



# Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 08:22 PM JST

PDB ID : 9KZR / pdb\_00009kzr  
Title : Anti-CRISPR protein AcrIIA7  
Authors : Lee, S.Y.; Park, H.H.  
Deposited on : 2024-12-11  
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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

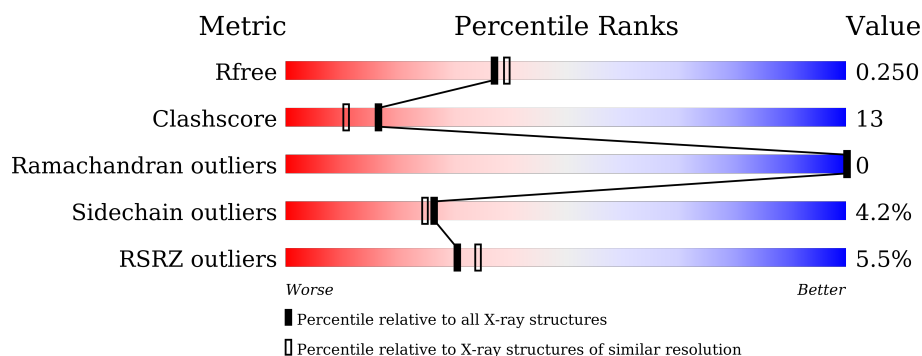
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	158	<div> <div>8%</div> <div>70% 21% .. 7%</div> </div>
1	B	158	<div> <div>%</div> <div>65% 24% 6% ..</div> </div>
1	C	158	<div> <div>3%</div> <div>79% 16% ...</div> </div>
1	D	158	<div> <div>8%</div> <div>62% 25% 5% • 6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4808 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 AcrIIA7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	Se	0	0	0
			1143	720	193	222	2	6			
1	B	152	Total	C	N	O	S	Se	0	0	0
			1189	749	200	231	2	7			
1	C	155	Total	C	N	O	S	Se	0	0	0
			1216	766	209	232	2	7			
1	D	149	Total	C	N	O	S	Se	0	0	0
			1158	730	194	226	2	6			

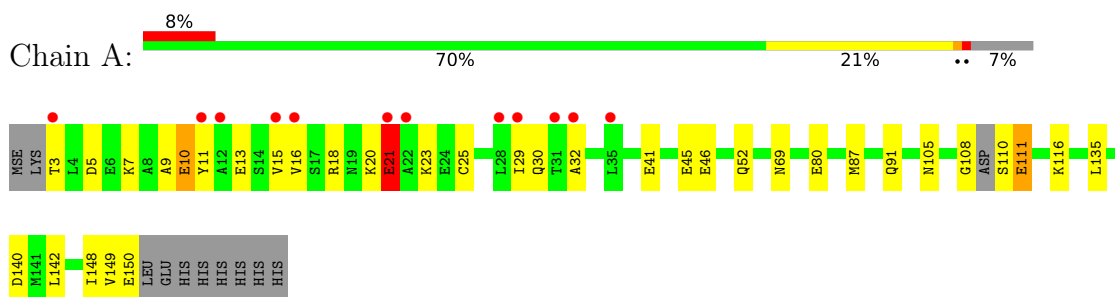
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	24	Total	O	0	0
			24	24		
2	C	31	Total	O	0	0
			31	31		
2	D	16	Total	O	0	0
			16	16		

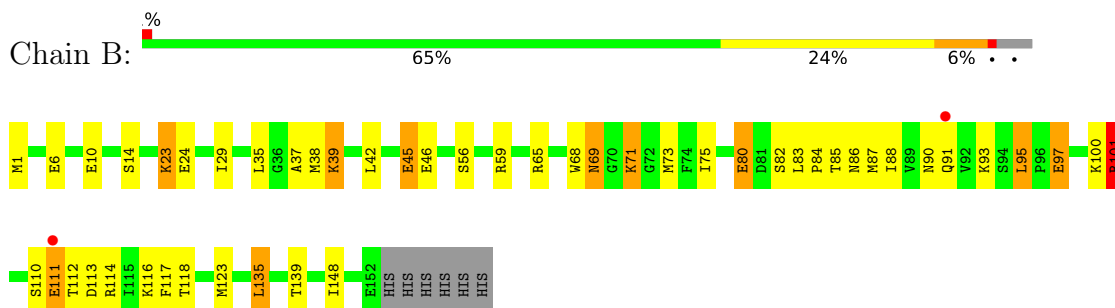
### 3 Residue-property plots [i](#)

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.

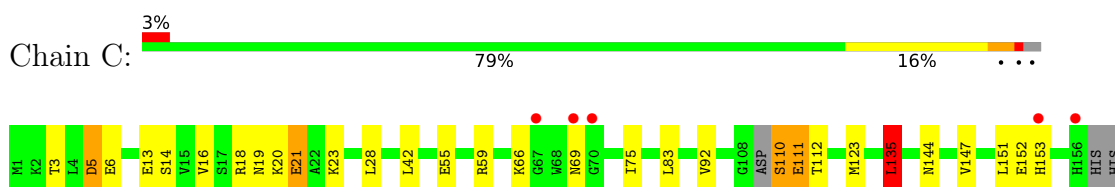
#### • Molecule 1: AcrIIA7



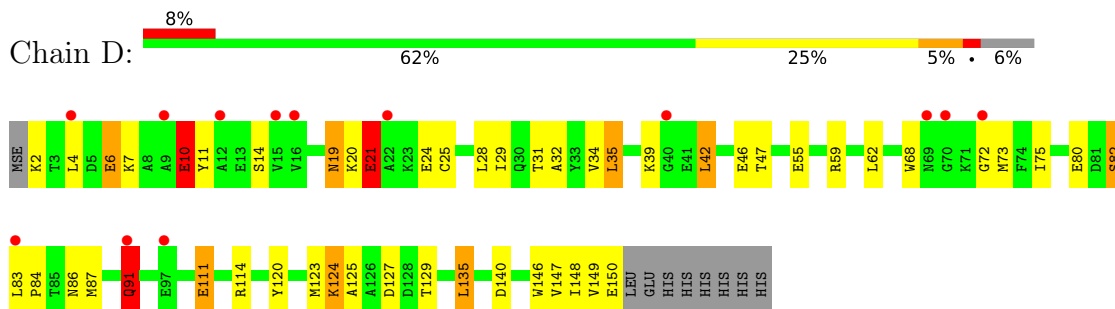
#### • Molecule 1: AcrIIA7



#### • Molecule 1: AcrIIA7



#### • Molecule 1: AcrIIA7



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.79Å 77.83Å 133.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 2.16 29.32 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.32-2.16) 99.9 (29.32-2.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.201 , 0.251 0.201 , 0.250	Depositor DCC
$R_{free}$ test set	1571 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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

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	1.10	0/1156	1.38	9/1549 (0.6%)
1	B	1.12	1/1203 (0.1%)	1.42	25/1611 (1.6%)
1	C	1.13	2/1232 (0.2%)	1.26	7/1649 (0.4%)
1	D	1.09	1/1172 (0.1%)	1.41	14/1571 (0.9%)
All	All	1.11	4/4763 (0.1%)	1.37	55/6380 (0.9%)

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	2
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	LEU	CA-C	-7.86	1.45	1.52
1	B	38	MSE	CA-C	-5.97	1.44	1.52
1	C	135	LEU	CB-CG	5.83	1.65	1.53
1	D	135	LEU	CB-CG	5.37	1.64	1.53

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	CG-CD-NE	14.48	143.85	112.00
1	A	21	GLU	CB-CG-CD	-13.21	90.14	112.60
1	D	10	GLU	CA-CB-CG	10.97	136.04	114.10
1	A	21	GLU	CA-CB-CG	10.42	134.95	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	GLU	CB-CA-C	-10.25	91.94	110.70
1	A	21	GLU	N-CA-CB	-9.94	94.93	110.44
1	D	10	GLU	CB-CA-C	-9.82	95.09	110.81
1	D	20	LYS	CA-C-N	9.73	135.41	120.82
1	D	20	LYS	C-N-CA	9.73	135.41	120.82
1	A	18	ARG	CA-CB-CG	9.53	133.17	114.10
1	C	111	GLU	CA-CB-CG	9.19	132.48	114.10
1	D	21	GLU	CB-CG-CD	-9.06	97.20	112.60
1	B	39	LYS	CB-CA-C	8.88	124.95	109.15
1	A	46	GLU	CB-CA-C	-8.68	94.92	110.36
1	C	6	GLU	CA-CB-CG	-8.56	96.98	114.10
1	B	97	GLU	CA-CB-CG	8.54	131.18	114.10
1	D	91	GLN	CB-CA-C	-8.28	97.75	110.83
1	B	39	LYS	N-CA-CB	-8.05	98.90	110.81
1	B	111	GLU	CA-CB-CG	8.05	130.20	114.10
1	B	45	GLU	CB-CG-CD	8.00	126.20	112.60
1	B	71	LYS	CB-CG-CD	7.70	129.00	111.30
1	B	23	LYS	CA-C-N	7.26	130.73	120.28
1	B	23	LYS	C-N-CA	7.26	130.73	120.28
1	D	10	GLU	CB-CG-CD	-7.08	100.57	112.60
1	A	46	GLU	N-CA-C	-7.06	99.77	110.14
1	A	46	GLU	CB-CG-CD	6.86	124.26	112.60
1	B	45	GLU	N-CA-C	-6.78	104.90	113.72
1	D	21	GLU	CB-CA-C	-6.65	99.70	110.74
1	B	111	GLU	CB-CG-CD	6.44	123.55	112.60
1	B	111	GLU	CB-CA-C	-6.44	99.73	110.68
1	D	6	GLU	CA-CB-CG	-6.22	101.66	114.10
1	C	135	LEU	CD1-CG-CD2	-6.11	97.36	110.80
1	D	19	ASN	N-CA-C	-6.01	99.27	108.76
1	D	80	GLU	CA-CB-CG	5.96	126.01	114.10
1	B	97	GLU	CB-CA-C	5.93	120.64	110.79
1	D	10	GLU	CG-CD-OE1	-5.86	104.91	118.40
1	B	95	LEU	CA-C-N	-5.82	114.27	120.03
1	B	95	LEU	C-N-CA	-5.82	114.27	120.03
1	B	110	SER	CA-C-N	5.78	128.30	120.38
1	B	110	SER	C-N-CA	5.78	128.30	120.38
1	B	80	GLU	CB-CG-CD	-5.55	103.16	112.60
1	B	101	ARG	CD-NE-CZ	5.53	132.14	124.40
1	B	45	GLU	CA-C-N	5.52	132.09	122.82
1	B	45	GLU	C-N-CA	5.52	132.09	122.82
1	C	13	GLU	CB-CG-CD	-5.41	103.40	112.60
1	B	38	MSE	CA-C-N	-5.40	112.86	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	MSE	C-N-CA	-5.40	112.86	122.42
1	A	46	GLU	CG-CD-OE1	-5.25	106.32	118.40
1	B	69	ASN	CA-C-N	-5.25	110.81	122.00
1	B	69	ASN	C-N-CA	-5.25	110.81	122.00
1	D	83	LEU	CD1-CG-CD2	-5.16	99.45	110.80
1	C	92	VAL	CA-C-N	-5.15	114.51	122.49
1	C	92	VAL	C-N-CA	-5.15	114.51	122.49
1	D	19	ASN	CB-CA-C	5.14	119.58	110.16
1	B	45	GLU	CA-CB-CG	-5.07	103.96	114.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	GLU	Sidechain
1	A	45	GLU	Sidechain
1	B	101	ARG	Sidechain
1	B	24	GLU	Sidechain
1	C	110	SER	Peptide
1	C	21	GLU	Peptide
1	D	10	GLU	Sidechain

## 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	1143	0	1119	38	1
1	B	1189	0	1177	39	0
1	C	1216	0	1195	19	1
1	D	1158	0	1137	43	0
2	A	31	0	0	2	0
2	B	24	0	0	3	0
2	C	31	0	0	0	0
2	D	16	0	0	3	0
All	All	4808	0	4628	119	1

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 13.

All (119) 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:110:SER:HB2	1:C:112:THR:H	1.30	0.94
1:A:105:ASN:ND2	1:C:152:GLU:O	2.04	0.90
1:A:140:ASP:OD2	2:A:201:HOH:O	1.96	0.82
1:A:111:GLU:OE2	1:A:111:GLU:HA	1.84	0.78
1:B:90:ASN:OD1	2:B:201:HOH:O	2.04	0.76
1:A:148:ILE:HG23	1:A:150:GLU:OE2	1.87	0.75
1:B:88:ILE:O	1:B:100:LYS:NZ	2.20	0.75
1:A:16:VAL:HG11	1:A:23:LYS:HD2	1.70	0.73
1:A:9:ALA:HA	1:A:30:GLN:HE21	1.51	0.72
1:B:86:ASN:O	2:B:201:HOH:O	2.08	0.72
1:A:69:ASN:C	1:A:69:ASN:HD22	1.99	0.71
1:A:105:ASN:HD21	1:C:153:HIS:HA	1.57	0.70
1:D:124:LYS:HE2	1:D:125:ALA:O	1.92	0.70
1:D:19:ASN:HB3	1:D:21:GLU:OE1	1.92	0.69
1:D:127:ASP:OD2	1:D:129:THR:HG23	1.94	0.68
1:C:16:VAL:HG11	1:C:23:LYS:HD3	1.77	0.67
1:D:84:PRO:HD3	1:D:114:ARG:NH2	2.10	0.67
1:D:120:TYR:OH	2:D:201:HOH:O	2.12	0.67
1:D:72:GLY:O	1:D:124:LYS:NZ	2.26	0.65
1:D:140:ASP:OD2	2:D:202:HOH:O	2.16	0.62
1:B:68:TRP:HZ3	1:B:75:ILE:HG12	1.64	0.61
1:B:6:GLU:OE2	1:B:10:GLU:OE2	2.19	0.60
1:A:25:CYS:CB	1:D:25:CYS:HG	2.14	0.60
1:C:66:LYS:HE3	1:C:147:VAL:HG11	1.84	0.60
1:D:31:THR:HG22	1:D:35:LEU:CD2	2.33	0.58
1:A:25:CYS:HB2	1:D:25:CYS:HG	1.67	0.58
1:B:111:GLU:HB2	1:B:112:THR:HG23	1.86	0.58
1:B:83:LEU:HD13	1:B:117:PHE:CE1	2.38	0.58
1:D:62:LEU:HB2	1:D:149:VAL:HG22	1.86	0.57
1:B:29:ILE:HD11	1:C:28:LEU:HB3	1.86	0.57
1:A:10:GLU:O	1:A:13:GLU:HB2	2.04	0.57
1:A:108:GLY:O	1:A:110:SER:N	2.38	0.56
1:A:87:MSE:HE3	1:A:91:GLN:HB3	1.87	0.56
1:D:147:VAL:HG23	2:D:206:HOH:O	2.05	0.56
1:D:21:GLU:O	1:D:24:GLU:OE2	2.23	0.56
1:A:135:LEU:HB3	1:B:135:LEU:HD11	1.88	0.55
1:B:114:ARG:HG2	1:B:114:ARG:NH1	2.22	0.55
1:B:37:ALA:C	1:B:39:LYS:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD11	1:D:135:LEU:HB2	1.89	0.55
1:B:42:LEU:HD21	1:B:59:ARG:HD3	1.90	0.54
1:B:85:THR:HG23	1:B:113:ASP:O	2.08	0.54
1:A:9:ALA:CA	1:A:30:GLN:HE21	2.17	0.53
1:A:29:ILE:HG23	1:D:32:ALA:HB2	1.91	0.53
1:D:68:TRP:HH2	1:D:75:ILE:HG12	1.73	0.53
1:D:86:ASN:ND2	1:D:111:GLU:HB3	2.23	0.53
1:A:11:TYR:CZ	1:D:35:LEU:HD23	2.44	0.52
1:D:11:TYR:O	1:D:14:SER:HB3	2.09	0.52
1:B:37:ALA:C	1:B:39:LYS:N	2.68	0.51
1:C:3:THR:HG22	1:C:5:ASP:H	1.75	0.51
1:D:31:THR:O	1:D:35:LEU:HD22	2.08	0.51
1:D:42:LEU:HD11	1:D:59:ARG:HD2	1.92	0.51
1:A:3:THR:HG22	1:A:5:ASP:H	1.75	0.50
1:B:97:GLU:OE2	1:B:101:ARG:NE	2.44	0.50
1:D:4:LEU:HG	1:D:34:VAL:HG13	1.93	0.50
1:A:69:ASN:C	1:A:69:ASN:ND2	2.69	0.49
1:A:116:LYS:NZ	2:A:204:HOH:O	2.43	0.49
1:D:147:VAL:HG22	1:D:148:ILE:O	2.12	0.49
1:A:25:CYS:HB2	1:D:25:CYS:SG	2.53	0.49
1:A:15:VAL:CG1	1:D:28:LEU:HD22	2.42	0.49
1:D:31:THR:HG22	1:D:35:LEU:HD22	1.93	0.49
1:C:110:SER:HB2	1:C:112:THR:N	2.12	0.48
1:A:87:MSE:HE3	1:A:87:MSE:HB3	1.74	0.48
1:B:90:ASN:N	2:B:201:HOH:O	2.47	0.48
1:C:14:SER:O	1:C:18:ARG:HD2	2.13	0.48
1:C:75:ILE:HD11	1:C:123:MSE:HE3	1.95	0.48
1:D:2:LYS:HB2	1:D:7:LYS:HD3	1.95	0.48
1:D:75:ILE:HD11	1:D:123:MSE:HE3	1.95	0.48
1:B:69:ASN:C	1:B:71:LYS:N	2.72	0.48
1:C:135:LEU:HD11	1:D:135:LEU:CB	2.44	0.48
1:A:149:VAL:O	1:A:150:GLU:C	2.57	0.48
1:B:29:ILE:CD1	1:C:28:LEU:HB3	2.44	0.47
1:C:55:GLU:O	1:C:59:ARG:HG2	2.13	0.47
1:A:3:THR:N	1:A:7:LYS:HE3	2.29	0.47
1:C:19:ASN:OD1	1:C:21:GLU:HG3	2.14	0.47
1:A:32:ALA:HB2	1:D:29:ILE:HG23	1.96	0.47
1:A:15:VAL:HG11	1:D:28:LEU:HD22	1.95	0.47
1:B:45:GLU:N	1:B:46:GLU:OE1	2.46	0.47
1:B:68:TRP:CZ3	1:B:75:ILE:HG12	2.49	0.47
1:B:42:LEU:HD21	1:B:59:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLU:H	1:D:46:GLU:CD	2.23	0.47
1:B:80:GLU:HG2	1:B:118:THR:HA	1.96	0.46
1:B:23:LYS:HD2	1:B:23:LYS:O	2.16	0.46
1:A:80:GLU:CD	1:A:116:LYS:HD2	2.40	0.46
1:C:151:LEU:HA	1:C:151:LEU:HD23	1.66	0.46
1:B:56:SER:HB3	1:B:148:ILE:HD11	1.98	0.46
1:D:82:SER:HB2	1:D:114:ARG:HE	1.80	0.46
1:B:75:ILE:HD13	1:B:75:ILE:HA	1.56	0.45
1:B:42:LEU:HD21	1:B:59:ARG:NE	2.32	0.45
1:B:65:ARG:HH12	1:B:139:THR:HG22	1.82	0.45
1:B:73:MSE:HE3	1:B:123:MSE:SE	2.67	0.45
1:C:20:LYS:HA	1:C:20:LYS:HD3	1.74	0.44
1:A:9:ALA:CB	1:A:30:GLN:HE21	2.30	0.44
1:A:11:TYR:OH	1:D:35:LEU:HD23	2.18	0.44
1:B:1:MSE:SE	1:C:144:ASN:HB3	2.68	0.44
1:B:69:ASN:C	1:B:71:LYS:H	2.25	0.44
1:D:87:MSE:HG2	1:D:91:GLN:OE1	2.18	0.43
1:A:25:CYS:SG	1:D:25:CYS:SG	3.08	0.43
1:B:84:PRO:O	1:B:87:MSE:HB2	2.18	0.43
1:A:135:LEU:CB	1:B:135:LEU:HD11	2.49	0.43
1:A:142:LEU:HA	1:A:142:LEU:HD23	1.84	0.43
1:B:42:LEU:HD21	1:B:59:ARG:CD	2.48	0.43
1:D:42:LEU:HD12	1:D:55:GLU:HB3	2.00	0.43
1:B:116:LYS:HE2	1:B:116:LYS:HB2	1.87	0.43
1:D:7:LYS:O	1:D:10:GLU:OE2	2.37	0.43
1:D:47:THR:HA	1:D:146:TRP:O	2.19	0.43
1:A:20:LYS:O	1:A:23:LYS:CB	2.68	0.42
1:A:87:MSE:HE3	1:A:91:GLN:CB	2.49	0.42
1:B:75:ILE:HD12	1:B:75:ILE:HG23	1.66	0.42
1:B:45:GLU:H	1:B:45:GLU:HG3	1.50	0.41
1:D:147:VAL:HG22	1:D:148:ILE:N	2.35	0.41
1:A:41:GLU:O	1:A:52:GLN:HA	2.19	0.41
1:A:20:LYS:O	1:A:23:LYS:HB3	2.21	0.41
1:D:6:GLU:O	1:D:10:GLU:HB2	2.21	0.41
1:B:88:ILE:HG23	1:B:95:LEU:CD1	2.51	0.40
1:D:84:PRO:HD3	1:D:114:ARG:HH22	1.84	0.40
1:D:73:MSE:H	1:D:73:MSE:HG3	1.67	0.40
1:B:35:LEU:O	1:B:39:LYS:HB2	2.22	0.40
1:A:105:ASN:ND2	1:C:153:HIS:HA	2.31	0.40
1:B:23:LYS:HD2	1:B:23:LYS:C	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:OE2	1:C:59:ARG:NE[2_554]	2.13	0.07

## 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	143/158 (90%)	142 (99%)	1 (1%)	0	100	100
1	B	150/158 (95%)	149 (99%)	1 (1%)	0	100	100
1	C	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
1	D	147/158 (93%)	143 (97%)	4 (3%)	0	100	100
All	All	591/632 (94%)	583 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	120/125 (96%)	118 (98%)	2 (2%)	53	60
1	B	126/125 (101%)	121 (96%)	5 (4%)	28	27
1	C	128/125 (102%)	123 (96%)	5 (4%)	28	28
1	D	122/125 (98%)	113 (93%)	9 (7%)	13	8
All	All	496/500 (99%)	475 (96%)	21 (4%)	26	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	111	GLU
1	B	14	SER
1	B	82	SER
1	B	91	GLN
1	B	93	LYS
1	B	135	LEU
1	C	5	ASP
1	C	42	LEU
1	C	69	ASN
1	C	111	GLU
1	C	135	LEU
1	D	21	GLU
1	D	35	LEU
1	D	39	LYS
1	D	42	LEU
1	D	82	SER
1	D	91	GLN
1	D	111	GLU
1	D	124	LYS
1	D	150	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	69	ASN
1	A	90	ASN
1	A	105	ASN
1	C	90	ASN
1	C	156	HIS
1	D	86	ASN
1	D	106	ASN

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	141/158 (89%)	0.30	12 (8%) 16 18	29, 44, 101, 108	0
1	B	145/158 (91%)	0.34	2 (1%) 73 77	29, 49, 79, 91	0
1	C	148/158 (93%)	0.22	5 (3%) 48 52	30, 44, 73, 83	0
1	D	143/158 (90%)	0.69	13 (9%) 15 16	31, 56, 88, 98	0
All	All	577/632 (91%)	0.38	32 (5%) 30 34	29, 48, 90, 108	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	VAL	4.2
1	C	70	GLY	4.0
1	D	9	ALA	3.9
1	D	91	GLN	3.4
1	A	16	VAL	3.3
1	A	32	ALA	3.3
1	D	12	ALA	3.3
1	A	29	ILE	3.1
1	A	12	ALA	3.1
1	A	28	LEU	2.8
1	A	21	GLU	2.8
1	A	11	TYR	2.7
1	D	40	GLY	2.7
1	A	3	THR	2.6
1	D	83	LEU	2.6
1	A	22	ALA	2.6
1	A	31	THR	2.6
1	D	4	LEU	2.6
1	B	111	GLU	2.5
1	A	15	VAL	2.4
1	C	67	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	69	ASN	2.4
1	D	97	GLU	2.4
1	D	15	VAL	2.4
1	C	156	HIS	2.4
1	B	91	GLN	2.4
1	D	70	GLY	2.4
1	C	69	ASN	2.3
1	D	72	GLY	2.3
1	D	22	ALA	2.3
1	A	35	LEU	2.3
1	C	153	HIS	2.2

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.