



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:18 am GMT

PDB ID : 1CT8
Title : CATALYTIC ANTIBODY 7C8 COMPLEX
Authors : Gigant, B.; Tsumuraya, T.; Fujii, I.; Knossow, M.
Deposited on : 1999-08-20
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

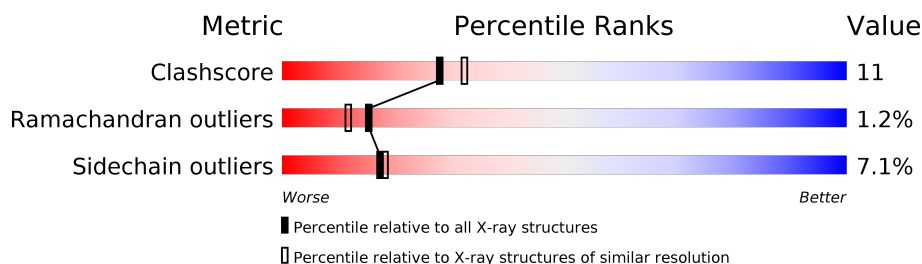
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
1	C	214	
2	B	220	
2	D	220	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TAA	B	550	X	-	-	-
4	TAA	D	551	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6921 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 7C8 FAB FRAGMENT; SHORT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1654	1027	284	336	7			
1	C	214	Total	C	N	O	S	0	0	0
			1654	1027	284	336	7			

- Molecule 2 is a protein called 7C8 FAB FRAGMENT; LONG CHAIN.

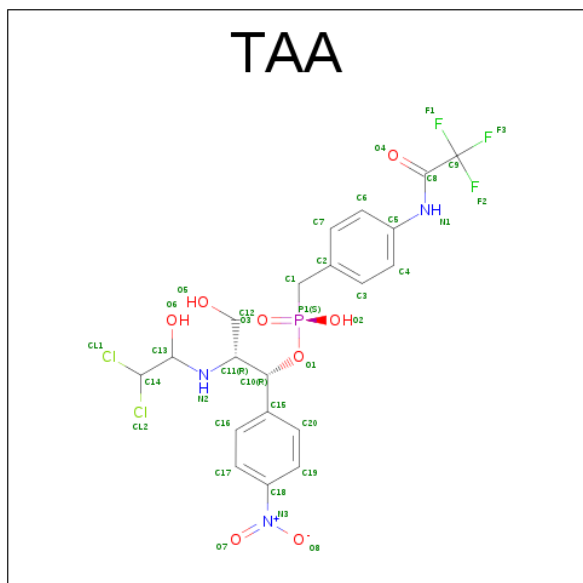
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	220	Total	C	N	O	S	0	0	0
			1667	1063	269	328	7			
2	D	220	Total	C	N	O	S	0	0	0
			1667	1063	269	328	7			

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is [4-(2,2,2-TRIFLUORO-ACETYLAMINO)-BENZYL]-PHOSPHONIC ACID MONO-[2-(2,2-DICHLORO-1-HYDROXY-ETHYLAMINO)-3-HYDROXY-1-(4-NITRO-PHENYL)-PROPYL] ESTER (three-letter code: TAA) (formula: C₂₀H₂₁Cl₂F₃N₃O₈P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C Cl F N O P 37 20 2 3 3 8 1	0	0
4	D	1	Total C Cl F N O P 37 20 2 3 3 8 1	0	0

- Molecule 5 is water.

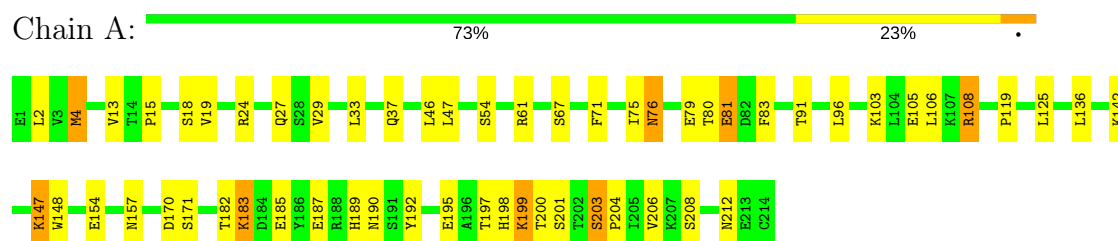
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	57	Total O 57 57	0	0
5	B	62	Total O 62 62	0	0
5	C	30	Total O 30 30	0	0
5	D	46	Total O 46 46	0	0

3 Residue-property plots

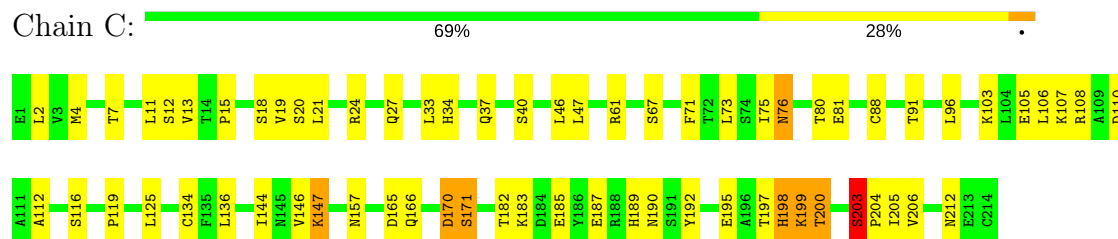
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

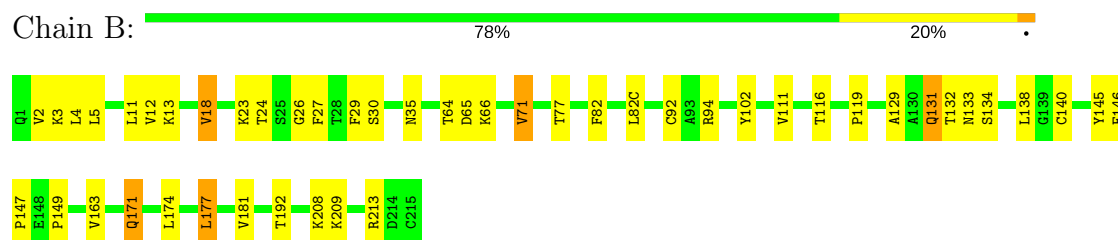
• Molecule 1: 7C8 FAB FRAGMENT; SHORT CHAIN



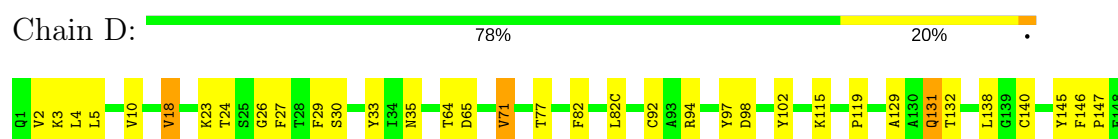
• Molecule 1: 7C8 FAB FRAGMENT; SHORT CHAIN

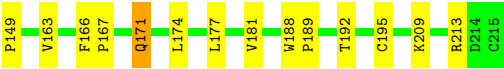


• Molecule 2: 7C8 FAB FRAGMENT; LONG CHAIN



• Molecule 2: 7C8 FAB FRAGMENT; LONG CHAIN





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.56Å 65.61Å 117.76Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	14.30 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (14.30-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.211 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6921	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: SO4, TAA

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	0.54	0/1692	0.79	0/2294
1	C	0.54	0/1692	0.79	0/2294
2	B	0.55	0/1713	0.80	1/2343 (0.0%)
2	D	0.54	0/1713	0.78	0/2343
All	All	0.54	0/6810	0.79	1/9274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	LEU	CA-CB-CG	5.89	128.85	115.30

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	1654	0	1589	37	0
1	C	1654	0	1589	47	0
2	B	1667	0	1628	33	0
2	D	1667	0	1628	32	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	37	0	17	1	0
4	D	37	0	17	2	0
5	A	57	0	0	1	0
5	B	62	0	0	0	0
5	C	30	0	0	0	0
5	D	46	0	0	0	0
All	All	6921	0	6468	148	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 11.

All (148) 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:C:11:LEU:HD21	1:C:19:VAL:HG21	1.24	1.11
1:A:203:SER:HB2	1:A:204:PRO:HD2	1.31	1.06
1:A:203:SER:HB2	1:A:204:PRO:CD	2.08	0.82
2:B:18:VAL:HG22	2:B:82(C):LEU:HD11	1.63	0.81
2:B:4:LEU:HD21	2:B:27:PHE:CZ	2.17	0.80
2:B:2:VAL:HG12	2:B:27:PHE:HD1	1.48	0.78
1:C:110:ASP:HB3	1:C:200:THR:HG23	1.64	0.77
2:D:4:LEU:HD21	2:D:27:PHE:CZ	2.20	0.76
1:C:190:ASN:HD21	1:C:212:ASN:H	1.31	0.75
2:D:4:LEU:HD22	2:D:24:THR:HG22	1.67	0.75
1:C:15:PRO:HG3	1:C:106:LEU:HD23	1.71	0.73
2:B:12:VAL:HG11	2:B:18:VAL:HG13	1.70	0.72
1:C:7:THR:HG23	1:C:24:ARG:HH22	1.53	0.72
1:C:195:GLU:HB3	1:C:206:VAL:HG22	1.72	0.72
2:B:2:VAL:CG1	2:B:27:PHE:HD1	2.03	0.71
2:D:2:VAL:HG12	2:D:27:PHE:HD1	1.55	0.70
1:A:13:VAL:HG11	1:A:19:VAL:HG11	1.73	0.70
2:D:2:VAL:CG1	2:D:27:PHE:HD1	2.03	0.70
2:D:18:VAL:HG22	2:D:82(C):LEU:HD11	1.73	0.70
1:A:195:GLU:HB3	1:A:206:VAL:HG22	1.74	0.69
2:B:4:LEU:HD21	2:B:27:PHE:HZ	1.57	0.69
2:B:2:VAL:HB	2:B:102:TYR:CE1	2.28	0.69
1:A:190:ASN:HD21	1:A:212:ASN:H	1.38	0.69
2:B:4:LEU:HD22	2:B:24:THR:HG22	1.75	0.68
1:C:103:LYS:NZ	1:C:105:GLU:HG2	2.09	0.68
1:A:83:PHE:HE1	1:A:103:LYS:HZ1	1.42	0.67
1:C:11:LEU:HD21	1:C:19:VAL:CG2	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:HD21	2:D:27:PHE:CE1	2.31	0.65
1:C:203:SER:HB3	1:C:204:PRO:HD2	1.78	0.65
1:C:203:SER:CB	1:C:204:PRO:HD2	2.27	0.65
1:C:147:LYS:HE2	1:C:147:LYS:HA	1.79	0.64
2:B:3:LYS:HE2	2:B:5:LEU:HB2	1.79	0.64
2:B:2:VAL:HG12	2:B:27:PHE:CD1	2.31	0.63
1:C:199:LYS:HA	1:C:199:LYS:HE2	1.81	0.63
2:D:2:VAL:HB	2:D:102:TYR:CE1	2.34	0.62
2:D:3:LYS:HE2	2:D:5:LEU:HB2	1.82	0.62
1:A:15:PRO:HG3	1:A:106:LEU:HD23	1.82	0.62
1:C:144:ILE:HD12	1:C:198:HIS:HB3	1.82	0.62
1:A:147:LYS:HE2	1:A:147:LYS:HA	1.82	0.61
1:A:199:LYS:HE2	1:A:199:LYS:HA	1.81	0.61
2:D:192:THR:HG23	2:D:209:LYS:HG3	1.84	0.60
1:C:80:THR:HA	1:C:106:LEU:HD22	1.82	0.60
2:D:4:LEU:HD21	2:D:27:PHE:HZ	1.66	0.60
2:B:12:VAL:HG11	2:B:18:VAL:CG1	2.31	0.60
2:B:4:LEU:HD21	2:B:27:PHE:CE1	2.36	0.59
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.83	0.59
1:A:2:LEU:HD22	1:A:27:GLN:CG	2.32	0.59
1:A:18:SER:OG	1:A:76:ASN:HA	2.03	0.59
2:D:2:VAL:HA	2:D:26:GLY:HA3	1.84	0.58
1:C:103:LYS:HZ1	1:C:105:GLU:HG2	1.68	0.57
1:C:61:ARG:HG3	1:C:75:ILE:HG23	1.86	0.57
1:C:40:SER:HB2	1:C:165:ASP:OD1	2.05	0.57
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.86	0.57
1:A:108:ARG:HG3	1:A:171:SER:HB2	1.86	0.56
1:A:190:ASN:ND2	1:A:212:ASN:H	2.02	0.56
1:A:80:THR:HA	1:A:106:LEU:HD22	1.87	0.56
1:C:12:SER:HB3	1:C:107:LYS:HE3	1.88	0.56
2:D:10:VAL:HG21	2:D:18:VAL:HG11	1.87	0.56
2:D:2:VAL:HG13	2:D:26:GLY:C	2.27	0.56
2:B:2:VAL:CG1	2:B:27:PHE:CD1	2.89	0.55
2:D:119:PRO:HB3	2:D:145:TYR:HB3	1.87	0.54
1:A:119:PRO:HG2	2:B:213:ARG:CZ	2.37	0.54
1:C:108:ARG:HD2	1:C:170:ASP:O	2.07	0.53
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.90	0.53
1:C:110:ASP:HB3	1:C:200:THR:CG2	2.36	0.53
1:C:7:THR:CG2	1:C:24:ARG:HH22	2.19	0.53
1:A:142:LYS:NZ	1:A:142:LYS:HB3	2.24	0.53
2:D:18:VAL:CG2	2:D:82(C):LEU:HD11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:VAL:HG13	2:B:26:GLY:C	2.29	0.52
1:C:190:ASN:ND2	1:C:212:ASN:H	2.03	0.52
2:B:192:THR:HG23	2:B:209:LYS:HG3	1.91	0.52
2:D:2:VAL:HG12	2:D:27:PHE:CD1	2.39	0.52
1:C:136:LEU:HD12	1:C:136:LEU:N	2.25	0.52
1:C:182:THR:OG1	1:C:185:GLU:HG3	2.10	0.52
2:B:23:LYS:HD2	2:B:77:THR:CG2	2.40	0.52
2:D:2:VAL:CG1	2:D:27:PHE:CD1	2.90	0.51
1:C:144:ILE:HG23	1:C:144:ILE:O	2.09	0.51
1:C:119:PRO:HG2	2:D:213:ARG:CZ	2.41	0.51
1:A:61:ARG:HG3	1:A:75:ILE:HG23	1.92	0.51
1:A:189:HIS:HA	5:A:578:HOH:O	2.09	0.51
1:A:189:HIS:HB2	1:A:192:TYR:OH	2.11	0.51
1:C:18:SER:OG	1:C:76:ASN:HA	2.11	0.51
2:D:171:GLN:HE22	2:D:174:LEU:HB2	1.75	0.51
2:B:23:LYS:HD2	2:B:77:THR:HG23	1.92	0.51
2:B:35:ASN:O	2:B:92:CYS:HA	2.10	0.51
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.46	0.51
1:A:108:ARG:HD2	1:A:170:ASP:O	2.11	0.50
1:C:24:ARG:HG3	1:C:24:ARG:HH11	1.76	0.50
1:C:91:THR:HA	1:C:96:LEU:HD22	1.94	0.50
2:B:171:GLN:HE22	2:B:174:LEU:HB2	1.77	0.50
1:C:166:GLN:HG2	1:C:171:SER:HA	1.92	0.50
2:D:64:THR:O	2:D:65:ASP:HB2	2.12	0.50
1:C:112:ALA:HB1	1:C:205:ILE:HD11	1.94	0.49
1:A:2:LEU:HD22	1:A:27:GLN:HG2	1.95	0.49
2:B:64:THR:O	2:B:65:ASP:HB2	2.13	0.49
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.47	0.49
1:C:136:LEU:HD21	1:C:146:VAL:HG22	1.96	0.48
1:A:103:LYS:NZ	1:A:105:GLU:HG2	2.28	0.48
1:C:2:LEU:HD22	1:C:27:GLN:CG	2.43	0.48
2:B:2:VAL:HB	2:B:102:TYR:HE1	1.77	0.48
4:B:550:TAA:O4	4:B:550:TAA:HC6	2.14	0.47
2:D:29:PHE:HZ	2:D:71:VAL:HG22	1.80	0.47
1:C:189:HIS:HB2	1:C:192:TYR:OH	2.14	0.47
1:C:11:LEU:CD2	1:C:19:VAL:HG21	2.18	0.47
2:D:163:VAL:HG22	2:D:181:VAL:HG23	1.96	0.47
1:A:182:THR:OG1	1:A:185:GLU:HG3	2.14	0.47
1:A:183:LYS:O	1:A:187:GLU:HG2	2.14	0.47
1:C:203:SER:CB	1:C:204:PRO:CD	2.92	0.47
1:C:20:SER:HA	1:C:73:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:TRP:CG	2:D:189:PRO:HA	2.50	0.47
2:B:208:LYS:HA	2:B:208:LYS:HD3	1.79	0.46
1:A:79:GLU:HB2	1:A:81:GLU:OE1	2.16	0.46
1:A:201:SER:HB2	1:A:203:SER:O	2.16	0.46
1:C:183:LYS:O	1:C:187:GLU:HG2	2.16	0.45
1:A:192:TYR:O	1:A:208:SER:HA	2.16	0.45
2:B:163:VAL:HG22	2:B:181:VAL:HG23	1.97	0.45
2:B:171:GLN:NE2	2:B:174:LEU:HB2	2.32	0.45
1:A:91:THR:HA	1:A:96:LEU:HD22	1.99	0.45
2:D:213:ARG:O	2:D:213:ARG:HG3	2.17	0.45
1:A:13:VAL:HG11	1:A:19:VAL:CG1	2.45	0.45
2:D:35:ASN:O	2:D:92:CYS:HA	2.17	0.44
2:B:11:LEU:HD23	2:B:116:THR:HG23	1.99	0.43
2:D:166:PHE:HA	2:D:167:PRO:HD3	1.88	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.99	0.43
2:B:29:PHE:HZ	2:B:71:VAL:HG22	1.83	0.43
1:A:148:TRP:O	1:A:154:GLU:HA	2.19	0.43
2:D:23:LYS:HD2	2:D:77:THR:CG2	2.49	0.43
1:A:136:LEU:HD12	1:A:136:LEU:N	2.34	0.42
2:B:133:ASN:CG	2:B:134:SER:H	2.22	0.42
1:C:21:LEU:HD12	1:C:21:LEU:N	2.35	0.42
1:C:12:SER:HA	1:C:105:GLU:O	2.20	0.42
1:A:67:SER:HA	1:A:71:PHE:CE1	2.55	0.42
1:C:116:SER:O	1:C:134:CYS:HA	2.20	0.42
1:A:4:MET:HA	1:A:24:ARG:O	2.20	0.41
1:C:144:ILE:O	1:C:144:ILE:CG2	2.68	0.41
1:C:203:SER:HB3	1:C:204:PRO:CD	2.48	0.41
2:D:171:GLN:NE2	2:D:174:LEU:HB2	2.35	0.41
2:D:23:LYS:HD2	2:D:77:THR:HG23	2.01	0.41
1:A:2:LEU:HD13	1:A:29:VAL:HG12	2.03	0.41
2:B:2:VAL:HG11	2:B:102:TYR:CZ	2.56	0.41
2:B:146:PHE:HA	2:B:147:PRO:HA	1.77	0.41
1:A:147:LYS:CE	1:A:147:LYS:HA	2.49	0.41
2:D:33:TYR:CD2	4:D:551:TAA:H17	2.56	0.40
2:D:146:PHE:HA	2:D:147:PRO:HA	1.76	0.40
1:C:11:LEU:HG	1:C:13:VAL:HG13	2.04	0.40
1:C:34:HIS:O	1:C:88:CYS:HA	2.22	0.40
2:D:97:TYR:HD1	4:D:551:TAA:O4	2.05	0.40
2:B:12:VAL:O	2:B:111:VAL:HA	2.22	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	212/214 (99%)	202 (95%)	8 (4%)	2 (1%)	20	18
1	C	212/214 (99%)	199 (94%)	11 (5%)	2 (1%)	20	18
2	B	218/220 (99%)	203 (93%)	12 (6%)	3 (1%)	13	10
2	D	218/220 (99%)	197 (90%)	18 (8%)	3 (1%)	13	10
All	All	860/868 (99%)	801 (93%)	49 (6%)	10 (1%)	15	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	132	THR
1	C	203	SER
2	D	132	THR
2	B	129	ALA
2	B	131	GLN
2	D	129	ALA
2	D	131	GLN
1	A	203	SER
1	C	200	THR
1	A	200	THR

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	192/192 (100%)	179 (93%)	13 (7%)	18	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	192/192 (100%)	178 (93%)	14 (7%)	16	17
2	B	188/188 (100%)	175 (93%)	13 (7%)	18	19
2	D	188/188 (100%)	174 (93%)	14 (7%)	16	17
All	All	760/760 (100%)	706 (93%)	54 (7%)	17	18

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	46	LEU
1	A	54	SER
1	A	76	ASN
1	A	81	GLU
1	A	108	ARG
1	A	125	LEU
1	A	147	LYS
1	A	157	ASN
1	A	183	LYS
1	A	197	THR
1	A	198	HIS
1	A	199	LYS
2	B	13	LYS
2	B	18	VAL
2	B	30	SER
2	B	66	LYS
2	B	71	VAL
2	B	82	PHE
2	B	94	ARG
2	B	131	GLN
2	B	138	LEU
2	B	140	CYS
2	B	149	PRO
2	B	171	GLN
2	B	177	LEU
1	C	4	MET
1	C	46	LEU
1	C	67	SER
1	C	76	ASN
1	C	81	GLU
1	C	125	LEU
1	C	147	LYS

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Mol	Chain	Res	Type
1	C	157	ASN
1	C	170	ASP
1	C	171	SER
1	C	197	THR
1	C	198	HIS
1	C	199	LYS
1	C	203	SER
2	D	18	VAL
2	D	30	SER
2	D	71	VAL
2	D	82	PHE
2	D	94	ARG
2	D	98	ASP
2	D	115	LYS
2	D	131	GLN
2	D	138	LEU
2	D	140	CYS
2	D	149	PRO
2	D	171	GLN
2	D	177	LEU
2	D	195	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	161	ASN
1	A	190	ASN
1	C	161	ASN
1	C	190	ASN
1	C	198	HIS
2	D	171	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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$
3	SO4	A	540	-	4,4,4	0.68	0	6,6,6	0.72	0
4	TAA	B	550	-	37,38,38	2.34	11 (29%)	41,55,55	1.84	8 (19%)
3	SO4	C	541	-	4,4,4	0.29	0	6,6,6	0.77	0
4	TAA	D	551	-	37,38,38	2.39	10 (27%)	41,55,55	1.87	8 (19%)

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
3	SO4	A	540	-	-	0/0/0/0	0/0/0/0
4	TAA	B	550	-	1/1/8/10	0/33/42/42	0/2/2/2
3	SO4	C	541	-	-	0/0/0/0	0/0/0/0
4	TAA	D	551	-	1/1/8/10	0/33/42/42	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	551	TAA	O6-C13	-8.75	1.23	1.40
4	B	550	TAA	O6-C13	-7.61	1.25	1.40
4	B	550	TAA	C10-C11	-6.49	1.46	1.53
4	D	551	TAA	P1-O2	-4.60	1.45	1.56
4	B	550	TAA	P1-O2	-4.24	1.46	1.56
4	D	551	TAA	C10-C11	-3.76	1.49	1.53
4	B	550	TAA	P1-C1	-3.30	1.71	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	551	TAA	P1-C1	-2.95	1.72	1.80
4	D	551	TAA	C11-N2	-2.30	1.43	1.47
4	B	550	TAA	C1-C2	-2.21	1.46	1.51
4	B	550	TAA	F3-C9	2.07	1.41	1.32
4	B	550	TAA	F1-C9	2.20	1.41	1.32
4	D	551	TAA	C6-C5	2.23	1.43	1.39
4	D	551	TAA	F1-C9	2.29	1.42	1.32
4	B	550	TAA	C6-C5	2.33	1.43	1.39
4	B	550	TAA	C18-N3	2.35	1.50	1.45
4	B	550	TAA	O7-N3	2.75	1.27	1.22
4	B	550	TAA	C5-N1	3.22	1.47	1.41
4	D	551	TAA	P1-O1	3.37	1.61	1.57
4	D	551	TAA	C12-C11	4.27	1.61	1.52
4	D	551	TAA	C5-N1	4.31	1.50	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	550	TAA	C5-N1-C8	-4.09	119.40	126.81
4	D	551	TAA	O1-P1-O3	-3.92	108.54	115.61
4	B	550	TAA	O1-P1-O3	-2.75	110.65	115.61
4	D	551	TAA	C5-N1-C8	-2.73	121.86	126.81
4	B	550	TAA	C17-C16-C15	-2.58	118.58	121.20
4	D	551	TAA	C1-C2-C3	-2.41	116.58	120.85
4	D	551	TAA	C6-C7-C2	-2.25	117.91	121.02
4	D	551	TAA	C17-C16-C15	-2.10	119.06	121.20
4	B	550	TAA	C6-C7-C2	-2.01	118.24	121.02
4	B	550	TAA	C7-C2-C3	2.36	121.91	118.16
4	D	551	TAA	C20-C15-C16	2.38	121.29	118.30
4	B	550	TAA	C20-C15-C16	3.41	122.58	118.30
4	B	550	TAA	O6-C13-C14	3.78	120.51	108.41
4	D	551	TAA	O6-C13-C14	4.48	122.72	108.41
4	B	550	TAA	O6-C13-N2	5.80	122.59	111.00
4	D	551	TAA	O6-C13-N2	6.57	124.12	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	550	TAA	C13
4	D	551	TAA	C13

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	550	TAA	1	0
4	D	551	TAA	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.