



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 09:24 AM BST

PDB ID : 5ZAC
Title : Crystal structure of ConA-R2M
Authors : Gan, J.H.; Chen, G.S.; Hu, R.T.
Deposited on : 2018-02-07
Resolution : 2.59 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

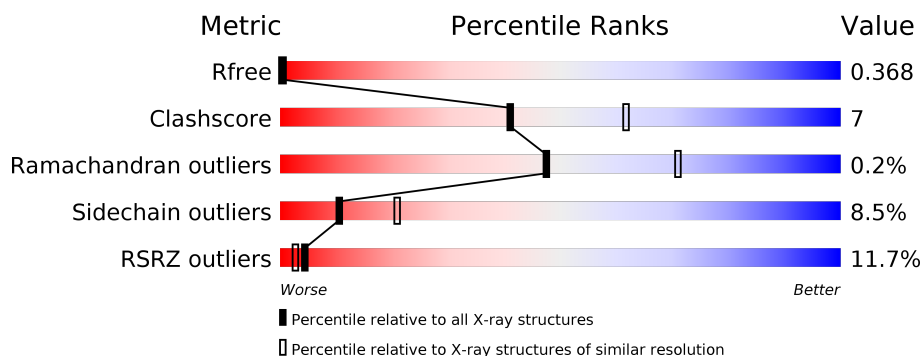
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	237	<div> <div>11%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	237	<div> <div>9%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	C	237	<div> <div>12%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	237	<div> <div>14%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TA5	D	305	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7348 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 Concanavalin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1760	1113	292	353	2			
1	B	232	Total	C	N	O	S	0	1	0
			1772	1121	294	355	2			
1	C	231	Total	C	N	O	S	0	1	0
			1763	1116	293	352	2			
1	D	231	Total	C	N	O	S	0	1	0
			1763	1116	293	352	2			

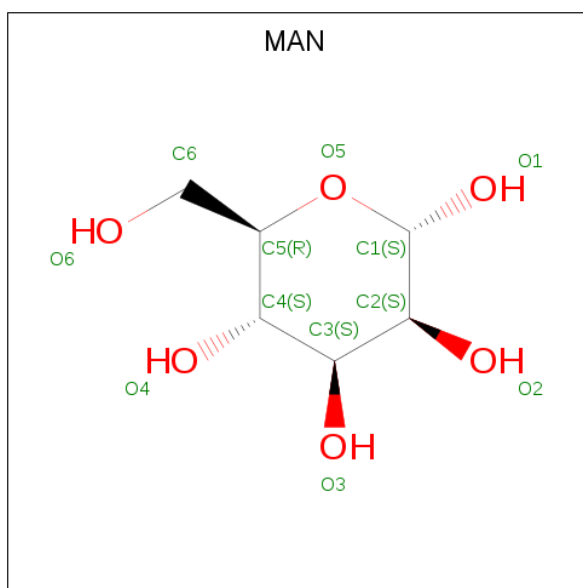
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

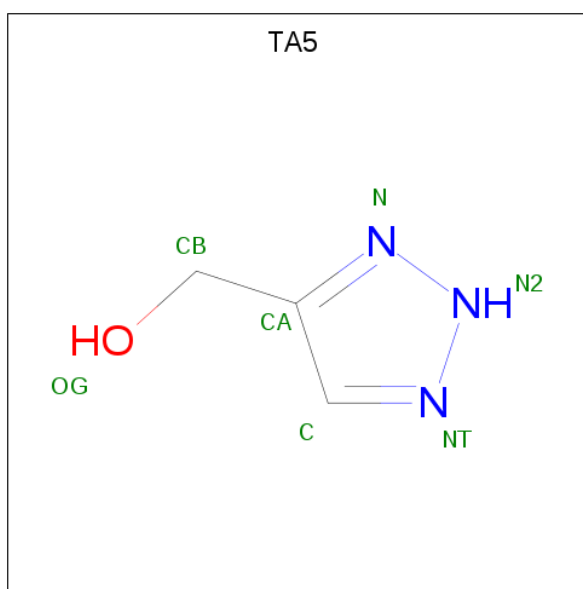
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 2H-1,2,3-TRIAZOL-4-YLMETHANOL (three-letter code: TA5) (formula: $C_3H_5N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			7	3	3	1		
5	D	1	Total	C	N	O	0	0
			7	3	3	1		

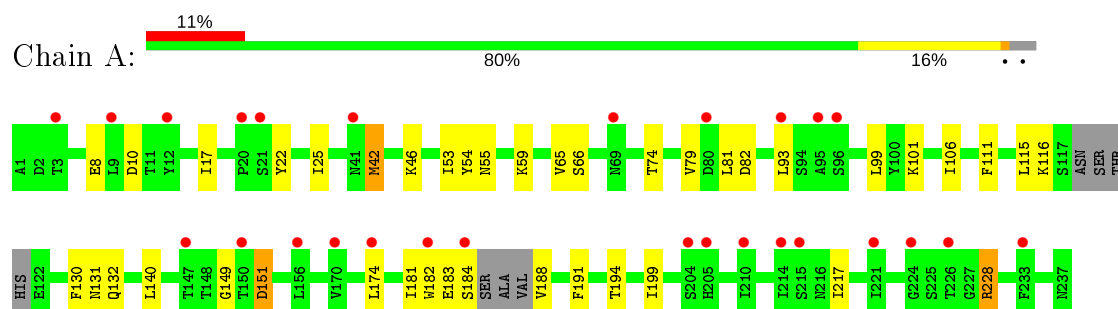
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total	O	0	0
			57	57		
6	B	64	Total	O	0	0
			64	64		
6	C	58	Total	O	0	0
			58	58		
6	D	65	Total	O	0	0
			65	65		

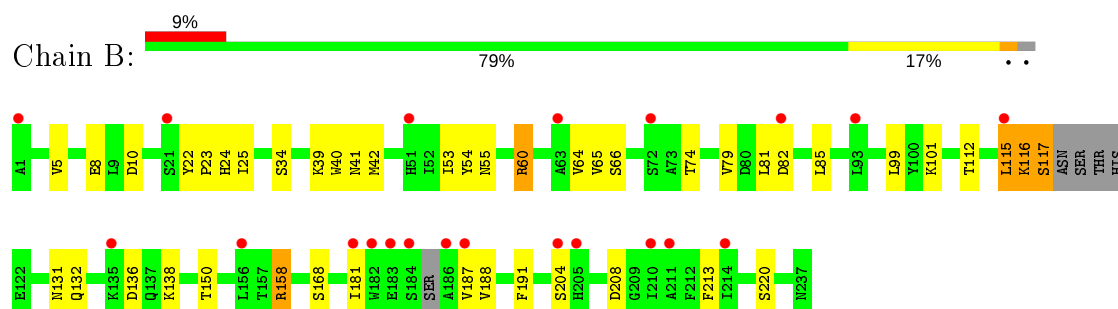
3 Residue-property plots

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.

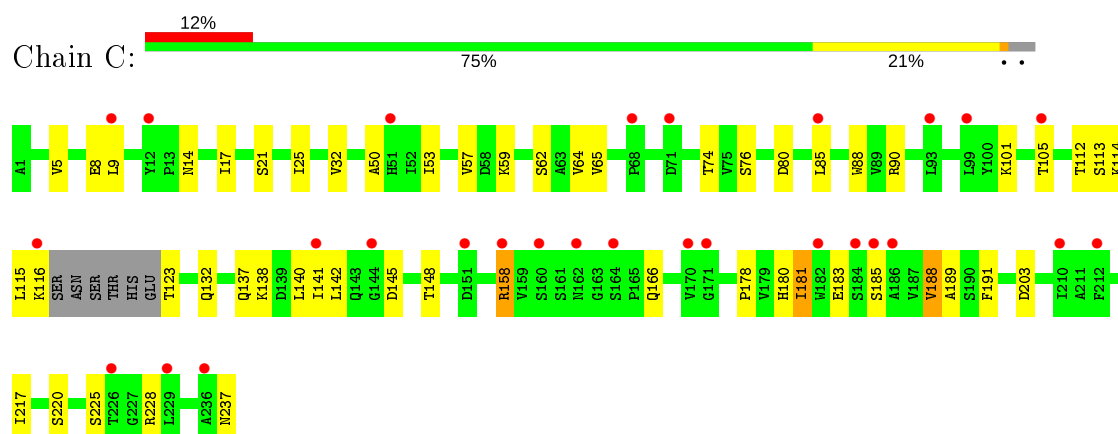
• Molecule 1: Concanavalin-A



• Molecule 1: Concanavalin-A

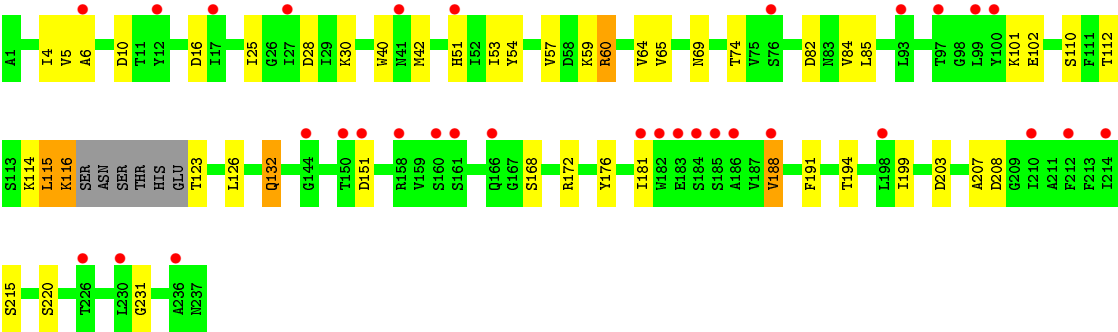


• Molecule 1: Concanavalin-A



• Molecule 1: Concanavalin-A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.23Å 119.89Å 125.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.59 29.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (30.00-2.59) 94.3 (29.83-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.278 , 0.372 0.280 , 0.368	Depositor DCC
R_{free} test set	1619 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7348	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1124e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TA5, CA, MN, MAN

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	0.66	0/1799	0.85	1/2447 (0.0%)
1	B	0.67	0/1811	0.84	1/2464 (0.0%)
1	C	0.67	0/1803	0.84	0/2455
1	D	0.66	0/1803	0.82	0/2455
All	All	0.67	0/7216	0.84	2/9821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	79	VAL	CB-CA-C	-5.43	101.07	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	150	THR	Peptide
1	D	115	LEU	Peptide

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	1760	0	1709	25	0
1	B	1772	0	1723	25	0
1	C	1763	0	1718	27	0
1	D	1763	0	1718	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	C	11	0	10	0	0
4	D	11	0	10	0	0
5	C	7	0	2	0	0
5	D	7	0	2	0	0
6	A	57	0	0	5	0
6	B	64	0	0	8	0
6	C	58	0	0	6	0
6	D	65	0	0	7	0
All	All	7348	0	6892	100	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 (100) 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:110:SER:OG	1:D:194:THR:OG1	1.80	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:VAL:HG23	1:D:85:LEU:HD21	1.53	0.90
1:C:88:TRP:HB3	1:C:217:ILE:HD11	1.56	0.86
1:D:116:LYS:HG3	1:D:188:VAL:O	1.82	0.80
1:B:5:VAL:HG23	1:B:85:LEU:HD21	1.62	0.80
1:D:208:ASP:O	6:D:401:HOH:O	2.00	0.79
1:C:123:THR:N	6:C:402:HOH:O	2.17	0.76
1:D:10:ASP:OD1	6:D:401:HOH:O	2.04	0.75
1:C:32:VAL:HG23	6:C:433:HOH:O	1.89	0.71
1:A:17:ILE:CD1	1:A:228:ARG:HD2	2.22	0.69
1:C:5:VAL:HG23	1:C:85:LEU:HD21	1.74	0.68
1:B:25:ILE:HG21	1:B:65:VAL:HG21	1.76	0.68
1:D:25:ILE:HG21	1:D:65:VAL:HG21	1.76	0.67
1:C:113:SER:OG	6:C:401:HOH:O	1.85	0.66
1:B:131:ASN:ND2	1:D:123:THR:O	2.28	0.66
1:A:111:PHE:HD2	6:A:426:HOH:O	1.77	0.65
1:A:82:ASP:OD1	6:A:401:HOH:O	2.15	0.65
1:B:24:HIS:ND1	6:B:401:HOH:O	2.29	0.64
1:A:42:MET:HE3	1:A:199:ILE:HB	1.81	0.62
1:D:132:GLN:HE21	1:D:132:GLN:C	2.03	0.61
1:B:115:LEU:HD12	1:B:116:LYS:N	2.15	0.61
1:B:8:GLU:OE1	1:B:34:SER:OG	2.19	0.61
1:C:90:ARG:HG3	1:C:217:ILE:HG23	1.83	0.60
1:B:5:VAL:CG2	1:B:85:LEU:HD21	2.32	0.59
1:B:136:ASP:OD2	1:B:138:LYS:NZ	2.37	0.57
1:B:158:ARG:NH2	6:B:402:HOH:O	2.27	0.57
1:A:17:ILE:HD13	1:A:228:ARG:HD2	1.86	0.56
1:A:53:ILE:HD13	6:A:402:HOH:O	2.05	0.56
1:A:131:ASN:ND2	1:C:123:THR:O	2.37	0.56
1:B:60:ARG:NH2	6:B:404:HOH:O	2.38	0.56
1:C:25:ILE:HG21	1:C:65:VAL:HG21	1.86	0.56
1:D:176:TYR:OH	6:D:402:HOH:O	2.11	0.55
1:D:112:THR:O	1:D:191:PHE:HA	2.06	0.55
1:C:145:ASP:OD2	1:C:158:ARG:NH1	2.37	0.55
1:D:60:ARG:NH1	6:D:408:HOH:O	2.41	0.54
1:D:126:LEU:HD22	6:D:405:HOH:O	2.07	0.54
1:B:25:ILE:CG2	1:B:65:VAL:HG21	2.38	0.54
1:D:5:VAL:CG2	1:D:85:LEU:HD21	2.33	0.54
1:B:25:ILE:HG21	1:B:65:VAL:CG2	2.39	0.53
1:D:116:LYS:CG	1:D:188:VAL:O	2.53	0.53
1:A:17:ILE:HD13	1:A:228:ARG:CD	2.39	0.52
1:A:42:MET:CE	1:A:199:ILE:HB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:CD2	6:A:426:HOH:O	2.52	0.51
1:B:10:ASP:O	6:B:401:HOH:O	2.19	0.51
1:A:82:ASP:HB3	1:A:182:TRP:CG	2.45	0.50
1:D:30:LYS:HD2	1:D:84:VAL:HG13	1.93	0.50
1:A:55:ASN:ND2	6:A:402:HOH:O	2.31	0.50
1:C:112:THR:O	1:C:191:PHE:HA	2.11	0.49
1:A:59:LYS:HB3	1:A:79:VAL:O	2.14	0.48
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.96	0.48
1:C:115:LEU:HD12	1:C:189:ALA:HB1	1.96	0.48
1:C:137:GLN:HG2	1:C:140:LEU:HD12	1.95	0.47
1:B:24:HIS:N	6:B:401:HOH:O	2.45	0.47
1:B:54:TYR:CD2	1:B:81:LEU:HD12	2.50	0.47
1:C:14:ASN:ND2	1:C:228:ARG:HB3	2.30	0.47
1:B:23:PRO:HA	6:B:401:HOH:O	2.14	0.46
1:B:24:HIS:CE1	6:B:401:HOH:O	2.64	0.46
1:C:62:SER:HG	1:C:76:SER:HG	1.60	0.46
1:B:40:TRP:O	1:B:42:MET:N	2.48	0.46
1:B:8:GLU:OE2	1:B:10:ASP:OD2	2.33	0.46
1:C:17:ILE:CD1	6:C:420:HOH:O	2.63	0.46
1:B:112:THR:O	1:B:191:PHE:HA	2.15	0.46
1:D:181:ILE:HD12	6:D:449:HOH:O	2.15	0.46
1:A:25:ILE:HG21	1:A:65:VAL:HG21	1.98	0.46
1:C:50:ALA:HA	1:C:64:VAL:O	2.15	0.46
1:C:178:PRO:HB3	1:C:217:ILE:HD13	1.99	0.45
1:C:5:VAL:CG2	1:C:85:LEU:HD21	2.44	0.45
1:D:25:ILE:HG23	1:D:40:TRP:HB2	1.99	0.45
1:C:181:ILE:HG13	6:C:439:HOH:O	2.16	0.45
1:A:149:GLY:O	1:A:151:ASP:HA	2.17	0.44
1:A:115:LEU:HD11	1:A:183:GLU:HB2	1.99	0.44
1:A:188:VAL:HG22	1:B:64:VAL:HG21	2.00	0.44
1:A:79:VAL:HG11	1:A:81:LEU:HD23	1.99	0.44
1:A:54:TYR:HB3	1:A:191:PHE:CE2	2.53	0.44
1:A:82:ASP:HA	1:A:182:TRP:CD1	2.52	0.44
1:D:207:ALA:HB1	1:D:208:ASP:CG	2.38	0.44
1:D:172:ARG:NH1	1:D:231:GLY:O	2.50	0.44
1:B:117:SER:O	1:B:117:SER:OG	2.36	0.44
1:B:187:VAL:HG12	1:B:188:VAL:HG23	2.00	0.43
1:C:59:LYS:HE2	1:C:80:ASP:OD1	2.19	0.43
1:D:54:TYR:CE1	1:D:59:LYS:HA	2.54	0.42
1:A:8:GLU:OE2	1:A:10:ASP:OD2	2.38	0.42
1:C:237:ASN:ND2	6:C:405:HOH:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:OE2	1:A:10:ASP:HB2	2.20	0.42
1:C:88:TRP:CH2	1:C:180:HIS:HB2	2.55	0.42
1:D:6:ALA:HB3	1:D:28:ASP:HB2	2.01	0.42
1:A:130:PHE:CE2	1:A:140:LEU:HD21	2.55	0.42
1:D:102:GLU:HB2	1:D:199:ILE:HG23	2.02	0.41
1:C:115:LEU:HD21	1:C:183:GLU:HB2	2.02	0.41
1:D:207:ALA:HA	1:D:208:ASP:HA	1.85	0.41
1:A:93:LEU:HD13	1:A:106:ILE:HD12	2.03	0.41
1:D:57:VAL:HG23	1:D:188:VAL:HG13	2.03	0.41
1:C:188:VAL:CG2	1:D:51:HIS:CD2	3.04	0.40
1:B:40:TRP:NE1	1:B:65:VAL:HG11	2.36	0.40
1:D:69:ASN:N	6:D:411:HOH:O	2.53	0.40
1:C:142:LEU:HD11	1:C:148:THR:HG23	2.04	0.40
1:B:55:ASN:ND2	6:B:406:HOH:O	2.43	0.40
1:C:9:LEU:HD12	1:C:9:LEU:N	2.37	0.40
1:A:174:LEU:HD12	1:A:174:LEU:N	2.36	0.40
1:C:57:VAL:HG21	1:D:64:VAL:CG2	2.52	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	224/237 (94%)	214 (96%)	10 (4%)	0	100	100
1	B	226/237 (95%)	208 (92%)	17 (8%)	1 (0%)	34	57
1	C	227/237 (96%)	212 (93%)	14 (6%)	1 (0%)	34	57
1	D	227/237 (96%)	216 (95%)	11 (5%)	0	100	100
All	All	904/948 (95%)	850 (94%)	52 (6%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ASN
1	C	225	SER

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	197/203 (97%)	184 (93%)	13 (7%)	16	33
1	B	198/203 (98%)	178 (90%)	20 (10%)	7	14
1	C	197/203 (97%)	179 (91%)	18 (9%)	9	18
1	D	197/203 (97%)	181 (92%)	16 (8%)	11	23
All	All	789/812 (97%)	722 (92%)	67 (8%)	10	21

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	TYR
1	A	42	MET
1	A	46	LYS
1	A	66	SER
1	A	74	THR
1	A	99	LEU
1	A	101	LYS
1	A	132	GLN
1	A	151	ASP
1	A	181	ILE
1	A	184	SER
1	A	194	THR
1	A	217	ILE
1	B	22	TYR
1	B	39	LYS
1	B	53	ILE
1	B	60	ARG
1	B	66	SER
1	B	74	THR
1	B	82	ASP

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Mol	Chain	Res	Type
1	B	99	LEU
1	B	101	LYS
1	B	115	LEU
1	B	116	LYS
1	B	117	SER
1	B	132	GLN
1	B	158	ARG
1	B	168	SER
1	B	181	ILE
1	B	204	SER
1	B	208	ASP
1	B	213	PHE
1	B	220	SER
1	C	8	GLU
1	C	21	SER
1	C	53	ILE
1	C	74	THR
1	C	101	LYS
1	C	105	THR
1	C	114	LYS
1	C	116	LYS
1	C	132	GLN
1	C	138	LYS
1	C	141	ILE
1	C	158	ARG
1	C	166	GLN
1	C	181	ILE
1	C	185	SER
1	C	188	VAL
1	C	203	ASP
1	C	220	SER
1	D	16	ASP
1	D	42	MET
1	D	53	ILE
1	D	60	ARG
1	D	74	THR
1	D	82	ASP
1	D	101	LYS
1	D	114	LYS
1	D	115	LEU
1	D	116	LYS
1	D	132	GLN

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Mol	Chain	Res	Type
1	D	151	ASP
1	D	168	SER
1	D	188	VAL
1	D	203	ASP
1	D	220	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	B	153	ASN
1	B	205	HIS
1	C	43	GLN
1	C	104	ASN
1	D	14	ASN
1	D	69	ASN
1	D	132	GLN
1	D	153	ASN
1	D	166	GLN
1	D	237	ASN

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](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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
4	MAN	C	303	5	11,11,12	0.61	0	15,15,17	1.35	1 (6%)
5	TA5	C	304	4	6,7,7	1.41	1 (16%)	4,8,8	2.14	2 (50%)
4	MAN	D	304	5	11,11,12	0.55	0	15,15,17	0.99	1 (6%)
5	TA5	D	305	4	6,7,7	1.38	1 (16%)	4,8,8	2.11	2 (50%)

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	MAN	C	303	5	-	0/2/19/22	0/1/1/1
5	TA5	C	304	4	-	0/0/2/2	0/1/1/1
4	MAN	D	304	5	-	0/2/19/22	0/1/1/1
5	TA5	D	305	4	-	0/0/2/2	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	305	TA5	N-N2	-2.56	1.31	1.34
5	C	304	TA5	N-N2	-2.49	1.31	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	MAN	C1-O5-C5	4.77	118.65	112.19
5	C	304	TA5	NT-N2-N	-3.30	107.13	111.24
5	D	305	TA5	NT-N2-N	-3.26	107.18	111.24
4	D	304	MAN	C1-O5-C5	2.76	115.93	112.19
5	D	305	TA5	C-CA-N	-2.31	107.90	111.34
5	C	304	TA5	C-CA-N	-2.29	107.93	111.34

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	230/237 (97%)	0.98	27 (11%) 4 3	13, 25, 47, 64	0
1	B	232/237 (97%)	0.97	21 (9%) 9 6	13, 26, 48, 61	0
1	C	231/237 (97%)	0.96	28 (12%) 4 2	15, 25, 42, 56	0
1	D	231/237 (97%)	1.03	32 (13%) 2 1	14, 25, 42, 57	0
All	All	924/948 (97%)	0.99	108 (11%) 4 3	13, 25, 46, 64	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	SER	5.4
1	C	182	TRP	4.5
1	C	185	SER	4.4
1	D	185	SER	4.4
1	A	204	SER	4.2
1	B	211	ALA	4.2
1	D	182	TRP	4.1
1	D	210	ILE	4.0
1	C	144	GLY	4.0
1	C	99	LEU	3.9
1	C	184	SER	3.9
1	D	166	GLN	3.9
1	B	182	TRP	3.7
1	B	210	ILE	3.7
1	A	182	TRP	3.6
1	A	205	HIS	3.6
1	D	181	ILE	3.5
1	A	69	ASN	3.5
1	A	21	SER	3.4
1	C	12	TYR	3.4
1	D	100	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	105	THR	3.2
1	A	93	LEU	3.2
1	D	93	LEU	3.2
1	D	99	LEU	3.1
1	B	184	SER	3.1
1	B	93	LEU	3.0
1	D	51	HIS	3.0
1	B	205	HIS	2.9
1	C	164	SER	2.9
1	D	183	GLU	2.9
1	C	162	ASN	2.9
1	A	150	THR	2.9
1	D	186	ALA	2.9
1	B	214	ILE	2.9
1	A	221	ILE	2.8
1	C	210	ILE	2.8
1	D	184	SER	2.8
1	B	181	ILE	2.8
1	B	1	ALA	2.8
1	A	80	ASP	2.7
1	C	170	VAL	2.7
1	A	147	THR	2.7
1	A	9	LEU	2.7
1	C	186	ALA	2.6
1	C	160	SER	2.6
1	C	229	LEU	2.6
1	C	141	ILE	2.6
1	D	150	THR	2.6
1	B	156	LEU	2.6
1	C	68	PRO	2.6
1	B	183	GLU	2.6
1	A	41	ASN	2.5
1	A	224	GLY	2.5
1	A	215	SER	2.5
1	B	187	VAL	2.5
1	D	198	LEU	2.5
1	A	226	THR	2.5
1	B	51	HIS	2.5
1	C	93	LEU	2.5
1	D	160	SER	2.4
1	D	230	LEU	2.4
1	D	236	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	212	PHE	2.4
1	D	151	ASP	2.4
1	C	212	PHE	2.4
1	B	186	ALA	2.4
1	C	151	ASP	2.3
1	A	12	TYR	2.3
1	B	63	ALA	2.3
1	D	12	TYR	2.3
1	A	184	SER	2.3
1	C	9	LEU	2.3
1	D	188	VAL	2.3
1	C	226	THR	2.3
1	A	156	LEU	2.3
1	A	170	VAL	2.3
1	D	144	GLY	2.3
1	A	174	LEU	2.3
1	B	115	LEU	2.3
1	A	3	THR	2.2
1	C	85	LEU	2.2
1	D	76	SER	2.2
1	C	236	ALA	2.2
1	C	158	ARG	2.2
1	D	158	ARG	2.2
1	B	21	SER	2.2
1	C	51	HIS	2.2
1	B	135	LYS	2.1
1	B	82	ASP	2.1
1	D	214	ILE	2.1
1	C	171	GLY	2.1
1	D	161	SER	2.1
1	A	210	ILE	2.1
1	A	214	ILE	2.1
1	B	72	SER	2.1
1	C	116	LYS	2.1
1	D	97	THR	2.1
1	D	17	ILE	2.1
1	A	233	PHE	2.1
1	A	95	ALA	2.0
1	D	6	ALA	2.0
1	D	41	ASN	2.0
1	C	71	ASP	2.0
1	D	226	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	27	ILE	2.0
1	A	20	PRO	2.0
1	A	96	SER	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, 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(\AA^2)	Q<0.9
5	TA5	D	305	7/7	0.58	0.40	35,43,47,48	0
4	MAN	D	304	11/12	0.76	0.30	24,28,29,30	0
5	TA5	C	304	7/7	0.77	0.30	30,40,44,44	0
3	CA	A	303	1/1	0.81	0.12	48,48,48,48	0
4	MAN	C	303	11/12	0.82	0.19	24,26,27,27	0
3	CA	A	302	1/1	0.84	0.06	32,32,32,32	0
3	CA	C	302	1/1	0.90	0.11	33,33,33,33	0
2	MN	D	301	1/1	0.90	0.10	35,35,35,35	0
3	CA	D	302	1/1	0.91	0.09	27,27,27,27	0
2	MN	B	301	1/1	0.94	0.06	39,39,39,39	0
3	CA	B	302	1/1	0.95	0.07	25,25,25,25	0
3	CA	D	303	1/1	0.96	0.07	40,40,40,40	0
2	MN	C	301	1/1	0.96	0.06	35,35,35,35	0
2	MN	A	301	1/1	0.97	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.