



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:44 AM GMT

PDB ID : 3W2V
Title : Crystal structure of the Cmr2dHD-Cmr3 subcomplex bound to 3'-AMP
Authors : Numata, T.; Osawa, T.
Deposited on : 2012-12-06
Resolution : 2.60 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>

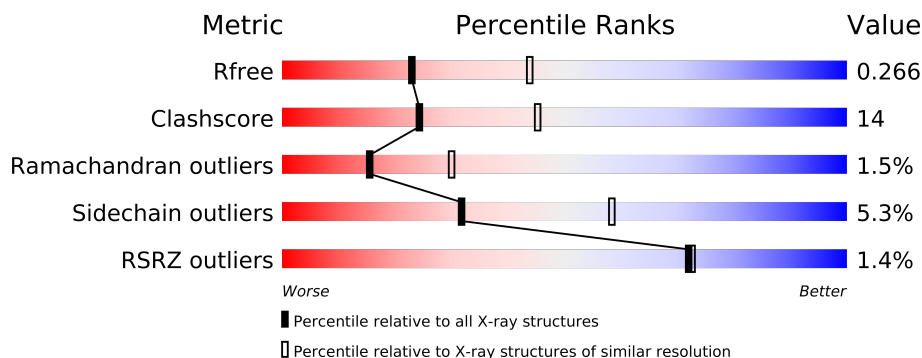
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	677	
2	B	322	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7096 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 CRISPR system Cmr subunit Cmr2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4832	3128	806	886	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	MET	-	EXPRESSION TAG	UNP Q8U1S6
A	196	GLY	-	EXPRESSION TAG	UNP Q8U1S6
A	197	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	198	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	199	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	200	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	201	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	202	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	203	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	204	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	205	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	206	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	207	GLY	-	EXPRESSION TAG	UNP Q8U1S6
A	208	LEU	-	EXPRESSION TAG	UNP Q8U1S6
A	209	VAL	-	EXPRESSION TAG	UNP Q8U1S6
A	210	PRO	-	EXPRESSION TAG	UNP Q8U1S6
A	211	ARG	-	EXPRESSION TAG	UNP Q8U1S6
A	212	GLY	-	EXPRESSION TAG	UNP Q8U1S6
A	213	SER	-	EXPRESSION TAG	UNP Q8U1S6
A	214	HIS	-	EXPRESSION TAG	UNP Q8U1S6
A	215	MET	-	EXPRESSION TAG	UNP Q8U1S6

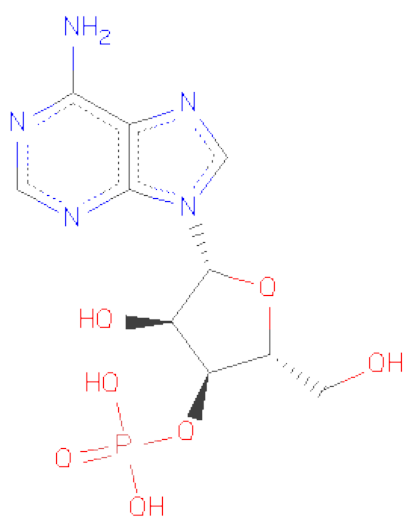
- Molecule 2 is a protein called CRISPR system Cmr subunit Cmr3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	281	Total	C	N	O	S	0	0	0
			2214	1454	350	406	4			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-4-HYDROXY-2-(HYDROXYMETHYL)OXOLAN-3-YL]DIHYDROGEN PHOSPHATE (three-letter code: 3AM) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

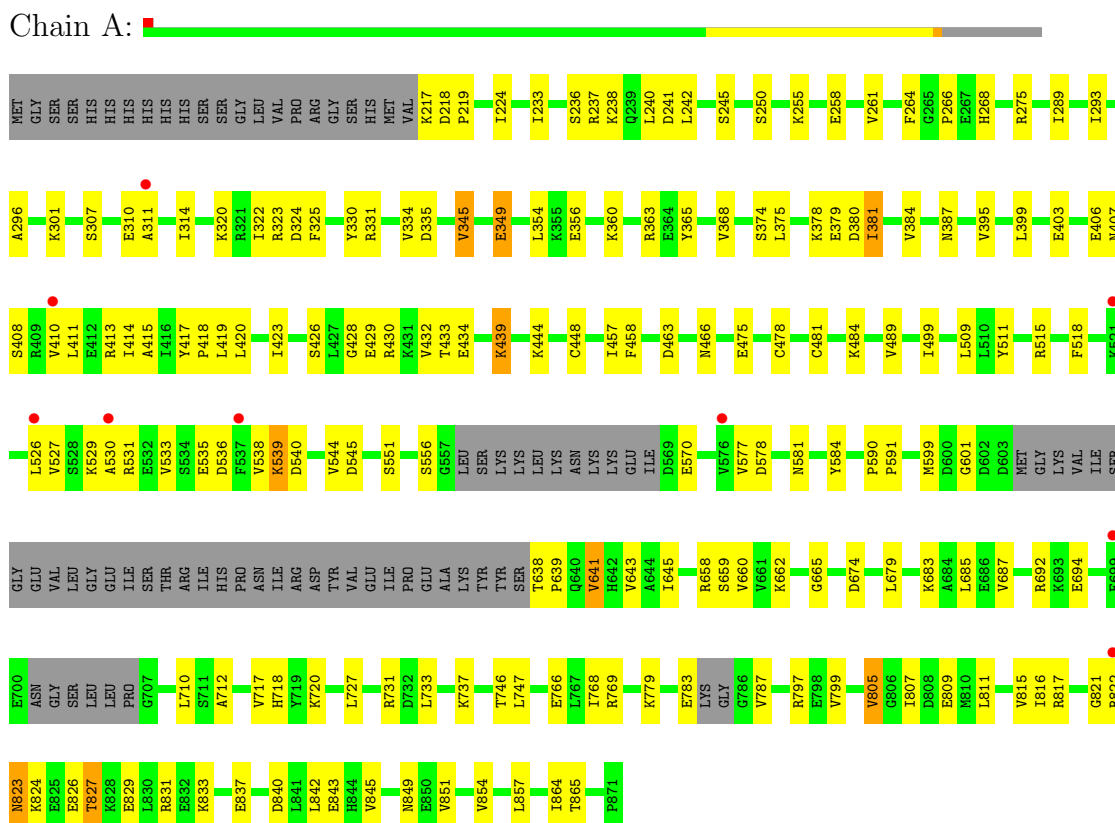
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	7	Total	O	0	0
			7	7		

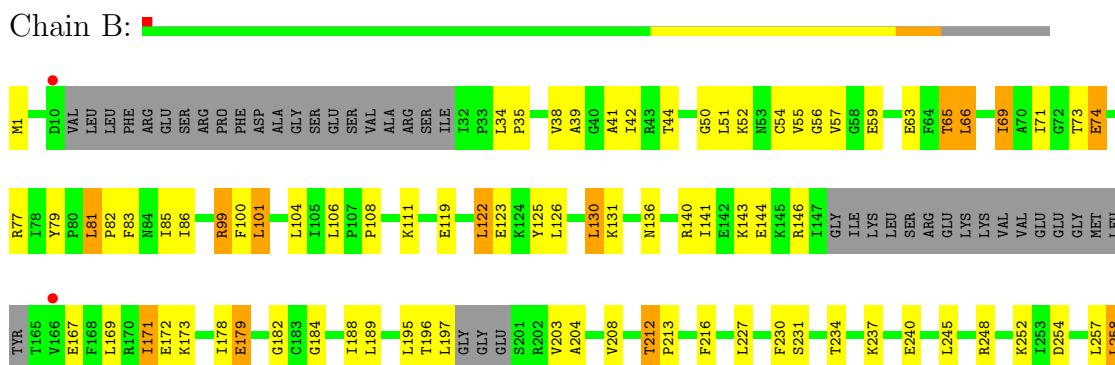
3 Residue-property plots

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.

• Molecule 1: CRISPR system Cmr subunit Cmr2



• Molecule 2: CRISPR system Cmr subunit Cmr3



V259	S260	D270	S287	V288	L289	E292	F293	K294	E295	E296	I303	K304	L305	L308	K309	K310	L311	G312	V313	G314	L315	G319	I320	W321	E322
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	103.94Å 136.67Å 191.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.73 – 2.60 41.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.73-2.60) 99.6 (41.72-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 2.61Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.259 0.223 , 0.266	Depositor DCC
R_{free} test set	2077 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42206 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7096	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 3AM

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	0.38	0/4929	0.59	0/6660
2	B	0.39	0/2262	0.64	1/3054 (0.0%)
All	All	0.38	0/7191	0.61	1/9714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	LEU	CA-CB-CG	5.97	129.03	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4832	0	4825	127	0
2	B	2214	0	2265	77	0
3	A	1	0	0	0	0
4	A	23	0	12	0	0
5	A	19	0	0	1	0
5	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7096	0	7102	200	0

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 14.

All (200) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:577:VAL:HG12	1:A:581:ASN:HD21	1.33	0.90
1:A:805:VAL:HG13	1:A:809:GLU:HB3	1.58	0.85
1:A:816:ILE:HG23	1:A:831:ARG:NH1	1.94	0.83
2:B:71:ILE:HD12	2:B:171:ILE:HD11	1.63	0.80
1:A:448:CYS:HB2	1:A:478:CYS:HB3	1.64	0.78
1:A:849:ASN:OD1	1:A:851:VAL:HG22	1.82	0.78
2:B:195:LEU:HD23	2:B:196:THR:N	1.99	0.77
2:B:230:PHE:HD1	2:B:234:THR:HG21	1.50	0.76
1:A:638:THR:O	1:A:641:VAL:HG22	1.87	0.75
1:A:769:ARG:HH11	1:A:769:ARG:HB3	1.51	0.74
2:B:140:ARG:HH11	2:B:140:ARG:HG3	1.52	0.74
1:A:380:ASP:O	1:A:384:VAL:HG23	1.89	0.73
2:B:237:LYS:HB2	2:B:240:GLU:HG3	1.70	0.73
1:A:665:GLY:HA3	1:A:679:LEU:HD23	1.71	0.72
1:A:577:VAL:HG12	1:A:581:ASN:ND2	2.04	0.71
2:B:308:LEU:HG	2:B:311:LEU:HD12	1.72	0.71
1:A:381:ILE:HG23	1:A:399:LEU:HD22	1.72	0.70
2:B:230:PHE:CD1	2:B:234:THR:HG21	2.26	0.70
2:B:143:LYS:HD3	2:B:169:LEU:HD23	1.74	0.70
1:A:718:HIS:HD2	1:A:720:LYS:H	1.40	0.69
1:A:531:ARG:HD3	1:A:535:GLU:OE1	1.93	0.68
1:A:779:LYS:O	1:A:783:GLU:HG2	1.93	0.68
2:B:234:THR:HG22	2:B:314:GLY:HA2	1.77	0.67
2:B:65:THR:HG23	2:B:179:GLU:HB3	1.77	0.66
1:A:864:ILE:HD12	1:A:865:THR:HG23	1.78	0.66
2:B:99:ARG:HH12	2:B:292:GLU:CD	1.98	0.66
1:A:578:ASP:HA	1:A:581:ASN:HD22	1.59	0.65
1:A:322:ILE:HD12	1:A:368:VAL:HG21	1.76	0.65
2:B:172:GLU:HG2	2:B:173:LYS:HG2	1.78	0.65
1:A:233:ILE:HG23	1:A:242:LEU:HD12	1.79	0.65
1:A:601:GLY:HA2	1:A:710:LEU:HD12	1.77	0.64
1:A:538:VAL:HG12	1:A:539:LYS:N	2.11	0.64
1:A:331:ARG:O	1:A:334:VAL:HG22	1.98	0.63
1:A:718:HIS:CD2	1:A:720:LYS:H	2.16	0.63
1:A:417:TYR:HB3	1:A:418:PRO:HD3	1.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:195:LEU:HD23	2:B:196:THR:H	1.64	0.62
1:A:769:ARG:NH1	1:A:769:ARG:HB3	2.15	0.61
1:A:217:LYS:O	1:A:219:PRO:HD3	2.01	0.60
1:A:766:GLU:OE1	1:A:769:ARG:NH1	2.34	0.59
1:A:236:SER:HB3	1:A:241:ASP:HB2	1.84	0.59
2:B:258:LEU:HD22	2:B:260:SER:HB2	1.84	0.59
1:A:816:ILE:HA	1:A:831:ARG:HD3	1.84	0.58
2:B:208:VAL:HG23	2:B:208:VAL:O	2.03	0.58
2:B:52:LYS:O	2:B:55:VAL:HG12	2.04	0.57
1:A:822:ARG:HG3	1:A:826:GLU:OE2	2.05	0.57
1:A:381:ILE:CG2	1:A:399:LEU:HD22	2.35	0.57
2:B:82:PRO:HD2	2:B:85:ILE:HD12	1.87	0.57
1:A:289:ILE:HD11	1:A:293:ILE:HD13	1.85	0.57
1:A:381:ILE:HD11	1:A:411:LEU:CD1	2.33	0.57
1:A:481:CYS:O	1:A:484:LYS:HB3	2.04	0.57
2:B:184:GLY:O	2:B:188:ILE:HG12	2.05	0.56
1:A:840:ASP:O	1:A:843:GLU:HB2	2.04	0.56
1:A:659:SER:O	1:A:662:LYS:HG3	2.05	0.56
1:A:833:LYS:O	1:A:837:GLU:HG3	2.07	0.55
1:A:428:GLY:O	1:A:432:VAL:HG13	2.07	0.55
2:B:54:CYS:HA	2:B:63:GLU:HB2	1.88	0.55
1:A:399:LEU:HD21	1:A:419:LEU:CD1	2.36	0.55
1:A:381:ILE:HG22	1:A:399:LEU:HD13	1.88	0.55
2:B:38:VAL:HG11	2:B:69:ILE:HD11	1.88	0.55
1:A:387:ASN:O	2:B:99:ARG:N	2.39	0.55
1:A:426:SER:OG	2:B:108:PRO:HD3	2.07	0.54
1:A:821:GLY:H	1:A:827:THR:HB	1.72	0.54
2:B:304:LYS:O	2:B:305:LEU:HD23	2.08	0.54
1:A:811:LEU:O	1:A:815:VAL:HG23	2.07	0.54
2:B:99:ARG:NH1	2:B:292:GLU:OE1	2.40	0.54
1:A:845:VAL:HG21	1:A:857:LEU:HB2	1.90	0.54
2:B:213:PRO:HG2	2:B:216:PHE:CD2	2.42	0.53
1:A:310:GLU:O	1:A:314:ILE:HG13	2.08	0.53
2:B:140:ARG:NH1	2:B:140:ARG:HG3	2.22	0.53
1:A:331:ARG:HG2	1:A:354:LEU:CD2	2.39	0.53
2:B:125:TYR:HB2	2:B:130:LEU:HD12	1.91	0.53
1:A:379:GLU:OE2	1:A:384:VAL:HG22	2.09	0.52
1:A:539:LYS:O	1:A:540:ASP:HB2	2.08	0.52
2:B:141:ILE:HG21	2:B:169:LEU:HB3	1.90	0.52
2:B:254:ASP:OD2	2:B:294:LYS:HA	2.09	0.52
1:A:805:VAL:CG1	1:A:809:GLU:HB3	2.36	0.52
1:A:807:ILE:HD11	1:A:851:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:692:ARG:HD3	1:A:710:LEU:HB3	1.92	0.52
1:A:475:GLU:HG3	1:A:475:GLU:O	2.09	0.52
2:B:56:GLY:O	2:B:59:GLU:HB2	2.10	0.52
2:B:77:ARG:HD2	2:B:119:GLU:OE2	2.09	0.52
1:A:509:LEU:HB3	1:A:515:ARG:HB2	1.91	0.52
2:B:65:THR:CG2	2:B:179:GLU:HB3	2.39	0.51
1:A:323:ARG:HG3	1:A:363:ARG:HG3	1.93	0.51
1:A:264:PHE:HB3	1:A:268:HIS:CD2	2.46	0.51
2:B:143:LYS:HD2	2:B:167:GLU:HG2	1.91	0.51
1:A:307:SER:HB2	1:A:310:GLU:CG	2.41	0.51
2:B:141:ILE:CG2	2:B:169:LEU:HD22	2.41	0.50
1:A:374:SER:O	1:A:413:ARG:HD2	2.12	0.49
2:B:119:GLU:O	2:B:123:GLU:HG3	2.11	0.49
1:A:255:LYS:O	1:A:258:GLU:HG2	2.11	0.49
1:A:539:LYS:HE3	1:A:540:ASP:OD2	2.12	0.49
1:A:783:GLU:HB3	1:A:787:VAL:HB	1.94	0.49
1:A:599:MET:HG2	1:A:712:ALA:HB2	1.94	0.49
1:A:658:ARG:HG3	1:A:658:ARG:HH11	1.78	0.49
1:A:330:TYR:O	1:A:334:VAL:HG13	2.13	0.49
1:A:429:GLU:O	1:A:432:VAL:HG22	2.13	0.49
2:B:65:THR:HB	2:B:310:LYS:HD3	1.94	0.48
1:A:403:GLU:HG3	1:A:408:SER:O	2.13	0.48
1:A:403:GLU:O	1:A:406:GLU:O	2.31	0.48
1:A:365:TYR:HA	1:A:439:LYS:NZ	2.27	0.48
1:A:538:VAL:HG12	1:A:539:LYS:H	1.74	0.48
1:A:536:ASP:O	1:A:544:VAL:HG21	2.13	0.48
2:B:252:LYS:HG2	2:B:294:LYS:HD2	1.94	0.48
1:A:423:ILE:HG21	2:B:100:PHE:CD2	2.50	0.47
1:A:410:VAL:C	1:A:411:LEU:HD23	2.34	0.47
2:B:141:ILE:HG22	2:B:169:LEU:HD22	1.95	0.47
1:A:406:GLU:O	1:A:408:SER:N	2.47	0.47
2:B:73:THR:HB	2:B:74:GLU:OE2	2.14	0.47
2:B:79:TYR:CD2	2:B:122:LEU:HD12	2.49	0.47
1:A:237:ARG:NH2	1:A:238:LYS:HD2	2.29	0.47
2:B:39:ALA:HB2	2:B:66:LEU:HD12	1.97	0.47
1:A:733:LEU:O	1:A:737:LYS:HB2	2.15	0.47
1:A:766:GLU:HB3	1:A:769:ARG:HH12	1.80	0.47
2:B:122:LEU:O	2:B:126:LEU:HG	2.15	0.47
1:A:665:GLY:HA3	1:A:679:LEU:CD2	2.44	0.47
1:A:538:VAL:CG1	1:A:539:LYS:N	2.77	0.47
1:A:320:LYS:HG2	1:A:324:ASP:OD2	2.15	0.47
1:A:323:ARG:CD	1:A:363:ARG:HG3	2.45	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:641:VAL:O	1:A:645:ILE:HG13	2.16	0.46
1:A:395:VAL:O	1:A:399:LEU:HG	2.16	0.46
2:B:74:GLU:H	2:B:74:GLU:CD	2.19	0.46
1:A:381:ILE:HD11	1:A:411:LEU:HD11	1.96	0.46
1:A:240:LEU:HD13	1:A:499:ILE:HD11	1.98	0.45
1:A:432:VAL:HG23	1:A:433:THR:N	2.31	0.45
1:A:518:PHE:CE2	1:A:526:LEU:HD22	2.52	0.45
1:A:551:SER:HG	1:A:584:TYR:HE2	1.64	0.45
2:B:66:LEU:HD21	2:B:69:ILE:CD1	2.46	0.45
1:A:345:VAL:HG21	1:A:458:PHE:CZ	2.51	0.45
1:A:511:TYR:HB3	1:A:591:PRO:HG2	1.96	0.45
1:A:240:LEU:CD1	1:A:499:ILE:HD11	2.46	0.45
2:B:234:THR:CG2	2:B:314:GLY:HA2	2.46	0.45
1:A:307:SER:HB2	1:A:310:GLU:HG2	1.98	0.45
2:B:86:ILE:HG23	2:B:111:LYS:O	2.17	0.45
2:B:227:LEU:C	2:B:227:LEU:HD12	2.36	0.45
1:A:823:ASN:ND2	1:A:826:GLU:H	2.14	0.44
2:B:227:LEU:CD1	2:B:319:GLY:HA3	2.47	0.44
1:A:233:ILE:HG23	1:A:242:LEU:CD1	2.45	0.44
1:A:717:VAL:HG23	5:A:1012:HOH:O	2.16	0.44
1:A:747:LEU:CD2	1:A:768:ILE:HD11	2.47	0.44
2:B:237:LYS:HB2	2:B:240:GLU:CG	2.42	0.44
2:B:34:LEU:N	2:B:35:PRO:CD	2.81	0.43
2:B:41:ALA:HB2	2:B:197:LEU:HD23	2.00	0.43
2:B:140:ARG:NH1	2:B:140:ARG:CG	2.81	0.43
2:B:65:THR:HG23	2:B:179:GLU:CB	2.47	0.43
1:A:799:VAL:HG11	1:A:854:VAL:HG11	2.00	0.43
1:A:746:THR:HG22	1:A:747:LEU:N	2.33	0.43
1:A:261:VAL:HG13	1:A:266:PRO:HD3	2.00	0.43
1:A:805:VAL:HG13	1:A:805:VAL:O	2.19	0.43
2:B:65:THR:HB	2:B:310:LYS:CD	2.48	0.43
1:A:307:SER:O	1:A:310:GLU:N	2.45	0.43
2:B:143:LYS:HD3	2:B:169:LEU:CD2	2.47	0.43
1:A:250:SER:OG	1:A:296:ALA:HB1	2.19	0.43
1:A:375:LEU:HD13	1:A:414:ILE:HD12	2.00	0.43
1:A:527:VAL:O	1:A:530:ALA:HB3	2.19	0.43
1:A:334:VAL:HG23	1:A:335:ASP:N	2.33	0.43
2:B:55:VAL:HG13	2:B:57:VAL:HG23	1.99	0.43
1:A:399:LEU:HD21	1:A:419:LEU:HD12	2.00	0.43
1:A:264:PHE:HB3	1:A:268:HIS:HD2	1.84	0.43
1:A:255:LYS:HE3	1:A:325:PHE:CD1	2.54	0.43
1:A:345:VAL:HG22	1:A:349:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:457:ILE:O	1:A:458:PHE:HB2	2.18	0.43
1:A:590:PRO:HA	1:A:591:PRO:HD3	1.86	0.43
2:B:101:LEU:HA	2:B:101:LEU:HD22	1.91	0.42
1:A:356:GLU:HA	1:A:356:GLU:OE1	2.19	0.42
1:A:674:ASP:N	1:A:674:ASP:OD2	2.47	0.42
2:B:50:GLY:O	2:B:52:LYS:N	2.46	0.42
2:B:234:THR:HG22	2:B:314:GLY:CA	2.48	0.42
2:B:99:ARG:NH1	2:B:292:GLU:OE2	2.48	0.42
1:A:529:LYS:O	1:A:533:VAL:HG23	2.20	0.42
1:A:463:ASP:OD1	1:A:466:ASN:ND2	2.53	0.42
1:A:658:ARG:NH1	1:A:658:ARG:HG3	2.34	0.42
2:B:42:ILE:CD1	2:B:178:ILE:HD11	2.50	0.42
2:B:189:LEU:CB	2:B:208:VAL:HG11	2.49	0.42
2:B:66:LEU:O	2:B:312:GLY:HA2	2.20	0.42
1:A:224:ILE:O	1:A:301:LYS:HA	2.20	0.42
2:B:248:ARG:HG2	2:B:303:ILE:HD11	2.02	0.42
2:B:83:PHE:HD1	2:B:287:SER:HA	1.85	0.42
1:A:683:LYS:O	1:A:687:VAL:HG23	2.19	0.42
1:A:378:LYS:HA	1:A:411:LEU:O	2.20	0.42
2:B:320:ILE:HG22	2:B:321:TRP:N	2.35	0.41
1:A:444:LYS:HE2	2:B:270:ASP:OD1	2.20	0.41
2:B:203:VAL:HG22	2:B:204:ALA:N	2.36	0.41
1:A:430:ARG:O	1:A:434:GLU:HG3	2.20	0.41
1:A:864:ILE:HD12	1:A:865:THR:CG2	2.48	0.41
1:A:694:GLU:OE2	1:A:694:GLU:HA	2.21	0.41
1:A:245:SER:OG	1:A:484:LYS:HD2	2.19	0.41
2:B:100:PHE:CE1	2:B:101:LEU:HB2	2.55	0.41
2:B:248:ARG:HG3	2:B:248:ARG:HH11	1.85	0.41
2:B:1:MET:HB3	2:B:212:THR:HG22	2.02	0.41
1:A:538:VAL:CG1	1:A:539:LYS:H	2.34	0.41
1:A:639:PRO:O	1:A:643:VAL:HG23	2.21	0.41
1:A:413:ARG:C	1:A:415:ALA:H	2.24	0.40
2:B:79:TYR:CG	2:B:122:LEU:HD12	2.56	0.40
1:A:420:LEU:HA	1:A:420:LEU:HD12	1.99	0.40
1:A:535:GLU:HA	1:A:535:GLU:OE1	2.22	0.40
2:B:99:ARG:HE	2:B:99:ARG:HB2	1.70	0.40
2:B:131:LYS:HA	2:B:131:LYS:HD3	1.93	0.40
2:B:231:SER:OG	2:B:315:LEU:HD13	2.21	0.40
2:B:144:GLU:OE1	2:B:146:ARG:NH2	2.55	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	592/677 (87%)	548 (93%)	34 (6%)	10 (2%)	14	26
2	B	273/322 (85%)	254 (93%)	16 (6%)	3 (1%)	21	42
All	All	865/999 (87%)	802 (93%)	50 (6%)	13 (2%)	15	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	ILE
2	B	296	GLU
1	A	311	ALA
1	A	570	GLU
2	B	51	LEU
1	A	275	ARG
1	A	349	GLU
1	A	407	ASN
1	A	824	LYS
1	A	439	LYS
1	A	539	LYS
1	A	556	SER
2	B	182	GLY

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	512/604 (85%)	495 (97%)	17 (3%)	50	79
2	B	238/280 (85%)	215 (90%)	23 (10%)	12	22
All	All	750/884 (85%)	710 (95%)	40 (5%)	32	58

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASP
1	A	345	VAL
1	A	360	LYS
1	A	489	VAL
1	A	545	ASP
1	A	641	VAL
1	A	660	VAL
1	A	685	LEU
1	A	727	LEU
1	A	731	ARG
1	A	797	ARG
1	A	805	VAL
1	A	817	ARG
1	A	823	ASN
1	A	827	THR
1	A	829	GLU
1	A	842	LEU
2	B	44	THR
2	B	65	THR
2	B	66	LEU
2	B	69	ILE
2	B	74	GLU
2	B	81	LEU
2	B	99	ARG
2	B	101	LEU
2	B	104	LEU
2	B	106	LEU
2	B	122	LEU
2	B	130	LEU
2	B	136	ASN
2	B	171	ILE
2	B	179	GLU
2	B	212	THR
2	B	245	LEU
2	B	257	LEU
2	B	258	LEU
2	B	289	LEU
2	B	295	GLU
2	B	308	LEU
2	B	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	ASN
1	A	268	HIS
1	A	383	GLN
1	A	581	ASN
1	A	718	HIS
1	A	735	ASN
1	A	794	HIS
1	A	823	ASN
1	A	848	ASN
2	B	136	ASN
2	B	217	ASN

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	3AM	A	902	-	25,25,25	1.67	5 (20%)	38,38,38	2.68	8 (21%)

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	3AM	A	902	-	-	0/11/27/27	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	3AM	C2-N3	4.11	1.40	1.32
4	A	902	3AM	C2-N1	3.32	1.40	1.33
4	A	902	3AM	C5-C4	-3.04	1.33	1.40
4	A	902	3AM	C4-N9	-3.03	1.33	1.37
4	A	902	3AM	C8-N9	-2.14	1.33	1.36

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	3AM	N3-C2-N1	-12.91	117.92	128.71
4	A	902	3AM	C4'-O4'-C1'	-5.78	103.47	109.75
4	A	902	3AM	N3-C4-N9	3.21	131.23	125.43
4	A	902	3AM	O4'-C4'-C3'	-2.47	99.27	104.88
4	A	902	3AM	O4'-C1'-N9	2.38	110.65	108.44
4	A	902	3AM	N7-C8-N9	-2.35	107.71	114.36
4	A	902	3AM	C5-C4-N3	-2.21	120.89	125.70
4	A	902	3AM	C2-N3-C4	2.03	119.78	114.01

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 ⓘ

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, 95th 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	602/677 (88%)	0.07	9 (1%) 70 71	33, 61, 97, 119	0
2	B	281/322 (87%)	-0.13	2 (0%) 84 86	36, 60, 89, 104	0
All	All	883/999 (88%)	0.00	11 (1%) 72 77	33, 61, 96, 119	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	526	LEU	3.2
1	A	576	VAL	3.1
1	A	410	VAL	3.0
2	B	166	VAL	3.0
1	A	822	ARG	2.7
1	A	699	PHE	2.5
1	A	521	LYS	2.4
1	A	537	PHE	2.4
1	A	311	ALA	2.3
2	B	10	ASP	2.3
1	A	530	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	901	1/1	0.16	1.56	53,53,53,53	0
4	3AM	A	902	23/23	0.18	-0.67	43,53,70,71	0

6.5 Other polymers

There are no such residues in this entry.