Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2023 – 10:21 AM JST

PDB ID	:	7Y5K
Title	:	Crystal structure of human CAF-1 core complex in spacegroup C2221
Authors	:	Liu, C.P.; Wang, M.Z.; Xu, R.M.
Deposited on	:	2022-06-17
Resolution	:	3.48 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 (i) 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 (1)) were used in the production of this report:

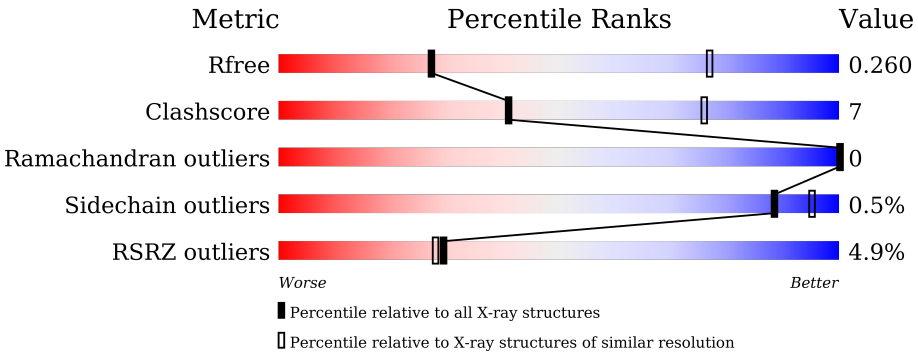
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 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	273	4% 62% 12% 27%
2	C	425	5% 76% 19% 5%
3	B	419	4% 73% 18% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7788 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 Chromatin assembly factor 1 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1607	1013	297	289	8	0	0	0

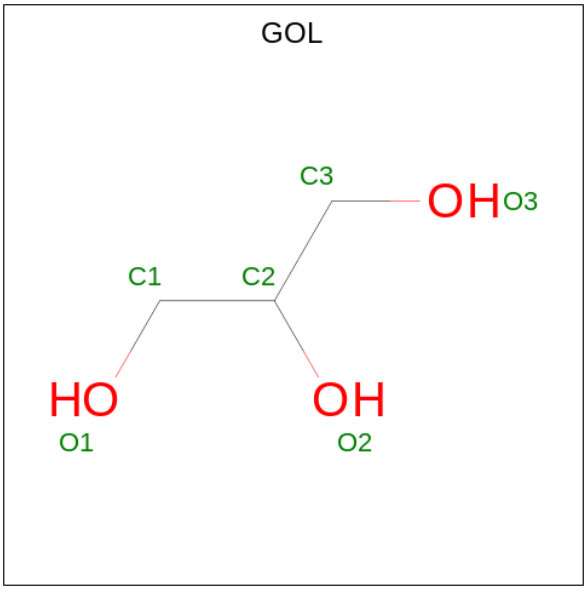
- Molecule 2 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	405	3191	2012	543	626	10	0	0	0

- Molecule 3 is a protein called Chromatin assembly factor 1 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	382	2982	1904	515	547	16	0	0	0

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



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

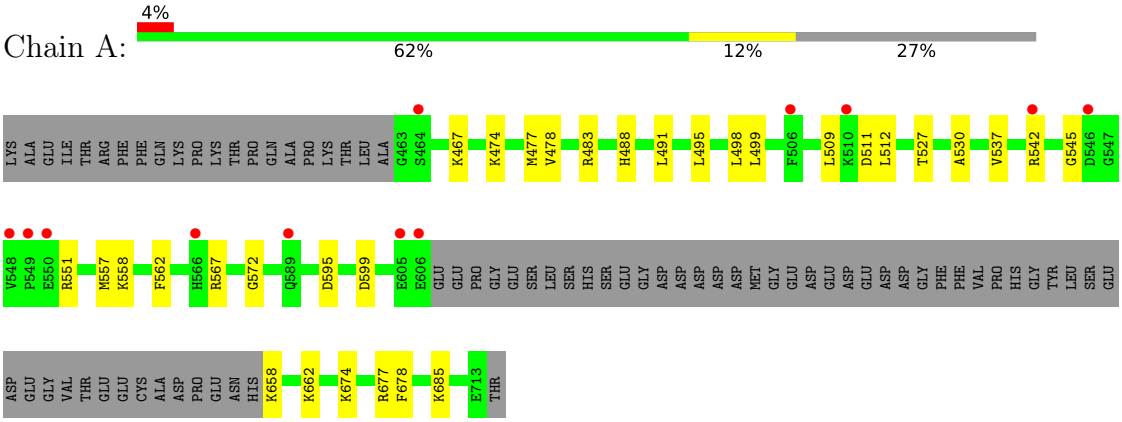
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0

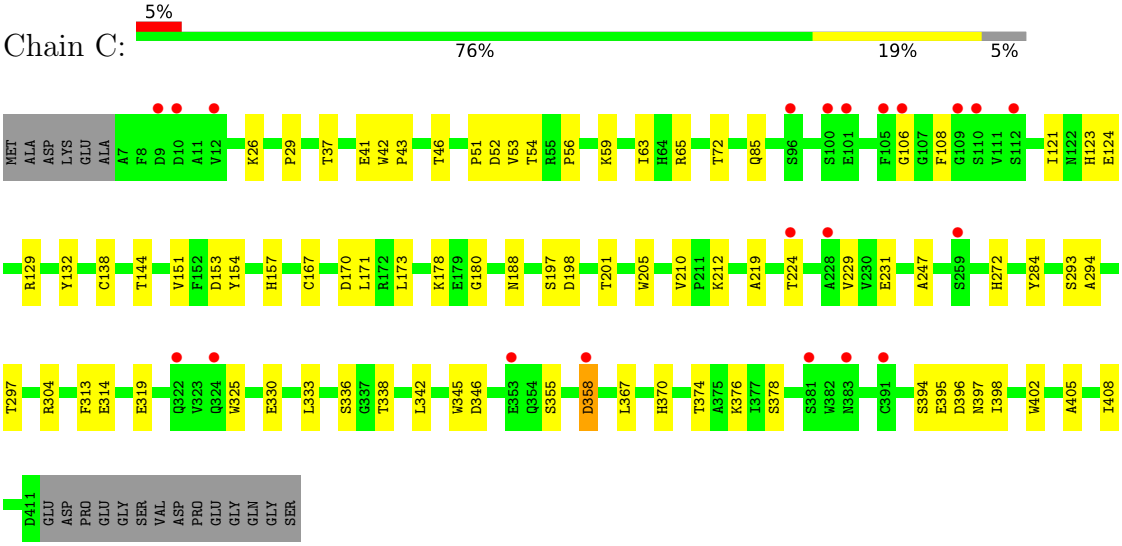
3 Residue-property plots (i)

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.

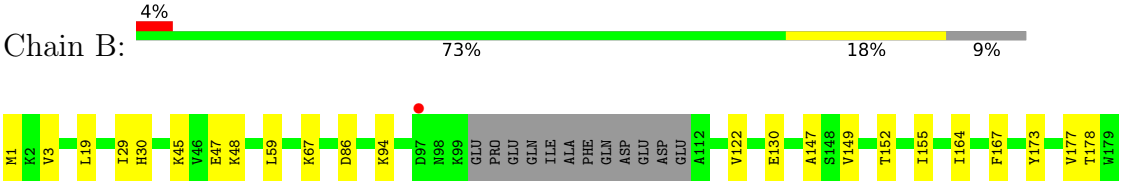
• Molecule 1: Chromatin assembly factor 1 subunit A

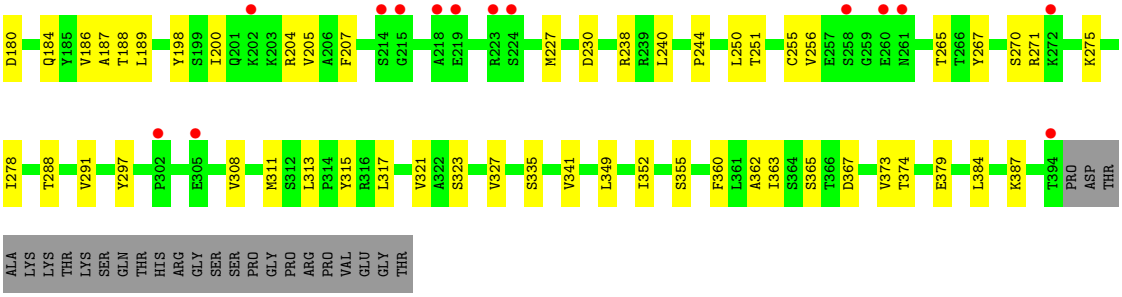


• Molecule 2: Histone-binding protein RBBP4



• Molecule 3: Chromatin assembly factor 1 subunit B




D180 Q184 Y185 V186 A187 T188 L189 Y198 S199 I200 Q201 K202 K203 R204 V205 A206 F207 S214 G215 A218 E219 R223 S224 M227 D230 R238 R239 L240 P244 L250 T251 C255 V256 E257 S258 G259 E260 N261 T265 T266 Y267 S270 R271 K272 K275
I278 T288 V291 Y297 P302 E305 V308 M311 S312 L313 P314 Y315 R316 L317 V321 A322 S323 V327 S335 V341 L349 I352 S355 F360 L361 A362 I363 S364 S365 T366 D367 V373 T374 E379 L384 K387 T394 PRO ASP THR
ALA LYS LYS THR LYS SER GLN THR HIS ARG GLY SER SER PRO GLY PRO ARG PRO VAL GLU GLY THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	108.87Å 169.84Å 153.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.33 – 3.48 39.33 – 3.48	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.33-3.48) 94.2 (39.33-3.48)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.225 , 0.257 0.227 , 0.260	Depositor DCC
R_{free} test set	1746 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 23.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7788	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/1642	0.48	0/2207
2	C	0.24	0/3280	0.45	0/4474
3	B	0.24	0/3051	0.49	0/4141
All	All	0.24	0/7973	0.47	0/10822

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	1607	0	1570	22	0
2	C	3191	0	3002	53	0
3	B	2982	0	2959	45	0
4	C	6	0	8	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	7788	0	7539	109	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 7.

All (109) 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)
3:B:270:SER:HB2	3:B:278:ILE:HD11	1.58	0.82
1:A:674:LYS:HE3	1:A:677:ARG:HH21	1.56	0.70
2:C:346:ASP:HB2	2:C:367:LEU:HD12	1.73	0.69
2:C:297:THR:HG22	2:C:314:GLU:HG2	1.77	0.67
2:C:342:LEU:HB3	2:C:370:HIS:HB3	1.79	0.64
2:C:46:THR:HB	2:C:129:ARG:HA	1.79	0.64
1:A:595:ASP:O	2:C:26:LYS:NZ	2.30	0.63
2:C:151:VAL:HB	2:C:171:LEU:HB2	1.79	0.63
2:C:294:ALA:HA	2:C:319:GLU:HG3	1.80	0.62
2:C:336:SER:HB3	2:C:342:LEU:HD13	1.83	0.60
3:B:311:MET:HE1	3:B:313:LEU:HD12	1.84	0.59
3:B:1:MET:N	3:B:379:GLU:OE2	2.32	0.59
3:B:178:THR:HG22	3:B:187:ALA:HB3	1.84	0.59
3:B:189:LEU:HD23	3:B:238:ARG:HB3	1.85	0.58
3:B:29:ILE:HG23	3:B:47:GLU:HB3	1.85	0.58
3:B:29:ILE:HG21	3:B:45:LYS:HE3	1.85	0.58
1:A:527:THR:HB	1:A:530:ALA:HB2	1.85	0.57
1:A:572:GLY:HA3	2:C:106:GLY:HA2	1.86	0.57
3:B:291:VAL:HG22	3:B:321:VAL:HG22	1.87	0.57
1:A:674:LYS:HB3	1:A:678:PHE:HB2	1.87	0.57
2:C:121:ILE:HD13	2:C:157:HIS:HD2	1.70	0.55
3:B:250:LEU:HB2	3:B:291:VAL:HG11	1.88	0.55
3:B:315:TYR:HB3	3:B:384:LEU:HD11	1.89	0.55
3:B:177:VAL:HG22	3:B:188:THR:HG22	1.90	0.54
1:A:567:ARG:HH22	1:A:599:ASP:HB2	1.72	0.54
3:B:147:ALA:HB2	3:B:177:VAL:HG23	1.88	0.54
1:A:537:VAL:HG11	1:A:662:LYS:HB3	1.88	0.53
2:C:178:LYS:HD3	2:C:198:ASP:HB2	1.89	0.53
3:B:48:LYS:HE2	3:B:374:THR:HB	1.90	0.53
3:B:297:TYR:HD1	3:B:387:LYS:HD2	1.74	0.53
2:C:198:ASP:HA	2:C:229:VAL:HG13	1.90	0.53
2:C:338:THR:HG22	2:C:376:LYS:HD2	1.89	0.53
3:B:355:SER:HB3	3:B:360:PHE:HB2	1.91	0.52
2:C:173:LEU:HB3	2:C:205:TRP:CE2	2.45	0.52
3:B:288:THR:HA	3:B:323:SER:HA	1.91	0.52
2:C:338:THR:HA	2:C:376:LYS:HG3	1.90	0.52
1:A:567:ARG:HD2	2:C:108:PHE:CE2	2.44	0.52
3:B:308:VAL:HG13	3:B:335:SER:HB3	1.91	0.52
3:B:184:GLN:OE1	3:B:271:ARG:NH2	2.42	0.51
2:C:342:LEU:HD23	2:C:402:TRP:HZ2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:152:THR:HA	3:B:167:PHE:O	2.11	0.50
2:C:63:ILE:HG12	2:C:85:GLN:HG2	1.93	0.50
2:C:138:CYS:HA	2:C:154:TYR:CE2	2.47	0.50
3:B:255:CYS:O	3:B:267:TYR:OH	2.28	0.50
2:C:201:THR:HG22	2:C:224:THR:HG22	1.94	0.50
3:B:149:VAL:HG13	3:B:173:TYR:CD1	2.47	0.49
3:B:365:SER:OG	3:B:367:ASP:OD1	2.29	0.49
2:C:374:THR:OG1	2:C:396:ASP:OD2	2.27	0.49
2:C:284:TYR:HB2	2:C:330:GLU:HB3	1.96	0.48
2:C:205:TRP:CD1	2:C:219:ALA:HA	2.48	0.48
3:B:45:LYS:HB2	3:B:59:LEU:HD11	1.95	0.47
3:B:207:PHE:HD1	3:B:275:LYS:HE3	1.80	0.47
2:C:378:SER:H	2:C:394:SER:HA	1.79	0.47
2:C:171:LEU:HD21	2:C:210:VAL:HG11	1.95	0.47
2:C:51:PRO:HD3	2:C:132:TYR:CZ	2.50	0.47
1:A:474:LYS:HB2	1:A:477:MET:HG3	1.96	0.47
3:B:327:VAL:HG21	3:B:363:ILE:HD13	1.98	0.46
1:A:558:LYS:NZ	2:C:29:PRO:O	2.39	0.46
3:B:256:VAL:HG23	3:B:265:THR:HG21	1.97	0.46
3:B:19:LEU:HD13	3:B:362:ALA:HB1	1.97	0.46
1:A:498:LEU:HB3	2:C:304:ARG:HG2	1.98	0.46
3:B:230:ASP:OD1	3:B:230:ASP:N	2.44	0.46
2:C:41:GLU:HG2	2:C:42:TRP:CD1	2.51	0.46
2:C:325:TRP:CD2	2:C:333:LEU:HD13	2.51	0.45
2:C:54:THR:OG1	2:C:63:ILE:HB	2.17	0.45
2:C:56:PRO:HG2	2:C:59:LYS:HB2	1.99	0.45
3:B:198:TYR:CE2	3:B:205:VAL:HG22	2.52	0.45
1:A:483:ARG:NH2	2:C:188:ASN:OD1	2.49	0.45
3:B:3:VAL:HG22	3:B:373:VAL:HG22	1.98	0.45
2:C:405:ALA:HB3	2:C:408:ILE:HG13	1.99	0.45
1:A:488:HIS:HB2	1:A:491:LEU:HB2	1.99	0.45
2:C:65:ARG:NH2	2:C:154:TYR:OH	2.34	0.44
3:B:130:GLU:HB3	3:B:149:VAL:HB	1.98	0.44
2:C:197:SER:OG	2:C:198:ASP:N	2.50	0.44
2:C:153:ASP:N	2:C:170:ASP:OD2	2.46	0.44
3:B:227:MET:O	3:B:255:CYS:N	2.33	0.44
2:C:52:ASP:OD2	2:C:65:ARG:NH2	2.51	0.44
1:A:562:PHE:HA	2:C:37:THR:HB	1.98	0.44
2:C:42:TRP:CD2	2:C:72:THR:HG22	2.53	0.43
2:C:43:PRO:HA	2:C:397:ASN:HA	2.00	0.43
3:B:180:ASP:OD1	3:B:271:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:123:HIS:CE1	2:C:144:THR:HG22	2.54	0.43
3:B:67:LYS:HB3	3:B:86:ASP:HB2	2.00	0.43
3:B:240:LEU:HB3	3:B:251:THR:HA	2.01	0.43
3:B:244:PRO:HD2	3:B:317:LEU:HD13	2.01	0.42
1:A:551:ARG:HH21	1:A:557:MET:HG3	1.83	0.42
2:C:272:HIS:CG	2:C:293:SER:HB2	2.54	0.42
1:A:478:VAL:HB	2:C:53:VAL:HG13	2.02	0.42
3:B:155:ILE:O	3:B:164:ILE:HG22	2.19	0.42
3:B:352:ILE:HG22	3:B:363:ILE:HG12	2.01	0.42
1:A:685:LYS:HG3	3:B:341:VAL:HG22	2.02	0.42
2:C:376:LYS:HD3	2:C:395:GLU:OE2	2.19	0.42
1:A:495:LEU:O	1:A:499:LEU:N	2.50	0.42
3:B:30:HIS:CD2	3:B:355:SER:HB2	2.54	0.42
2:C:231:GLU:H	2:C:247:ALA:HA	1.85	0.42
1:A:509:LEU:HD23	1:A:512:LEU:HD12	2.01	0.41
2:C:313:PHE:HB3	2:C:345:TRP:CZ3	2.55	0.41
2:C:355:SER:OG	2:C:358:ASP:HB2	2.21	0.41
3:B:349:LEU:HD23	3:B:365:SER:HB3	2.01	0.41
1:A:467:LYS:HB2	2:C:212:LYS:HA	2.01	0.41
1:A:545:GLY:HA2	1:A:658:LYS:HG3	2.03	0.41
2:C:398:ILE:HD13	2:C:398:ILE:HA	1.94	0.41
2:C:180:GLY:HA3	2:C:197:SER:HA	2.02	0.41
3:B:186:VAL:HG23	3:B:200:ILE:HD13	2.03	0.41
3:B:200:ILE:HD12	3:B:200:ILE:HA	1.90	0.41
1:A:477:MET:HG2	2:C:54:THR:HG22	2.03	0.41
2:C:124:GLU:HG2	2:C:167:CYS:SG	2.62	0.40
3:B:94:LYS:HD3	3:B:122:VAL:HG21	2.03	0.40
3:B:189:LEU:HD12	3:B:189:LEU:HA	1.94	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	196/273 (72%)	189 (96%)	7 (4%)	0	100	100
2	C	403/425 (95%)	392 (97%)	11 (3%)	0	100	100
3	B	378/419 (90%)	365 (97%)	13 (3%)	0	100	100
All	All	977/1117 (88%)	946 (97%)	31 (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	166/235 (71%)	164 (99%)	2 (1%)	71	87
2	C	353/375 (94%)	352 (100%)	1 (0%)	92	97
3	B	325/363 (90%)	324 (100%)	1 (0%)	92	97
All	All	844/973 (87%)	840 (100%)	4 (0%)	88	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	ASP
1	A	542	ARG
2	C	358	ASP
3	B	204	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

1 ligand is 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	$\#\|Z\| > 2$
4	GOL	C	501	-	5,5,5	0.92	0	5,5,5	1.01	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
4	GOL	C	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

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 (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	200/273 (73%)	0.60	12 (6%)	21	21	47, 76, 108, 127	0
2	C	405/425 (95%)	0.42	21 (5%)	27	26	42, 66, 99, 116	0
3	B	382/419 (91%)	0.29	15 (3%)	39	36	39, 58, 95, 117	0
All	All	987/1117 (88%)	0.41	48 (4%)	29	28	39, 64, 103, 127	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	218	ALA	4.5
3	B	215	GLY	4.4
1	A	606	GLU	3.8
2	C	324	GLN	3.3
3	B	258	SER	3.3
3	B	219	GLU	3.3
2	C	110	SER	3.2
2	C	259	SER	3.2
3	B	394	THR	3.1
3	B	261	ASN	3.1
2	C	101	GLU	3.0
2	C	105	PHE	2.8
2	C	10	ASP	2.8
2	C	358	ASP	2.7
2	C	381	SER	2.7
3	B	302	PRO	2.7
3	B	214	SER	2.7
1	A	549	PRO	2.7
1	A	506	PHE	2.6
2	C	109	GLY	2.6
1	A	542	ARG	2.5
1	A	550	GLU	2.5
1	A	510	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	224	THR	2.4
2	C	96	SER	2.4
1	A	566	HIS	2.4
2	C	353	GLU	2.4
3	B	97	ASP	2.3
1	A	605	GLU	2.3
1	A	548	VAL	2.3
1	A	589	GLN	2.3
1	A	546	ASP	2.3
3	B	202	LYS	2.3
1	A	464	SER	2.2
2	C	9	ASP	2.2
2	C	106	GLY	2.2
2	C	112	SER	2.1
2	C	12	VAL	2.1
3	B	305	GLU	2.1
2	C	383	ASN	2.1
3	B	223	ARG	2.1
3	B	224	SER	2.1
3	B	260	GLU	2.1
2	C	391	CYS	2.1
2	C	322	GLN	2.1
2	C	100	SER	2.1
2	C	228	ALA	2.1
3	B	272	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	C	501	6/6	0.90	0.18	59,60,61,62	0

6.5 Other polymers (i)

There are no such residues in this entry.