Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 PM GMT

PDB ID	:	3UR3
Title	:	Structure of the Cmr2 subunit of the CRISPR RNA silencing complex
Authors	:	Cocozaki, A.I.; Ramia, N.F.; Shao, Y.; Hale, C.R.; Terns, R.M.; Terns, M.P.; Li, H.
Deposited on	:	2011-11-21
Resolution	:	2.40 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:

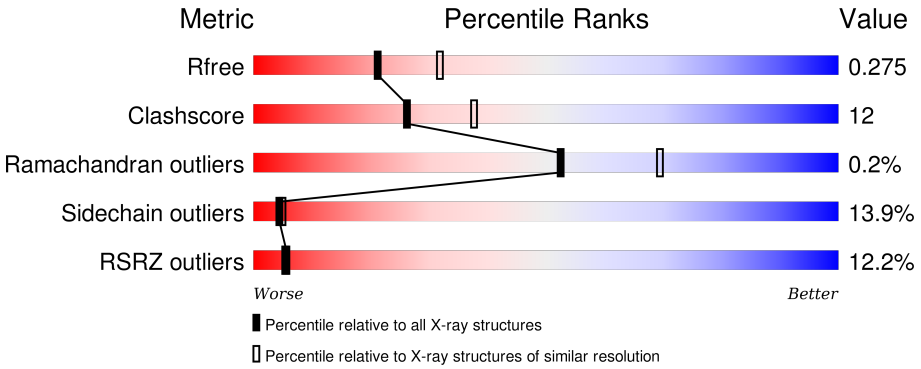
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	C	693	10% 53% 23% 21%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4502 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 Cmr2dHD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	548	4470	2907	740	810	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	179	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	180	ARG	-	EXPRESSION TAG	UNP Q8U1S6
C	181	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	182	SER	-	EXPRESSION TAG	UNP Q8U1S6
C	183	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	184	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	185	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	186	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	187	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	188	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	189	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	190	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	191	ALA	-	EXPRESSION TAG	UNP Q8U1S6
C	192	SER	-	EXPRESSION TAG	UNP Q8U1S6
C	193	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	194	THR	-	EXPRESSION TAG	UNP Q8U1S6
C	195	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	196	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	197	GLN	-	EXPRESSION TAG	UNP Q8U1S6
C	198	GLN	-	EXPRESSION TAG	UNP Q8U1S6
C	199	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	200	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	201	ARG	-	EXPRESSION TAG	UNP Q8U1S6
C	202	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	203	LEU	-	EXPRESSION TAG	UNP Q8U1S6
C	204	TYR	-	EXPRESSION TAG	UNP Q8U1S6
C	205	ASP	-	EXPRESSION TAG	UNP Q8U1S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	207	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	208	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	209	LYS	-	EXPRESSION TAG	UNP Q8U1S6
C	210	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	211	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	212	PRO	-	EXPRESSION TAG	UNP Q8U1S6
C	213	PHE	-	EXPRESSION TAG	UNP Q8U1S6
C	214	THR	-	EXPRESSION TAG	UNP Q8U1S6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Ca 2 2	0	0

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

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

- Molecule 4 is water.

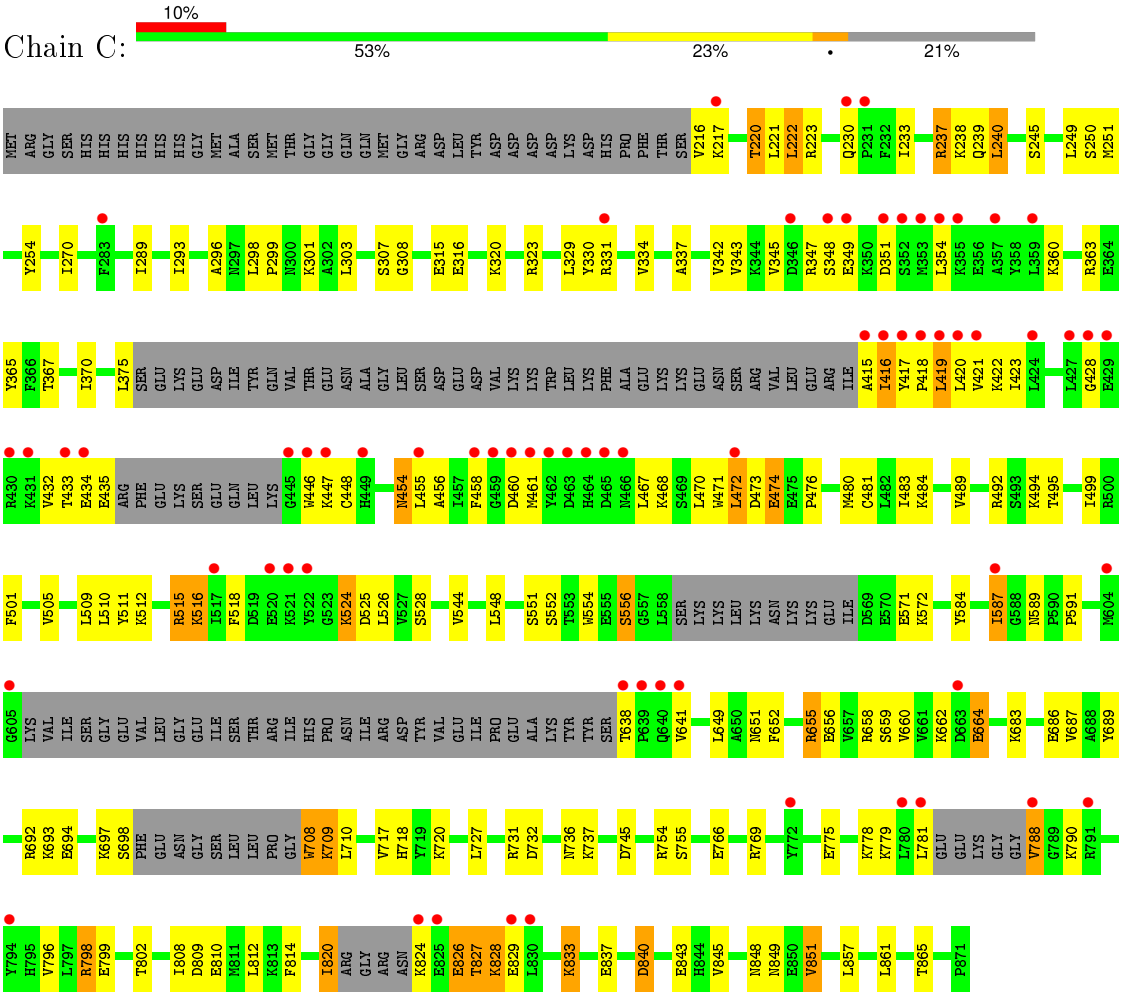
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	29	Total O 29 29	0	0

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: Cmr2dHD

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.64Å 80.21Å 143.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 2.40 49.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.9 (42.68-2.40) 82.8 (49.74-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.76 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.218 , 0.273 0.214 , 0.275	Depositor DCC
R_{free} test set	1870 reflections (6.85%)	DCC
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29245 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: 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	C	0.40	0/4559	0.53	0/6147

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	556	SER	Peptide
1	C	788	VAL	Peptide

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	C	4470	0	4571	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
3	C	1	0	0	0	0
4	C	29	0	0	1	0
All	All	4502	0	4571	111	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 12.

All (111) 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:C:233:ILE:HG12	1:C:245:SER:HB3	1.67	0.77
1:C:584:TYR:HB3	1:C:589:ASN:HD22	1.50	0.74
1:C:238:LYS:HD2	1:C:239:GLN:H	1.53	0.72
1:C:337:ALA:HA	1:C:342:VAL:HG13	1.70	0.71
1:C:516:LYS:N	1:C:516:LYS:HD2	2.06	0.71
1:C:820:ILE:HD11	1:C:827:THR:HG21	1.73	0.68
1:C:220:THR:HG21	1:C:308:GLY:HA2	1.75	0.68
1:C:289:ILE:HD11	1:C:293:ILE:HD13	1.75	0.68
1:C:238:LYS:HD2	1:C:239:GLN:N	2.10	0.67
1:C:417:TYR:N	1:C:418:PRO:HD2	2.11	0.66
1:C:448:CYS:HB2	1:C:476:PRO:O	1.98	0.64
1:C:468:LYS:HG3	1:C:474:GLU:HB3	1.79	0.63
1:C:584:TYR:HB3	1:C:589:ASN:ND2	2.15	0.62
1:C:238:LYS:CD	1:C:239:GLN:H	2.13	0.62
1:C:766:GLU:HB3	1:C:769:ARG:HH22	1.64	0.62
1:C:828:LYS:HG3	1:C:829:GLU:N	2.15	0.61
1:C:775:GLU:HA	1:C:778:LYS:HG3	1.82	0.61
1:C:331:ARG:O	1:C:334:VAL:HG22	2.01	0.61
1:C:509:LEU:HB3	1:C:515:ARG:HB2	1.83	0.60
1:C:718:HIS:CD2	1:C:754:ARG:HD3	2.36	0.59
1:C:709:LYS:HE2	1:C:745:ASP:HB2	1.85	0.59
1:C:511:TYR:HB3	1:C:591:PRO:HG3	1.86	0.58
1:C:342:VAL:HA	1:C:472:LEU:HD23	1.85	0.57
1:C:516:LYS:HD2	1:C:516:LYS:H	1.68	0.56
1:C:492:ARG:O	1:C:495:THR:O	2.24	0.56
1:C:694:GLU:OE1	1:C:697:LYS:HD3	2.06	0.56
1:C:718:HIS:HD2	1:C:720:LYS:HB2	1.70	0.55
1:C:840:ASP:O	1:C:843:GLU:HB3	2.05	0.55
1:C:471:TRP:CD2	1:C:476:PRO:HA	2.42	0.55
1:C:501:PHE:CE1	1:C:510:LEU:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:LYS:HG3	1:C:474:GLU:CB	2.38	0.53
1:C:315:GLU:HA	1:C:370:ILE:HD12	1.90	0.53
1:C:548:LEU:HD22	1:C:554:TRP:CZ2	2.44	0.53
1:C:692:ARG:HD3	1:C:710:LEU:HB3	1.91	0.53
1:C:468:LYS:HG3	1:C:474:GLU:HA	1.90	0.53
1:C:421:VAL:HG23	1:C:422:LYS:HD2	1.91	0.52
1:C:447:LYS:HA	1:C:455:LEU:HA	1.93	0.51
1:C:828:LYS:HG3	1:C:829:GLU:H	1.75	0.50
1:C:698:SER:C	1:C:708:TRP:HZ3	2.14	0.50
1:C:845:VAL:HG21	1:C:857:LEU:HB2	1.93	0.50
1:C:343:VAL:O	1:C:345:VAL:HG13	2.12	0.50
1:C:718:HIS:CD2	1:C:720:LYS:HB2	2.48	0.49
1:C:551:SER:HG	1:C:584:TYR:HE2	1.60	0.49
1:C:524:LYS:HZ3	1:C:524:LYS:H	1.59	0.49
1:C:238:LYS:HD2	1:C:238:LYS:HA	1.43	0.49
1:C:480:MET:CE	1:C:483:ILE:HD12	2.42	0.49
1:C:217:LYS:HB2	1:C:307:SER:HB3	1.95	0.48
1:C:323:ARG:HG2	1:C:363:ARG:HG2	1.94	0.48
1:C:471:TRP:CG	1:C:476:PRO:HA	2.48	0.48
1:C:251:MET:O	1:C:254:TYR:HB3	2.14	0.48
1:C:419:LEU:O	1:C:423:ILE:HG13	2.14	0.48
1:C:238:LYS:CD	1:C:239:GLN:N	2.75	0.47
1:C:480:MET:HE2	1:C:483:ILE:HD12	1.96	0.47
1:C:432:VAL:HG13	1:C:433:THR:H	1.79	0.47
1:C:551:SER:OG	1:C:584:TYR:CE2	2.66	0.47
1:C:417:TYR:O	1:C:421:VAL:HG13	2.14	0.47
1:C:240:LEU:HD13	1:C:499:ILE:HD11	1.96	0.47
1:C:320:LYS:HE2	1:C:320:LYS:HB2	1.72	0.47
1:C:833:LYS:HE3	1:C:837:GLU:HG3	1.96	0.47
1:C:861:LEU:O	1:C:865:THR:HG23	2.15	0.46
1:C:820:ILE:HD11	1:C:827:THR:CG2	2.43	0.46
1:C:468:LYS:HG3	1:C:474:GLU:CA	2.46	0.46
1:C:799:GLU:O	1:C:802:THR:O	2.33	0.46
1:C:808:ILE:O	1:C:812:LEU:HG	2.16	0.46
1:C:505:VAL:O	1:C:509:LEU:HG	2.16	0.46
1:C:222:LEU:O	1:C:303:LEU:HA	2.16	0.46
1:C:447:LYS:HB3	1:C:454:ASN:O	2.16	0.45
1:C:250:SER:OG	1:C:296:ALA:HB1	2.15	0.45
1:C:587:ILE:HD12	1:C:587:ILE:HA	1.78	0.45
1:C:652:PHE:HA	1:C:656:GLU:HG3	1.97	0.45
1:C:365:TYR:CD1	1:C:480:MET:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:TYR:N	1:C:418:PRO:CD	2.80	0.45
1:C:428:GLY:O	1:C:432:VAL:HG12	2.17	0.45
1:C:223:ARG:HD3	4:C:1018:HOH:O	2.17	0.45
1:C:448:CYS:HA	1:C:456:ALA:HB2	1.99	0.45
1:C:649:LEU:HA	1:C:649:LEU:HD23	1.84	0.44
1:C:329:LEU:HA	1:C:329:LEU:HD23	1.74	0.44
1:C:798:ARG:HA	1:C:798:ARG:HD3	1.45	0.44
1:C:415:ALA:C	1:C:417:TYR:H	2.21	0.44
1:C:418:PRO:O	1:C:421:VAL:HG22	2.18	0.44
1:C:216:VAL:HG12	1:C:217:LYS:HG3	2.00	0.44
1:C:420:LEU:HA	1:C:423:ILE:HD12	2.00	0.43
1:C:230:GLN:HG3	1:C:365:TYR:CE1	2.54	0.43
1:C:651:ASN:OD1	1:C:655:ARG:HG3	2.19	0.43
1:C:270:ILE:HB	1:C:303:LEU:HD12	2.00	0.43
1:C:221:LEU:HB2	1:C:375:LEU:HD11	2.00	0.43
1:C:420:LEU:HA	1:C:423:ILE:CG1	2.49	0.43
1:C:779:LYS:HE2	1:C:779:LYS:HB2	1.88	0.43
1:C:481:CYS:HA	1:C:484:LYS:HD3	2.01	0.42
1:C:455:LEU:HG	1:C:456:ALA:O	2.18	0.42
1:C:432:VAL:HG13	1:C:433:THR:N	2.34	0.42
1:C:766:GLU:HB3	1:C:769:ARG:HH12	1.84	0.42
1:C:494:LYS:HD2	1:C:494:LYS:HA	1.51	0.42
1:C:664:GLU:HG2	1:C:683:LYS:HG3	2.02	0.42
1:C:717:VAL:HG22	1:C:718:HIS:N	2.35	0.41
1:C:689:TYR:CE2	1:C:693:LYS:HE3	2.55	0.41
1:C:683:LYS:O	1:C:687:VAL:HG23	2.20	0.41
1:C:458:PHE:O	1:C:467:LEU:HD13	2.20	0.41
1:C:298:LEU:HA	1:C:299:PRO:HD3	1.82	0.41
1:C:849:ASN:OD1	1:C:851:VAL:HG13	2.21	0.41
1:C:237:ARG:HE	1:C:237:ARG:HB3	1.64	0.41
1:C:518:PHE:CZ	1:C:526:LEU:HD22	2.55	0.41
1:C:697:LYS:HG2	1:C:698:SER:N	2.34	0.41
1:C:810:GLU:HG2	1:C:814:PHE:CZ	2.55	0.41
1:C:330:TYR:O	1:C:334:VAL:HG13	2.21	0.41
1:C:766:GLU:HB3	1:C:769:ARG:NH2	2.34	0.40
1:C:824:LYS:HD2	1:C:824:LYS:HA	1.74	0.40
1:C:826:GLU:HG2	1:C:826:GLU:O	2.20	0.40
1:C:551:SER:OG	1:C:584:TYR:HE2	2.05	0.40
1:C:732:ASP:O	1:C:736:ASN:HB2	2.21	0.40
1:C:293:ILE:HA	1:C:293:ILE:HD12	1.92	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	C	532/693 (77%)	500 (94%)	31 (6%)	1 (0%)	52 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	ILE

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	C	489/617 (79%)	421 (86%)	68 (14%)	4 5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	220	THR
1	C	222	LEU
1	C	237	ARG
1	C	240	LEU
1	C	249	LEU
1	C	301	LYS
1	C	316	GLU
1	C	347	ARG
1	C	348	SER
1	C	349	GLU

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Mol	Chain	Res	Type
1	C	351	ASP
1	C	354	LEU
1	C	360	LYS
1	C	367	THR
1	C	416	ILE
1	C	419	LEU
1	C	434	GLU
1	C	435	GLU
1	C	446	TRP
1	C	454	ASN
1	C	460	ASP
1	C	461	MET
1	C	470	LEU
1	C	472	LEU
1	C	473	ASP
1	C	474	GLU
1	C	489	VAL
1	C	512	LYS
1	C	515	ARG
1	C	516	LYS
1	C	524	LYS
1	C	525	ASP
1	C	528	SER
1	C	544	VAL
1	C	552	SER
1	C	556	SER
1	C	571	GLU
1	C	572	LYS
1	C	587	ILE
1	C	638	THR
1	C	641	VAL
1	C	655	ARG
1	C	658	ARG
1	C	659	SER
1	C	660	VAL
1	C	662	LYS
1	C	664	GLU
1	C	686	GLU
1	C	708	TRP
1	C	709	LYS
1	C	727	LEU
1	C	731	ARG

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Mol	Chain	Res	Type
1	C	737	LYS
1	C	755	SER
1	C	781	LEU
1	C	788	VAL
1	C	790	LYS
1	C	796	VAL
1	C	798	ARG
1	C	809	ASP
1	C	820	ILE
1	C	826	GLU
1	C	827	THR
1	C	828	LYS
1	C	833	LYS
1	C	840	ASP
1	C	848	ASN
1	C	851	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	581	ASN
1	C	589	ASN
1	C	718	HIS

5.3.3 RNA (i)

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	C	548/693 (79%)	0.73	67 (12%) 5 5	46, 75, 132, 165	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	605	GLY	10.3
1	C	446	TRP	7.8
1	C	641	VAL	7.0
1	C	461	MET	6.6
1	C	230	GLN	5.9
1	C	420	LEU	5.6
1	C	464	HIS	5.6
1	C	417	TYR	5.5
1	C	460	ASP	5.4
1	C	427	LEU	5.3
1	C	353	MET	5.1
1	C	419	LEU	5.1
1	C	465	ASP	4.5
1	C	416	ILE	4.3
1	C	418	PRO	4.2
1	C	352	SER	4.2
1	C	604	MET	4.1
1	C	463	ASP	3.9
1	C	447	LYS	3.9
1	C	517	ILE	3.8
1	C	434	GLU	3.5
1	C	421	VAL	3.4
1	C	348	SER	3.4
1	C	640	GLN	3.3
1	C	587	ILE	3.3
1	C	433	THR	3.2
1	C	231	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	349	GLU	3.0
1	C	462	TYR	3.0
1	C	830	LEU	2.9
1	C	459	GLY	2.8
1	C	466	ASN	2.8
1	C	351	ASP	2.8
1	C	794	TYR	2.8
1	C	357	ALA	2.7
1	C	472	LEU	2.7
1	C	780	LEU	2.6
1	C	791	ARG	2.6
1	C	346	ASP	2.6
1	C	354	LEU	2.5
1	C	825	GLU	2.5
1	C	424	LEU	2.5
1	C	772	TYR	2.5
1	C	430	ARG	2.4
1	C	359	LEU	2.4
1	C	638	THR	2.4
1	C	663	ASP	2.3
1	C	829	GLU	2.3
1	C	824	LYS	2.3
1	C	781	LEU	2.3
1	C	520	GLU	2.3
1	C	355	LYS	2.2
1	C	522	TYR	2.2
1	C	788	VAL	2.2
1	C	429	GLU	2.2
1	C	639	PRO	2.1
1	C	449	HIS	2.1
1	C	283	PHE	2.1
1	C	445	GLY	2.1
1	C	431	LYS	2.1
1	C	415	ALA	2.1
1	C	217	LYS	2.1
1	C	428	GLY	2.0
1	C	331	ARG	2.0
1	C	455	LEU	2.0
1	C	521	LYS	2.0
1	C	458	PHE	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	CA	C	901	1/1	0.96	0.17	-0.20	81,81,81,81	0
3	ZN	C	903	1/1	0.98	0.14	-0.37	96,96,96,96	0
2	CA	C	902	1/1	0.89	0.20	-	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.