN:OD1	1:D:252:ARG:NH2	2.51	0.42
1:C:324:CYS:HB3	1:C:332:LEU:HD13	2.03	0.41
1:D:104:MET:O	1:D:107:ILE:HG12	2.21	0.41
1:B:311:ILE:O	1:B:368:LEU:HA	2.20	0.41
1:C:275:LEU:HD13	1:C:311:ILE:HG21	2.02	0.41
1:D:156:ASN:HA	1:D:157:PRO:HA	1.78	0.41
1:A:257:LEU:HB3	1:A:258:PRO:HD3	2.03	0.41
1:D:69:VAL:HG11	1:D:218:MET:HG2	2.03	0.41
1:C:168:ALA:O	1:C:172:LYS:HD2	2.20	0.41
1:D:92:ILE:HD13	1:D:92:ILE:HA	1.89	0.41
1:D:308:ILE:HD11	1:D:336:LEU:HD13	2.01	0.41
1:C:57:THR:HA	2:C:467:HOH:O	2.21	0.40
1:C:143:THR:HG21	2:C:505:HOH:O	2.21	0.40
1:D:114:LEU:C	1:D:114:LEU:CD2	2.89	0.40
1:D:33:PRO:HA	1:D:34:PRO:HD3	2.00	0.40
1:B:69:VAL:HG11	1:B:218:MET:HG2	2.03	0.40
1:C:33:PRO:HA	1:C:34:PRO:HD3	2.01	0.40
1:B:119:ARG:HB3	1:B:125:LEU:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD13	1:B:287:PRO:HD3	2.04	0.40
1:C:182:ASN:HB3	1:C:202:HIS:CE1	2.57	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	364/392 (93%)	350 (96%)	14 (4%)	0	100	100
1	B	367/392 (94%)	355 (97%)	12 (3%)	0	100	100
1	C	365/392 (93%)	354 (97%)	11 (3%)	0	100	100
1	D	366/392 (93%)	356 (97%)	10 (3%)	0	100	100
All	All	1462/1568 (93%)	1415 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	280/306 (92%)	277 (99%)	3 (1%)	73	73
1	B	282/306 (92%)	279 (99%)	3 (1%)	73	73
1	C	279/306 (91%)	277 (99%)	2 (1%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	279/306 (91%)	273 (98%)	6 (2%)	52 46
All	All	1120/1224 (92%)	1106 (99%)	14 (1%)	69 67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	GLU
1	A	300	LYS
1	A	353	SER
1	B	108	TYR
1	B	117	ARG
1	B	313	LEU
1	C	112	PHE
1	C	227	LEU
1	D	108	TYR
1	D	113	ARG
1	D	117	ARG
1	D	194	GLU
1	D	312	VAL
1	D	349	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	361	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

There are no ligands in this entry.

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, 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	368/392 (93%)	0.02	20 (5%)	25	28	25, 41, 75, 118	0
1	B	371/392 (94%)	-0.06	18 (4%)	29	31	22, 38, 90, 135	0
1	C	369/392 (94%)	0.00	17 (4%)	32	35	24, 41, 80, 128	0
1	D	370/392 (94%)	0.01	15 (4%)	37	40	20, 42, 89, 144	0
All	All	1478/1568 (94%)	-0.01	70 (4%)	31	33	20, 41, 86, 144	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	108	TYR	10.2
1	C	108	TYR	6.8
1	D	44	SER	6.0
1	A	356	VAL	6.0
1	B	355	PRO	5.8
1	B	357	ALA	5.2
1	A	108	TYR	4.9
1	C	357	ALA	4.9
1	A	357	ALA	4.8
1	C	10	ALA	4.8
1	B	361	GLN	4.5
1	A	354	ILE	4.2
1	A	42	ALA	4.2
1	B	317	PHE	4.0
1	A	353	SER	4.0
1	B	108	TYR	3.8
1	D	312	VAL	3.6
1	C	356	VAL	3.5
1	D	390	LYS	3.4
1	C	9	ARG	3.4
1	B	353	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	353	SER	3.4
1	A	352	ALA	3.4
1	A	360	GLU	3.4
1	D	115	PHE	3.3
1	C	348	VAL	3.3
1	B	318	ASP	3.2
1	C	183	THR	3.2
1	A	226	GLU	3.2
1	D	354	ILE	3.2
1	D	279	PRO	3.2
1	C	317	PHE	3.2
1	B	316	GLY	3.1
1	B	362	LEU	3.1
1	B	356	VAL	3.1
1	D	352	ALA	3.1
1	B	115	PHE	3.1
1	B	358	ARG	3.0
1	C	184	PHE	2.9
1	D	353	SER	2.8
1	D	355	PRO	2.8
1	B	348	VAL	2.7
1	D	23	SER	2.7
1	C	27	SER	2.6
1	C	207	TYR	2.6
1	D	107	ILE	2.6
1	A	355	PRO	2.6
1	D	318	ASP	2.5
1	A	361	GLN	2.5
1	A	112	PHE	2.5
1	A	223	ASP	2.5
1	C	112	PHE	2.5
1	A	225	ALA	2.4
1	C	115	PHE	2.4
1	D	313	LEU	2.4
1	C	114	LEU	2.3
1	B	386	GLY	2.3
1	B	23	SER	2.2
1	C	204	ALA	2.2
1	A	56	ARG	2.2
1	A	208	LEU	2.2
1	C	239	GLY	2.2
1	A	358	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	369	VAL	2.1
1	B	184	PHE	2.1
1	A	207	TYR	2.1
1	A	390	LYS	2.0
1	D	114	LEU	2.0
1	A	115	PHE	2.0
1	B	354	ILE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.