



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:06 AM UTC

PDB ID : 7OFP / pdb_00007ofp
Title : Apo Structure of Mu2 Adaptin Subunit (Ap50) Of AP2 Clathrin Adaptor
Authors : Zaccai, N.R.; Kelly, B.T.; Evans, P.R.; Owen, D.J.
Deposited on : 2021-05-05
Resolution : 1.92 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

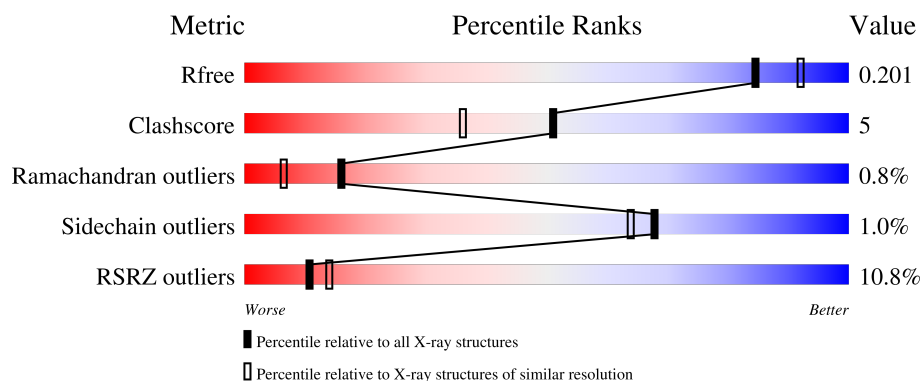
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. 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	285	11% 80% 11% 8%
1	B	285	9% 81% 12% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9111 atoms, of which 4512 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 AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	H	N	O	S	0	1	0
			4314	1359	2200	372	369	14			
1	B	266	Total	C	H	N	O	S	0	0	0
			4385	1378	2239	377	377	14			

There are 14 discrepancies between the modelled and reference sequences:

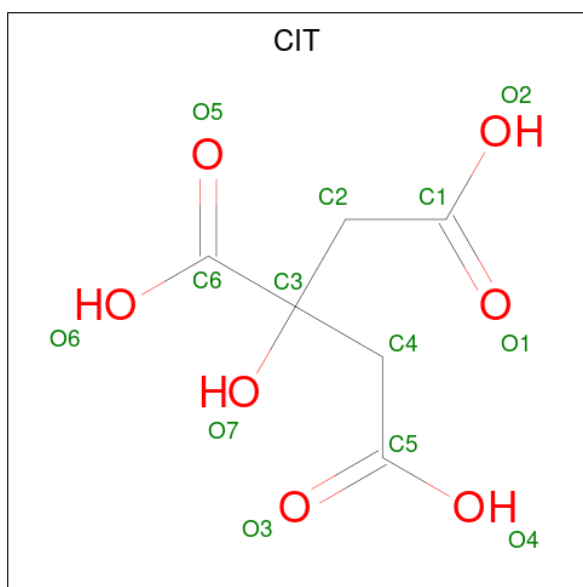
Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	initiating methionine	UNP P84092
A	152	HIS	-	expression tag	UNP P84092
A	153	HIS	-	expression tag	UNP P84092
A	154	HIS	-	expression tag	UNP P84092
A	155	HIS	-	expression tag	UNP P84092
A	156	HIS	-	expression tag	UNP P84092
A	157	HIS	-	expression tag	UNP P84092
B	151	MET	-	initiating methionine	UNP P84092
B	152	HIS	-	expression tag	UNP P84092
B	153	HIS	-	expression tag	UNP P84092
B	154	HIS	-	expression tag	UNP P84092
B	155	HIS	-	expression tag	UNP P84092
B	156	HIS	-	expression tag	UNP P84092
B	157	HIS	-	expression tag	UNP P84092

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			13	3	7	3		
2	B	1	Total	C	H	O	0	0
			13	3	7	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			18	6	5	7		

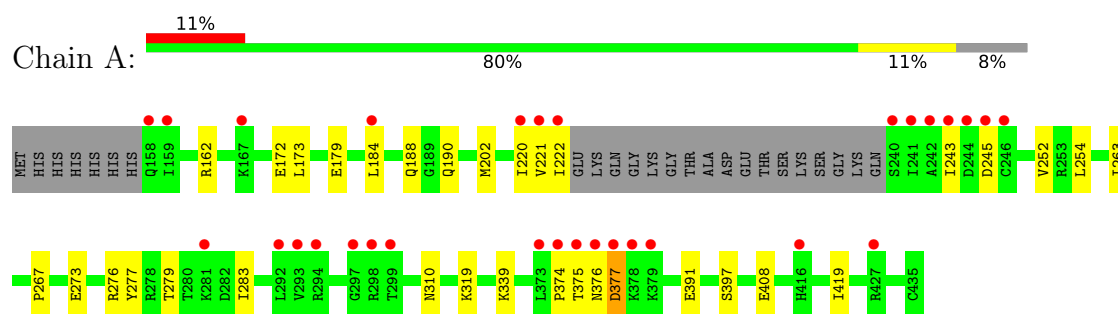
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	132	Total	O	0	0
			132	132		

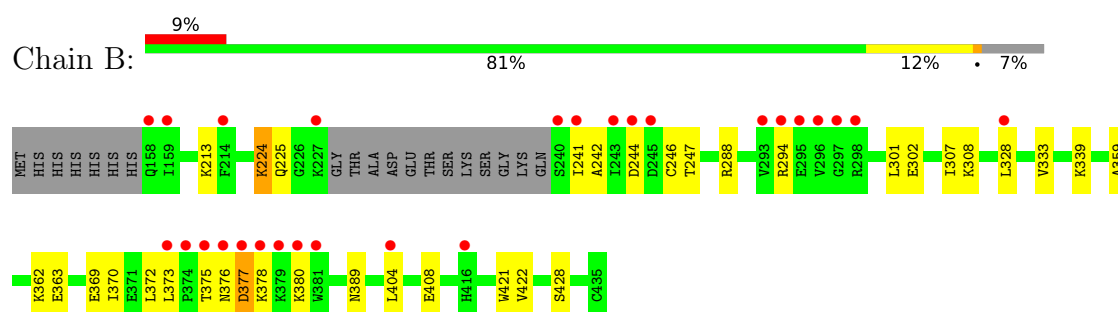
3 Residue-property plots [i](#)

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: AP-2 complex subunit mu



- Molecule 1: AP-2 complex subunit mu



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	123.83Å 123.83Å 112.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	77.68 – 1.92 77.68 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (77.68-1.92) 99.9 (77.68-1.92)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.92Å)	Xtriage
Refinement program	REFMAC 1.19rc1_4016, PHENIX 1.19rc1_4016	Depositor
R, R_{free}	0.188 , 0.210 (Not available) , 0.201	Depositor DCC
R_{free} test set	3820 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9111	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 5.95% 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, 0.333 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: GOL, CIT

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	0/2160	0.71	0/2904
1	B	0.81	2/2189 (0.1%)	0.76	1/2941 (0.0%)
All	All	0.79	2/4349 (0.0%)	0.74	1/5845 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	CYS	CB-SG	-5.59	1.62	1.81
1	B	224	LYS	CE-NZ	5.09	1.64	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	THR	CA-CB-OG1	-5.09	101.96	109.60

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	2114	2200	2211	23	0
1	B	2146	2239	2241	23	0
2	A	36	46	47	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	22	24	0	0
3	A	13	5	5	2	0
4	A	140	0	0	1	0
4	B	132	0	0	1	0
All	All	4599	4512	4528	46	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 5.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LYS:HG2	1:B:363:GLU:HG2	1.59	0.81
1:A:173:LEU:HD11	1:A:202:MET:HE3	1.66	0.76
1:B:376:ASN:O	1:B:377:ASP:HB2	1.94	0.66
1:B:225:GLN:H	1:B:225:GLN:CD	2.05	0.65
1:A:220:ILE:HG22	1:A:243:ILE:HG13	1.82	0.62
1:A:319:LYS:HD3	1:A:391:GLU:OE1	2.02	0.59
1:B:302:GLU:HG3	1:B:369:GLU:OE1	2.04	0.57
1:B:376:ASN:O	1:B:377:ASP:CB	2.54	0.56
1:A:243:ILE:HG21	1:A:277:TYR:HB2	1.87	0.56
1:B:213:LYS:HE3	4:B:703:HOH:O	2.07	0.55
3:A:507:CIT:O6	1:B:339:LYS:NZ	2.40	0.54
1:B:328:LEU:HD22	1:B:328:LEU:N	2.25	0.52
1:A:273:GLU:OE2	1:A:276:ARG:HG3	2.10	0.50
1:A:310:ASN:HB2	4:A:714:HOH:O	2.11	0.50
1:B:288:ARG:HH11	1:B:288:ARG:HG3	1.77	0.50
1:A:283:ILE:H	2:A:503:GOL:H12	1.78	0.47
1:A:374:PRO:O	1:A:375:THR:C	2.58	0.47
1:A:376:ASN:O	1:A:377:ASP:CB	2.63	0.47
1:A:339:LYS:NZ	2:A:505:GOL:H31	2.31	0.46
3:A:507:CIT:O5	3:A:507:CIT:C1	2.65	0.45
1:A:188:GLN:OE1	1:A:190:GLN:NE2	2.50	0.45
1:B:373:LEU:HD12	1:B:375:THR:HG23	1.99	0.45
1:B:328:LEU:HD22	1:B:328:LEU:H	1.82	0.44
1:A:162:ARG:HD2	1:A:267:PRO:O	2.19	0.43
1:B:294:ARG:HG3	1:B:294:ARG:HH11	1.84	0.43
1:B:301:LEU:HG	1:B:372:LEU:HD11	2.00	0.43
1:B:359:ALA:HB3	1:B:362:LYS:HD2	2.01	0.43
1:A:179:GLU:OE2	1:A:397:SER:OG	2.30	0.42
1:B:288:ARG:HG3	1:B:288:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASP:O	1:B:378:LYS:CB	2.67	0.42
1:A:184:LEU:HB3	1:B:421:TRP:CZ3	2.55	0.42
1:A:243:ILE:HG23	1:A:279:THR:HG22	2.01	0.41
1:A:376:ASN:O	1:A:377:ASP:CG	2.63	0.41
1:A:221:VAL:HG11	1:A:254:LEU:HD22	2.01	0.41
1:A:221:VAL:O	1:A:222:ILE:C	2.63	0.41
1:B:241:ILE:CG2	1:B:242:ALA:N	2.84	0.41
1:B:294:ARG:HG3	1:B:294:ARG:NH1	2.36	0.41
1:B:307:ILE:HG21	1:B:307:ILE:HD13	1.89	0.41
1:A:172:GLU:HG2	1:A:419:ILE:HB	2.03	0.41
1:A:339:LYS:NZ	2:A:505:GOL:C3	2.84	0.41
1:A:339:LYS:HZ2	2:A:505:GOL:H31	1.85	0.40
1:B:389:ASN:HA	1:B:428:SER:OG	2.22	0.40
1:B:404:LEU:HD11	1:B:422:VAL:CG2	2.52	0.40
1:A:252:VAL:HG13	1:A:263:ILE:HB	2.03	0.40
1:B:301:LEU:HB2	1:B:370:ILE:HB	2.02	0.40
1:A:377:ASP:OD1	1:A:377:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	258/285 (90%)	251 (97%)	6 (2%)	1 (0%)	30	19
1	B	262/285 (92%)	251 (96%)	8 (3%)	3 (1%)	11	3
All	All	520/570 (91%)	502 (96%)	14 (3%)	4 (1%)	16	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	377	ASP

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Mol	Chain	Res	Type
1	A	377	ASP
1	B	244	ASP
1	B	380	LYS

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	238/257 (93%)	236 (99%)	2 (1%)	73	71
1	B	241/257 (94%)	238 (99%)	3 (1%)	63	57
All	All	479/514 (93%)	474 (99%)	5 (1%)	68	64

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	ASP
1	A	408	GLU
1	B	224	LYS
1	B	333	VAL
1	B	408	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	349	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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$
2	GOL	A	501	-	5,5,5	0.85	0	5,5,5	0.77	0
2	GOL	B	502	-	5,5,5	1.04	0	5,5,5	0.82	0
2	GOL	A	503	-	5,5,5	0.73	0	5,5,5	0.89	0
2	GOL	A	505	-	5,5,5	1.45	2 (40%)	5,5,5	1.08	0
2	GOL	B	501	-	5,5,5	1.40	1 (20%)	5,5,5	1.21	1 (20%)
2	GOL	A	506	-	5,5,5	1.23	1 (20%)	5,5,5	1.15	1 (20%)
2	GOL	B	503	-	5,5,5	1.40	1 (20%)	5,5,5	1.38	1 (20%)
2	GOL	A	504	-	5,5,5	1.12	1 (20%)	5,5,5	1.16	0
3	CIT	A	507	-	12,12,12	1.20	0	17,17,17	1.28	3 (17%)
2	GOL	A	502	-	5,5,5	1.08	0	5,5,5	1.17	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
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	503	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	505	-	-	3/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	506	-	-	2/4/4/4	-
2	GOL	B	503	-	-	3/4/4/4	-
2	GOL	A	504	-	-	2/4/4/4	-
3	CIT	A	507	-	-	7/16/16/16	-
2	GOL	A	502	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	505	GOL	C3-C2	2.42	1.61	1.51
2	A	504	GOL	O1-C1	-2.26	1.33	1.42
2	B	503	GOL	O1-C1	2.21	1.51	1.42
2	A	506	GOL	O2-C2	-2.16	1.37	1.43
2	A	505	GOL	C1-C2	2.04	1.59	1.51
2	B	501	GOL	O2-C2	-2.01	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	CIT	O4-C5-C4	2.59	122.55	114.35
2	A	506	GOL	C3-C2-C1	-2.30	103.38	111.80
2	B	503	GOL	C3-C2-C1	-2.28	103.43	111.80
2	B	501	GOL	C3-C2-C1	-2.17	103.85	111.80
3	A	507	CIT	O4-C5-O3	-2.13	117.86	123.33
3	A	507	CIT	O6-C6-C3	2.00	116.98	113.14

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	GOL	C1-C2-C3-O3
2	B	501	GOL	C1-C2-C3-O3
3	A	507	CIT	O7-C3-C4-C5
3	A	507	CIT	C2-C3-C6-O5
3	A	507	CIT	C2-C3-C6-O6
3	A	507	CIT	O7-C3-C6-O5
3	A	507	CIT	O7-C3-C6-O6
3	A	507	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	A	506	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	503	GOL	O1-C1-C2-C3
2	B	501	GOL	O2-C2-C3-O3
3	A	507	CIT	C2-C3-C4-C5
2	A	505	GOL	O2-C2-C3-O3
2	A	506	GOL	O1-C1-C2-O2
2	A	504	GOL	O2-C2-C3-O3
2	A	505	GOL	O1-C1-C2-O2
2	A	503	GOL	O2-C2-C3-O3
2	B	502	GOL	O2-C2-C3-O3
2	B	503	GOL	O2-C2-C3-O3
2	A	501	GOL	O2-C2-C3-O3
2	B	503	GOL	O1-C1-C2-O2
2	A	504	GOL	C1-C2-C3-O3
2	A	502	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	1	0
2	A	505	GOL	3	0
3	A	507	CIT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/285 (91%)	0.36	30 (11%) 9 12	26, 39, 78, 146	1 (0%)
1	B	266/285 (93%)	0.36	27 (10%) 12 16	26, 39, 77, 165	0
All	All	527/570 (92%)	0.36	57 (10%) 11 14	26, 39, 78, 165	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	ILE	7.5
1	A	294[A]	ARG	7.4
1	B	374	PRO	7.2
1	A	241	ILE	6.0
1	A	375	THR	5.6
1	A	243	ILE	5.6
1	B	378	LYS	5.6
1	B	375	THR	5.4
1	B	373	LEU	4.8
1	B	380	LYS	4.5
1	B	294	ARG	4.4
1	B	377	ASP	4.4
1	A	245	ASP	4.2
1	B	379	LYS	4.2
1	A	220	ILE	4.1
1	A	374	PRO	4.1
1	A	242	ALA	4.0
1	A	158	GLN	3.8
1	A	378	LYS	3.5
1	A	373	LEU	3.5
1	A	376	ASN	3.4
1	A	246	CYS	3.3
1	A	292	LEU	3.3
1	B	240	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	377	ASP	3.1
1	B	227	LYS	3.0
1	A	427	ARG	3.0
1	B	376	ASN	3.0
1	A	221	VAL	3.0
1	B	158	GLN	2.9
1	B	293	VAL	2.9
1	A	159	ILE	2.9
1	B	296	VAL	2.8
1	B	381	TRP	2.7
1	B	328	LEU	2.7
1	B	297	GLY	2.6
1	B	159	ILE	2.6
1	A	379	LYS	2.6
1	A	244	ASP	2.5
1	B	214	PHE	2.5
1	B	404	LEU	2.5
1	B	244	ASP	2.5
1	B	416	HIS	2.5
1	A	281	LYS	2.5
1	B	298	ARG	2.4
1	B	241	ILE	2.4
1	B	243	ILE	2.3
1	B	245	ASP	2.3
1	A	416	HIS	2.3
1	A	297	GLY	2.2
1	A	298	ARG	2.2
1	B	295	GLU	2.1
1	A	299	THR	2.1
1	A	167	LYS	2.1
1	A	184	LEU	2.1
1	A	240	SER	2.0
1	A	293	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	CIT	A	507	13/13	0.77	0.19	60,83,98,107	0
2	GOL	A	505	6/6	0.78	0.20	45,60,83,95	0
2	GOL	B	502	6/6	0.79	0.23	53,79,107,107	0
2	GOL	A	503	6/6	0.82	0.18	47,72,87,88	0
2	GOL	A	502	6/6	0.84	0.20	48,65,85,85	0
2	GOL	A	504	6/6	0.89	0.17	41,62,79,88	0
2	GOL	B	503	6/6	0.90	0.14	39,50,67,80	0
2	GOL	A	506	6/6	0.90	0.16	44,62,74,76	0
2	GOL	A	501	6/6	0.91	0.15	42,66,81,88	0
2	GOL	B	501	6/6	0.94	0.11	32,51,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.