Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:58 PM GMT

PDB ID	:	3VMA
Title	:	Crystal Structure of the Full-Length Transglycosylase PBP1b from Escherichia coli
Authors	:	Huang, C.Y.; Sung, M.T.; Lai, Y.T.; Chou, L.Y.; Shih, H.W.; Cheng, W.C.; Wong, C.H.; Ma, C.
Deposited on	:	2011-12-09
Resolution	:	2.16 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:

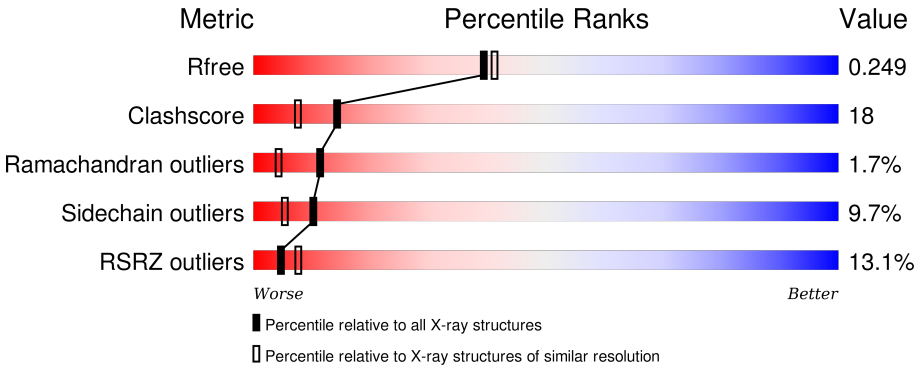
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	768	12% 63% 24% 5% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5855 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.

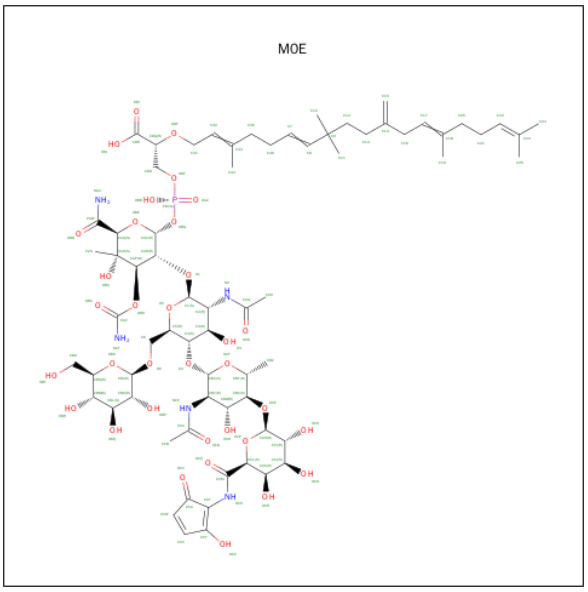
- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	708	5561	3524	981	1030	26	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	EXPRESSION TAG	UNP P02919
A	38	GLY	-	EXPRESSION TAG	UNP P02919
A	39	SER	-	EXPRESSION TAG	UNP P02919
A	40	SER	-	EXPRESSION TAG	UNP P02919
A	41	HIS	-	EXPRESSION TAG	UNP P02919
A	42	HIS	-	EXPRESSION TAG	UNP P02919
A	43	HIS	-	EXPRESSION TAG	UNP P02919
A	44	HIS	-	EXPRESSION TAG	UNP P02919
A	45	HIS	-	EXPRESSION TAG	UNP P02919
A	46	HIS	-	EXPRESSION TAG	UNP P02919
A	47	SER	-	EXPRESSION TAG	UNP P02919
A	48	SER	-	EXPRESSION TAG	UNP P02919
A	49	GLY	-	EXPRESSION TAG	UNP P02919
A	50	LEU	-	EXPRESSION TAG	UNP P02919
A	51	VAL	-	EXPRESSION TAG	UNP P02919
A	52	PRO	-	EXPRESSION TAG	UNP P02919
A	53	ARG	-	EXPRESSION TAG	UNP P02919
A	54	GLY	-	EXPRESSION TAG	UNP P02919
A	55	SER	-	EXPRESSION TAG	UNP P02919
A	56	HIS	-	EXPRESSION TAG	UNP P02919
A	57	MET	-	EXPRESSION TAG	UNP P02919

- Molecule 2 is MOENOMYCIN (three-letter code: M0E) (formula: $C_{69}H_{106}N_5O_{34}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			77	39	5	32	1		

- Molecule 3 is water.

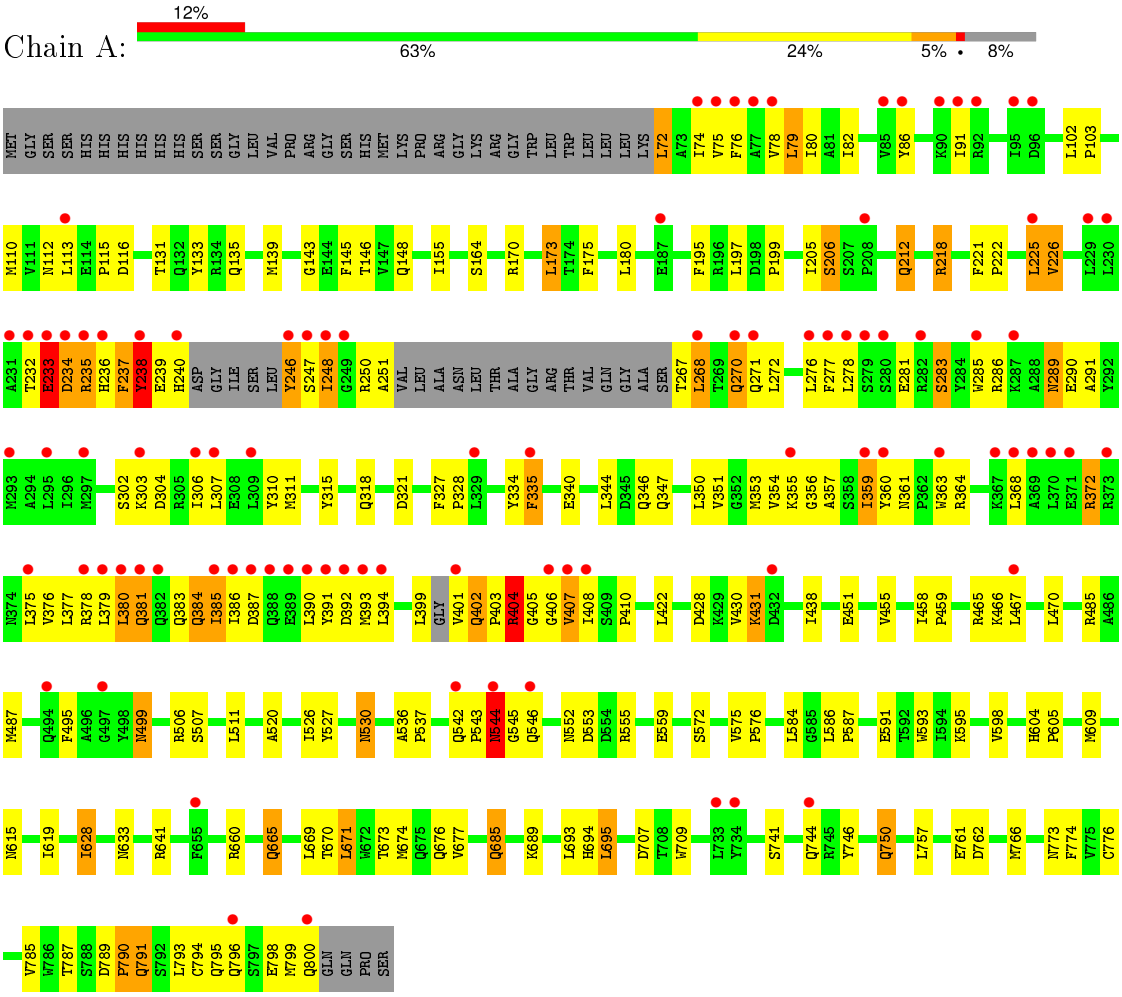
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	217	Total	O	0	0
			217	217		

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: Penicillin-binding protein 1B

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	62.90Å 289.53Å 62.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.84 – 2.16 28.84 – 2.16	Depositor EDS
% Data completeness (in resolution range)	97.0 (28.84-2.16) 97.0 (28.84-2.16)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.212 , 0.250 0.213 , 0.249	Depositor DCC
R_{free} test set	3072 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.063 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 60720 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5855	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: M0E

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	0.30	0/5672	0.49	0/7694

There are no bond length outliers.

There are no bond angle outliers.

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	5561	0	5598	202	0
2	A	77	0	60	7	0
3	A	217	0	0	4	0
All	All	5855	0	5658	204	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 18.

All (204) 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:A:278:LEU:HD11	1:A:290:GLU:HB3	1.41	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLN:HE21	1:A:791:GLN:N	1.61	0.96
1:A:380:LEU:HD13	1:A:386:ILE:HG13	1.49	0.95
1:A:787:THR:HG22	1:A:789:ASP:H	1.39	0.88
1:A:110:MET:HG2	1:A:199:PRO:HG3	1.53	0.88
1:A:671:LEU:HD13	1:A:674:MET:HE3	1.56	0.88
1:A:674:MET:HA	1:A:677:VAL:HG13	1.59	0.83
1:A:665:GLN:H	1:A:665:GLN:HE21	1.25	0.82
1:A:235:ARG:HD2	1:A:235:ARG:H	1.47	0.79
1:A:791:GLN:HE21	1:A:791:GLN:CA	1.97	0.77
1:A:110:MET:CG	1:A:199:PRO:HG3	2.14	0.76
1:A:303:LYS:HG3	1:A:304:ASP:H	1.51	0.75
1:A:665:GLN:H	1:A:665:GLN:NE2	1.84	0.75
1:A:307:LEU:O	1:A:311:MET:HG3	1.87	0.74
1:A:789:ASP:O	1:A:791:GLN:N	2.20	0.73
1:A:386:ILE:HG23	1:A:390:LEU:HD11	1.71	0.73
1:A:671:LEU:CD1	1:A:674:MET:HE3	2.21	0.70
1:A:674:MET:SD	3:A:1172:HOH:O	2.49	0.70
1:A:270:GLN:HE22	1:A:291:ALA:HA	1.56	0.70
1:A:355:LYS:HG2	2:A:901:M0E:HAS1	1.73	0.70
1:A:401:VAL:HG12	1:A:402:GLN:H	1.58	0.69
1:A:790:PRO:O	1:A:793:LEU:HG	1.92	0.69
1:A:359:ILE:HD12	2:A:901:M0E:HCB1	1.73	0.69
1:A:384:GLN:HE21	1:A:384:GLN:H	1.41	0.69
1:A:375:LEU:O	1:A:378:ARG:HG3	1.93	0.69
1:A:380:LEU:HD13	1:A:386:ILE:CG1	2.23	0.67
1:A:670:THR:HG22	1:A:674:MET:HE1	1.75	0.67
1:A:384:GLN:NE2	1:A:384:GLN:H	1.93	0.66
1:A:741:SER:O	1:A:744:GLN:HG2	1.96	0.66
1:A:670:THR:HG22	1:A:674:MET:CE	2.26	0.65
1:A:506:ARG:HD2	1:A:707:ASP:OD1	1.94	0.65
1:A:766:MET:HE3	1:A:793:LEU:HD23	1.77	0.65
1:A:359:ILE:H	1:A:359:ILE:HD13	1.62	0.64
1:A:238:TYR:O	1:A:240:HIS:N	2.30	0.64
1:A:381:GLN:HA	1:A:386:ILE:HB	1.78	0.64
1:A:385:ILE:H	1:A:385:ILE:HD13	1.63	0.64
1:A:72:LEU:HD23	1:A:74:ILE:HB	1.79	0.64
1:A:222:PRO:HD2	1:A:225:LEU:HD22	1.80	0.63
1:A:791:GLN:HG3	1:A:794:CYS:SG	2.39	0.63
1:A:234:ASP:OD1	1:A:268:LEU:HB2	1.99	0.63
1:A:363:TRP:HH2	1:A:403:PRO:HB2	1.64	0.62
1:A:628:ILE:HD11	1:A:671:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:PRO:C	1:A:791:GLN:HE21	2.02	0.62
1:A:173:LEU:N	1:A:173:LEU:HD12	2.15	0.61
1:A:593:TRP:O	1:A:598:VAL:HG22	2.00	0.60
1:A:387:ASP:HB2	1:A:390:LEU:HG	1.83	0.60
1:A:344:LEU:HD21	1:A:386:ILE:HD11	1.84	0.60
1:A:407:VAL:HG13	1:A:410:PRO:HG3	1.84	0.60
1:A:363:TRP:HZ3	1:A:404:ARG:HA	1.67	0.59
1:A:221:PHE:HB3	1:A:225:LEU:HD21	1.84	0.59
1:A:694:HIS:HD2	3:A:1146:HOH:O	1.86	0.59
1:A:377:LEU:HA	1:A:380:LEU:HD11	1.84	0.59
1:A:670:THR:O	1:A:674:MET:HE2	2.03	0.58
1:A:222:PRO:HG3	1:A:340:GLU:HA	1.84	0.58
1:A:785:VAL:HG12	1:A:787:THR:OG1	2.03	0.58
1:A:75:VAL:O	1:A:79:LEU:HD13	2.02	0.58
1:A:303:LYS:HG3	1:A:304:ASP:N	2.18	0.58
1:A:206:SER:HA	1:A:212:GLN:HE22	1.68	0.58
1:A:526:ILE:HG13	1:A:527:TYR:CD2	2.39	0.58
1:A:402:GLN:O	1:A:404:ARG:HG3	2.02	0.58
1:A:139:MET:HG3	1:A:146:THR:HG23	1.86	0.57
1:A:795:GLN:O	1:A:798:GLU:HG2	2.03	0.57
1:A:356:GLY:O	1:A:360:TYR:HD2	1.88	0.57
1:A:79:LEU:HA	1:A:82:ILE:HG12	1.86	0.57
1:A:693:LEU:HB3	1:A:695:LEU:HD13	1.86	0.56
1:A:799:MET:HG3	1:A:800:GLN:H	1.70	0.56
1:A:789:ASP:C	1:A:791:GLN:H	2.08	0.56
1:A:304:ASP:HA	1:A:307:LEU:HD21	1.87	0.56
1:A:175:PHE:HB3	3:A:1161:HOH:O	2.05	0.56
1:A:363:TRP:HZ3	1:A:404:ARG:CA	2.19	0.55
1:A:422:LEU:HD11	1:A:438:ILE:HD13	1.88	0.55
1:A:530:ASN:HD22	1:A:530:ASN:H	1.54	0.55
1:A:791:GLN:NE2	1:A:791:GLN:CA	2.69	0.55
1:A:685:GLN:HE21	1:A:689:LYS:NZ	2.04	0.55
1:A:276:LEU:HD22	1:A:277:PHE:CZ	2.42	0.54
1:A:351:VAL:O	1:A:354:VAL:HG12	2.06	0.54
1:A:401:VAL:HG12	1:A:402:GLN:N	2.22	0.53
1:A:75:VAL:O	1:A:78:VAL:HB	2.09	0.53
1:A:350:LEU:HA	1:A:353:MET:HE2	1.91	0.53
1:A:283:SER:HB3	1:A:286:ARG:H	1.74	0.53
1:A:542:GLN:HB2	1:A:543:PRO:HD2	1.90	0.53
1:A:267:THR:O	1:A:271:GLN:HG3	2.09	0.52
1:A:799:MET:HG3	1:A:800:GLN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:MET:CE	1:A:793:LEU:HD23	2.38	0.52
1:A:402:GLN:NE2	1:A:403:PRO:HD2	2.25	0.52
1:A:356:GLY:HA3	1:A:359:ILE:HD11	1.91	0.52
1:A:361:ASN:HD21	1:A:363:TRP:HD1	1.58	0.52
1:A:278:LEU:CD1	1:A:290:GLU:HB3	2.28	0.52
1:A:334:TYR:O	1:A:335:PHE:CG	2.63	0.52
1:A:741:SER:HA	1:A:744:GLN:CD	2.30	0.51
2:A:901:M0E:ODI	2:A:901:M0E:HAQ	2.11	0.51
1:A:307:LEU:HA	1:A:310:TYR:HB3	1.91	0.51
1:A:377:LEU:O	1:A:381:GLN:HB3	2.10	0.51
1:A:235:ARG:HD2	1:A:235:ARG:N	2.22	0.51
1:A:403:PRO:O	1:A:404:ARG:HD3	2.10	0.51
1:A:376:VAL:O	1:A:380:LEU:HG	2.11	0.51
1:A:372:ARG:O	1:A:376:VAL:HG23	2.11	0.51
1:A:364:ARG:N	1:A:364:ARG:HD2	2.26	0.51
1:A:776:CYS:HA	1:A:793:LEU:HD13	1.93	0.51
1:A:307:LEU:H	1:A:307:LEU:HD23	1.74	0.51
1:A:431:LYS:HE2	1:A:431:LYS:H	1.76	0.51
1:A:250:ARG:O	1:A:250:ARG:HD2	2.10	0.51
1:A:315:TYR:OH	1:A:318:GLN:HB2	2.10	0.51
1:A:591:GLU:HG2	1:A:595:LYS:HE3	1.93	0.50
1:A:246:TYR:HE1	1:A:250:ARG:HB2	1.77	0.50
1:A:286:ARG:O	1:A:290:GLU:HG2	2.12	0.50
1:A:173:LEU:CD1	1:A:173:LEU:N	2.74	0.50
1:A:355:LYS:O	2:A:901:M0E:H5	2.11	0.50
1:A:520:ALA:HB2	1:A:584:LEU:HD11	1.92	0.49
1:A:674:MET:HA	1:A:677:VAL:CG1	2.37	0.49
1:A:131:THR:HG22	1:A:131:THR:O	2.12	0.49
1:A:327:PHE:N	1:A:328:PRO:CD	2.75	0.49
1:A:536:ALA:HB1	1:A:537:PRO:HD2	1.93	0.49
1:A:776:CYS:SG	1:A:793:LEU:HD13	2.53	0.49
1:A:633:ASN:HD22	1:A:660:ARG:HA	1.77	0.49
1:A:72:LEU:HD23	1:A:74:ILE:H	1.77	0.49
1:A:428:ASP:O	1:A:431:LYS:HE3	2.12	0.49
1:A:76:PHE:O	1:A:80:ILE:HG23	2.13	0.48
1:A:552:ASN:ND2	1:A:575:VAL:H	2.11	0.48
2:A:901:M0E:H61	2:A:901:M0E:CCA	2.44	0.48
1:A:403:PRO:O	1:A:405:GLY:N	2.46	0.48
1:A:385:ILE:HG12	1:A:386:ILE:HG12	1.95	0.48
1:A:392:ASP:OD1	1:A:393:MET:N	2.46	0.48
1:A:670:THR:C	1:A:674:MET:HE2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LEU:HB3	1:A:757:LEU:HD11	1.96	0.47
1:A:470:LEU:N	3:A:1170:HOH:O	2.48	0.47
1:A:344:LEU:HD23	1:A:394:LEU:HD11	1.97	0.46
1:A:774:PHE:N	1:A:796:GLN:HG2	2.30	0.46
1:A:72:LEU:CD2	1:A:74:ILE:HB	2.45	0.46
1:A:487:MET:HE1	1:A:619:ILE:HD12	1.98	0.46
1:A:380:LEU:HD12	1:A:381:GLN:N	2.30	0.46
1:A:302:SER:O	1:A:306:ILE:HG12	2.15	0.46
1:A:91:ILE:HG22	1:A:91:ILE:O	2.16	0.46
1:A:340:GLU:O	1:A:340:GLU:HG2	2.15	0.46
1:A:375:LEU:HD23	1:A:379:LEU:HG	1.97	0.46
1:A:237:PHE:O	1:A:238:TYR:HB3	2.16	0.46
1:A:451:GLU:O	1:A:455:VAL:HG23	2.16	0.45
1:A:407:VAL:O	1:A:407:VAL:HG12	2.15	0.45
1:A:467:LEU:HD12	1:A:470:LEU:HD22	1.98	0.45
1:A:511:LEU:HD22	1:A:709:TRP:CB	2.47	0.45
1:A:350:LEU:HA	1:A:353:MET:CE	2.46	0.45
1:A:315:TYR:HD1	1:A:357:ALA:CB	2.30	0.45
1:A:344:LEU:HD21	1:A:386:ILE:CD1	2.47	0.45
1:A:665:GLN:O	1:A:669:LEU:HG	2.16	0.45
1:A:685:GLN:NE2	1:A:689:LYS:NZ	2.65	0.45
1:A:135:GLN:HB2	1:A:145:PHE:CZ	2.52	0.45
1:A:344:LEU:HA	1:A:347:GLN:OE1	2.17	0.44
1:A:76:PHE:HA	1:A:79:LEU:CD1	2.47	0.44
1:A:530:ASN:N	1:A:530:ASN:HD22	2.09	0.44
1:A:685:GLN:HE21	1:A:689:LYS:HZ2	1.65	0.44
1:A:304:ASP:HA	1:A:307:LEU:CD2	2.46	0.44
1:A:359:ILE:CD1	1:A:359:ILE:H	2.30	0.44
1:A:553:ASP:OD1	1:A:553:ASP:C	2.56	0.44
1:A:586:LEU:N	1:A:587:PRO:CD	2.80	0.44
1:A:276:LEU:HD23	1:A:276:LEU:O	2.18	0.44
1:A:458:ILE:HB	1:A:459:PRO:HD3	2.00	0.43
1:A:248:ILE:HD13	1:A:248:ILE:O	2.17	0.43
1:A:221:PHE:HB3	1:A:225:LEU:CD2	2.47	0.43
1:A:393:MET:HE2	1:A:393:MET:O	2.18	0.43
1:A:383:GLN:HB2	1:A:385:ILE:CD1	2.49	0.43
1:A:79:LEU:HD13	1:A:79:LEU:H	1.83	0.43
1:A:390:LEU:HD12	1:A:391:TYR:N	2.33	0.43
1:A:238:TYR:N	1:A:238:TYR:CD2	2.87	0.43
1:A:76:PHE:HA	1:A:79:LEU:HD11	1.99	0.43
1:A:507:SER:HA	1:A:615:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:THR:O	1:A:676:GLN:HB2	2.19	0.43
1:A:789:ASP:OD2	1:A:791:GLN:HB2	2.18	0.43
1:A:218:ARG:HG3	1:A:304:ASP:HB3	2.01	0.43
1:A:113:LEU:HD12	1:A:195:PHE:HD1	1.83	0.43
1:A:761:GLU:O	1:A:762:ASP:HB2	2.18	0.43
1:A:115:PRO:O	1:A:116:ASP:HB2	2.19	0.42
1:A:575:VAL:HB	1:A:576:PRO:HD3	2.01	0.42
1:A:403:PRO:C	1:A:404:ARG:HD3	2.40	0.42
1:A:315:TYR:HD1	1:A:357:ALA:HB1	1.85	0.42
1:A:487:MET:CE	1:A:619:ILE:HD12	2.49	0.42
1:A:544:ASN:N	1:A:544:ASN:HD22	2.17	0.42
1:A:225:LEU:HD23	1:A:226:VAL:N	2.33	0.42
1:A:355:LYS:O	2:A:901:M0E:H1	2.20	0.42
1:A:285:TRP:O	1:A:289:ASN:HB2	2.20	0.42
1:A:746:TYR:CE2	1:A:750:GLN:NE2	2.87	0.42
1:A:791:GLN:NE2	1:A:791:GLN:N	2.46	0.41
1:A:335:PHE:CE1	1:A:346:GLN:HG2	2.54	0.41
1:A:271:GLN:OE1	2:A:901:M0E:HAH2	2.20	0.41
1:A:234:ASP:CG	1:A:238:TYR:HB3	2.41	0.41
1:A:102:LEU:HA	1:A:103:PRO:HD2	1.90	0.41
1:A:741:SER:HA	1:A:744:GLN:OE1	2.20	0.41
1:A:205:ILE:O	1:A:206:SER:C	2.59	0.41
1:A:250:ARG:O	1:A:251:ALA:HB2	2.21	0.41
1:A:773:ASN:HB3	1:A:796:GLN:CG	2.50	0.41
1:A:399:LEU:HD22	1:A:399:LEU:N	2.36	0.41
1:A:232:THR:O	1:A:233:GLU:C	2.59	0.41
1:A:155:ILE:HG12	1:A:170:ARG:HG3	2.02	0.41
1:A:544:ASN:HA	1:A:545:GLY:HA2	1.42	0.41
1:A:385:ILE:O	1:A:386:ILE:HD13	2.20	0.41
1:A:356:GLY:O	1:A:360:TYR:CD2	2.72	0.41
1:A:378:ARG:HD2	1:A:378:ARG:C	2.41	0.41
1:A:392:ASP:OD1	1:A:392:ASP:C	2.59	0.41
1:A:604:HIS:HA	1:A:605:PRO:HD3	1.94	0.41
1:A:238:TYR:C	1:A:238:TYR:CD2	2.91	0.41
1:A:133:TYR:CE1	1:A:143:GLY:HA2	2.56	0.41
1:A:406:GLY:O	1:A:407:VAL:C	2.59	0.40
1:A:499:ASN:ND2	1:A:499:ASN:C	2.74	0.40
1:A:334:TYR:O	1:A:403:PRO:HD3	2.21	0.40
1:A:552:ASN:HD21	1:A:575:VAL:H	1.68	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	700/768 (91%)	645 (92%)	43 (6%)	12 (2%)	11 4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	TYR
1	A	239	GLU
1	A	404	ARG
1	A	790	PRO
1	A	233	GLU
1	A	283	SER
1	A	544	ASN
1	A	407	VAL
1	A	164	SER
1	A	206	SER
1	A	335	PHE
1	A	430	VAL

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	597/645 (93%)	539 (90%)	58 (10%)	10 5

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	79	LEU
1	A	86	TYR
1	A	112	ASN
1	A	148	GLN
1	A	173	LEU
1	A	180	LEU
1	A	197	LEU
1	A	212	GLN
1	A	218	ARG
1	A	225	LEU
1	A	226	VAL
1	A	233	GLU
1	A	234	ASP
1	A	235	ARG
1	A	236	HIS
1	A	237	PHE
1	A	238	TYR
1	A	246	TYR
1	A	247	SER
1	A	248	ILE
1	A	268	LEU
1	A	270	GLN
1	A	272	LEU
1	A	281	GLU
1	A	289	ASN
1	A	321	ASP
1	A	359	ILE
1	A	368	LEU
1	A	372	ARG
1	A	380	LEU
1	A	381	GLN
1	A	384	GLN
1	A	385	ILE
1	A	402	GLN
1	A	404	ARG
1	A	408	ILE
1	A	431	LYS
1	A	465	ARG
1	A	466	LYS
1	A	485	ARG
1	A	495	PHE
1	A	499	ASN

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Mol	Chain	Res	Type
1	A	530	ASN
1	A	544	ASN
1	A	546	GLN
1	A	555	ARG
1	A	559	GLU
1	A	572	SER
1	A	609	MET
1	A	628	ILE
1	A	641	ARG
1	A	665	GLN
1	A	671	LEU
1	A	685	GLN
1	A	695	LEU
1	A	750	GLN
1	A	791	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	112	ASN
1	A	179	HIS
1	A	191	GLN
1	A	212	GLN
1	A	240	HIS
1	A	270	GLN
1	A	275	ASN
1	A	289	ASN
1	A	318	GLN
1	A	381	GLN
1	A	383	GLN
1	A	384	GLN
1	A	388	GLN
1	A	402	GLN
1	A	411	GLN
1	A	423	GLN
1	A	499	ASN
1	A	503	GLN
1	A	523	GLN
1	A	530	ASN
1	A	544	ASN
1	A	552	ASN

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Mol	Chain	Res	Type
1	A	615	ASN
1	A	633	ASN
1	A	657	GLN
1	A	665	GLN
1	A	685	GLN
1	A	703	ASN
1	A	791	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	M0E	A	901	-	75,81,114	1.93	14 (18%)	94,122,166	2.40	45 (47%)

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	M0E	A	901	-	-	0/47/158/206	0/5/5/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	M0E	OBH-CAP	-3.08	1.39	1.45
2	A	901	M0E	CAO-CAP	-2.84	1.49	1.53
2	A	901	M0E	OBA-CAO	-2.68	1.39	1.44
2	A	901	M0E	OBE-CAX	2.30	1.47	1.41
2	A	901	M0E	CBU-CBV	2.38	1.57	1.53
2	A	901	M0E	CAG-N2	2.79	1.45	1.34
2	A	901	M0E	CCA-NCC	2.79	1.45	1.34
2	A	901	M0E	CAX-CAR	2.87	1.60	1.52
2	A	901	M0E	OBC-CAV	3.22	1.26	1.21
2	A	901	M0E	C1-C2	4.68	1.61	1.53
2	A	901	M0E	CAV-NAT	4.98	1.44	1.33
2	A	901	M0E	C3-C2	5.12	1.63	1.53
2	A	901	M0E	CAW-NAU	5.54	1.43	1.32
2	A	901	M0E	CCM-NCS	5.61	1.44	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	M0E	C1-O1-CAR	-3.11	109.88	118.01
2	A	901	M0E	OBC-CAV-NAT	-2.67	120.23	125.34
2	A	901	M0E	C1-O5-C5	-2.39	109.11	113.75
2	A	901	M0E	OBD-CAW-NAU	-2.34	119.61	123.08
2	A	901	M0E	CCH-OCE-CBX	-2.09	112.55	118.01
2	A	901	M0E	OCN-CCI-CCJ	2.04	114.94	110.34
2	A	901	M0E	OCE-CCH-OCP	2.08	115.94	110.68
2	A	901	M0E	OCD-CBW-CBX	2.09	114.81	109.87
2	A	901	M0E	CBU-CBV-NCC	2.10	114.96	111.01
2	A	901	M0E	C6-C5-C4	2.17	118.84	113.35
2	A	901	M0E	C3-C2-N2	2.20	115.23	110.66
2	A	901	M0E	C1-C2-N2	2.30	115.33	111.01
2	A	901	M0E	OCO-CCJ-CCK	2.36	115.66	110.34
2	A	901	M0E	O4-C4-C5	2.41	115.67	109.32
2	A	901	M0E	OCD-CBW-CBV	2.43	114.61	109.66
2	A	901	M0E	O3-C3-C4	2.43	115.62	109.87
2	A	901	M0E	OCR-CCK-CCJ	2.53	116.04	110.34
2	A	901	M0E	OBA-CAO-CAS	2.65	112.83	107.46
2	A	901	M0E	OBR-CBM-CBN	2.68	116.35	109.24
2	A	901	M0E	OCE-CBX-CBY	2.76	114.07	106.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	M0E	OCE-CCH-CCI	2.77	114.83	108.10
2	A	901	M0E	OCR-CCK-CCL	2.82	116.01	109.81
2	A	901	M0E	OBQ-CBL-CBK	2.83	116.70	110.34
2	A	901	M0E	OBR-CBM-CBL	2.87	116.81	110.34
2	A	901	M0E	OBE-CAQ-CAW	2.92	116.70	109.63
2	A	901	M0E	OBS-CBJ-O6	2.93	117.11	110.05
2	A	901	M0E	OCO-CCJ-CCI	2.98	117.06	110.34
2	A	901	M0E	OCE-CBX-CBW	3.00	114.91	107.17
2	A	901	M0E	OBQ-CBL-CBM	3.09	117.28	110.34
2	A	901	M0E	O3-C3-C2	3.10	115.98	109.66
2	A	901	M0E	OBG-CAX-CAR	3.37	114.68	108.39
2	A	901	M0E	C6-O6-CBJ	3.38	120.91	113.82
2	A	901	M0E	OBP-CBK-CBL	3.52	118.25	110.34
2	A	901	M0E	OBP-CBK-CBJ	3.62	117.96	110.02
2	A	901	M0E	O1-CAR-CAP	3.70	116.53	106.83
2	A	901	M0E	OBE-CAX-OBG	3.79	116.36	111.36
2	A	901	M0E	O6-C6-C5	3.96	116.25	109.08
2	A	901	M0E	OBH-CAP-CAR	3.98	116.53	107.96
2	A	901	M0E	O4-C4-C3	4.04	117.58	107.17
2	A	901	M0E	OCF-CBY-CBZ	4.17	115.76	106.64
2	A	901	M0E	CAS-CAO-CAP	4.20	115.94	111.71
2	A	901	M0E	OBS-CBN-CBO	4.44	117.57	106.36
2	A	901	M0E	OBH-CAP-CAO	4.98	115.51	108.16
2	A	901	M0E	O5-C5-C6	6.03	118.94	106.61
2	A	901	M0E	O6-CBJ-CBK	6.27	115.96	108.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	M0E	7	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	708/768 (92%)	0.78	93 (13%) 5 8	32, 62, 152, 182	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	TRP	7.3
1	A	544	ASN	7.3
1	A	406	GLY	6.6
1	A	386	ILE	6.5
1	A	282	ARG	6.2
1	A	76	PHE	5.6
1	A	235	ARG	5.6
1	A	734	TYR	5.3
1	A	407	VAL	5.1
1	A	408	ILE	5.0
1	A	360	TYR	4.9
1	A	295	LEU	4.8
1	A	236	HIS	4.8
1	A	432	ASP	4.7
1	A	233	GLU	4.3
1	A	394	LEU	4.3
1	A	229	LEU	4.2
1	A	369	ALA	4.1
1	A	382	GLN	4.0
1	A	270	GLN	4.0
1	A	77	ALA	3.9
1	A	86	TYR	3.9
1	A	297	MET	3.9
1	A	387	ASP	3.8
1	A	234	ASP	3.8
1	A	368	LEU	3.8
1	A	401	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	371	GLU	3.7
1	A	75	VAL	3.7
1	A	85	VAL	3.6
1	A	381	GLN	3.5
1	A	335	PHE	3.4
1	A	390	LEU	3.4
1	A	208	PRO	3.4
1	A	293	MET	3.4
1	A	378	ARG	3.4
1	A	78	VAL	3.3
1	A	391	TYR	3.2
1	A	379	LEU	3.2
1	A	271	GLN	3.1
1	A	248	ILE	3.0
1	A	355	LYS	3.0
1	A	393	MET	3.0
1	A	74	ILE	3.0
1	A	240	HIS	2.9
1	A	800	GLN	2.9
1	A	231	ALA	2.9
1	A	329	LEU	2.8
1	A	232	THR	2.8
1	A	92	ARG	2.8
1	A	225	LEU	2.8
1	A	90	LYS	2.8
1	A	230	LEU	2.8
1	A	268	LEU	2.8
1	A	467	LEU	2.8
1	A	277	PHE	2.7
1	A	307	LEU	2.7
1	A	309	LEU	2.7
1	A	385	ILE	2.7
1	A	363	TRP	2.7
1	A	370	LEU	2.6
1	A	238	TYR	2.6
1	A	392	ASP	2.6
1	A	187	GLU	2.6
1	A	375	LEU	2.6
1	A	380	LEU	2.6
1	A	246	TYR	2.6
1	A	249	GLY	2.6
1	A	388	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	655	PHE	2.5
1	A	276	LEU	2.4
1	A	497	GLY	2.3
1	A	96	ASP	2.3
1	A	280	SER	2.3
1	A	279	SER	2.3
1	A	247	SER	2.3
1	A	287	LYS	2.3
1	A	542	GLN	2.2
1	A	796	GLN	2.2
1	A	91	ILE	2.2
1	A	306	ILE	2.1
1	A	113	LEU	2.1
1	A	733	LEU	2.1
1	A	744	GLN	2.1
1	A	494	GLN	2.1
1	A	367	LYS	2.1
1	A	359	ILE	2.1
1	A	373	ARG	2.1
1	A	95	ILE	2.0
1	A	303	LYS	2.0
1	A	278	LEU	2.0
1	A	389	GLU	2.0
1	A	546	GLN	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	M0E	A	901	77/109	0.89	0.15	-0.60	87,121,171,181	0

6.5 Other polymers (i)

There are no such residues in this entry.