



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:49 PM GMT

PDB ID : 2PJT
Title : Crystal structure of the catalytic domain of MMP-13 complexed with WAY-344
Authors : Xu, Z.; Huang, A.; Lovering, F.; Levin, J.I.; Mosyak, L.
Deposited on : 2007-04-16
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

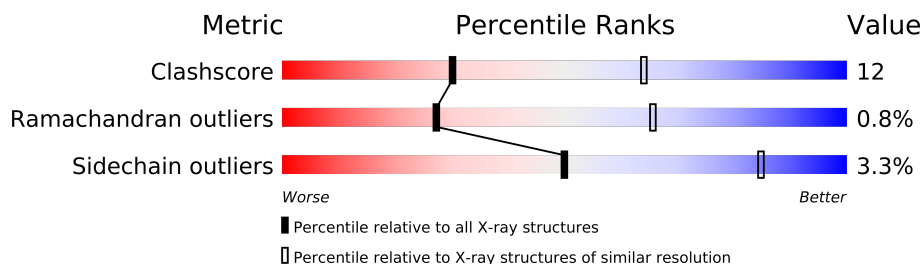
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	
1	B	165	
1	C	165	
1	D	165	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5412 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1292	840	207	241	4			
1	B	164	Total	C	N	O	S	0	0	0
			1307	849	209	244	5			
1	C	159	Total	C	N	O	S	0	0	0
			1271	827	201	238	5			
1	D	161	Total	C	N	O	S	0	0	0
			1284	835	205	240	4			

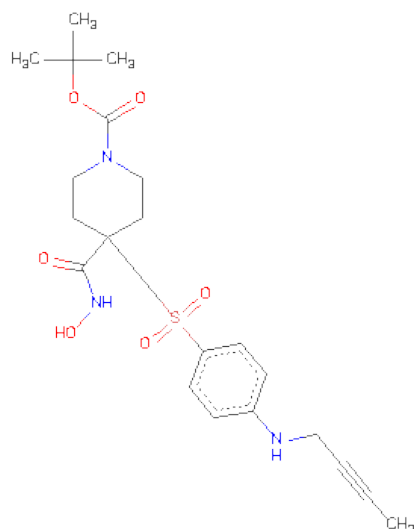
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is TERT-BUTYL 4-({[4-(BUT-2-YN-1-YLAMINO)PHENYL]SULFONYL} METHYL)-4-[(HYDROXYAMINO)CARBONYL]PIPERIDINE-1-CARBOXYLATE (three-letter code: 347) (formula: C₂₂H₃₁N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			32	22	3	6	1		
4	B	1	Total	C	N	O	S	0	0
			32	22	3	6	1		
4	C	1	Total	C	N	O	S	0	0
			32	22	3	6	1		
4	D	1	Total	C	N	O	S	0	0
			32	22	3	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	33	Total	O	0	0
			33	33		
5	C	25	Total	O	0	0
			25	25		
5	D	29	Total	O	0	0
			29	29		

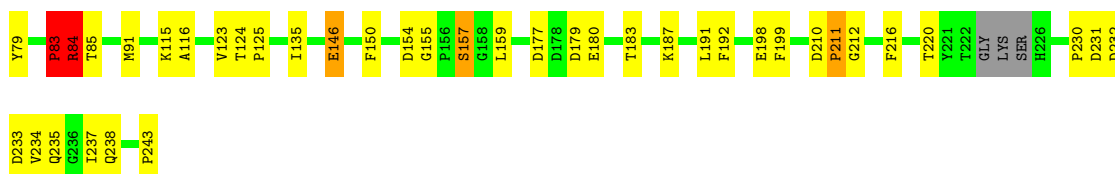
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

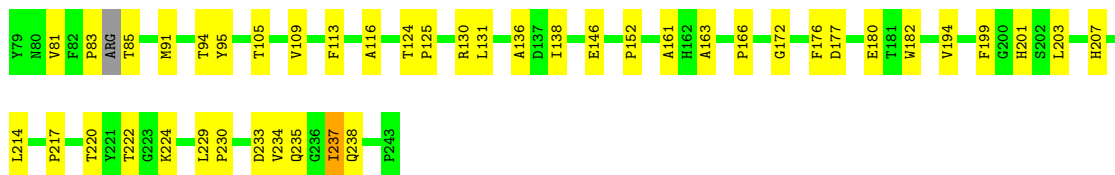
• Molecule 1: Collagenase 3

Chain A: 



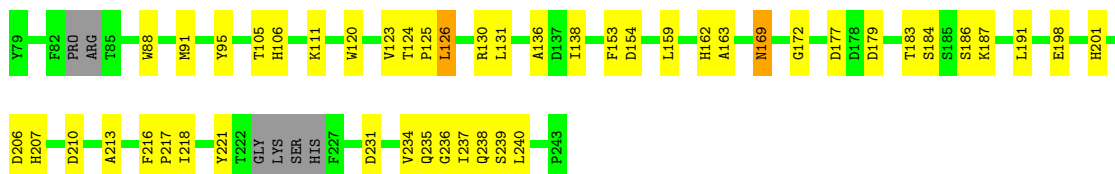
• Molecule 1: Collagenase 3

Chain B: 



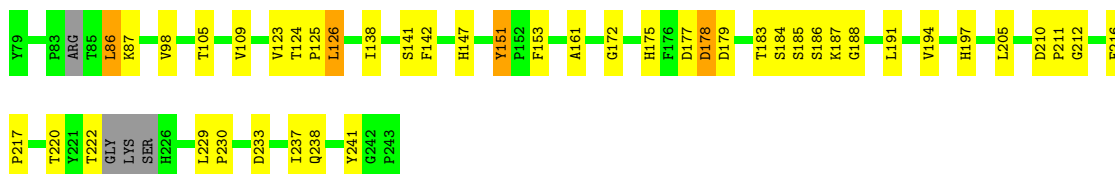
• Molecule 1: Collagenase 3

Chain C: 



• Molecule 1: Collagenase 3

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 35.79Å 139.41Å 90.00° 108.94° 90.00°	Depositor
Resolution (Å)	19.95 – 2.80	Depositor
% Data completeness (in resolution range)	92.5 (19.95-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5412	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 347, CA

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	0.55	1/1339 (0.1%)	0.73	3/1820 (0.2%)
1	B	0.44	0/1354	0.63	0/1839
1	C	0.45	0/1315	0.63	0/1785
1	D	0.42	0/1330	0.60	0/1807
All	All	0.47	1/5338 (0.0%)	0.65	3/7251 (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	1	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ARG	CD-NE	-9.60	1.30	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	N-CA-C	9.33	136.20	111.00
1	A	83	PRO	N-CA-C	8.20	133.43	112.10
1	A	83	PRO	C-N-CA	5.82	136.25	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	85	THR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	A	84	ARG	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1292	0	1198	24	8
1	B	1307	0	1219	27	4
1	C	1271	0	1183	34	0
1	D	1284	0	1189	34	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	30	2	0
4	B	32	0	31	2	0
4	C	32	0	30	2	0
4	D	32	0	30	2	0
5	A	25	0	0	1	1
5	B	33	0	0	1	4
5	C	25	0	0	0	1
5	D	29	0	0	0	0
All	All	5412	0	4910	122	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:183:THR:HG21	1:C:187:LYS:O	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:85:THR:N	5:B:408:HOH:O	2.09	0.86
1:A:243:PRO:OXT	5:A:405:HOH:O	2.02	0.78
1:A:237:ILE:HD12	1:A:238:GLN:H	1.52	0.74
1:D:153:PHE:HB3	1:D:177:ASP:OD2	1.88	0.74
1:D:86:LEU:HD23	1:D:87:LYS:H	1.53	0.74
1:D:237:ILE:HD12	1:D:238:GLN:H	1.53	0.73
1:D:237:ILE:HD12	1:D:238:GLN:N	2.04	0.72
1:B:131:LEU:HD12	1:B:136:ALA:HB2	1.72	0.72
1:C:231:ASP:O	1:C:235:GLN:HG2	1.91	0.70
1:D:183:THR:HG23	1:D:185:SER:H	1.55	0.70
1:C:236:GLY:O	1:C:239:SER:HB3	1.92	0.69
1:D:185:SER:OG	1:D:186:SER:N	2.25	0.69
1:C:131:LEU:HD12	1:C:136:ALA:HB2	1.78	0.65
1:B:229:LEU:HD12	1:B:230:PRO:HD2	1.77	0.65
1:A:237:ILE:HD12	1:A:238:GLN:N	2.13	0.62
1:B:81:VAL:O	1:B:83:PRO:HD3	1.99	0.62
1:C:91:MET:SD	1:C:125:PRO:HG2	2.39	0.62
1:A:177:ASP:OD1	1:A:179:ASP:HB2	1.99	0.61
1:C:123:VAL:HG11	1:C:234:VAL:HG22	1.83	0.61
1:B:124:THR:HB	1:B:125:PRO:HD2	1.82	0.60
1:C:124:THR:OG1	1:C:126:LEU:HB2	2.01	0.59
1:C:154:ASP:OD2	1:C:159:LEU:HG	2.03	0.59
1:B:234:VAL:O	1:B:238:GLN:HG3	2.02	0.59
1:D:229:LEU:HD12	1:D:230:PRO:HD2	1.84	0.58
1:A:211:PRO:HA	1:A:216:PHE:CD2	2.38	0.58
1:A:146:GLU:OE2	1:A:150:PHE:HA	2.04	0.58
1:D:205:LEU:HD11	1:D:237:ILE:HG23	1.85	0.57
1:B:177:ASP:HB3	1:B:180:GLU:HG2	1.88	0.55
1:D:86:LEU:HD23	1:D:87:LYS:HG2	1.88	0.55
1:D:124:THR:HB	1:D:125:PRO:HD2	1.89	0.55
1:C:124:THR:HB	1:C:125:PRO:HD2	1.89	0.54
1:D:230:PRO:HB2	1:D:233:ASP:OD1	2.08	0.53
1:C:216:PHE:CD2	1:C:217:PRO:HD2	2.44	0.53
1:B:91:MET:SD	1:B:125:PRO:HG2	2.49	0.53
1:C:120:TRP:CE3	1:C:237:ILE:HG12	2.44	0.53
1:D:123:VAL:O	1:D:124:THR:HG23	2.08	0.53
1:D:86:LEU:CD2	1:D:87:LYS:H	2.20	0.52
1:A:91:MET:SD	1:A:125:PRO:HG2	2.49	0.52
1:A:183:THR:HG21	1:A:187:LYS:HG3	1.91	0.52
1:C:163:ALA:HB3	1:C:201:HIS:HB2	1.91	0.51
1:A:230:PRO:HB2	1:A:233:ASP:OD2	2.11	0.51
1:B:180:GLU:OE1	1:B:180:GLU:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:LYS:HG2	1:A:192:PHE:CE1	2.45	0.51
1:C:217:PRO:O	1:C:218:ILE:HD13	2.11	0.51
1:C:210:ASP:HB3	1:C:213:ALA:HB2	1.93	0.51
1:A:230:PRO:O	1:A:234:VAL:HG23	2.11	0.51
1:C:234:VAL:HA	1:C:237:ILE:HD11	1.92	0.51
1:A:79:TYR:HB3	1:A:232:ASP:OD1	2.11	0.51
1:B:95:TYR:CZ	1:B:130:ARG:HB2	2.46	0.50
1:C:186:SER:HB3	1:C:221:TYR:CE2	2.46	0.50
1:A:123:VAL:HG23	1:A:124:THR:HG23	1.93	0.50
1:C:169:ASN:HD22	1:C:169:ASN:N	2.10	0.49
1:C:234:VAL:O	1:C:237:ILE:HD12	2.13	0.49
1:C:120:TRP:HE3	1:C:237:ILE:HG12	1.77	0.48
1:B:182:TRP:HZ3	1:B:194:VAL:HG21	1.77	0.48
1:D:123:VAL:O	1:D:124:THR:CG2	2.62	0.48
1:C:206:ASP:OD1	1:C:207:HIS:N	2.42	0.48
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.14	0.48
1:C:186:SER:HB3	1:C:221:TYR:CZ	2.49	0.48
1:D:98:VAL:HB	1:D:141:SER:HB3	1.96	0.48
1:B:194:VAL:HG13	4:B:401:347:H6	1.97	0.47
1:D:183:THR:OG1	1:D:184:SER:N	2.46	0.47
1:B:230:PRO:O	1:B:234:VAL:HG23	2.14	0.47
1:A:177:ASP:HB3	1:A:180:GLU:HG2	1.96	0.47
4:D:401:347:H131	4:D:401:347:O1	2.14	0.47
1:D:183:THR:CG2	1:D:187:LYS:O	2.64	0.46
4:C:401:347:H131	4:C:401:347:O1	2.15	0.46
1:A:157:SER:N	1:A:180:GLU:OE1	2.44	0.46
1:B:138:ILE:HG23	1:B:172:GLY:O	2.16	0.46
1:A:154:ASP:OD2	1:A:159:LEU:HG	2.16	0.46
1:D:105:THR:O	1:D:109:VAL:HG23	2.16	0.45
1:C:237:ILE:HD12	1:C:238:GLN:H	1.81	0.45
1:D:220:THR:O	4:D:401:347:H12	2.17	0.45
1:B:214:LEU:HB3	1:B:233:ASP:OD2	2.16	0.44
1:A:234:VAL:O	1:A:238:GLN:HG3	2.18	0.44
1:C:111:LYS:HD3	1:C:111:LYS:HA	1.77	0.44
1:B:105:THR:O	1:B:109:VAL:HG23	2.16	0.44
1:B:199:PHE:O	1:B:203:LEU:HG	2.16	0.44
1:B:113:PHE:O	1:B:116:ALA:HB3	2.17	0.44
1:D:142:PHE:HB3	1:D:178:ASP:OD2	2.17	0.44
1:D:87:LYS:HB2	1:D:241:TYR:CZ	2.52	0.44
1:C:88:TRP:HZ2	1:C:172:GLY:HA3	1.83	0.43
1:B:161:ALA:HB2	1:B:176:PHE:HA	1.99	0.43
1:C:237:ILE:HG13	1:C:237:ILE:H	1.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:161:ALA:HB1	1:D:175:HIS:O	2.19	0.43
1:B:234:VAL:HA	1:B:237:ILE:HD11	2.00	0.43
1:A:231:ASP:O	1:A:235:GLN:HG2	2.18	0.43
1:D:183:THR:HG21	1:D:187:LYS:O	2.18	0.43
1:B:163:ALA:HB3	1:B:201:HIS:HB2	1.99	0.43
1:D:216:PHE:CD2	1:D:217:PRO:HD2	2.54	0.43
1:C:138:ILE:HG23	1:C:172:GLY:O	2.18	0.42
1:C:105:THR:O	1:C:106:HIS:C	2.57	0.42
1:C:237:ILE:HD12	1:C:238:GLN:N	2.34	0.42
1:D:124:THR:OG1	1:D:126:LEU:HB2	2.20	0.42
1:C:198:GLU:OE2	4:C:401:347:O6	2.38	0.42
1:A:155:GLY:HA2	1:A:179:ASP:OD2	2.20	0.42
1:B:220:THR:O	4:B:401:347:H12	2.18	0.42
1:B:146:GLU:CD	1:B:152:PRO:HB3	2.39	0.42
1:A:198:GLU:OE2	4:A:401:347:O6	2.38	0.42
1:D:177:ASP:OD1	1:D:179:ASP:HB2	2.20	0.42
1:C:183:THR:CG2	1:C:187:LYS:O	2.58	0.42
1:A:238:GLN:NE2	1:A:243:PRO:HA	2.35	0.42
1:A:116:ALA:HB3	1:A:199:PHE:CE2	2.54	0.42
1:A:210:ASP:C	1:A:212:GLY:H	2.23	0.42
1:B:161:ALA:CB	1:B:176:PHE:HA	2.50	0.41
1:D:147:HIS:CE1	1:D:151:TYR:O	2.73	0.41
1:D:237:ILE:CD1	1:D:238:GLN:HG3	2.51	0.41
1:C:183:THR:OG1	1:C:184:SER:N	2.54	0.41
1:D:194:VAL:O	1:D:197:HIS:HB3	2.20	0.41
1:B:94:THR:HB	1:B:131:LEU:HG	2.02	0.41
1:D:187:LYS:O	1:D:188:GLY:C	2.59	0.41
1:D:229:LEU:HA	1:D:230:PRO:HD3	1.92	0.41
1:D:151:TYR:N	1:D:151:TYR:CD1	2.89	0.41
1:C:153:PHE:HE1	1:C:162:HIS:HD1	1.68	0.41
1:B:207:HIS:HB3	1:B:217:PRO:HD3	2.03	0.41
1:C:95:TYR:CZ	1:C:130:ARG:HB2	2.56	0.41
1:B:124:THR:HB	1:B:125:PRO:CD	2.50	0.41
1:D:210:ASP:O	1:D:212:GLY:N	2.54	0.40
1:D:138:ILE:HG23	1:D:172:GLY:O	2.22	0.40
1:A:116:ALA:HB3	1:A:199:PHE:HE2	1.85	0.40
4:A:401:347:O1	4:A:401:347:H131	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:PRO:C	5:B:408:HOH:O[2.667]	0.57	1.63
5:A:421:HOH:O	5:C:417:HOH:O[3.546]	0.78	1.42
1:A:83:PRO:O	5:B:408:HOH:O[2.667]	1.14	1.06
1:A:83:PRO:O	1:B:85:THR:N[2.667]	1.15	1.05
1:A:84:ARG:O	1:B:83:PRO:C[2.667]	1.42	0.78
1:A:84:ARG:N	5:B:408:HOH:O[2.667]	1.45	0.75
1:A:83:PRO:CA	5:B:408:HOH:O[2.667]	1.87	0.33
1:A:84:ARG:O	1:B:83:PRO:O[2.667]	1.87	0.33
1:A:83:PRO:O	1:B:85:THR:CA[2.667]	2.18	0.02

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	158/165 (96%)	142 (90%)	14 (9%)	2 (1%)	18	51
1	B	160/165 (97%)	141 (88%)	17 (11%)	2 (1%)	18	51
1	C	153/165 (93%)	141 (92%)	12 (8%)	0	100	100
1	D	155/165 (94%)	143 (92%)	11 (7%)	1 (1%)	33	72
All	All	626/660 (95%)	567 (91%)	54 (9%)	5 (1%)	27	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR
1	B	224	LYS
1	B	166	PRO
1	D	211	PRO
1	A	211	PRO

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	137/141 (97%)	132 (96%)	5 (4%)	47	82
1	B	140/141 (99%)	137 (98%)	3 (2%)	66	93
1	C	136/141 (96%)	132 (97%)	4 (3%)	55	88
1	D	137/141 (97%)	131 (96%)	6 (4%)	39	75
All	All	550/564 (98%)	532 (97%)	18 (3%)	50	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	ILE
1	A	146	GLU
1	A	157	SER
1	A	191	LEU
1	A	220	THR
1	B	222	THR
1	B	235	GLN
1	B	237	ILE
1	C	126	LEU
1	C	169	ASN
1	C	191	LEU
1	C	240	LEU
1	D	86	LEU
1	D	126	LEU
1	D	151	TYR
1	D	178	ASP
1	D	191	LEU
1	D	222	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	238	GLN
1	B	127	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	235	GLN
1	C	80	ASN
1	C	92	ASN
1	C	169	ASN
1	D	80	ASN
1	D	207	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 18 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	347	A	401	2	33,33,33	2.12	13 (39%)	48,48,48	1.81	2 (4%)
4	347	B	401	2	33,33,33	2.55	17 (51%)	48,48,48	1.78	10 (20%)
4	347	C	401	2	33,33,33	2.43	15 (45%)	48,48,48	1.58	5 (10%)
4	347	D	401	2	33,33,33	2.10	13 (39%)	48,48,48	1.90	5 (10%)

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	347	A	401	2	-	0/33/46/46	0/2/2/2
4	347	B	401	2	-	0/33/46/46	0/2/2/2
4	347	C	401	2	-	0/33/46/46	0/2/2/2
4	347	D	401	2	-	0/33/46/46	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	347	C17-N2	5.58	1.46	1.35
4	C	401	347	C17-N2	5.24	1.45	1.35
4	B	401	347	C16-C12	5.16	1.61	1.54
4	B	401	347	O4-C17	4.90	1.42	1.34
4	C	401	347	O4-C17	4.72	1.42	1.34
4	A	401	347	C13-C12	4.49	1.60	1.54
4	C	401	347	C16-C12	4.43	1.60	1.54
4	C	401	347	C13-C12	4.39	1.60	1.54
4	B	401	347	C13-C12	4.23	1.60	1.54
4	A	401	347	O4-C17	3.92	1.41	1.34
4	D	401	347	C17-N2	3.85	1.43	1.35
4	B	401	347	C16-C15	3.83	1.58	1.52
4	D	401	347	C13-C12	3.81	1.59	1.54
4	A	401	347	C17-N2	3.72	1.42	1.35
4	D	401	347	O3-C17	3.66	1.26	1.21
4	D	401	347	O4-C17	3.59	1.40	1.34
4	D	401	347	C16-C12	3.57	1.59	1.54
4	C	401	347	O3-C17	3.55	1.26	1.21
4	C	401	347	C16-C15	3.42	1.57	1.52
4	A	401	347	C16-C12	3.42	1.58	1.54
4	A	401	347	C10-C9	3.39	1.45	1.38
4	A	401	347	O3-C17	3.30	1.26	1.21
4	B	401	347	O3-C17	3.18	1.26	1.21
4	D	401	347	C10-C9	3.15	1.44	1.38
4	B	401	347	O4-C18	3.08	1.54	1.48
4	D	401	347	C16-C15	2.94	1.57	1.52
4	C	401	347	O4-C18	2.93	1.54	1.48
4	C	401	347	C22-N3	2.87	1.39	1.34
4	B	401	347	C11-S1	2.84	1.82	1.78
4	C	401	347	C11-S1	2.83	1.82	1.78
4	A	401	347	C16-C15	2.83	1.56	1.52
4	B	401	347	C22-N3	2.83	1.39	1.34
4	B	401	347	C15-N2	2.79	1.52	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	347	C10-C5	2.77	1.43	1.39
4	C	401	347	C15-N2	2.73	1.52	1.47
4	C	401	347	C10-C9	2.70	1.43	1.38
4	B	401	347	C10-C9	2.70	1.43	1.38
4	A	401	347	C10-C5	2.64	1.43	1.39
4	A	401	347	C6-C5	2.57	1.43	1.39
4	B	401	347	C7-C8	2.54	1.43	1.38
4	D	401	347	C15-N2	2.40	1.51	1.47
4	B	401	347	C10-C5	2.39	1.43	1.39
4	A	401	347	C22-N3	2.38	1.38	1.34
4	C	401	347	C10-C5	2.36	1.43	1.39
4	B	401	347	C7-C6	2.36	1.43	1.38
4	B	401	347	C8-S1	2.35	1.81	1.76
4	C	401	347	C9-C8	2.34	1.42	1.38
4	C	401	347	C6-C5	2.32	1.43	1.39
4	D	401	347	C14-N2	-2.31	1.42	1.47
4	D	401	347	C7-C8	2.28	1.42	1.38
4	A	401	347	C7-C8	2.27	1.42	1.38
4	D	401	347	C6-C5	2.26	1.43	1.39
4	B	401	347	C6-C5	2.22	1.42	1.39
4	A	401	347	C15-N2	2.20	1.51	1.47
4	D	401	347	C9-C8	2.19	1.42	1.38
4	C	401	347	O2-S1	2.13	1.47	1.44
4	B	401	347	O2-S1	2.08	1.47	1.44
4	A	401	347	C7-C6	2.06	1.42	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	347	C18-O4-C17	10.40	133.29	121.06
4	D	401	347	C18-O4-C17	9.63	132.38	121.06
4	B	401	347	C18-O4-C17	7.62	130.02	121.06
4	C	401	347	C18-O4-C17	6.88	129.15	121.06
4	D	401	347	O1-S1-C8	-5.33	102.75	108.39
4	C	401	347	O1-S1-C8	-4.21	103.94	108.39
4	B	401	347	O1-S1-C8	-3.90	104.27	108.39
4	A	401	347	O1-S1-C8	-3.32	104.88	108.39
4	D	401	347	C3-C4-N1	-2.94	109.78	113.17
4	B	401	347	C12-C22-N3	2.93	119.55	115.97
4	B	401	347	O6-N3-C22	-2.57	116.34	119.80
4	B	401	347	C6-C5-N1	2.50	126.11	121.02
4	B	401	347	C3-C4-N1	-2.48	110.31	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	347	O6-N3-C22	-2.30	116.70	119.80
4	C	401	347	C6-C5-N1	2.14	125.39	121.02
4	C	401	347	O4-C17-N2	2.10	114.28	110.98
4	B	401	347	C4-N1-C5	2.09	126.76	122.42
4	B	401	347	O4-C17-N2	2.06	114.23	110.98
4	B	401	347	C19-C18-C20	-2.06	105.44	111.19
4	B	401	347	C9-C10-C5	2.06	122.67	120.27
4	C	401	347	O6-N3-C22	-2.06	117.04	119.80
4	D	401	347	C6-C5-N1	2.05	125.20	121.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.