



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:03 PM UTC

PDB ID : 5BYG / pdb_00005byg
Title : X-ray structure of AAV2 OBD-AAVS1 complex 2:1
Authors : Musayev, F.N.; Escalante, C.R.
Deposited on : 2015-06-10
Resolution : 2.50 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

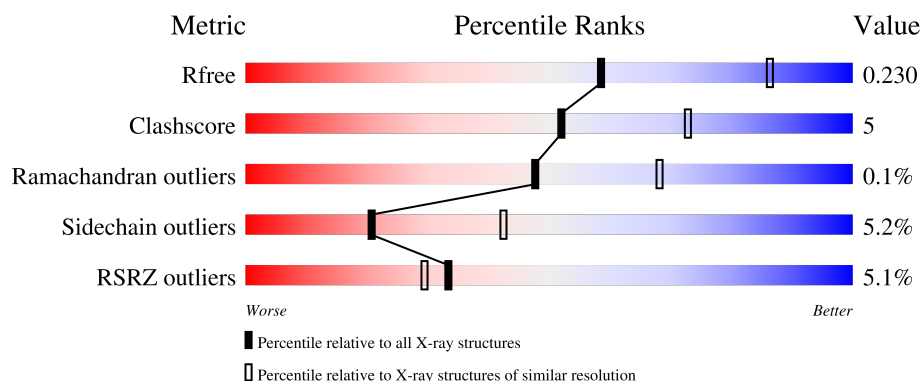
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	213	2% 75% 10% 15%
1	B	213	% 82% 12% 6%
1	C	213	2% 72% 17% 9%
1	D	213	14% 73% 11% 15%
2	E	21	90% 10%

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Mol	Chain	Length	Quality of chain
2	G	21	 81%19%
3	F	21	 5%90%10%
3	H	21	 76%24%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7847 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 Protein Rep78.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1457	940	249	263	5			
1	B	201	Total	C	N	O	S	0	0	0
			1635	1048	279	302	6			
1	C	193	Total	C	N	O	S	0	0	0
			1559	1005	265	284	5			
1	D	180	Total	C	N	O	S	0	0	0
			1329	852	228	245	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q89268
A	-1	SER	-	expression tag	UNP Q89268
A	0	HIS	-	expression tag	UNP Q89268
A	151	SER	CYS	engineered mutation	UNP Q89268
A	156	PHE	TYR	engineered mutation	UNP Q89268
B	-2	GLY	-	expression tag	UNP Q89268
B	-1	SER	-	expression tag	UNP Q89268
B	0	HIS	-	expression tag	UNP Q89268
B	151	SER	CYS	engineered mutation	UNP Q89268
B	156	PHE	TYR	engineered mutation	UNP Q89268
C	-2	GLY	-	expression tag	UNP Q89268
C	-1	SER	-	expression tag	UNP Q89268
C	0	HIS	-	expression tag	UNP Q89268
C	151	SER	CYS	engineered mutation	UNP Q89268
C	156	PHE	TYR	engineered mutation	UNP Q89268
D	-2	GLY	-	expression tag	UNP Q89268
D	-1	SER	-	expression tag	UNP Q89268
D	0	HIS	-	expression tag	UNP Q89268
D	151	SER	CYS	engineered mutation	UNP Q89268
D	156	PHE	TYR	engineered mutation	UNP Q89268

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*CP*TP*CP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	P	0	0	0
			419	200	70	129	20			
2	G	21	Total	C	N	O	P	0	0	0
			419	200	70	129	20			

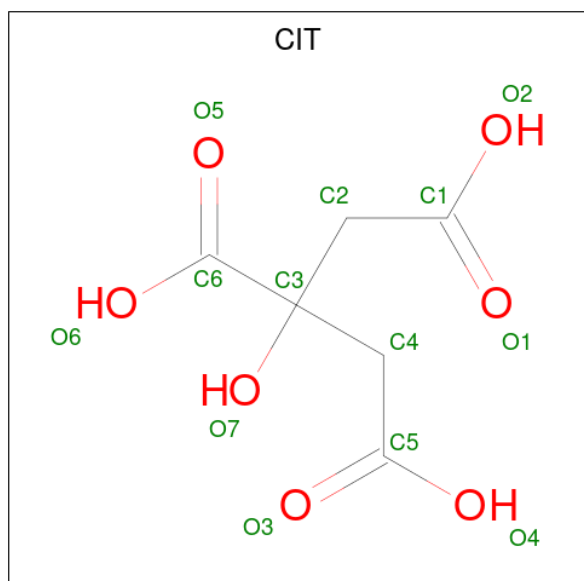
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*AP*GP*CP*GP*AP*GP*CP*GP*AP*GP*CP*GP*AP*GP*CP*GP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	21	Total	C	N	O	P	0	0	0
			436	204	93	119	20			
3	H	21	Total	C	N	O	P	0	0	0
			436	204	93	119	20			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	C	1	Total	C	O	0	0
			13	6	7		

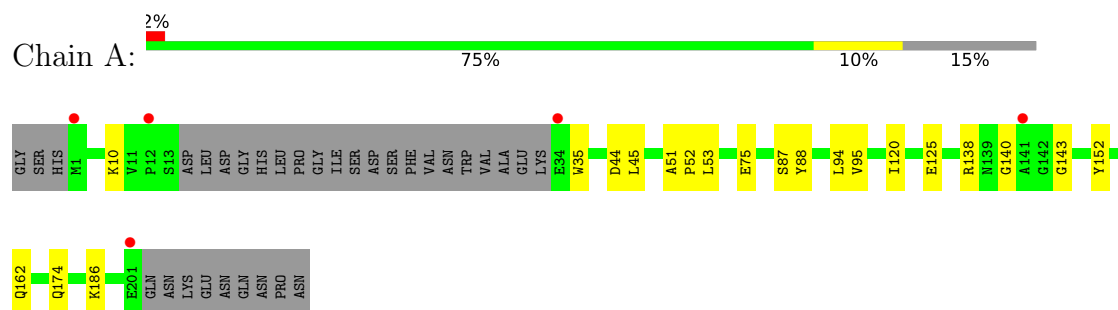
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	36	Total	O	0	0
			36	36		
6	C	33	Total	O	0	0
			33	33		
6	D	10	Total	O	0	0
			10	10		
6	E	6	Total	O	0	0
			6	6		
6	F	6	Total	O	0	0
			6	6		
6	G	3	Total	O	0	0
			3	3		
6	H	3	Total	O	0	0
			3	3		

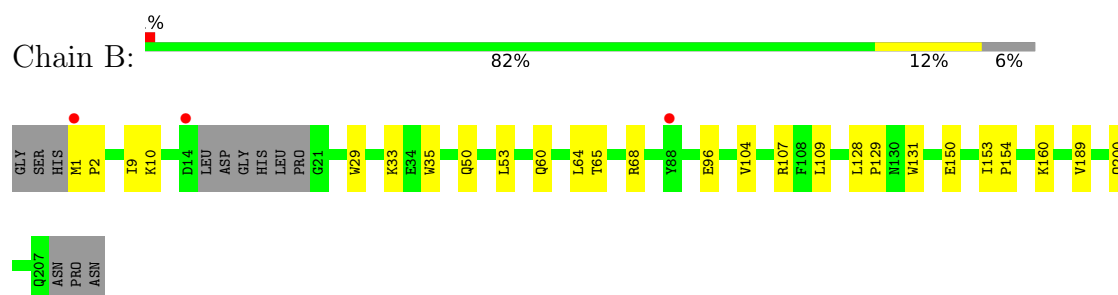
3 Residue-property plots [i](#)

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.

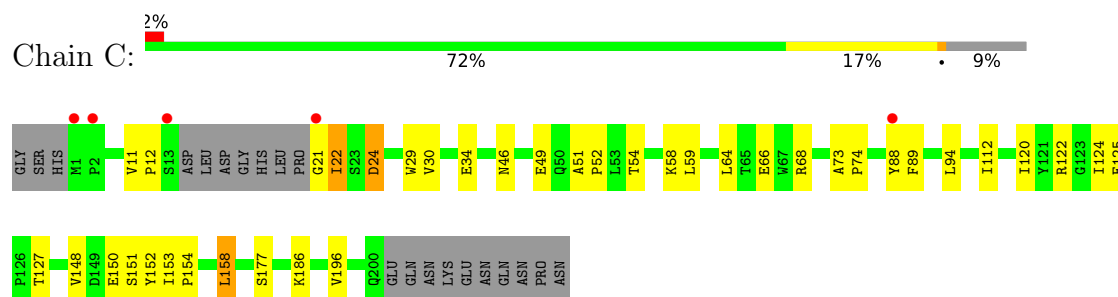
• Molecule 1: Protein Rep78



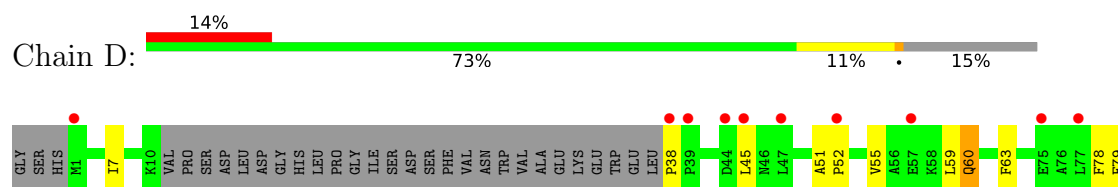
• Molecule 1: Protein Rep78

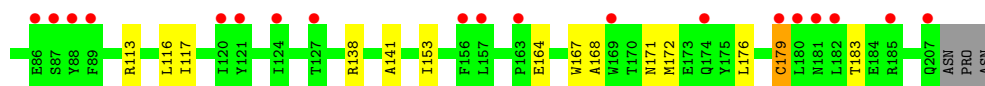


• Molecule 1: Protein Rep78



• Molecule 1: Protein Rep78





- Molecule 2: DNA (5'-D(*CP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*CP*TP*CP*GP*CP*TP*CP*GP*CP*T)-3')

Chain E: 90% 10%



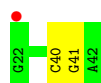
- Molecule 2: DNA (5'-D(*CP*TP*CP*GP*GP*CP*GP*CP*TP*CP*GP*CP*TP*CP*GP*CP*TP*CP*GP*CP*T)-3')

Chain G: 81% 19%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*AP*GP*CP*GP*AP*GP*CP*GP*AP*GP*CP*GP*CP*CP*GP*A)-3')

Chain F: 5% 90% 10%



- Molecule 3: DNA (5'-D(*GP*AP*GP*CP*GP*AP*GP*CP*GP*AP*GP*CP*GP*AP*GP*CP*GP*CP*CP*GP*A)-3')

Chain H: 76% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.14Å 79.59Å 139.50Å 90.00° 98.12° 90.00°	Depositor
Resolution (Å)	29.40 – 2.50 29.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.40-2.50) 94.9 (29.40-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.189 , 0.227 0.198 , 0.230	Depositor DCC
R_{free} test set	3317 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7847	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.56	0/1494	0.87	0/2030
1	B	0.59	0/1675	0.90	2/2273 (0.1%)
1	C	0.57	0/1599	0.85	2/2174 (0.1%)
1	D	0.48	0/1361	0.88	0/1862
2	E	0.41	0/466	0.61	0/716
2	G	0.32	0/466	0.53	0/716
3	F	0.38	0/492	0.56	0/759
3	H	0.37	0/492	0.52	0/759
All	All	0.52	0/8045	0.80	4/11289 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	LEU	CA-C-N	6.60	125.83	118.97
1	B	128	LEU	C-N-CA	6.60	125.83	118.97
1	C	158	LEU	CA-C-N	-5.01	114.66	119.87
1	C	158	LEU	C-N-CA	-5.01	114.66	119.87

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	1457	0	1440	13	0
1	B	1635	0	1610	15	0
1	C	1559	0	1535	19	0
1	D	1329	0	1201	13	0
2	E	419	0	238	2	0
2	G	419	0	238	2	0
3	F	436	0	233	1	0
3	H	436	0	233	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	13	0	5	1	0
5	C	13	0	5	1	0
6	A	31	0	0	0	0
6	B	36	0	0	2	0
6	C	33	0	0	1	0
6	D	10	0	0	0	0
6	E	6	0	0	0	0
6	F	6	0	0	0	0
6	G	3	0	0	0	0
6	H	3	0	0	0	0
All	All	7847	0	6738	73	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 (73) 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:138:ARG:HD3	1:A:143:GLY:CA	2.13	0.79
1:A:138:ARG:HD3	1:A:143:GLY:N	2.03	0.74
3:H:22:DG:H2''	3:H:23:DA:H5'	1.72	0.70
3:H:37:DC:H2'	3:H:38:DG:C8	2.30	0.67
1:C:94:LEU:HD11	1:C:152:TYR:HD2	1.60	0.67
1:A:138:ARG:CG	1:A:143:GLY:HA3	2.26	0.66
1:C:64:LEU:O	1:C:68:ARG:HG3	1.98	0.63
1:D:38:PRO:HG2	1:D:45:LEU:HD11	1.81	0.63
1:C:29:TRP:CZ3	1:C:58:LYS:HG3	2.34	0.62
1:D:138:ARG:NH1	1:D:141:ALA:O	2.31	0.62
5:C:302:CIT:O1	5:C:302:CIT:O7	2.19	0.59
1:C:22:ILE:HG13	1:C:30:VAL:HB	1.87	0.57
1:D:168:ALA:HB3	1:D:179:CYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:22:DG:H5''	3:H:22:DG:H8	1.71	0.56
1:A:174:GLN:NE2	5:A:302:CIT:O5	2.40	0.55
1:A:138:ARG:HG2	1:A:143:GLY:HA3	1.89	0.55
1:C:66:GLU:HB3	1:C:112:ILE:HG12	1.88	0.54
3:H:38:DG:H5''	3:H:38:DG:H8	1.74	0.53
1:A:138:ARG:HD3	1:A:143:GLY:HA2	1.90	0.53
1:D:79:PHE:HB2	1:D:172:MET:HE2	1.91	0.53
1:B:35:TRP:HD1	1:B:50:GLN:OE1	1.92	0.52
1:A:10:LYS:HE2	1:A:88:TYR:CZ	2.45	0.52
1:D:78:PHE:CE1	1:D:171:ASN:HB2	2.46	0.51
1:D:7:ILE:HD13	1:D:63:PHE:CZ	2.46	0.51
1:A:138:ARG:CD	1:A:143:GLY:CA	2.86	0.50
1:B:35:TRP:CD1	1:B:53:LEU:HD23	2.47	0.50
1:C:21:GLY:HA2	1:C:122:ARG:NH1	2.27	0.49
1:D:167:TRP:CD1	1:D:168:ALA:H	2.30	0.49
1:D:153:ILE:HD13	1:D:172:MET:HE1	1.93	0.49
1:B:10:LYS:NZ	1:B:129:PRO:HG2	2.27	0.48
1:C:153:ILE:HB	1:C:154:PRO:HD3	1.96	0.48
1:C:49:GLU:HG3	1:C:89:PHE:HZ	1.77	0.48
1:C:59:LEU:HD23	1:C:120:ILE:HD12	1.95	0.48
2:G:8:DC:C6	2:G:9:DT:H72	2.48	0.47
1:C:46:ASN:HB3	6:C:417:HOH:O	2.15	0.47
1:C:68:ARG:HD3	1:C:74:PRO:O	2.14	0.47
1:B:33:LYS:HE3	1:B:35:TRP:CH2	2.49	0.46
1:D:51:ALA:HB3	1:D:52:PRO:HD3	1.98	0.46
2:E:12:DC:H2''	2:E:13:DT:O5'	2.15	0.46
1:A:51:ALA:HB3	1:A:52:PRO:HD3	1.96	0.46
1:D:113:ARG:O	1:D:117:ILE:HG13	2.15	0.46
1:C:24:ASP:OD2	1:C:24:ASP:N	2.49	0.46
1:A:138:ARG:CG	1:A:143:GLY:CA	2.95	0.45
1:B:2:PRO:HB3	1:B:96:GLU:OE2	2.17	0.45
1:C:94:LEU:HD11	1:C:152:TYR:CD2	2.47	0.45
3:H:22:DG:H5''	3:H:22:DG:C8	2.52	0.45
1:D:7:ILE:HD13	1:D:63:PHE:HZ	1.81	0.45
1:C:151:SER:C	1:C:154:PRO:HD2	2.42	0.44
2:G:5:DG:H1'	2:G:6:DC:H5'	1.98	0.44
3:H:38:DG:C8	3:H:38:DG:H5''	2.51	0.44
1:B:64:LEU:O	1:B:68:ARG:HG3	2.16	0.44
1:B:109:LEU:HA	1:B:109:LEU:HD23	1.70	0.44
1:B:104:VAL:HG12	1:B:107:ARG:HH11	1.83	0.44
2:E:12:DC:C6	2:E:13:DT:H72	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ALA:HB3	1:C:52:PRO:HD3	2.00	0.43
1:C:49:GLU:HG3	1:C:89:PHE:CZ	2.53	0.43
3:F:40:DC:H2"	3:F:41:DG:C8	2.53	0.43
1:D:167:TRP:CD1	1:D:168:ALA:N	2.87	0.43
1:A:35:TRP:CD1	1:A:53:LEU:HD23	2.54	0.43
1:D:60:GLN:HE21	1:D:60:GLN:HB3	1.72	0.42
1:B:104:VAL:HG12	1:B:107:ARG:NH1	2.35	0.42
1:B:160:LYS:NZ	6:B:406:HOH:O	2.52	0.42
1:B:29:TRP:O	6:B:401:HOH:O	2.22	0.42
1:B:10:LYS:HZ2	1:B:129:PRO:HG2	1.85	0.42
3:H:41:DG:H8	3:H:41:DG:OP2	2.03	0.41
1:C:73:ALA:HA	1:C:74:PRO:HD2	1.89	0.41
1:C:30:VAL:HA	1:C:54:THR:HG21	2.02	0.41
1:A:44:ASP:H	1:A:162:GLN:HE22	1.69	0.41
1:B:9:ILE:HA	1:B:131:TRP:O	2.21	0.41
1:A:94:LEU:HD11	1:A:152:TYR:HD2	1.87	0.40
1:C:11:VAL:HA	1:C:12:PRO:HD3	1.89	0.40
1:B:60:GLN:O	1:B:64:LEU:HG	2.22	0.40
1:B:153:ILE:HB	1:B:154:PRO:HD3	2.02	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	177/213 (83%)	174 (98%)	2 (1%)	1 (1%)	21	38
1	B	197/213 (92%)	193 (98%)	4 (2%)	0	100	100
1	C	189/213 (89%)	186 (98%)	3 (2%)	0	100	100
1	D	176/213 (83%)	171 (97%)	5 (3%)	0	100	100
All	All	739/852 (87%)	724 (98%)	14 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	GLY

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	157/191 (82%)	150 (96%)	7 (4%)	24	49
1	B	179/191 (94%)	174 (97%)	5 (3%)	38	66
1	C	169/191 (88%)	156 (92%)	13 (8%)	12	25
1	D	125/191 (65%)	117 (94%)	8 (6%)	16	33
All	All	630/764 (82%)	597 (95%)	33 (5%)	21	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	75	GLU
1	A	87	SER
1	A	95	VAL
1	A	120	ILE
1	A	125	GLU
1	A	186	LYS
1	B	1	MET
1	B	65	THR
1	B	150	GLU
1	B	189	VAL
1	B	200	GLN
1	C	22	ILE
1	C	24	ASP
1	C	34	GLU
1	C	88	TYR
1	C	124	ILE
1	C	125	GLU
1	C	127	THR

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Mol	Chain	Res	Type
1	C	148	VAL
1	C	150	GLU
1	C	158	LEU
1	C	177	SER
1	C	186	LYS
1	C	196	VAL
1	D	55	VAL
1	D	59	LEU
1	D	60	GLN
1	D	116	LEU
1	D	164	GLU
1	D	176	LEU
1	D	179	CYS
1	D	183	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	118	GLN
1	B	192	HIS
1	C	198	GLN
1	D	90	HIS
1	D	130	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
5	CIT	A	302	-	12,12,12	1.20	0	17,17,17	1.57	3 (17%)
5	CIT	C	302	-	12,12,12	1.10	0	17,17,17	1.47	2 (11%)

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
5	CIT	A	302	-	-	3/16/16/16	-
5	CIT	C	302	-	-	8/16/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	302	CIT	O6-C6-C3	3.98	120.78	113.14
5	A	302	CIT	C3-C4-C5	-3.16	105.27	113.92
5	A	302	CIT	O2-C1-O1	-2.38	117.20	123.33
5	C	302	CIT	O4-C5-C4	2.16	121.19	114.35
5	A	302	CIT	C2-C3-C6	2.01	114.47	110.03

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	CIT	C1-C2-C3-O7
5	A	302	CIT	C1-C2-C3-C4
5	A	302	CIT	C1-C2-C3-C6

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Mol	Chain	Res	Type	Atoms
5	C	302	CIT	O7-C3-C6-O5
5	C	302	CIT	O7-C3-C6-O6
5	C	302	CIT	C4-C3-C6-O5
5	C	302	CIT	C4-C3-C6-O6
5	C	302	CIT	C1-C2-C3-C6
5	C	302	CIT	C1-C2-C3-O7
5	C	302	CIT	C1-C2-C3-C4
5	C	302	CIT	C2-C3-C6-O5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	CIT	1	0
5	C	302	CIT	1	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	181/213 (84%)	0.01	5 (2%) 55 50	50, 71, 111, 127	0
1	B	201/213 (94%)	-0.06	3 (1%) 72 68	53, 72, 110, 151	0
1	C	193/213 (90%)	0.11	5 (2%) 57 52	53, 77, 116, 139	0
1	D	180/213 (84%)	0.99	29 (16%) 4 4	81, 124, 164, 179	0
2	E	21/21 (100%)	-0.44	0 100 100	64, 87, 126, 146	0
2	G	21/21 (100%)	-0.19	0 100 100	77, 98, 137, 152	0
3	F	21/21 (100%)	-0.18	1 (4%) 35 31	67, 88, 125, 155	0
3	H	21/21 (100%)	-0.16	0 100 100	79, 104, 163, 164	0
All	All	839/936 (89%)	0.20	43 (5%) 33 29	50, 84, 151, 179	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	ASN	5.5
1	D	44	ASP	5.3
1	C	2	PRO	4.4
1	B	14	ASP	4.3
1	A	34	GLU	4.2
1	D	180	LEU	4.2
1	A	201	GLU	4.1
1	D	86	GLU	3.9
1	C	21	GLY	3.7
1	D	89	PHE	3.7
1	D	207	GLN	3.6
1	D	185	ARG	3.6
1	D	45	LEU	3.6
1	D	47	LEU	3.5
1	D	38	PRO	3.1
1	D	182	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	169	TRP	3.0
1	C	13	SER	2.9
1	A	12	PRO	2.7
1	A	1	MET	2.7
1	D	127	THR	2.7
1	D	39	PRO	2.6
1	D	75	GLU	2.6
1	D	124	ILE	2.6
1	D	77	LEU	2.5
1	D	174	GLN	2.5
1	D	157	LEU	2.5
1	D	87	SER	2.5
1	D	1	MET	2.5
1	D	120	ILE	2.4
1	D	88	TYR	2.4
1	D	52	PRO	2.4
1	B	1	MET	2.4
1	D	121	TYR	2.3
1	C	1	MET	2.3
3	F	22	DG	2.2
1	A	141	ALA	2.1
1	D	179	CYS	2.1
1	B	88	TYR	2.1
1	D	156	PHE	2.1
1	C	88	TYR	2.1
1	D	163	PRO	2.1
1	D	57	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 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(Å ²)	Q<0.9
4	MG	B	301	1/1	0.76	0.16	110,110,110,110	0
5	CIT	C	302	13/13	0.84	0.16	108,123,129,134	0
4	MG	C	301	1/1	0.91	0.20	97,97,97,97	0
5	CIT	A	302	13/13	0.94	0.09	65,79,96,108	0
4	MG	A	301	1/1	0.97	0.25	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.