



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:47 PM GMT

PDB ID : 4W8J
Title : Structure of the full-length insecticidal protein Cry1Ac reveals intriguing details of toxin packaging into in vivo formed crystals
Authors : Evdokimov, A.G.; Moshiri, F.; Sturman, E.J.; Rydel, T.J.; Zheng, M.; Seale, J.W.; Franklin, S.
Deposited on : 2014-08-25
Resolution : 2.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

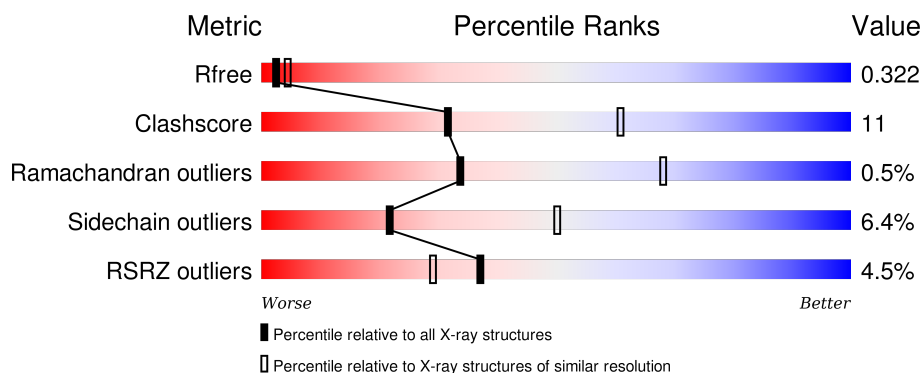
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1184	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8206 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 Pesticidal crystal protein cry1Ac.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			8152	5170	1406	1567	9			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	LEU	PHE	conflict	UNP M4LET9
A	462	VAL	PHE	conflict	UNP M4LET9
A	661	SER	CYS	engineered mutation	UNP M4LET9
A	730	SER	CYS	engineered mutation	UNP M4LET9
A	796	SER	CYS	engineered mutation	UNP M4LET9
A	802	SER	CYS	engineered mutation	UNP M4LET9
A	814	SER	CYS	engineered mutation	UNP M4LET9
A	816	SER	CYS	engineered mutation	UNP M4LET9
A	822	SER	CYS	engineered mutation	UNP M4LET9
A	837	SER	CYS	engineered mutation	UNP M4LET9
A	990	SER	CYS	engineered mutation	UNP M4LET9
A	1025	SER	CYS	engineered mutation	UNP M4LET9
A	1045	SER	CYS	engineered mutation	UNP M4LET9
A	1063	SER	CYS	engineered mutation	UNP M4LET9
A	1076	SER	CYS	engineered mutation	UNP M4LET9
A	1125	SER	CYS	engineered mutation	UNP M4LET9
A	1179	HIS	-	expression tag	UNP M4LET9
A	1180	HIS	-	expression tag	UNP M4LET9
A	1181	HIS	-	expression tag	UNP M4LET9
A	1182	HIS	-	expression tag	UNP M4LET9
A	1183	HIS	-	expression tag	UNP M4LET9
A	1184	HIS	-	expression tag	UNP M4LET9

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	K	0	0
			3	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

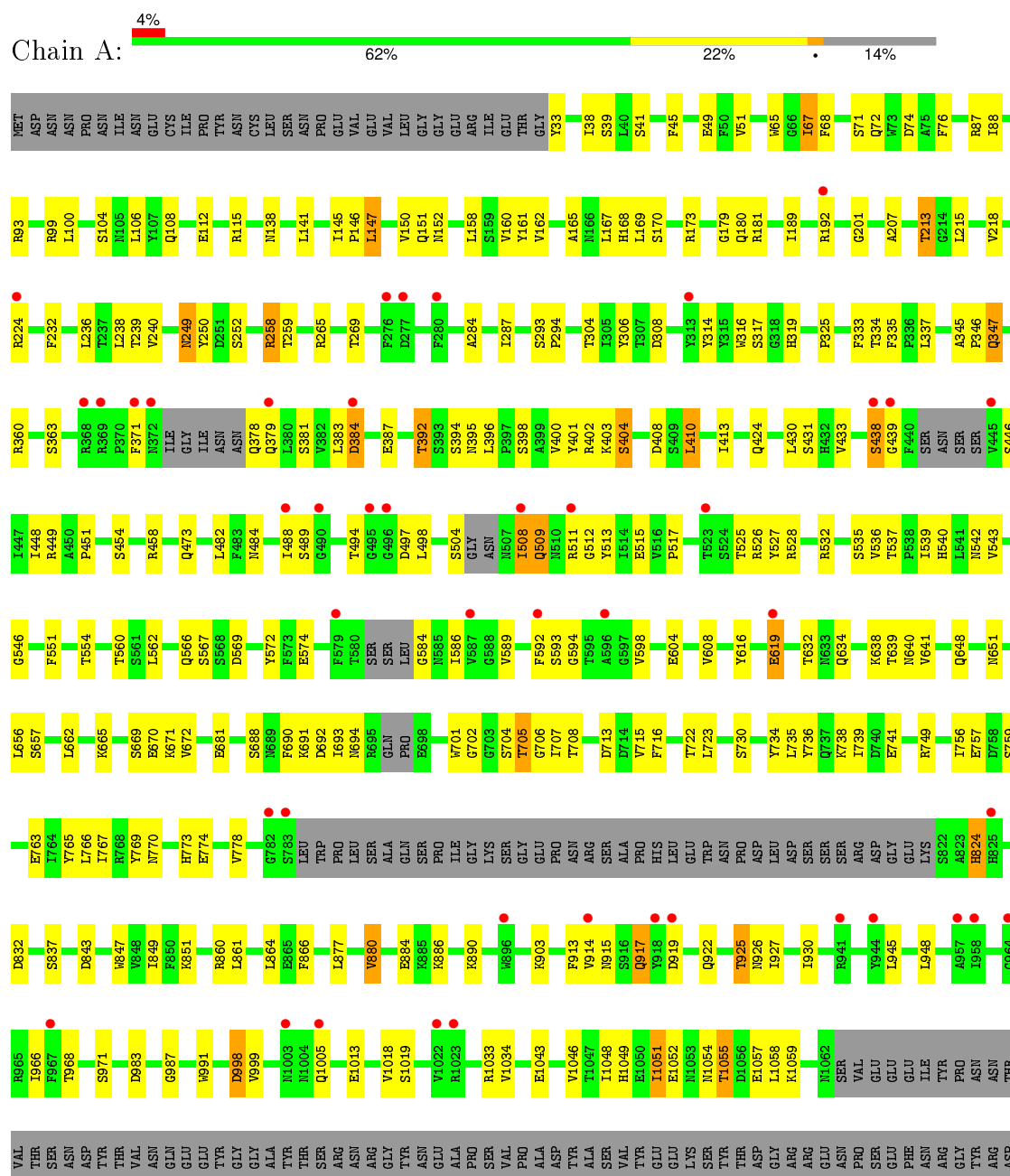
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		

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: Pesticidal crystal protein cry1Ac





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.31Å 87.31Å 266.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 2.78 39.18 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.8 (82.97-2.78) 98.9 (39.18-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.332 0.217 , 0.322	Depositor DCC
R_{free} test set	1340 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 26541 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8206	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: K, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/8335	0.71	0/11317

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	8152	0	7896	171	0
2	A	3	0	0	0	0
3	A	1	0	0	0	0
4	A	50	0	0	8	0
All	All	8206	0	7896	171	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 11.

All (171) 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:922:GLN:HB2	1:A:925:THR:CG2	2.03	0.88
1:A:722:THR:HG22	1:A:860:ARG:HG2	1.54	0.87
1:A:100:LEU:HD11	1:A:160:VAL:HG11	1.56	0.86
1:A:715:VAL:HG21	1:A:757:GLU:HG3	1.57	0.84
1:A:213:THR:HG22	4:A:1329:HOH:O	1.80	0.80
1:A:922:GLN:HB2	1:A:925:THR:HG23	1.63	0.78
1:A:74:ASP:OD1	1:A:93:ARG:NH2	2.15	0.78
1:A:1033:ARG:HB3	1:A:1172:GLU:HG2	1.68	0.76
1:A:508:ILE:HG12	1:A:511:ARG:HH21	1.49	0.75
1:A:346:PRO:O	1:A:347:GLN:HB3	1.86	0.75
1:A:100:LEU:HD11	1:A:160:VAL:CG1	2.17	0.75
1:A:713:ASP:HB3	1:A:716:PHE:H	1.52	0.73
1:A:927:ILE:HA	1:A:930:ILE:HD12	1.68	0.72
1:A:987:GLY:HA2	1:A:999:VAL:HG11	1.72	0.72
1:A:708:THR:HB	1:A:722:THR:OG1	1.91	0.71
1:A:707:ILE:HG12	1:A:723:LEU:HD22	1.71	0.70
1:A:917:GLN:HA	1:A:917:GLN:NE2	2.11	0.65
1:A:756:ILE:HG21	1:A:759:SER:HB2	1.77	0.65
1:A:566:GLN:O	1:A:569:ASP:HB2	1.97	0.65
1:A:1051:ILE:HD12	1:A:1051:ILE:H	1.62	0.64
1:A:394:SER:OG	1:A:395:ASN:N	2.31	0.64
1:A:1162:THR:HG22	1:A:1163:GLU:HG2	1.81	0.63
1:A:539:ILE:HG23	1:A:593:SER:HB2	1.81	0.63
1:A:656:LEU:HB2	1:A:665:LYS:HD2	1.79	0.62
1:A:151:GLN:O	1:A:152:ASN:HB2	1.99	0.62
1:A:713:ASP:OD1	1:A:715:VAL:N	2.30	0.61
1:A:517:PRO:HA	1:A:586:ILE:HG22	1.81	0.61
1:A:513:TYR:OH	1:A:515:GLU:HG3	2.01	0.60
1:A:861:LEU:HD13	1:A:864:LEU:HD21	1.83	0.59
1:A:917:GLN:HA	1:A:917:GLN:HE21	1.67	0.59
1:A:383:LEU:HD12	1:A:451:PRO:HG2	1.83	0.59
1:A:546:GLY:HA3	1:A:584:GLY:HA3	1.84	0.59
1:A:33:TYR:CD1	1:A:33:TYR:N	2.67	0.59
1:A:504:SER:OG	1:A:511:ARG:NH1	2.36	0.58
1:A:112:GLU:HG3	1:A:115:ARG:HH21	1.69	0.58
1:A:430:LEU:HD12	1:A:454:SER:O	2.04	0.58
1:A:1048:ILE:HA	1:A:1156:TRP:O	2.04	0.57
1:A:690:PHE:HB3	1:A:693:ILE:HD11	1.87	0.57
1:A:778:VAL:HG22	1:A:824:HIS:HB2	1.85	0.57
1:A:158:LEU:HD11	1:A:207:ALA:HA	1.87	0.56
1:A:948:LEU:HA	4:A:1320:HOH:O	2.06	0.56
1:A:45:PHE:CE1	1:A:49:GLU:HG3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:TYR:HB2	1:A:849:ILE:HB	1.87	0.55
1:A:1049:HIS:HB3	1:A:1055:THR:HB	1.87	0.55
1:A:41:SER:HA	4:A:1304:HOH:O	2.06	0.55
1:A:535:SER:HB3	1:A:598:VAL:HG23	1.89	0.54
1:A:536:VAL:HG13	1:A:562:LEU:HG	1.88	0.54
1:A:138:ASN:HD22	1:A:192:ARG:HH11	1.56	0.54
1:A:922:GLN:HB2	1:A:925:THR:HG22	1.89	0.54
1:A:314:TYR:HB2	1:A:402:ARG:NH2	2.23	0.53
1:A:1034:VAL:HG23	1:A:1058:LEU:HD12	1.89	0.53
1:A:769:TYR:N	4:A:1346:HOH:O	2.42	0.52
1:A:739:ILE:HD13	1:A:866:PHE:CD2	2.44	0.52
1:A:112:GLU:CD	1:A:115:ARG:HH21	2.12	0.52
1:A:269:THR:HG21	1:A:413:ILE:HD11	1.92	0.51
1:A:360:ARG:NH2	1:A:408:ASP:OD2	2.38	0.51
1:A:914:VAL:HG12	1:A:914:VAL:O	2.10	0.51
1:A:269:THR:CG2	1:A:413:ILE:HD11	2.40	0.51
1:A:1046:VAL:HG22	1:A:1159:ILE:HG12	1.92	0.51
1:A:87:ARG:HG3	1:A:88:ILE:N	2.25	0.51
1:A:360:ARG:HD2	1:A:410:LEU:HD13	1.92	0.51
1:A:616:TYR:O	1:A:619:GLU:HG3	2.10	0.51
1:A:384:ASP:OD1	1:A:384:ASP:N	2.43	0.51
1:A:439:GLY:HA2	1:A:449:ARG:NH1	2.25	0.51
1:A:100:LEU:HD21	1:A:160:VAL:HG13	1.92	0.50
1:A:378:GLN:HA	1:A:378:GLN:OE1	2.12	0.50
1:A:158:LEU:O	1:A:161:TYR:HB3	2.11	0.50
1:A:387:GLU:HG2	1:A:398:SER:OG	2.11	0.50
1:A:987:GLY:CA	1:A:999:VAL:HG11	2.42	0.50
1:A:488:ILE:HD12	1:A:489:SER:H	1.77	0.50
1:A:431:SER:HB3	1:A:454:SER:HB2	1.93	0.50
1:A:162:VAL:HG21	1:A:240:VAL:HG13	1.94	0.49
1:A:112:GLU:CG	1:A:115:ARG:HH21	2.25	0.49
1:A:236:LEU:O	1:A:240:VAL:HB	2.11	0.49
1:A:509:GLN:OE1	1:A:509:GLN:HA	2.13	0.49
1:A:99:ARG:HD2	1:A:147:LEU:HD13	1.94	0.49
1:A:138:ASN:HD22	1:A:192:ARG:NH1	2.10	0.48
1:A:634:GLN:HE22	1:A:671:LYS:HE3	1.78	0.48
1:A:39:SER:OG	1:A:239:THR:HG22	2.14	0.48
1:A:484:ASN:HB3	1:A:512:GLY:HA2	1.96	0.48
1:A:346:PRO:O	1:A:347:GLN:CB	2.58	0.48
1:A:998:ASP:OD1	1:A:998:ASP:N	2.47	0.48
1:A:345:ALA:HB1	1:A:346:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:THR:O	1:A:259:THR:HG23	2.14	0.47
1:A:991:TRP:CE3	1:A:1018:VAL:HG12	2.49	0.47
1:A:741:GLU:HG3	1:A:843:ASP:HA	1.96	0.47
1:A:738:LYS:HB2	1:A:847:TRP:CZ3	2.49	0.47
1:A:543:VAL:HG22	1:A:589:VAL:HG22	1.97	0.47
1:A:525:THR:HB	1:A:527:TYR:CE1	2.49	0.47
1:A:511:ARG:NH1	1:A:592:PHE:O	2.47	0.47
1:A:767:ILE:HB	1:A:847:TRP:HB2	1.95	0.47
1:A:201:GLY:HA2	1:A:567:SER:OG	2.15	0.47
1:A:1146:LEU:HD12	1:A:1146:LEU:C	2.35	0.47
1:A:38:ILE:HD12	1:A:76:PHE:HE1	1.78	0.47
1:A:693:ILE:O	1:A:694:ASN:HB2	2.15	0.46
1:A:968:THR:O	1:A:971:SER:HB2	2.16	0.46
1:A:1043:GLU:H	1:A:1162:THR:HB	1.80	0.46
1:A:319:HIS:NE2	1:A:433:VAL:O	2.44	0.45
1:A:232:PHE:CZ	1:A:236:LEU:HD22	2.52	0.45
1:A:51:VAL:HB	1:A:258:ARG:HG2	1.98	0.45
1:A:33:TYR:HD1	1:A:33:TYR:N	2.13	0.45
1:A:334:THR:OG1	1:A:335:PHE:N	2.49	0.45
1:A:67:ILE:HD12	1:A:67:ILE:HA	1.86	0.45
1:A:489:SER:HA	1:A:497:ASP:OD1	2.17	0.45
1:A:1057:GLU:OE1	1:A:1059:LYS:HE3	2.17	0.45
1:A:65:TRP:CE2	1:A:167:LEU:HD22	2.52	0.45
1:A:1033:ARG:HB3	1:A:1172:GLU:CG	2.44	0.45
1:A:504:SER:HB2	1:A:594:GLY:HA2	1.99	0.45
1:A:345:ALA:HB1	1:A:346:PRO:CD	2.47	0.44
1:A:215:LEU:HD13	1:A:232:PHE:HD1	1.81	0.44
1:A:387:GLU:HG3	1:A:400:VAL:HG22	2.00	0.44
1:A:335:PHE:HB2	4:A:1341:HOH:O	2.18	0.44
1:A:494:THR:HG21	1:A:498:LEU:HD21	1.98	0.44
1:A:532:ARG:CG	1:A:572:TYR:CE2	3.00	0.44
1:A:713:ASP:HB3	1:A:716:PHE:N	2.26	0.44
1:A:877:LEU:O	1:A:880:VAL:HG12	2.18	0.44
1:A:542:ASN:HA	1:A:551:PHE:O	2.18	0.44
1:A:705:THR:HG23	1:A:706:GLY:N	2.32	0.44
1:A:913:PHE:C	1:A:915:ASN:H	2.20	0.44
1:A:763:GLU:HB3	1:A:851:LYS:HB3	1.99	0.44
1:A:616:TYR:HB3	4:A:1345:HOH:O	2.17	0.44
1:A:141:LEU:HD13	1:A:168:HIS:HA	1.99	0.44
1:A:308:ASP:HB2	1:A:317:SER:HB3	1.99	0.44
1:A:638:LYS:HB2	1:A:641:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:SER:HB2	1:A:1158:GLU:HG2	2.00	0.44
1:A:387:GLU:HB2	1:A:404:SER:OG	2.17	0.44
1:A:504:SER:CB	1:A:594:GLY:HA2	2.48	0.43
1:A:438:SER:HB2	1:A:448:ILE:HD12	2.00	0.43
1:A:886:LYS:HE2	1:A:890:LYS:HD2	2.00	0.43
1:A:526:ARG:O	1:A:608:VAL:HG12	2.18	0.43
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.80	0.43
1:A:284:ALA:HA	1:A:287:ILE:HD12	2.00	0.43
1:A:473:GLN:HG2	1:A:604:GLU:HG2	1.99	0.43
1:A:173:ARG:O	1:A:173:ARG:HG2	2.18	0.43
1:A:293:SER:HB2	1:A:294:PRO:HD2	2.00	0.43
1:A:215:LEU:HD13	1:A:232:PHE:CD1	2.54	0.43
1:A:173:ARG:HD2	1:A:250:TYR:HD1	1.83	0.43
1:A:68:PHE:HA	1:A:72:GLN:HG3	2.00	0.43
1:A:536:VAL:HG23	1:A:537:THR:HG23	2.00	0.43
1:A:392:THR:HG21	1:A:396:LEU:HD13	2.01	0.43
1:A:532:ARG:HG2	1:A:572:TYR:CE2	2.54	0.43
1:A:648:GLN:O	1:A:651:ASN:HB2	2.19	0.42
1:A:528:ARG:HD3	1:A:574:GLU:HB3	2.01	0.42
1:A:539:ILE:HG22	1:A:540:HIS:N	2.34	0.42
1:A:702:GLY:HA3	1:A:736:TYR:CE1	2.55	0.42
1:A:851:LYS:HD2	1:A:948:LEU:HD13	2.01	0.42
1:A:379:GLN:HB2	1:A:446:SER:HB3	2.00	0.42
1:A:837:SER:OG	1:A:884:GLU:OE2	2.37	0.42
1:A:926:ASN:HB2	4:A:1347:HOH:O	2.19	0.42
1:A:749:ARG:HD3	1:A:832:ASP:HB3	2.00	0.42
1:A:165:ALA:O	1:A:169:LEU:HG	2.19	0.42
1:A:540:HIS:HA	1:A:554:THR:HA	2.02	0.42
1:A:45:PHE:CD1	1:A:49:GLU:HG3	2.54	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.87	0.41
1:A:104:SER:O	1:A:108:GLN:HG3	2.19	0.41
1:A:145:ILE:O	1:A:146:PRO:C	2.58	0.41
1:A:179:GLY:C	1:A:189:ILE:HD11	2.40	0.41
1:A:701:TRP:CE3	1:A:735:LEU:HG	2.56	0.41
1:A:662:LEU:HA	1:A:662:LEU:HD23	1.81	0.41
1:A:504:SER:OG	1:A:594:GLY:HA2	2.21	0.41
1:A:401:TYR:O	1:A:403:LYS:N	2.53	0.41
1:A:170:SER:HB3	1:A:250:TYR:CE1	2.55	0.41
1:A:639:THR:HG22	4:A:1309:HOH:O	2.21	0.41
1:A:325:PRO:HD3	1:A:333:PHE:HE1	1.86	0.41
1:A:316:TRP:CD1	1:A:316:TRP:C	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:OD1	1:A:249:ASN:N	2.52	0.41
1:A:306:TYR:CE2	1:A:337:LEU:HD11	2.56	0.41
1:A:702:GLY:HA3	1:A:736:TYR:CZ	2.56	0.40
1:A:704:SER:HB3	1:A:734:TYR:CE2	2.56	0.40
1:A:707:ILE:HG22	1:A:708:THR:N	2.36	0.40
1:A:669:SER:HA	1:A:672:VAL:HG12	2.04	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	1001/1184 (84%)	950 (95%)	46 (5%)	5 (0%)	34 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	917	GLN
1	A	1054	ASN
1	A	1052	GLU
1	A	1163	GLU

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	888/1036 (86%)	831 (94%)	57 (6%)	22	50

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	71	SER
1	A	147	LEU
1	A	150	VAL
1	A	180	GLN
1	A	181	ARG
1	A	213	THR
1	A	218	VAL
1	A	224	ARG
1	A	249	ASN
1	A	252	SER
1	A	258	ARG
1	A	265	ARG
1	A	304	THR
1	A	363	SER
1	A	371	PHE
1	A	381	SER
1	A	384	ASP
1	A	392	THR
1	A	404	SER
1	A	410	LEU
1	A	424	GLN
1	A	438	SER
1	A	458	ARG
1	A	482	LEU
1	A	508	ILE
1	A	509	GLN
1	A	560	THR
1	A	619	GLU
1	A	632	THR
1	A	640	ASN
1	A	657	SER
1	A	670	GLU
1	A	681	GLU
1	A	688	SER
1	A	691	LYS
1	A	692	ASP
1	A	705	THR

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Mol	Chain	Res	Type
1	A	730	SER
1	A	766	LEU
1	A	770	ASN
1	A	773	HIS
1	A	774	GLU
1	A	824	HIS
1	A	880	VAL
1	A	903	LYS
1	A	919	ASP
1	A	925	THR
1	A	945	LEU
1	A	966	ILE
1	A	983	ASP
1	A	998	ASP
1	A	1005	GLN
1	A	1013	GLU
1	A	1051	ILE
1	A	1055	THR
1	A	1155	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	194	ASN
1	A	301	ASN
1	A	770	ASN
1	A	855	GLN
1	A	917	GLN
1	A	1002	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	1017/1184 (85%)	0.41	46 (4%) 37 29	38, 52, 68, 92	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	PHE	6.8
1	A	783	SER	6.3
1	A	1138	PRO	5.6
1	A	379	GLN	4.9
1	A	369	ARG	4.5
1	A	508	ILE	4.3
1	A	592	PHE	4.1
1	A	280	PHE	3.7
1	A	277	ASP	3.4
1	A	825	HIS	3.3
1	A	1005	GLN	3.3
1	A	384	ASP	3.3
1	A	372	ASN	3.2
1	A	941	ARG	3.1
1	A	511	ARG	3.0
1	A	782	GLY	2.9
1	A	579	PHE	2.9
1	A	445	VAL	2.8
1	A	439	GLY	2.7
1	A	918	TYR	2.7
1	A	313	TYR	2.6
1	A	957	ALA	2.6
1	A	523	THR	2.6
1	A	488	ILE	2.6
1	A	1023	ARG	2.6
1	A	896	TRP	2.5
1	A	919	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	596	ALA	2.5
1	A	958	ILE	2.4
1	A	914	VAL	2.4
1	A	619	GLU	2.4
1	A	1153	ASP	2.4
1	A	967	PHE	2.3
1	A	490	GLY	2.3
1	A	1003	ASN	2.3
1	A	495	GLY	2.2
1	A	587	VAL	2.2
1	A	192	ARG	2.2
1	A	964	GLY	2.1
1	A	276	PHE	2.1
1	A	438	SER	2.1
1	A	496	GLY	2.1
1	A	224	ARG	2.1
1	A	944	TYR	2.1
1	A	368	ARG	2.1
1	A	1022	VAL	2.1

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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	A	1204	1/1	0.96	0.07	-3.03	90,90,90,90	0
2	K	A	1203	1/1	0.87	0.10	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	K	A	1201	1/1	0.91	0.19	-	84,84,84,84	0
2	K	A	1202	1/1	0.87	0.10	-	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.