Full wwPDB X-ray Structure Validation Report (i)

Dec 28, 2016 – 02:57 AM EST

PDB ID	:	5IE6
Title	:	Crystal structure of a lactonase mutant in complex with substrate b
Authors	:	Zheng, Y.Y.; Xu, Z.X.; Liu, W.D.; Chen, C.C.; Guo, R.T.
Deposited on	:	2016-02-25
Resolution	:	2.67 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

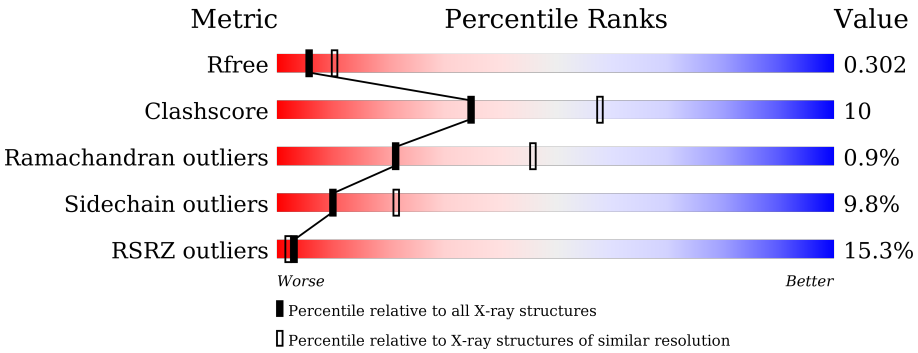
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	91344	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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 <=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	264	4% 77% 19% ·
1	B	264	5% 82% 16% ·
1	C	264	29% 30% 14% · 52%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5302 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.

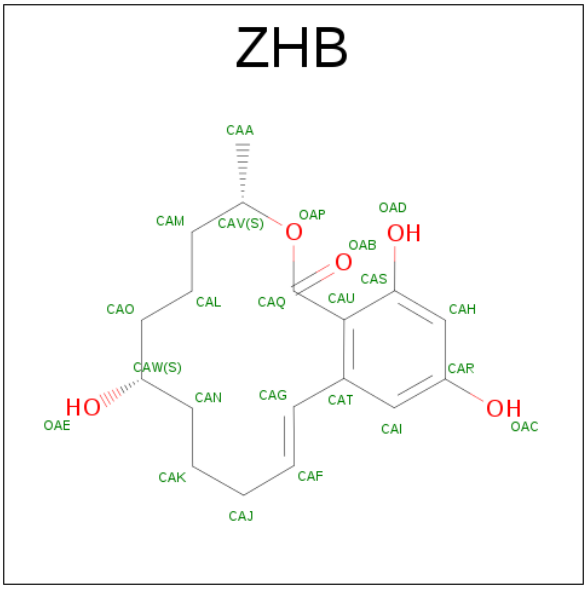
- Molecule 1 is a protein called Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2020	1282	341	386	11			
1	B	264	Total	C	N	O	S	0	0	0
			2020	1282	341	386	11			
1	C	127	Total	C	N	O	S	0	0	0
			988	639	159	185	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	SER	engineered mutation	UNP Q8NKB0
B	102	ALA	SER	engineered mutation	UNP Q8NKB0
C	102	ALA	SER	engineered mutation	UNP Q8NKB0

- Molecule 2 is (3S,7S,11E)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecin-1-one (three-letter code: ZHB) (formula: $C_{18}H_{24}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 18 5	0	0
2	B	1	Total C O 23 18 5	0	0

- Molecule 3 is water.

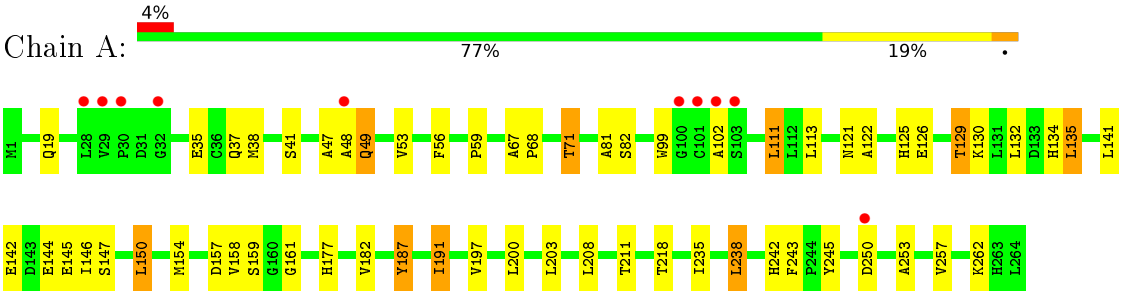
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total O 75 75	0	0
3	B	63	Total O 63 63	0	0
3	C	90	Total O 90 90	0	0

3 Residue-property plots (i)

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.

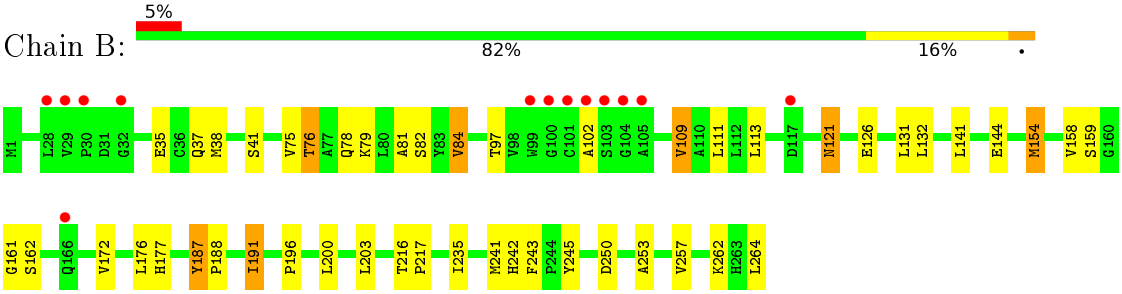
- Molecule 1: Zearalenone hydrolase

Chain A:



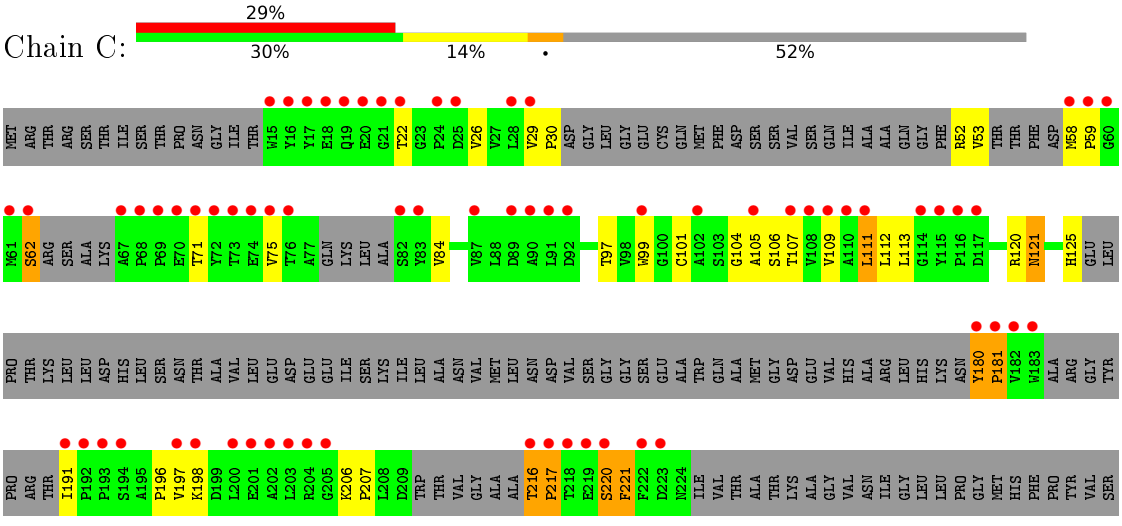
- Molecule 1: Zearalenone hydrolase

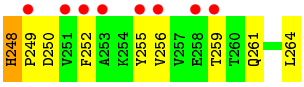
Chain B:



- Molecule 1: Zearalenone hydrolase

Chain C:




H248
P249
D250
V251
F252
A253
K254
Y255
V256
V257
E258
T259
T260
Q261
L264

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	86.04Å 86.04Å 470.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.94 – 2.67 24.94 – 2.67	Depositor EDS
% Data completeness (in resolution range)	98.2 (24.94-2.67) 98.4 (24.94-2.67)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.27 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.221 , 0.279 0.251 , 0.302	Depositor DCC
R_{free} test set	1513 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5302	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZHB

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	0.53	0/2071	0.76	1/2829 (0.0%)
1	B	0.52	0/2071	0.72	0/2829
1	C	0.53	1/1012 (0.1%)	0.61	0/1379
All	All	0.53	1/5154 (0.0%)	0.72	1/7037 (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	C	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	SER	C-O	5.63	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	GLN	N-CA-C	-6.15	94.40	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	216	THR	Peptide
1	C	217	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	221	PHE	Peptide

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	2020	0	1991	32	0
1	B	2020	0	1991	37	0
1	C	988	0	956	28	0
2	A	23	0	0	2	0
2	B	23	0	0	3	0
3	A	75	0	0	1	0
3	B	63	0	0	0	0
3	C	90	0	0	0	0
All	All	5302	0	4938	99	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 10.

All (99) 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:B:158:VAL:HG11	1:B:242:HIS:CD2	1.95	1.00
1:B:158:VAL:CG1	1:B:242:HIS:CD2	2.53	0.91
1:B:76:THR:HG22	1:B:79:LYS:H	1.36	0.90
1:B:154:MET:HE3	1:B:154:MET:HA	1.60	0.84
1:B:38:MET:HE2	1:B:245:TYR:HE1	1.43	0.82
1:B:154:MET:CE	1:B:154:MET:HA	2.10	0.81
1:A:38:MET:HE2	1:A:245:TYR:HE1	1.44	0.80
1:C:216:THR:HB	1:C:217:PRO:CD	2.11	0.80
1:B:38:MET:CE	1:B:245:TYR:HE1	1.99	0.74
1:C:255:TYR:O	1:C:259:THR:OG1	2.03	0.73
1:A:134:HIS:CE1	1:A:135:LEU:HD13	2.24	0.73
1:A:67:ALA:HB1	1:A:71:THR:HG21	1.71	0.71
1:C:248:HIS:N	1:C:249:PRO:HD3	2.06	0.70
1:B:109:VAL:HG22	1:B:196:PRO:HG2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:O	1:A:71:THR:HB	1.93	0.68
1:B:76:THR:CG2	1:B:79:LYS:H	2.06	0.68
1:A:38:MET:CE	1:A:245:TYR:HE1	2.07	0.68
1:A:59:PRO:HB2	1:A:71:THR:HG23	1.78	0.66
1:B:81:ALA:HB1	1:B:111:LEU:HD23	1.77	0.66
1:C:216:THR:HB	1:C:217:PRO:HD3	1.79	0.63
1:B:109:VAL:CG2	1:B:196:PRO:HG2	2.29	0.63
1:A:81:ALA:HB1	1:A:111:LEU:HD13	1.83	0.61
1:A:59:PRO:CB	1:A:71:THR:HG23	2.31	0.61
1:C:101:CYS:O	1:C:105:ALA:HB2	2.02	0.60
1:C:99:TRP:CE2	1:C:252:PHE:HE1	2.20	0.60
1:A:102:ALA:HB1	2:A:300:ZHB:CAQ	2.32	0.60
1:B:158:VAL:HG11	1:B:242:HIS:NE2	2.17	0.59
1:C:84:VAL:HG11	1:C:111:LEU:HD21	1.85	0.59
1:B:84:VAL:CG2	1:B:111:LEU:HD11	2.32	0.58
1:C:101:CYS:HA	1:C:125:HIS:HB2	1.87	0.57
1:B:38:MET:CE	1:B:245:TYR:CE1	2.85	0.56
1:B:158:VAL:O	1:B:158:VAL:HG12	2.05	0.56
1:B:84:VAL:HG21	1:B:111:LEU:HD11	1.89	0.55
1:A:129:THR:HG22	1:A:130:LYS:HG3	1.87	0.55
1:A:38:MET:CE	1:A:245:TYR:CE1	2.89	0.55
1:A:38:MET:HE1	1:A:243:PHE:CD1	2.42	0.55
1:B:38:MET:HE1	1:B:243:PHE:CD1	2.42	0.55
1:C:180:TYR:HB3	1:C:181:PRO:HD3	1.89	0.55
1:B:158:VAL:HG13	1:B:241:MET:HE2	1.89	0.54
1:B:144:GLU:OE2	1:B:177:HIS:CE1	2.61	0.54
1:A:81:ALA:CB	1:A:111:LEU:HD13	2.38	0.54
1:A:47:ALA:O	1:A:49:GLN:O	2.26	0.53
1:B:187:TYR:CD2	1:B:191:ILE:HD13	2.43	0.53
1:C:220:SER:HB2	1:C:221:PHE:CD2	2.44	0.53
1:B:35:GLU:OE2	1:B:37:GLN:HB3	2.09	0.52
1:C:261:GLN:HA	1:C:264:LEU:HG	1.92	0.51
1:A:144:GLU:OE2	1:A:177:HIS:CE1	2.65	0.50
1:C:101:CYS:HA	1:C:125:HIS:CB	2.42	0.50
1:C:59:PRO:HB2	1:C:71:THR:HG22	1.94	0.50
1:A:38:MET:HE1	1:A:243:PHE:HD1	1.77	0.49
1:B:76:THR:HG23	1:B:78:GLN:H	1.76	0.49
1:B:126:GLU:OE1	1:B:242:HIS:ND1	2.46	0.48
2:B:301:ZHB:OAP	2:B:301:ZHB:CAG	2.61	0.48
1:A:187:TYR:CD2	1:A:191:ILE:HD13	2.48	0.48
1:B:158:VAL:CG1	1:B:242:HIS:NE2	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:OE2	1:A:37:GLN:HB3	2.13	0.48
1:B:38:MET:HE1	1:B:243:PHE:HD1	1.78	0.48
1:C:29:VAL:HG23	1:C:99:TRP:O	2.14	0.47
1:A:81:ALA:HB1	1:A:111:LEU:CD1	2.45	0.47
1:A:129:THR:CG2	3:A:451:HOH:O	2.62	0.47
1:C:252:PHE:O	1:C:256:VAL:HG23	2.15	0.46
1:B:75:VAL:HG12	1:B:76:THR:N	2.31	0.45
1:B:216:THR:O	1:B:217:PRO:C	2.55	0.45
1:C:121:ASN:HA	1:C:207:PRO:HB2	1.97	0.45
1:B:154:MET:O	1:B:159:SER:HB3	2.16	0.45
1:A:48:ALA:C	1:A:49:GLN:O	2.48	0.44
1:A:99:TRP:CH2	1:A:125:HIS:HB2	2.53	0.44
1:C:30:PRO:HG2	1:C:58:MET:HG2	2.00	0.44
1:C:26:VAL:N	1:C:52:ARG:O	2.50	0.44
1:C:97:THR:HG1	1:C:120:ARG:HB3	1.83	0.44
2:A:300:ZHB:OAD	2:A:300:ZHB:OAB	2.34	0.44
1:C:58:MET:SD	1:C:59:PRO:HD3	2.57	0.44
1:B:102:ALA:HB1	2:B:301:ZHB:CAQ	2.48	0.43
1:A:253:ALA:O	1:A:257:VAL:HG13	2.19	0.43
1:C:112:LEU:HD21	1:C:206:LYS:HB3	2.01	0.43
1:A:126:GLU:OE1	1:A:242:HIS:ND1	2.52	0.43
2:B:301:ZHB:CAA	2:B:301:ZHB:OAB	2.67	0.43
1:A:122:ALA:O	1:A:208:LEU:HD12	2.20	0.42
1:A:146:ILE:CG2	1:A:150:LEU:HD22	2.49	0.42
1:A:147:SER:HB3	1:A:177:HIS:CD2	2.54	0.42
1:C:197:VAL:O	1:C:197:VAL:HG12	2.19	0.42
1:A:157:ASP:HB2	1:A:158:VAL:HG13	2.02	0.42
1:C:109:VAL:CG1	1:C:196:PRO:HG2	2.49	0.41
1:A:154:MET:O	1:A:159:SER:HB3	2.20	0.41
1:A:218:THR:OG1	1:B:216:THR:O	2.25	0.41
1:B:187:TYR:HB2	1:B:188:PRO:HD3	2.02	0.41
1:C:75:VAL:O	1:C:191:ILE:HG13	2.20	0.41
1:A:19:GLN:HA	1:A:53:VAL:O	2.21	0.41
1:B:76:THR:HG22	1:B:79:LYS:HB2	2.01	0.41
1:B:158:VAL:O	1:B:158:VAL:CG1	2.68	0.41
1:B:253:ALA:O	1:B:257:VAL:HG13	2.21	0.41
1:B:154:MET:CE	1:B:243:PHE:HE2	2.33	0.41
1:C:248:HIS:N	1:C:249:PRO:CD	2.79	0.41
1:B:35:GLU:OE2	1:B:37:GLN:CB	2.70	0.40
1:C:109:VAL:HG12	1:C:196:PRO:HG2	2.03	0.40
1:B:97:THR:OG1	1:B:121:ASN:ND2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLY:O	1:C:107:THR:HB	2.21	0.40
1:C:53:VAL:O	1:C:53:VAL:HG12	2.22	0.40
1:A:211:THR:HG21	1:A:238:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	262/264 (99%)	249 (95%)	11 (4%)	2 (1%)	24	49
1	B	262/264 (99%)	248 (95%)	12 (5%)	2 (1%)	24	49
1	C	109/264 (41%)	95 (87%)	12 (11%)	2 (2%)	11	25
All	All	633/792 (80%)	592 (94%)	35 (6%)	6 (1%)	21	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	106	SER
1	C	181	PRO
1	A	161	GLY
1	A	187	TYR
1	B	187	TYR
1	B	161	GLY

5.3.2 Protein sidechains (i)

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	220/220 (100%)	197 (90%)	23 (10%)	8 18
1	B	220/220 (100%)	199 (90%)	21 (10%)	11 23
1	C	109/220 (50%)	99 (91%)	10 (9%)	11 24
All	All	549/660 (83%)	495 (90%)	54 (10%)	10 21

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

Mol	Chain	Res	Type
1	A	41	SER
1	A	56	PHE
1	A	71	THR
1	A	82	SER
1	A	111	LEU
1	A	113	LEU
1	A	121	ASN
1	A	129	THR
1	A	132	LEU
1	A	135	LEU
1	A	141	LEU
1	A	142	GLU
1	A	145	GLU
1	A	150	LEU
1	A	182	VAL
1	A	191	ILE
1	A	197	VAL
1	A	200	LEU
1	A	203	LEU
1	A	235	ILE
1	A	238	LEU
1	A	250	ASP
1	A	262	LYS
1	B	41	SER
1	B	76	THR
1	B	82	SER
1	B	84	VAL
1	B	109	VAL
1	B	113	LEU
1	B	121	ASN
1	B	131	LEU
1	B	132	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	141	LEU
1	B	154	MET
1	B	162	SER
1	B	172	VAL
1	B	176	LEU
1	B	191	ILE
1	B	200	LEU
1	B	203	LEU
1	B	235	ILE
1	B	250	ASP
1	B	262	LYS
1	B	264	LEU
1	C	22	THR
1	C	62	SER
1	C	111	LEU
1	C	113	LEU
1	C	121	ASN
1	C	180	TYR
1	C	198	LYS
1	C	220	SER
1	C	248	HIS
1	C	250	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	134	HIS
1	A	152	ASN
1	A	156	ASN
1	A	166	GLN
1	A	177	HIS
1	B	121	ASN
1	B	137	ASN
1	B	166	GLN
1	B	177	HIS
1	B	261	GLN
1	C	121	ASN
1	C	224	ASN
1	C	248	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	$\#\|Z\| > 2$
2	ZHB	A	300	-	24,24,24	1.59	4 (16%)	32,32,32	1.56	8 (25%)
2	ZHB	B	301	-	24,24,24	1.37	3 (12%)	32,32,32	1.22	4 (12%)

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
2	ZHB	A	300	-	-	0/22/22/22	0/1/2/2
2	ZHB	B	301	-	-	1/22/22/22	0/1/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZHB	CAT-CAG	-4.96	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZHB	CAU-CAQ	-4.40	1.39	1.50
2	B	301	ZHB	CAT-CAG	-4.25	1.41	1.47
2	B	301	ZHB	CAU-CAQ	-3.65	1.41	1.50
2	A	300	ZHB	CAJ-CAF	-2.09	1.38	1.50
2	A	300	ZHB	CAG-CAF	2.46	1.39	1.31
2	B	301	ZHB	CAG-CAF	2.52	1.40	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	300	ZHB	CAT-CAG-CAF	-4.08	115.92	125.35
2	A	300	ZHB	CAN-CAK-CAJ	-3.44	109.06	114.61
2	A	300	ZHB	CAA-CAV-CAM	-3.07	105.91	113.98
2	A	300	ZHB	CAK-CAN-CAW	-3.02	104.44	114.95
2	B	301	ZHB	CAJ-CAF-CAG	-2.40	120.52	125.20
2	A	300	ZHB	CAL-CAO-CAW	-2.40	106.60	114.95
2	A	300	ZHB	OAD-CAS-CAU	-2.18	117.00	121.18
2	B	301	ZHB	CAN-CAK-CAJ	-2.14	111.16	114.61
2	A	300	ZHB	CAI-CAT-CAG	-2.06	116.10	120.80
2	A	300	ZHB	OAP-CAV-CAA	2.00	112.40	107.89
2	B	301	ZHB	OAP-CAV-CAA	2.81	114.21	107.89
2	B	301	ZHB	CAV-OAP-CAQ	3.06	123.70	117.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	ZHB	CAQ-OAP-CAV-CAA

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ZHB	2	0
2	B	301	ZHB	3	0

5.7 Other polymers (i)

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, 95^{th} 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	264/264 (100%)	-0.06	10 (3%) 44 43	24, 32, 55, 67	0
1	B	264/264 (100%)	0.04	13 (4%) 33 31	25, 36, 56, 74	0
1	C	127/264 (48%)	2.63	77 (60%) 0 0	50, 74, 91, 100	0
All	All	655/792 (82%)	0.50	100 (15%) 3 2	24, 37, 82, 100	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	ALA	7.2
1	C	219	GLU	7.2
1	C	24	PRO	7.0
1	C	220	SER	6.9
1	C	60	GLY	6.8
1	C	72	TYR	6.7
1	C	90	ALA	6.1
1	C	182	VAL	6.0
1	C	251	VAL	5.9
1	C	18	GLU	5.9
1	C	193	PRO	5.8
1	C	181	PRO	5.6
1	C	16	TYR	5.2
1	C	115	TYR	5.2
1	C	67	ALA	4.9
1	C	191	ILE	4.9
1	C	73	THR	4.8
1	C	253	ALA	4.6
1	C	252	PHE	4.5
1	C	192	PRO	4.5
1	C	218	THR	4.5
1	C	89	ASP	4.3
1	C	76	THR	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	200	LEU	4.2
1	C	183	TRP	4.1
1	B	29	VAL	4.1
1	C	217	PRO	3.9
1	C	74	GLU	3.9
1	C	180	TYR	3.8
1	C	69	PRO	3.8
1	C	222	PHE	3.8
1	A	29	VAL	3.7
1	C	75	VAL	3.7
1	C	87	VAL	3.7
1	C	70	GLU	3.7
1	C	19	GLN	3.7
1	C	17	TYR	3.5
1	C	110	ALA	3.5
1	C	61	MET	3.5
1	C	105	ALA	3.4
1	B	166	GLN	3.4
1	C	259	THR	3.4
1	C	108	VAL	3.4
1	A	48	ALA	3.3
1	C	249	PRO	3.3
1	C	71	THR	3.3
1	C	20	GLU	3.3
1	A	32	GLY	3.3
1	C	68	PRO	3.2
1	C	109	VAL	3.2
1	C	15	TRP	3.2
1	A	30	PRO	3.2
1	C	203	LEU	3.2
1	B	101	CYS	3.1
1	C	62	SER	3.1
1	C	83	TYR	3.0
1	C	223	ASP	3.0
1	C	92	ASP	3.0
1	C	256	VAL	2.9
1	A	102	ALA	2.9
1	C	21	GLY	2.9
1	C	29	VAL	2.9
1	C	58	MET	2.9
1	C	114	GLY	2.8
1	B	103	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	28	LEU	2.8
1	C	194	SER	2.8
1	C	117	ASP	2.8
1	C	204	ARG	2.7
1	B	100	GLY	2.7
1	C	205	GLY	2.7
1	C	22	THR	2.7
1	B	104	GLY	2.6
1	C	258	GLU	2.6
1	C	197	VAL	2.6
1	B	102	ALA	2.5
1	C	201	GLU	2.5
1	C	99	TRP	2.5
1	A	103	SER	2.5
1	A	101	CYS	2.4
1	C	116	PRO	2.4
1	A	28	LEU	2.4
1	C	91	LEU	2.4
1	B	32	GLY	2.4
1	C	111	LEU	2.4
1	C	82	SER	2.4
1	C	102	ALA	2.4
1	B	99	TRP	2.3
1	C	25	ASP	2.3
1	A	250	ASP	2.3
1	C	198	LYS	2.3
1	B	117	ASP	2.2
1	B	30	PRO	2.2
1	B	105	ALA	2.2
1	B	28	LEU	2.2
1	C	255	TYR	2.1
1	A	100	GLY	2.1
1	C	59	PRO	2.1
1	C	107	THR	2.0
1	C	216	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZHB	A	300	23/23	0.94	0.36	1.67	50,61,68,72	0
2	ZHB	B	301	23/23	0.95	0.28	0.83	39,50,76,78	0

6.5 Other polymers (i)

There are no such residues in this entry.