Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 01:19 AM EDT

PDB ID	:	5BJS
Title	:	Apo ctPRC2 in an autoinhibited state
Authors	:	Bratkowski, M.A.; Liu, X.
Deposited on	:	2016-10-22
Resolution	:	2.19 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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 2.19 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		1.1%
RSRZ outliers		10.4%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
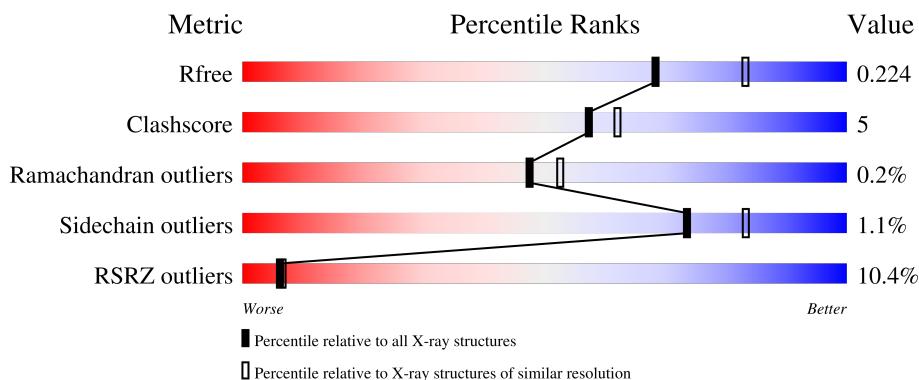
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	605	8% / 67% 9% 23%
2	B	937	9% / 79% 7% 15%
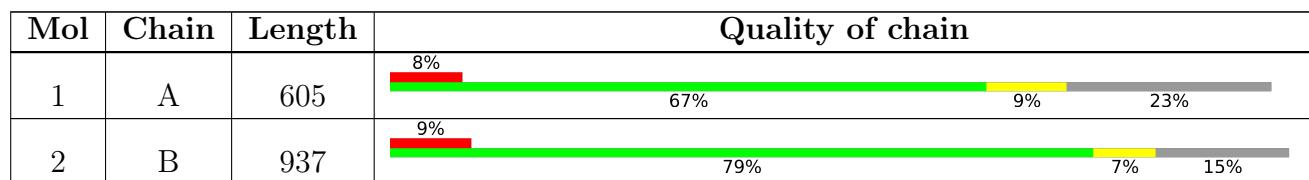
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10825 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 Polycomb Protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3654	2337	627	671	19	0	2	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	expression tag	UNP G0S8H7
A	-38	ALA	-	expression tag	UNP G0S8H7
A	-37	SER	-	expression tag	UNP G0S8H7
A	-36	ALA	-	expression tag	UNP G0S8H7
A	-35	TRP	-	expression tag	UNP G0S8H7
A	-34	SER	-	expression tag	UNP G0S8H7
A	-33	HIS	-	expression tag	UNP G0S8H7
A	-32	PRO	-	expression tag	UNP G0S8H7
A	-31	GLN	-	expression tag	UNP G0S8H7
A	-30	PHE	-	expression tag	UNP G0S8H7
A	-29	GLU	-	expression tag	UNP G0S8H7
A	-28	LYS	-	expression tag	UNP G0S8H7
A	-27	GLY	-	expression tag	UNP G0S8H7
A	-26	GLY	-	expression tag	UNP G0S8H7
A	-25	GLY	-	expression tag	UNP G0S8H7
A	-24	SER	-	expression tag	UNP G0S8H7
A	-23	GLY	-	expression tag	UNP G0S8H7
A	-22	GLY	-	expression tag	UNP G0S8H7
A	-21	GLY	-	expression tag	UNP G0S8H7
A	-20	SER	-	expression tag	UNP G0S8H7
A	-19	GLY	-	expression tag	UNP G0S8H7
A	-18	GLY	-	expression tag	UNP G0S8H7
A	-17	SER	-	expression tag	UNP G0S8H7
A	-16	ALA	-	expression tag	UNP G0S8H7
A	-15	TRP	-	expression tag	UNP G0S8H7
A	-14	SER	-	expression tag	UNP G0S8H7
A	-13	HIS	-	expression tag	UNP G0S8H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	PRO	-	expression tag	UNP G0S8H7
A	-11	GLN	-	expression tag	UNP G0S8H7
A	-10	PHE	-	expression tag	UNP G0S8H7
A	-9	GLU	-	expression tag	UNP G0S8H7
A	-8	LYS	-	expression tag	UNP G0S8H7
A	-7	LEU	-	expression tag	UNP G0S8H7
A	-6	GLU	-	expression tag	UNP G0S8H7
A	-5	VAL	-	expression tag	UNP G0S8H7
A	-4	LEU	-	expression tag	UNP G0S8H7
A	-3	PHE	-	expression tag	UNP G0S8H7
A	-2	GLN	-	expression tag	UNP G0S8H7
A	-1	GLY	-	expression tag	UNP G0S8H7
A	0	PRO	-	expression tag	UNP G0S8H7

- Molecule 2 is a protein called Histone-lysine N-methyltransferase EZH2, Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	801	6374	4015	1153	1165	41	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	expression tag	UNP G0SDW4
B	183	ASN	-	expression tag	UNP G0SDW4
B	184	HIS	-	expression tag	UNP G0SDW4
B	185	HIS	-	expression tag	UNP G0SDW4
B	186	HIS	-	expression tag	UNP G0SDW4
B	187	HIS	-	expression tag	UNP G0SDW4
B	188	HIS	-	expression tag	UNP G0SDW4
B	189	HIS	-	expression tag	UNP G0SDW4
B	190	ALA	-	expression tag	UNP G0SDW4
B	2524	LEU	-	linker	UNP G0SDW4
B	2525	VAL	-	linker	UNP G0SDW4
B	2526	PRO	-	linker	UNP G0SDW4
B	2527	ARG	-	linker	UNP G0SDW4
B	2528	GLY	-	linker	UNP G0SDW4
B	2529	SER	-	linker	UNP G0SDW4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	8	Total 8	Zn 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	298	Total 298	O 298	0	0
4	B	491	Total 491	O 491	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Polycomb Protein EED
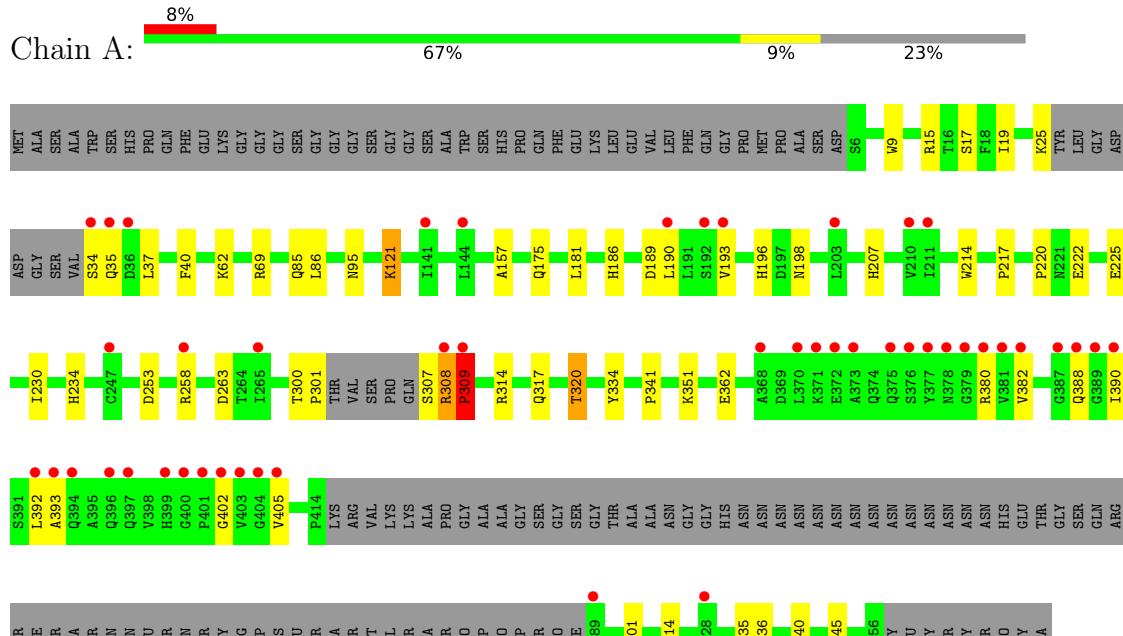
- Molecule 2: Histone-lysine N-methyltransferase EZH2, Polycomb protein SUZ12

S665 D666 I672 C685 D688 H705 E710 C713 Q738 G743 A806 V837 E840 V846 F847 D848 GLU GLU N851 F857 Y893 H896 T926 K927 K928 L929 V930 E931 R932 N933 GLU GLN SER GLY ALA GLU THR THR PRO GLN GLN PRO LYS

ARG ALA ASN GLY LEU VAL PRO ARG GLY SER GLU VAL MET LEU PRO GLY ARG GLY VAL PRO LYS LYS PRO LEU ARG ARG PRO LYS ARG R2549 I2580 L2585 F2629 V2633 A2655 R2661 V2668 L2682 R2683 E2684 GLN GLY VAL ILE GLU GLY GLY
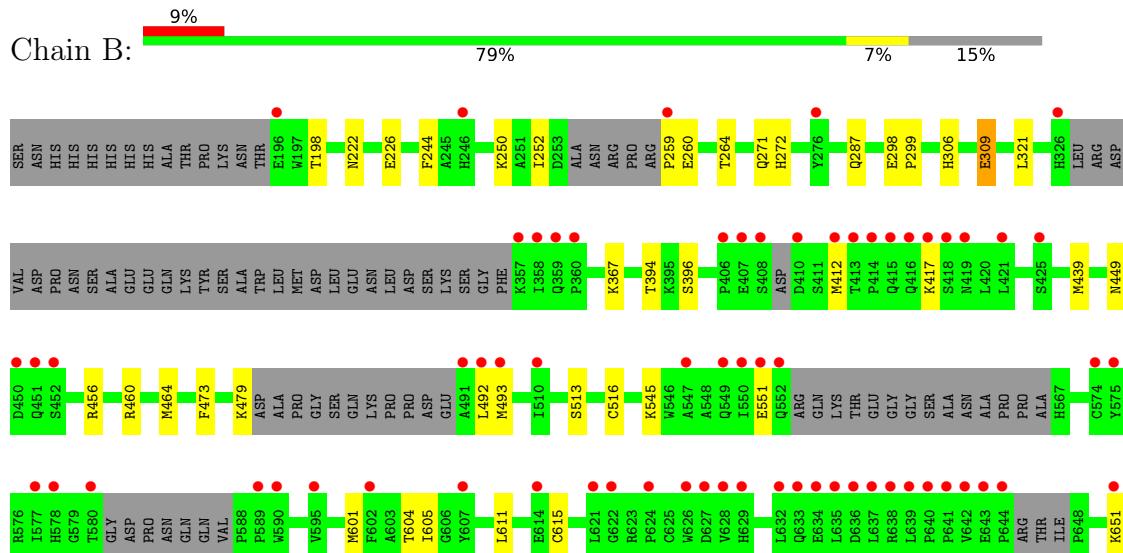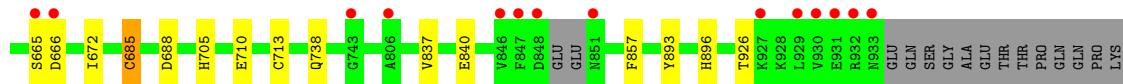
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	117.78Å 137.90Å 223.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.45 – 2.19 43.45 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.9 (43.45-2.19) 95.9 (43.45-2.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.173 , 0.224 0.173 , 0.224	Depositor DCC
R_{free} test set	4384 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å²)	33.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 54.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10825	wwPDB-VP
Average B, all atoms (Å²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/3766	0.59	0/5128
2	B	0.39	1/6518 (0.0%)	0.54	0/8810
All	All	0.41	1/10284 (0.0%)	0.56	0/13938

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	685	CYS	CB-SG	-7.20	1.70	1.82

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	PRO	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	A	3654	0	3514	46	0
2	B	6374	0	6213	55	0
3	B	8	0	0	0	0
4	A	298	0	0	6	0
4	B	491	0	0	4	0
All	All	10825	0	9727	96	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 5.

All (96) 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)
2:B:492:LEU:HD13	2:B:493:MET:CE	1.96	0.96
2:B:837:VAL:HG13	2:B:926:THR:HG22	1.52	0.90
1:A:196:HIS:HD2	1:A:198:ASN:H	1.19	0.89
2:B:492:LEU:CD1	2:B:493:MET:CE	2.52	0.86
1:A:15:ARG:HH22	2:B:271:GLN:HE21	1.27	0.83
2:B:604:THR:HG21	2:B:2655:ALA:HA	1.63	0.80
2:B:492:LEU:CD1	2:B:493:MET:HE3	2.12	0.78
2:B:493:MET:HA	2:B:493:MET:HE2	1.64	0.78
2:B:222:ASN:O	2:B:226:GLU:HG3	1.85	0.76
1:A:320:THR:HG21	4:A:617:HOH:O	1.85	0.76
2:B:492:LEU:CD1	2:B:493:MET:HE1	2.16	0.75
2:B:412:MET:HB3	2:B:417:LYS:HZ1	1.54	0.73
2:B:492:LEU:HD13	2:B:493:MET:HE3	1.72	0.72
2:B:198:THR:HA	2:B:439:MET:CE	2.20	0.71
2:B:840:GLU:OE1	2:B:926:THR:HG23	1.94	0.66
2:B:309:GLU:HG2	2:B:2580:ILE:HG12	1.76	0.66
2:B:492:LEU:HD13	2:B:493:MET:HE1	1.75	0.65
2:B:492:LEU:HD12	2:B:493:MET:CE	2.28	0.64
1:A:15:ARG:NH2	2:B:271:GLN:HE21	1.96	0.64
2:B:493:MET:CE	2:B:493:MET:HA	2.27	0.64
1:A:196:HIS:CD2	1:A:198:ASN:H	2.09	0.63
1:A:196:HIS:HE1	1:A:253:ASP:OD1	1.83	0.62
2:B:252:ILE:HD13	2:B:259:PRO:HG3	1.82	0.61
1:A:85:GLN:HE21	1:A:86:LEU:H	1.48	0.61
1:A:382:VAL:CG1	1:A:405:VAL:HG12	2.31	0.61
2:B:298:GLU:HG3	2:B:299:PRO:HD2	1.83	0.61
2:B:492:LEU:HD12	2:B:493:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:665:SER:OG	2:B:666:ASP:N	2.35	0.59
2:B:412:MET:HB3	2:B:417:LYS:NZ	2.17	0.59
2:B:264:THR:HG21	2:B:287:GLN:OE1	2.03	0.59
2:B:601:MET:O	2:B:605:ILE:HG12	2.04	0.58
1:A:95:ASN:HD21	1:A:121:LYS:NZ	2.03	0.57
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.40	0.56
1:A:234:HIS:HD2	4:A:737:HOH:O	1.89	0.56
1:A:220:PRO:HB2	1:A:222:GLU:HG2	1.88	0.55
2:B:394:THR:HG22	2:B:396:SER:N	2.22	0.55
1:A:217:PRO:HD3	1:A:230:ILE:HD11	1.88	0.54
1:A:380:ARG:NH2	1:A:402:GLY:O	2.38	0.54
2:B:611:LEU:HD11	2:B:2668:VAL:HB	1.89	0.54
2:B:412:MET:HB3	2:B:417:LYS:CE	2.38	0.53
2:B:545:LYS:HB2	2:B:2661:ARG:HD2	1.90	0.53
2:B:2684:GLU:N	2:B:2684:GLU:OE2	2.41	0.53
1:A:392:LEU:CD1	1:A:405:VAL:HG23	2.39	0.53
2:B:412:MET:HB3	2:B:417:LYS:HE3	1.91	0.53
2:B:198:THR:HA	2:B:439:MET:HE3	1.92	0.51
2:B:604:THR:HG21	2:B:2655:ALA:CA	2.36	0.51
1:A:25:LYS:HD2	1:A:35:GLN:HA	1.91	0.51
1:A:314:ARG:HH11	1:A:317:GLN:HE21	1.58	0.51
1:A:320:THR:CG2	1:A:320:THR:O	2.59	0.50
1:A:62:LYS:HE3	4:A:815:HOH:O	2.11	0.50
1:A:535:GLU:HG2	1:A:536:TRP:CD1	2.47	0.50
1:A:95:ASN:HD21	1:A:121:LYS:HZ1	1.61	0.49
1:A:181:LEU:HD13	1:A:214:TRP:CG	2.48	0.49
2:B:551:GLU:O	2:B:551:GLU:HG3	2.13	0.49
2:B:367:LYS:HG3	4:B:8545:HOH:O	2.11	0.48
2:B:306:HIS:HD2	4:B:8525:HOH:O	1.96	0.48
2:B:394:THR:HG22	2:B:396:SER:H	1.78	0.48
2:B:893:TYR:CE1	2:B:896:HIS:HA	2.50	0.46
2:B:710:GLU:HB2	4:B:8524:HOH:O	2.14	0.46
1:A:225:GLU:HG3	4:A:710:HOH:O	2.16	0.45
1:A:85:GLN:HE22	2:B:250:LYS:NZ	2.15	0.45
1:A:17:SER:HB2	2:B:272:HIS:NE2	2.32	0.44
1:A:263:ASP:C	1:A:320:THR:HG22	2.37	0.44
1:A:157:ALA:HB2	1:A:193:VAL:HB	1.99	0.44
2:B:685:CYS:HB2	2:B:713:CYS:HB3	1.99	0.44
2:B:651:LYS:HB2	2:B:651:LYS:HE3	1.85	0.44
1:A:300:THR:HA	1:A:301:PRO:HD3	1.83	0.44
1:A:388:GLN:C	1:A:390:ILE:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG12	1:A:545:ARG:HG2	2.00	0.43
1:A:234:HIS:CD2	4:A:737:HOH:O	2.69	0.43
1:A:382:VAL:HG13	1:A:405:VAL:HG12	2.01	0.43
2:B:493:MET:CE	2:B:493:MET:CA	2.94	0.43
2:B:2629:PHE:O	2:B:2633:VAL:HG23	2.18	0.43
1:A:189:ASP:HB2	1:A:207:HIS:CD2	2.54	0.42
1:A:308:ARG:N	1:A:309:PRO:HD2	2.34	0.42
2:B:460:ARG:O	2:B:464:MET:HG2	2.19	0.42
2:B:545:LYS:CB	2:B:2661:ARG:HD2	2.49	0.42
2:B:412:MET:HG2	2:B:473:PHE:HE2	1.83	0.42
1:A:9:TRP:CH2	1:A:362:GLU:HG3	2.54	0.42
2:B:513:SER:HB3	2:B:516:CYS:HB3	2.01	0.42
1:A:258:ARG:HG3	4:A:617:HOH:O	2.19	0.42
1:A:307:SER:C	1:A:309:PRO:HD2	2.40	0.42
1:A:308:ARG:HA	1:A:308:ARG:HD3	1.93	0.42
2:B:551:GLU:O	2:B:551:GLU:CG	2.66	0.42
1:A:334:TYR:O	1:A:341:PRO:HA	2.19	0.41
1:A:392:LEU:HA	1:A:392:LEU:HD12	1.76	0.41
1:A:392:LEU:HD11	1:A:405:VAL:HG23	2.03	0.41
2:B:615:CYS:HB2	4:B:8519:HOH:O	2.21	0.41
1:A:34:SER:OG	1:A:37:LEU:HD12	2.20	0.41
1:A:40:PHE:CB	1:A:540:VAL:HB	2.51	0.41
1:A:390:ILE:HD12	1:A:390:ILE:N	2.36	0.41
2:B:449:ASN:HA	2:B:456:ARG:HB2	2.03	0.41
2:B:321:LEU:HD12	2:B:321:LEU:HA	1.84	0.40
1:A:501:MET:CE	1:A:514:HIS:HA	2.51	0.40
2:B:672:ILE:HG23	2:B:705:HIS:HB2	2.02	0.40
1:A:69:ARG:NH2	2:B:244:PHE:O	2.54	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	458/605 (76%)	440 (96%)	16 (4%)	2 (0%)	34	35
2	B	781/937 (83%)	757 (97%)	24 (3%)	0	100	100
All	All	1239/1542 (80%)	1197 (97%)	40 (3%)	2 (0%)	47	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	PRO
1	A	393	ALA

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	389/495 (79%)	384 (99%)	5 (1%)	69	79
2	B	684/816 (84%)	677 (99%)	7 (1%)	76	85
All	All	1073/1311 (82%)	1061 (99%)	12 (1%)	73	83

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	175	GLN
1	A	308	ARG
1	A	320	THR
1	A	351	LYS
2	B	260	GLU
2	B	309	GLU
2	B	479	LYS
2	B	688	ASP
2	B	738	GLN
2	B	857	PHE
2	B	2549	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	95	ASN
1	A	142	ASN
1	A	196	HIS
1	A	234	HIS
1	A	317	GLN
1	A	375	GLN
1	A	544	ASN
1	A	550	GLN
2	B	271	GLN
2	B	306	HIS
2	B	752	ASN
2	B	895	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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, 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(Å²)	Q<0.9
1	A	464/605 (76%)	0.47	47 (10%)	7	7	19, 33, 87, 129	0
2	B	801/937 (85%)	0.38	85 (10%)	6	6	22, 44, 88, 114	0
All	All	1265/1542 (82%)	0.41	132 (10%)	6	6	19, 40, 88, 129	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	9.4
1	A	401	PRO	8.6
2	B	635	LEU	7.9
1	A	400	GLY	7.5
1	A	393	ALA	7.2
2	B	637	LEU	6.4
1	A	392	LEU	6.2
2	B	638	ARG	5.7
1	A	379	GLY	5.3
2	B	639	LEU	5.3
2	B	492	LEU	5.2
1	A	378	ASN	4.9
2	B	930	VAL	4.9
2	B	933	ASN	4.9
2	B	641	PRO	4.9
2	B	418	SER	4.8
2	B	626	TRP	4.7
2	B	326	HIS	4.7
2	B	929	LEU	4.6
2	B	607	TYR	4.6
2	B	580	THR	4.5
2	B	491	ALA	4.4
2	B	414	PRO	4.4
1	A	387	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	402	GLY	4.3
2	B	636	ASP	4.2
1	A	380	ARG	4.1
2	B	575	TYR	4.1
1	A	309	PRO	4.0
1	A	34	SER	4.0
1	A	389	GLY	4.0
2	B	547	ALA	4.0
2	B	931	GLU	4.0
2	B	640	PRO	3.9
2	B	589	PRO	3.9
2	B	644	PRO	3.9
2	B	421	LEU	3.9
2	B	358	ILE	3.8
2	B	412	MET	3.8
2	B	577	ILE	3.8
2	B	642	VAL	3.7
1	A	405	VAL	3.7
2	B	413	THR	3.7
1	A	375	GLN	3.6
2	B	408	SER	3.6
2	B	2682	LEU	3.6
1	A	397	GLN	3.6
1	A	372	GLU	3.5
2	B	629	HIS	3.5
1	A	377	TYR	3.5
2	B	634	GLU	3.4
2	B	632	LEU	3.4
1	A	36	ASP	3.4
2	B	2549	ARG	3.4
1	A	382	VAL	3.4
2	B	259	PRO	3.3
2	B	602	PHE	3.3
2	B	643	GLU	3.3
2	B	622	GLY	3.2
1	A	371	LYS	3.2
2	B	666	ASP	3.2
2	B	551	GLU	3.2
2	B	419	ASN	3.2
2	B	848	ASP	3.2
2	B	595	VAL	3.2
2	B	743	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	394	GLN	3.1
2	B	574	CYS	3.1
2	B	578	HIS	3.1
1	A	373	ALA	3.0
2	B	633	GLN	3.0
2	B	932	ARG	3.0
2	B	425	SER	3.0
2	B	550	ILE	2.9
2	B	628	VAL	2.9
1	A	190	LEU	2.9
1	A	308	ARG	2.9
1	A	376	SER	2.9
2	B	410	ASP	2.9
1	A	370	LEU	2.9
2	B	359	GLN	2.9
2	B	590	TRP	2.9
1	A	489	GLY	2.8
1	A	368	ALA	2.8
2	B	847	PHE	2.7
2	B	406	PRO	2.7
2	B	450	ASP	2.7
2	B	452	SER	2.7
2	B	651	LYS	2.7
2	B	417	LYS	2.6
2	B	806	ALA	2.6
1	A	399	HIS	2.6
2	B	196	GLU	2.6
2	B	851	ASN	2.6
1	A	390	ILE	2.6
2	B	624	PRO	2.6
1	A	265	ILE	2.6
2	B	614	GLU	2.5
1	A	141	ILE	2.5
2	B	627	ASP	2.5
1	A	388	GLN	2.5
2	B	552	GLN	2.5
2	B	357	LYS	2.5
1	A	203	LEU	2.4
2	B	846	VAL	2.4
2	B	2683	ARG	2.4
2	B	493	MET	2.4
2	B	665	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	404	GLY	2.4
1	A	144	LEU	2.4
2	B	415	GLN	2.3
2	B	246	HIS	2.3
1	A	211	ILE	2.3
1	A	35	GLN	2.3
2	B	416	GLN	2.2
2	B	2585	LEU	2.2
2	B	621	LEU	2.2
2	B	360	PRO	2.2
2	B	549	GLN	2.2
1	A	210	VAL	2.1
2	B	276	TYR	2.1
2	B	510	ILE	2.1
1	A	258	ARG	2.1
1	A	396	GLN	2.1
1	A	193	VAL	2.1
1	A	247	CYS	2.1
1	A	528	VAL	2.1
2	B	927	LYS	2.1
1	A	192	SER	2.0
2	B	451	GLN	2.0
2	B	407	GLU	2.0
1	A	381	VAL	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 monosaccharides 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. 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	B-factors($Å^2$)	Q<0.9
3	ZN	B	8008	1/1	0.98	0.04	67,67,67,67	0
3	ZN	B	8004	1/1	0.99	0.06	42,42,42,42	0
3	ZN	B	8006	1/1	0.99	0.07	37,37,37,37	0
3	ZN	B	8002	1/1	0.99	0.12	32,32,32,32	0
3	ZN	B	8005	1/1	1.00	0.06	41,41,41,41	0
3	ZN	B	8003	1/1	1.00	0.09	32,32,32,32	0
3	ZN	B	8007	1/1	1.00	0.15	28,28,28,28	0
3	ZN	B	8001	1/1	1.00	0.12	31,31,31,31	0

6.5   Other polymers ⓘ

There are no such residues in this entry.