



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:27 pm GMT

PDB ID : 1ZTQ
Title : Crystal structure of the catalytic domain of MMP-13 complexed with WAY-033
Authors : Wu, J.; Rush III, T.S.; Hotchandani, R.; Du, X.; Geck, M.; Collins, E.; Xu, Z.B.; Skotnicki, J.; Levin, J.I.; Lovering, F.
Deposited on : 2005-05-27
Resolution : 2.00 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

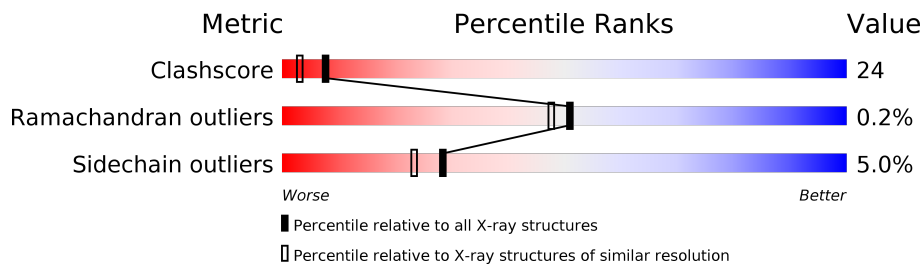
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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	165	
1	B	165	
1	C	165	
1	D	165	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5692 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1293	840	207	241	5			
1	B	160	Total	C	N	O	S	0	0	0
			1274	825	205	239	5			
1	C	153	Total	C	N	O	S	0	0	0
			1218	790	195	229	4			
1	D	156	Total	C	N	O	S	0	0	0
			1245	810	198	232	5			

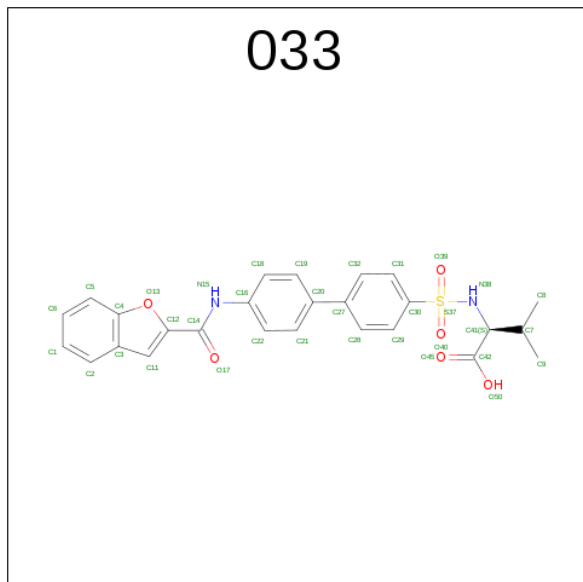
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		
3	D	3	Total	Ca	0	0
			3	3		
3	C	3	Total	Ca	0	0
			3	3		

- Molecule 4 is N-({4'-[(1-BENZOFURAN-2-YLCARBONYL)AMINO]-1,1'-BIPHENYL-4-YL}SULFONYL)-L-VALINE (three-letter code: 033) (formula: C₂₆H₂₄N₂O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			35	26	2	6	1		
4	B	1	Total	C	N	O	S	0	0
			35	26	2	6	1		
4	C	1	Total	C	N	O	S	0	0
			35	26	2	6	1		
4	D	1	Total	C	N	O	S	0	0
			35	26	2	6	1		

- Molecule 5 is water.

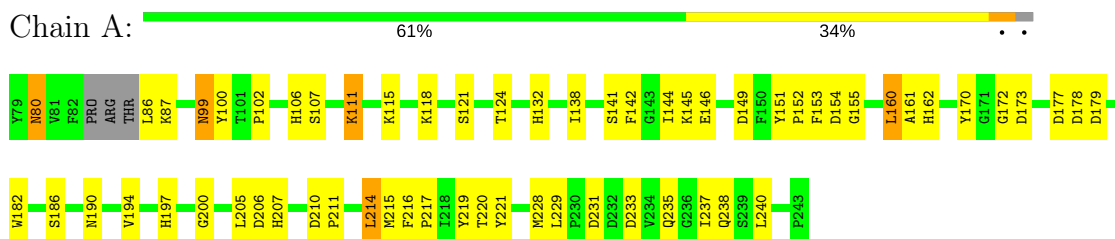
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	127	Total	O	0	0
			127	127		
5	C	135	Total	O	0	0
			135	135		
5	D	115	Total	O	0	0
			115	115		

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 ($RSRZ > 2$). 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.

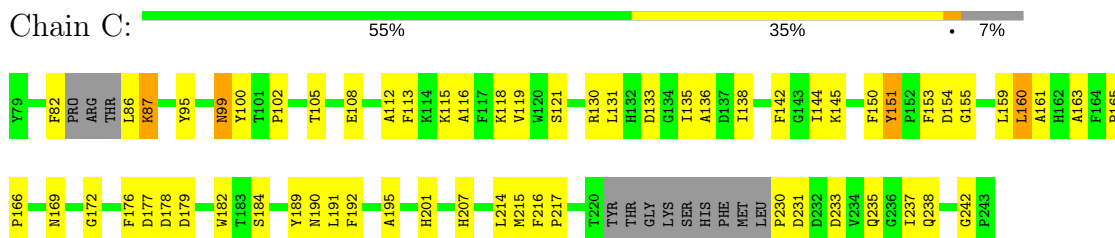
• Molecule 1: Collagenase 3



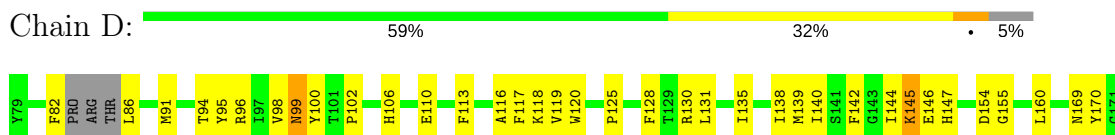
• Molecule 1: Collagenase 3

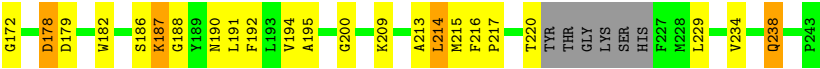


• Molecule 1: Collagenase 3



• Molecule 1: Collagenase 3





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	35.94Å 135.25Å 69.39Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	19.46 – 2.00	Depositor
% Data completeness (in resolution range)	86.0 (19.46-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5692	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: 033, ZN, 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	0.40	0/1339	0.62	1/1817 (0.1%)
1	B	0.37	0/1319	0.62	0/1790
1	C	0.35	0/1260	0.61	0/1709
1	D	0.45	1/1288 (0.1%)	0.63	1/1747 (0.1%)
All	All	0.40	1/5206 (0.0%)	0.62	2/7063 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	187	LYS	C-N	7.96	1.47	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	LYS	N-CA-CB	-5.27	101.11	110.60
1	A	228	MET	CG-SD-CE	-5.05	92.12	100.20

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	1293	0	1205	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1274	0	1185	63	0
1	C	1218	0	1132	64	0
1	D	1245	0	1160	67	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	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	35	0	23	2	0
4	B	35	0	23	3	0
4	C	35	0	23	1	0
4	D	35	0	23	0	0
5	A	125	0	0	10	0
5	B	127	0	0	22	0
5	C	135	0	0	23	1
5	D	115	0	0	21	1
All	All	5692	0	4774	242	1

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 24.

All (242) 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:138:ILE:HG22	5:D:632:HOH:O	1.59	1.00
1:B:230:PRO:HG2	5:B:682:HOH:O	1.62	0.97
1:D:99:ASN:HD21	1:D:142:PHE:H	1.04	0.97
1:C:161:ALA:HA	5:C:616:HOH:O	1.62	0.97
1:B:102:PRO:HB3	1:C:100:TYR:HE2	1.26	0.95
1:B:140:ILE:HG23	5:B:615:HOH:O	1.67	0.95
1:B:91:MET:HE2	1:B:125:PRO:HB2	1.51	0.91
1:A:99:ASN:HD21	1:A:142:PHE:H	1.18	0.90
1:A:194:VAL:HG22	5:A:626:HOH:O	1.73	0.87
1:B:222:THR:HB	1:B:224:LYS:HD3	1.57	0.87
1:B:123:VAL:HB	5:B:623:HOH:O	1.77	0.85
1:D:213:ALA:HB3	5:D:625:HOH:O	1.77	0.85
1:A:102:PRO:HB3	1:D:100:TYR:HE2	1.39	0.85
1:B:100:TYR:HE2	1:C:102:PRO:HB3	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PHE:HD1	5:C:666:HOH:O	1.63	0.81
1:C:99:ASN:HD21	1:C:142:PHE:H	1.26	0.81
1:A:160:LEU:HD23	1:A:161:ALA:N	1.97	0.80
1:A:144:ILE:HD12	1:D:98:VAL:HG13	1.65	0.79
1:A:118:LYS:HA	1:A:121:SER:OG	1.82	0.79
1:D:140:ILE:HG13	5:D:632:HOH:O	1.84	0.78
1:B:102:PRO:HB3	1:C:100:TYR:CE2	2.15	0.77
1:A:160:LEU:HD23	1:A:161:ALA:H	1.51	0.75
1:A:99:ASN:HD21	1:A:142:PHE:N	1.84	0.75
1:D:113:PHE:HA	5:D:616:HOH:O	1.87	0.75
1:B:242:GLY:HA2	5:B:626:HOH:O	1.87	0.75
1:A:102:PRO:HB3	1:D:100:TYR:CE2	2.21	0.74
1:D:144:ILE:HD11	1:D:178:ASP:C	2.08	0.74
1:A:99:ASN:ND2	1:A:142:PHE:H	1.84	0.74
1:A:182:TRP:HZ3	1:A:194:VAL:HG21	1.53	0.74
1:C:178:ASP:OD2	5:C:731:HOH:O	2.05	0.73
1:B:214:LEU:N	5:B:682:HOH:O	2.20	0.73
1:B:140:ILE:HG13	5:B:695:HOH:O	1.87	0.73
1:D:113:PHE:HD1	5:D:616:HOH:O	1.72	0.73
1:A:87:LYS:HD2	1:A:240:LEU:O	1.90	0.72
1:C:144:ILE:HD11	1:C:178:ASP:C	2.10	0.72
1:D:194:VAL:HB	5:D:675:HOH:O	1.90	0.72
1:C:144:ILE:HG22	1:C:145:LYS:HG2	1.72	0.71
1:C:182:TRP:HB3	5:C:631:HOH:O	1.89	0.71
1:C:207:HIS:ND1	1:C:217:PRO:HB3	2.05	0.71
1:C:144:ILE:HD11	1:C:179:ASP:N	2.06	0.71
1:B:216:PHE:HE1	1:B:218:ILE:HD12	1.55	0.70
1:C:138:ILE:HG23	1:C:172:GLY:O	1.91	0.70
1:D:209:LYS:HE2	5:D:684:HOH:O	1.91	0.69
1:C:113:PHE:HA	5:C:666:HOH:O	1.92	0.69
1:D:82:PHE:HB3	1:D:86:LEU:HD12	1.74	0.69
1:A:144:ILE:HG23	5:A:603:HOH:O	1.93	0.68
1:C:195:ALA:HB1	5:C:666:HOH:O	1.94	0.67
1:D:234:VAL:O	1:D:238:GLN:HB2	1.95	0.67
1:B:100:TYR:CE2	1:C:102:PRO:HB3	2.27	0.66
1:B:91:MET:HE2	1:B:125:PRO:CB	2.25	0.66
1:D:94:THR:HB	1:D:131:LEU:HD13	1.76	0.66
1:B:243:PRO:HD3	5:B:626:HOH:O	1.95	0.66
1:C:177:ASP:N	5:C:616:HOH:O	2.28	0.66
1:B:186:SER:HB3	1:B:221:TYR:CE2	2.30	0.66
1:A:99:ASN:HD21	1:A:141:SER:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:TRP:HZ3	5:B:677:HOH:O	1.78	0.65
1:B:133:ASP:OD1	5:B:716:HOH:O	2.15	0.65
1:A:186:SER:HB3	1:A:221:TYR:CE2	2.31	0.65
1:C:153:PHE:CZ	5:C:616:HOH:O	2.50	0.65
1:C:182:TRP:CD1	5:C:731:HOH:O	2.50	0.64
1:A:132:HIS:NE2	1:B:111:LYS:HE3	2.13	0.64
1:A:144:ILE:HG23	1:A:179:ASP:OD2	1.98	0.63
1:D:120:TRP:HZ2	5:D:643:HOH:O	1.81	0.63
1:C:182:TRP:HD1	5:C:731:HOH:O	1.81	0.63
1:D:144:ILE:HD11	1:D:179:ASP:N	2.14	0.63
1:D:182:TRP:HE3	5:D:663:HOH:O	1.81	0.63
1:A:99:ASN:ND2	1:A:141:SER:HA	2.14	0.63
1:D:216:PHE:CD2	1:D:217:PRO:HD2	2.34	0.62
1:C:99:ASN:ND2	1:C:142:PHE:H	1.97	0.62
1:A:220:THR:HG22	5:A:695:HOH:O	2.01	0.60
1:D:99:ASN:HD21	1:D:142:PHE:N	1.88	0.60
1:C:118:LYS:HA	1:C:121:SER:OG	2.01	0.60
1:C:115:LYS:HG2	1:C:192:PHE:CE1	2.36	0.60
1:B:222:THR:HG22	5:B:724:HOH:O	2.02	0.60
1:A:100:TYR:HE2	1:D:102:PRO:HB3	1.66	0.60
1:B:231:ASP:HB2	5:B:726:HOH:O	2.01	0.60
1:B:138:ILE:O	5:B:695:HOH:O	2.16	0.60
1:B:145:LYS:HB2	5:B:719:HOH:O	2.01	0.59
1:B:118:LYS:HE3	1:D:187:LYS:HD3	1.85	0.59
1:C:116:ALA:HB3	5:C:666:HOH:O	2.01	0.59
1:A:144:ILE:HD12	1:D:98:VAL:CG1	2.31	0.58
1:D:106:HIS:O	1:D:110:GLU:HG3	2.02	0.58
1:C:105:THR:OG1	1:C:108:GLU:HG3	2.03	0.58
1:D:200:GLY:HA3	5:D:643:HOH:O	2.03	0.58
1:B:234:VAL:O	1:B:237:ILE:HG22	2.04	0.57
1:B:238:GLN:NE2	5:B:623:HOH:O	2.37	0.57
5:A:607:HOH:O	1:D:144:ILE:HG21	2.02	0.57
1:A:138:ILE:HG23	1:A:172:GLY:O	2.04	0.57
1:C:87:LYS:HA	1:C:166:PRO:HG2	1.86	0.57
4:B:602:033:H5	5:B:682:HOH:O	2.03	0.56
1:C:86:LEU:N	5:C:659:HOH:O	2.39	0.56
1:D:138:ILE:HG23	1:D:172:GLY:O	2.05	0.56
1:A:160:LEU:HD21	4:A:601:033:C31	2.36	0.56
1:C:176:PHE:HA	5:C:616:HOH:O	2.05	0.56
1:D:119:VAL:CG1	1:D:229:LEU:HD13	2.35	0.55
1:C:82:PHE:CE2	1:C:165:PRO:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ASP:OD2	1:A:235:GLN:NE2	2.39	0.55
1:C:231:ASP:O	1:C:235:GLN:HG2	2.07	0.55
1:A:80:ASN:HB2	1:A:207:HIS:O	2.07	0.55
1:A:162:HIS:CD2	5:A:701:HOH:O	2.59	0.54
1:D:82:PHE:CB	1:D:86:LEU:HD12	2.37	0.54
1:B:87:LYS:HB2	1:B:241:TYR:CE1	2.43	0.54
1:D:186:SER:O	1:D:188:GLY:N	2.40	0.54
1:B:193:LEU:HD13	4:B:602:033:H11	1.88	0.54
1:A:207:HIS:ND1	1:A:217:PRO:HB3	2.23	0.53
1:A:111:LYS:HD3	1:A:111:LYS:C	2.29	0.53
1:B:187:LYS:HD3	5:B:669:HOH:O	2.09	0.53
1:A:144:ILE:HG21	5:A:672:HOH:O	2.07	0.53
1:A:107:SER:HA	5:A:613:HOH:O	2.07	0.53
5:A:648:HOH:O	1:D:135:ILE:HD11	2.08	0.53
1:D:155:GLY:HA2	1:D:179:ASP:OD2	2.08	0.52
1:D:144:ILE:HG23	5:D:610:HOH:O	2.07	0.52
1:C:154:ASP:OD1	1:C:159:LEU:HD13	2.09	0.52
1:D:91:MET:SD	1:D:125:PRO:HB2	2.50	0.51
1:B:160:LEU:N	1:B:160:LEU:HD23	2.25	0.51
1:A:207:HIS:CE1	1:A:217:PRO:HB3	2.45	0.51
1:B:140:ILE:HD11	1:B:199:PHE:CZ	2.46	0.51
1:C:160:LEU:HD22	1:C:189:TYR:CZ	2.45	0.51
1:C:95:TYR:CZ	1:C:130:ARG:HB2	2.46	0.51
1:A:99:ASN:HD21	1:A:141:SER:CA	2.21	0.51
1:D:99:ASN:ND2	1:D:142:PHE:H	1.89	0.50
1:C:155:GLY:HA2	1:C:179:ASP:OD2	2.10	0.50
1:A:154:ASP:OD2	1:A:154:ASP:N	2.44	0.50
1:A:205:LEU:N	1:A:205:LEU:HD12	2.27	0.50
1:C:182:TRP:HE3	5:C:631:HOH:O	1.94	0.50
1:A:145:LYS:HE3	5:A:648:HOH:O	2.11	0.50
1:B:200:GLY:O	1:B:205:LEU:HB2	2.11	0.50
1:B:233:ASP:C	5:B:677:HOH:O	2.50	0.50
1:C:216:PHE:CD2	1:C:217:PRO:HD2	2.47	0.50
1:B:211:PRO:HA	1:B:216:PHE:CD2	2.46	0.50
1:D:144:ILE:HG23	1:D:179:ASP:OD2	2.12	0.50
1:C:151:TYR:CD1	1:C:151:TYR:N	2.80	0.49
1:D:144:ILE:CD1	1:D:179:ASP:N	2.74	0.49
1:C:191:LEU:N	5:C:631:HOH:O	2.45	0.49
1:D:182:TRP:HB3	5:D:663:HOH:O	2.11	0.49
1:D:142:PHE:HB3	1:D:178:ASP:OD1	2.13	0.49
1:B:124:THR:HG21	1:B:237:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:HB2	5:C:683:HOH:O	2.12	0.49
1:C:191:LEU:HB2	5:C:631:HOH:O	2.13	0.49
1:D:118:LYS:CE	5:D:716:HOH:O	2.61	0.49
1:B:123:VAL:HG23	1:B:124:THR:HG23	1.95	0.49
1:C:207:HIS:CE1	1:C:217:PRO:HB3	2.47	0.48
1:B:120:TRP:CZ3	5:B:677:HOH:O	2.55	0.48
1:C:115:LYS:O	1:C:119:VAL:HG23	2.14	0.48
1:B:190:ASN:HD22	1:B:193:LEU:H	1.61	0.48
1:C:230:PRO:N	5:C:655:HOH:O	2.45	0.48
1:C:131:LEU:HD12	1:C:136:ALA:HB2	1.94	0.48
1:A:111:LYS:CE	1:A:115:LYS:HD3	2.43	0.48
1:A:214:LEU:HD23	4:A:601:033:H15	1.79	0.48
1:B:187:LYS:HE2	5:B:661:HOH:O	2.13	0.48
1:D:190:ASN:OD1	1:D:192:PHE:HB3	2.12	0.47
1:D:191:LEU:HD12	5:D:675:HOH:O	2.14	0.47
1:B:151:TYR:HD2	1:B:162:HIS:CD2	2.32	0.47
1:B:151:TYR:OH	4:B:602:033:H83	2.15	0.47
1:D:116:ALA:HB3	5:D:616:HOH:O	2.15	0.47
1:D:145:LYS:O	1:D:147:HIS:ND1	2.44	0.47
1:D:144:ILE:HD12	1:D:179:ASP:CG	2.35	0.47
1:A:190:ASN:O	1:A:194:VAL:HG23	2.14	0.47
1:A:206:ASP:CG	1:A:207:HIS:H	2.19	0.46
1:D:195:ALA:HB1	5:D:616:HOH:O	2.15	0.46
1:D:214:LEU:HD12	1:D:229:LEU:CD1	2.45	0.46
1:A:100:TYR:CE2	1:D:102:PRO:HB3	2.50	0.46
1:A:149:ASP:O	1:A:151:TYR:CD1	2.69	0.46
1:A:229:LEU:HD11	1:A:233:ASP:HB2	1.98	0.46
1:A:197:HIS:CE1	1:A:215:MET:HA	2.51	0.46
1:D:99:ASN:HD22	1:D:99:ASN:C	2.18	0.46
1:C:135:ILE:HD13	5:C:644:HOH:O	2.15	0.46
1:B:197:HIS:CE1	1:B:215:MET:HA	2.50	0.46
1:A:144:ILE:HG22	1:A:145:LYS:HD3	1.97	0.46
1:B:91:MET:HE3	1:B:125:PRO:C	2.37	0.45
1:B:234:VAL:O	1:B:238:GLN:HG3	2.16	0.45
1:C:144:ILE:CG2	1:C:145:LYS:HG2	2.42	0.45
1:D:118:LYS:NZ	5:D:716:HOH:O	2.46	0.45
1:D:169:ASN:OD1	1:D:170:TYR:N	2.49	0.45
1:A:219:TYR:HE1	5:A:707:HOH:O	1.98	0.45
1:C:191:LEU:CA	5:C:631:HOH:O	2.64	0.45
1:A:124:THR:HG21	1:A:237:ILE:HG13	1.97	0.45
1:A:153:PHE:CD1	1:A:177:ASP:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:PHE:CZ	1:D:140:ILE:HG21	2.52	0.45
1:B:115:LYS:HE2	1:B:192:PHE:CZ	2.51	0.45
1:D:95:TYR:CE2	1:D:130:ARG:HD3	2.52	0.45
1:B:210:ASP:HA	1:B:211:PRO:HD2	1.82	0.45
1:C:237:ILE:CG2	1:C:238:GLN:N	2.80	0.45
1:C:190:ASN:OD1	1:C:192:PHE:HB3	2.17	0.44
1:B:182:TRP:HZ3	1:B:194:VAL:HG21	1.80	0.44
1:A:100:TYR:CD1	1:A:106:HIS:HA	2.52	0.44
1:A:111:LYS:O	1:A:111:LYS:HD3	2.17	0.44
1:D:191:LEU:N	5:D:663:HOH:O	2.49	0.44
1:A:200:GLY:O	1:A:205:LEU:HD13	2.18	0.44
1:A:99:ASN:H	1:A:99:ASN:HD22	1.66	0.44
1:D:154:ASP:OD1	1:D:154:ASP:N	2.48	0.44
1:A:132:HIS:CD2	1:B:111:LYS:HE3	2.52	0.44
1:B:140:ILE:N	5:B:695:HOH:O	2.49	0.44
1:C:150:PHE:HD1	5:C:726:HOH:O	2.00	0.44
1:C:215:MET:HG2	1:C:233:ASP:OD2	2.18	0.44
1:D:117:PHE:HB3	1:D:128:PHE:CD1	2.53	0.44
1:D:139:MET:C	5:D:632:HOH:O	2.55	0.44
1:B:226:HIS:HE1	1:D:102:PRO:O	2.01	0.44
1:B:118:LYS:CE	1:D:187:LYS:HD3	2.48	0.43
1:D:119:VAL:HG11	1:D:229:LEU:HD13	2.00	0.43
1:B:87:LYS:HB2	1:B:241:TYR:CZ	2.53	0.43
1:C:95:TYR:HA	1:C:138:ILE:O	2.18	0.43
1:B:118:LYS:HA	1:B:121:SER:OG	2.18	0.43
1:A:170:TYR:HA	1:A:173:ASP:OD1	2.19	0.43
1:C:144:ILE:HG23	5:C:632:HOH:O	2.18	0.43
1:C:163:ALA:HB3	1:C:201:HIS:HB2	1.99	0.43
1:C:237:ILE:HG23	1:C:238:GLN:N	2.33	0.43
1:D:116:ALA:CB	5:D:616:HOH:O	2.67	0.43
1:D:190:ASN:O	1:D:194:VAL:HG23	2.19	0.43
1:D:216:PHE:N	5:D:625:HOH:O	2.52	0.43
1:D:144:ILE:HG22	1:D:145:LYS:HD3	2.01	0.43
1:A:145:LYS:HB3	1:A:146:GLU:H	1.64	0.42
1:A:155:GLY:HA2	1:A:179:ASP:OD2	2.18	0.42
1:B:115:LYS:HG2	1:B:192:PHE:CE1	2.54	0.42
1:B:95:TYR:HA	1:B:138:ILE:O	2.19	0.42
1:B:91:MET:HE3	1:B:126:LEU:N	2.33	0.42
1:D:145:LYS:HB3	1:D:146:GLU:H	1.52	0.42
1:B:133:ASP:OD1	1:B:134:GLY:N	2.53	0.42
1:B:99:ASN:HD21	1:B:141:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:HG23	1:A:238:GLN:N	2.34	0.42
1:B:207:HIS:CE1	1:B:217:PRO:HB3	2.54	0.42
1:C:105:THR:HG23	1:C:108:GLU:OE2	2.19	0.42
1:A:233:ASP:O	1:A:237:ILE:HG22	2.19	0.42
1:D:144:ILE:O	1:D:145:LYS:C	2.57	0.41
1:A:145:LYS:O	1:A:152:PRO:HA	2.20	0.41
1:B:135:ILE:HA	1:B:139:MET:CE	2.51	0.41
1:C:142:PHE:HB3	1:C:178:ASP:OD1	2.20	0.41
1:C:214:LEU:HA	4:C:603:033:O13	2.19	0.41
1:B:81:VAL:HG11	1:B:240:LEU:HD21	2.02	0.41
1:A:211:PRO:HA	1:A:216:PHE:CD2	2.55	0.41
1:A:144:ILE:HG22	1:A:145:LYS:CD	2.50	0.41
1:B:234:VAL:HG13	5:B:623:HOH:O	2.20	0.41
1:C:112:ALA:HB3	1:C:191:LEU:HD23	2.03	0.41
1:A:144:ILE:CD1	1:D:96:ARG:NH2	2.84	0.41
1:C:238:GLN:O	1:C:242:GLY:N	2.50	0.41
1:A:99:ASN:N	1:A:99:ASN:HD22	2.17	0.41
1:B:140:ILE:HD11	1:B:199:PHE:CE2	2.56	0.41
1:C:144:ILE:HG23	1:C:179:ASP:OD2	2.20	0.40
1:C:116:ALA:CB	5:C:666:HOH:O	2.66	0.40
5:B:667:HOH:O	1:C:144:ILE:HG21	2.20	0.40
1:C:154:ASP:N	1:C:154:ASP:OD2	2.52	0.40
1:A:210:ASP:HA	1:A:211:PRO:HD2	1.96	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:654:HOH:O	5:D:716:HOH:O[2_657]	2.17	0.03

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%)	150 (95%)	8 (5%)	0	100	100
1	B	156/165 (94%)	151 (97%)	5 (3%)	0	100	100
1	C	147/165 (89%)	137 (93%)	10 (7%)	0	100	100
1	D	150/165 (91%)	142 (95%)	7 (5%)	1 (1%)	25	18
All	All	611/660 (93%)	580 (95%)	30 (5%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	215	MET

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	138/141 (98%)	131 (95%)	7 (5%)	28	22
1	B	136/141 (96%)	129 (95%)	7 (5%)	28	22
1	C	130/141 (92%)	124 (95%)	6 (5%)	31	27
1	D	133/141 (94%)	126 (95%)	7 (5%)	26	21
All	All	537/564 (95%)	510 (95%)	27 (5%)	28	23

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	86	LEU
1	A	99	ASN
1	A	111	LYS
1	A	160	LEU
1	A	178	ASP
1	A	214	LEU
1	B	119	VAL
1	B	135	ILE
1	B	139	MET

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Mol	Chain	Res	Type
1	B	160	LEU
1	B	178	ASP
1	B	220	THR
1	B	228	MET
1	C	87	LYS
1	C	99	ASN
1	C	133	ASP
1	C	151	TYR
1	C	160	LEU
1	C	184	SER
1	D	99	ASN
1	D	145	LYS
1	D	160	LEU
1	D	178	ASP
1	D	214	LEU
1	D	220	THR
1	D	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	92	ASN
1	A	99	ASN
1	A	226	HIS
1	A	235	GLN
1	B	190	ASN
1	B	226	HIS
1	B	238	GLN
1	C	99	ASN
1	C	127	ASN
1	C	238	GLN
1	D	92	ASN
1	D	99	ASN
1	D	162	HIS
1	D	207	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 20 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	033	A	601	2	30,38,38	2.74	18 (60%)	41,55,55	1.10	3 (7%)
4	033	B	602	2	30,38,38	2.79	17 (56%)	41,55,55	1.02	3 (7%)
4	033	C	603	2	30,38,38	2.83	17 (56%)	41,55,55	0.94	2 (4%)
4	033	D	604	2	30,38,38	2.72	16 (53%)	41,55,55	0.90	2 (4%)

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	033	A	601	2	-	0/24/31/31	0/3/4/4
4	033	B	602	2	-	0/24/31/31	0/3/4/4
4	033	C	603	2	-	0/24/31/31	0/3/4/4
4	033	D	604	2	-	0/24/31/31	0/3/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	033	C12-C14	-5.41	1.40	1.49
4	A	601	033	C12-C14	-5.23	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	033	C12-C14	-5.14	1.41	1.49
4	B	602	033	C12-C14	-4.78	1.41	1.49
4	A	601	033	C21-C20	2.22	1.44	1.39
4	A	601	033	C19-C18	2.31	1.42	1.38
4	A	601	033	C18-C16	2.39	1.43	1.39
4	A	601	033	C22-C21	2.41	1.43	1.38
4	A	601	033	C32-C27	2.46	1.44	1.39
4	B	602	033	C6-C1	2.47	1.44	1.38
4	A	601	033	C32-C31	2.49	1.43	1.38
4	A	601	033	C6-C1	2.51	1.44	1.38
4	C	603	033	C22-C21	2.55	1.43	1.38
4	A	601	033	C19-C20	2.55	1.44	1.39
4	D	604	033	C28-C27	2.56	1.44	1.39
4	C	603	033	C32-C27	2.58	1.44	1.39
4	D	604	033	C6-C1	2.58	1.44	1.38
4	B	602	033	C22-C21	2.59	1.43	1.38
4	D	604	033	C29-C28	2.59	1.43	1.38
4	C	603	033	C29-C28	2.60	1.43	1.38
4	D	604	033	C32-C31	2.62	1.43	1.38
4	C	603	033	C6-C1	2.62	1.44	1.38
4	C	603	033	C19-C20	2.65	1.45	1.39
4	B	602	033	C18-C16	2.66	1.43	1.39
4	A	601	033	C30-S37	2.70	1.80	1.76
4	D	604	033	C19-C20	2.71	1.45	1.39
4	B	602	033	C21-C20	2.72	1.45	1.39
4	A	601	033	C28-C27	2.74	1.45	1.39
4	D	604	033	C21-C20	2.75	1.45	1.39
4	B	602	033	C32-C31	2.77	1.43	1.38
4	D	604	033	C32-C27	2.79	1.45	1.39
4	B	602	033	C32-C27	2.79	1.45	1.39
4	B	602	033	C19-C20	2.84	1.45	1.39
4	C	603	033	C21-C20	2.85	1.45	1.39
4	C	603	033	C28-C27	2.89	1.45	1.39
4	C	603	033	C18-C16	2.90	1.44	1.39
4	B	602	033	C29-C28	2.93	1.44	1.38
4	A	601	033	C29-C28	2.96	1.44	1.38
4	D	604	033	C18-C16	2.96	1.44	1.39
4	C	603	033	C29-C30	2.97	1.43	1.38
4	B	602	033	C19-C18	2.99	1.44	1.38
4	C	603	033	C19-C18	3.03	1.44	1.38
4	C	603	033	C31-C30	3.05	1.43	1.38
4	C	603	033	C32-C31	3.09	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	033	C6-C5	3.10	1.44	1.36
4	D	604	033	C31-C30	3.14	1.43	1.38
4	A	601	033	C31-C30	3.17	1.43	1.38
4	C	603	033	C1-C2	3.17	1.44	1.36
4	B	602	033	C28-C27	3.20	1.46	1.39
4	D	604	033	C1-C2	3.20	1.44	1.36
4	A	601	033	C1-C2	3.24	1.44	1.36
4	A	601	033	C29-C30	3.26	1.44	1.38
4	B	602	033	C6-C5	3.27	1.44	1.36
4	D	604	033	C6-C5	3.28	1.44	1.36
4	A	601	033	C22-C16	3.28	1.44	1.39
4	D	604	033	C19-C18	3.30	1.44	1.38
4	D	604	033	C29-C30	3.32	1.44	1.38
4	D	604	033	C22-C16	3.39	1.44	1.39
4	C	603	033	C6-C5	3.39	1.44	1.36
4	B	602	033	C1-C2	3.44	1.44	1.36
4	B	602	033	C29-C30	3.49	1.44	1.38
4	B	602	033	C31-C30	3.76	1.44	1.38
4	C	603	033	C22-C16	3.79	1.45	1.39
4	B	602	033	C22-C16	3.91	1.45	1.39
4	B	602	033	S37-N38	7.38	1.73	1.61
4	D	604	033	S37-N38	7.85	1.74	1.61
4	A	601	033	S37-N38	8.23	1.74	1.61
4	C	603	033	S37-N38	8.40	1.75	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	033	O39-S37-N38	-2.35	102.58	106.88
4	A	601	033	O40-S37-O39	-2.16	116.79	119.55
4	B	602	033	O39-S37-C30	2.18	110.65	107.95
4	D	604	033	C11-C3-C4	2.49	108.44	106.27
4	D	604	033	O40-S37-C30	2.52	111.07	107.95
4	C	603	033	C11-C3-C4	2.60	108.54	106.27
4	C	603	033	O40-S37-C30	2.65	111.24	107.95
4	A	601	033	C11-C3-C4	2.72	108.65	106.27
4	B	602	033	C11-C3-C4	2.93	108.83	106.27
4	A	601	033	O40-S37-C30	3.00	111.67	107.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	033	2	0
4	B	602	033	3	0
4	C	603	033	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

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.