



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:06 pm BST

PDB ID : 2ODO  
Title : Crystal structure of Pseudomonas Fluorescens alanine racemase  
Authors : Tsuge, H.; Ohnishi, K.; Yokoigawa, K.  
Deposited on : 2006-12-25  
Resolution : 2.80 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

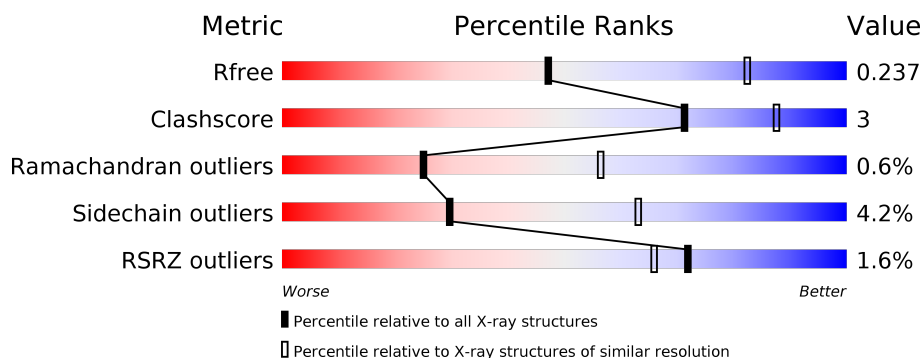
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	357	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> </div> </div> <div>88% 11% •</div> </div>
1	B	357	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 86%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> </div> </div> <div>86% 12% •</div> </div>
1	C	357	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> </div> </div> <div>88% 10% •</div> </div>
1	D	357	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 89%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> </div> </div> <div>89% 10% •</div> </div>

## 2 Entry composition [i](#)

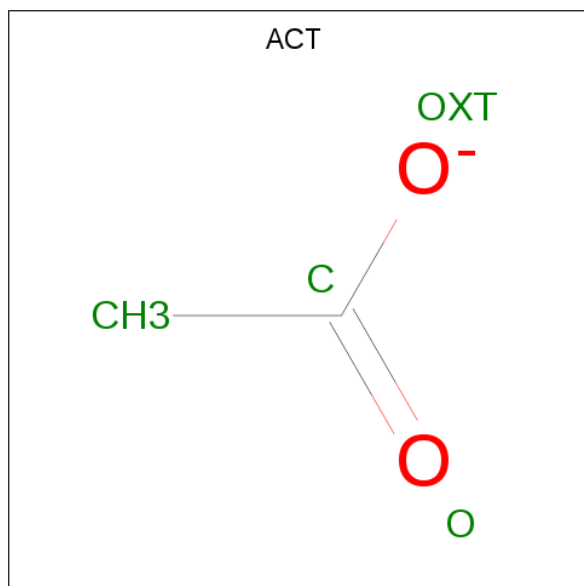
There are 3 unique types of molecules in this entry. The entry contains 11074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	P	S	0	0	0
			2750	1749	484	500	1	16			
1	B	356	Total	C	N	O	P	S	0	0	0
			2750	1749	484	500	1	16			
1	C	356	Total	C	N	O	P	S	0	0	0
			2750	1749	484	500	1	16			
1	D	356	Total	C	N	O	P	S	0	0	0
			2750	1749	484	500	1	16			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

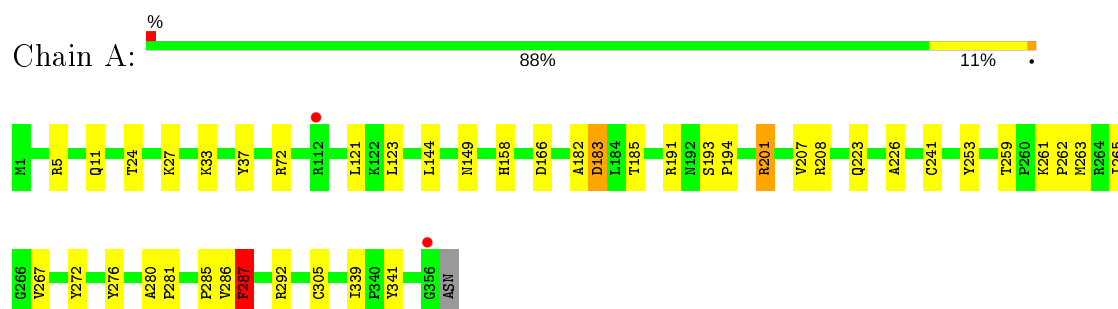
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	22	Total	O	0	0
			22	22		
3	C	8	Total	O	0	0
			8	8		
3	D	7	Total	O	0	0
			7	7		

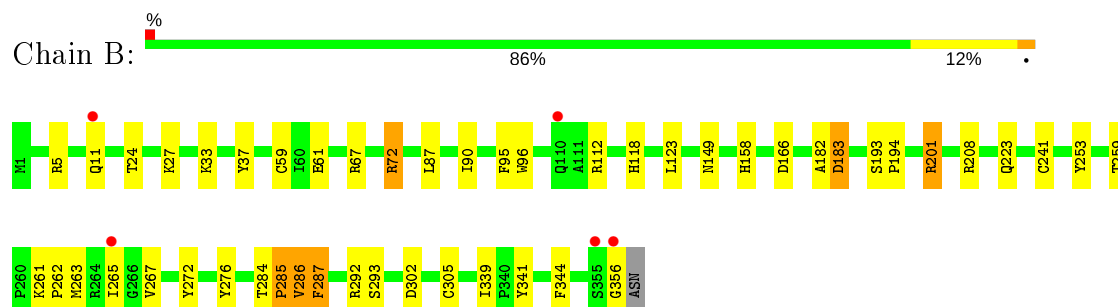
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

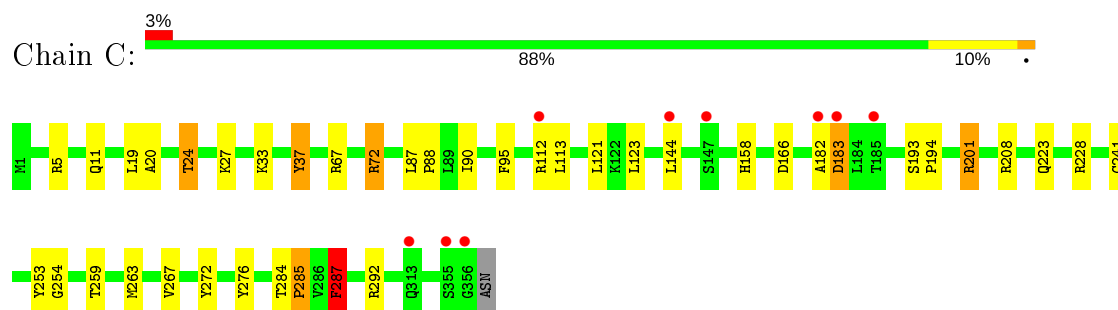
#### • Molecule 1: Alanine racemase



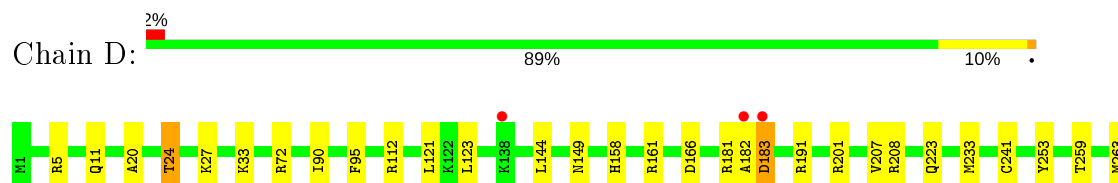
#### • Molecule 1: Alanine racemase



#### • Molecule 1: Alanine racemase



#### • Molecule 1: Alanine racemase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.74Å 186.74Å 103.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.80 45.32 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.32-2.80) 93.5 (45.32-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.247 0.204 , 0.237	Depositor DCC
$R_{free}$ test set	2076 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, KCX, ACT

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	0.30	0/2773	0.51	2/3774 (0.1%)
1	B	0.30	0/2773	0.51	1/3774 (0.0%)
1	C	0.31	0/2773	0.51	1/3774 (0.0%)
1	D	0.31	0/2773	0.51	1/3774 (0.0%)
All	All	0.30	0/11092	0.51	5/15096 (0.0%)

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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	286	VAL	N-CA-C	-5.33	96.60	111.00
1	D	286	VAL	N-CA-C	-5.23	96.88	111.00
1	A	287	PHE	N-CA-C	5.17	124.95	111.00
1	B	286	VAL	N-CA-C	-5.12	97.19	111.00
1	C	287	PHE	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	285	PRO	Peptide
1	B	285	PRO	Peptide
1	C	285	PRO	Peptide
1	D	285	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	2750	0	2758	19	0
1	B	2750	0	2759	26	0
1	C	2750	0	2759	23	0
1	D	2750	0	2759	16	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	1	0
2	D	4	0	3	1	0
3	A	21	0	0	0	0
3	B	22	0	0	0	0
3	C	8	0	0	0	0
3	D	7	0	0	0	0
All	All	11074	0	11047	77	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 3.

All (77) 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:B:201:ARG:HG2	1:B:201:ARG:HH21	1.46	0.80
1:B:201:ARG:HH21	1:B:201:ARG:CG	2.10	0.64
1:B:287:PHE:H	1:B:292:ARG:HA	1.66	0.60
2:C:3400:ACT:H1	1:D:33:LLP:H4'1	1.84	0.59
2:A:1400:ACT:H1	1:B:33:LLP:H4'1	1.84	0.58
1:C:201:ARG:HH21	1:C:201:ARG:HG2	1.68	0.57
1:C:201:ARG:CG	1:C:201:ARG:HH21	2.18	0.56
1:B:158:HIS:HD2	1:B:208:ARG:HH21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:PHE:H	1:A:292:ARG:HA	1.72	0.55
1:A:182:ALA:O	1:A:183:ASP:CB	2.55	0.55
1:C:90:ILE:HG23	1:C:95:PHE:HB2	1.90	0.54
1:A:265:ILE:HG23	1:A:305:CYS:SG	2.49	0.53
1:B:265:ILE:HG23	1:B:305:CYS:SG	2.49	0.53
1:D:287:PHE:H	1:D:292:ARG:HA	1.74	0.52
1:B:182:ALA:O	1:B:183:ASP:CB	2.57	0.52
1:C:287:PHE:H	1:C:292:ARG:HA	1.73	0.52
1:D:182:ALA:O	1:D:183:ASP:CB	2.57	0.52
1:C:259:THR:HG22	1:C:263:MET:HE2	1.92	0.50
1:C:182:ALA:O	1:C:183:ASP:CB	2.60	0.49
1:A:193:SER:HB2	1:A:194:PRO:HD3	1.93	0.49
1:B:356:GLY:N	1:D:313:GLN:HE22	2.10	0.49
1:B:67:ARG:NH1	1:B:72:ARG:HA	2.28	0.49
1:C:19:LEU:HD11	1:C:228:ARG:HB3	1.95	0.48
1:A:158:HIS:HD2	1:A:208:ARG:HH21	1.61	0.48
1:A:158:HIS:HE1	1:B:253:TYR:OH	1.97	0.48
1:B:259:THR:HG22	1:B:263:MET:HE2	1.95	0.48
1:A:201:ARG:CG	1:A:201:ARG:HH21	2.27	0.48
1:A:182:ALA:O	1:A:183:ASP:HB3	2.14	0.47
1:C:33:LLP:H4'1	2:D:2400:ACT:H1	1.96	0.47
1:A:253:TYR:OH	1:B:158:HIS:HE1	1.98	0.47
1:A:191:ARG:HB2	1:A:207:VAL:HG12	1.97	0.46
1:A:259:THR:HG22	1:A:263:MET:HE2	1.97	0.46
1:B:96:TRP:CD1	1:B:118:HIS:HB2	2.51	0.46
1:A:33:LLP:HD3	1:B:302:ASP:OD2	2.17	0.45
1:C:259:THR:HG22	1:C:263:MET:CE	2.47	0.45
1:C:253:TYR:OH	1:D:158:HIS:HE1	1.99	0.45
1:A:339:ILE:HD12	1:A:341:TYR:CD1	2.51	0.44
1:A:121:LEU:HD13	1:A:144:LEU:HD11	2.00	0.44
1:C:193:SER:HB2	1:C:194:PRO:HD3	1.98	0.44
1:D:158:HIS:HD2	1:D:208:ARG:HH21	1.66	0.44
1:D:233:MET:HE1	1:D:347:LEU:HD22	2.00	0.44
1:C:87:LEU:N	1:C:88:PRO:HD2	2.33	0.43
1:B:241:CYS:HB3	1:B:267:VAL:HB	2.00	0.43
1:C:158:HIS:HE1	1:D:253:TYR:OH	2.01	0.43
1:D:20:ALA:O	1:D:24:THR:HG22	2.18	0.43
1:B:193:SER:HB2	1:B:194:PRO:HD3	2.01	0.43
1:C:20:ALA:O	1:C:24:THR:HG22	2.19	0.42
1:D:121:LEU:HD13	1:D:144:LEU:HD11	2.02	0.42
1:C:67:ARG:NH1	1:C:72:ARG:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLN:HG3	1:A:226:ALA:H	1.85	0.42
1:A:241:CYS:HB3	1:A:267:VAL:HB	2.02	0.42
1:A:261:LYS:HB2	1:A:262:PRO:HD2	2.02	0.42
1:B:261:LYS:HB2	1:B:262:PRO:HD2	2.01	0.42
1:B:87:LEU:HA	1:B:90:ILE:HD12	2.02	0.42
1:B:284:THR:HA	1:B:285:PRO:HD3	1.83	0.42
1:B:90:ILE:HG23	1:B:95:PHE:HB2	2.02	0.42
1:D:241:CYS:HB3	1:D:267:VAL:HB	2.01	0.42
1:A:280:ALA:HA	1:A:281:PRO:HD3	1.91	0.42
1:D:191:ARG:HB2	1:D:207:VAL:HG12	2.01	0.41
1:B:272:TYR:HA	1:B:276:TYR:O	2.21	0.41
1:B:59:CYS:SG	1:B:61:GLU:HG2	2.61	0.41
1:D:259:THR:HG22	1:D:263:MET:HE2	2.01	0.41
1:B:286:VAL:O	1:B:293:SER:N	2.53	0.41
1:C:201:ARG:NH2	1:C:201:ARG:CG	2.80	0.41
1:D:272:TYR:HA	1:D:276:TYR:O	2.21	0.41
1:A:272:TYR:HA	1:A:276:TYR:O	2.21	0.41
1:C:121:LEU:HD13	1:C:144:LEU:HD11	2.02	0.41
1:C:254:GLY:HA2	1:D:161:ARG:HG2	2.03	0.41
1:C:272:TYR:HA	1:C:276:TYR:O	2.21	0.41
1:C:241:CYS:HB3	1:C:267:VAL:HB	2.03	0.41
1:C:284:THR:HA	1:C:285:PRO:HD3	1.83	0.41
1:D:90:ILE:HG23	1:D:95:PHE:HB2	2.02	0.40
1:B:201:ARG:CG	1:B:201:ARG:NH2	2.75	0.40
1:C:37:TYR:CD1	1:C:37:TYR:N	2.89	0.40
1:B:37:TYR:O	1:B:344:PHE:HB3	2.21	0.40
1:B:339:ILE:HD12	1:B:341:TYR:CD1	2.56	0.40
1:C:158:HIS:HD2	1:C:208:ARG:HH21	1.69	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	352/357 (99%)	340 (97%)	10 (3%)	2 (1%)	25	56
1	B	352/357 (99%)	336 (96%)	14 (4%)	2 (1%)	25	56
1	C	352/357 (99%)	334 (95%)	16 (4%)	2 (1%)	25	56
1	D	352/357 (99%)	335 (95%)	15 (4%)	2 (1%)	25	56
All	All	1408/1428 (99%)	1345 (96%)	55 (4%)	8 (1%)	25	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	ASP
1	A	183	ASP
1	C	183	ASP
1	D	183	ASP
1	A	287	PHE
1	B	287	PHE
1	C	287	PHE
1	D	287	PHE

### 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	281/282 (100%)	270 (96%)	11 (4%)	32	66
1	B	281/282 (100%)	270 (96%)	11 (4%)	32	66
1	C	281/282 (100%)	269 (96%)	12 (4%)	29	62
1	D	281/282 (100%)	268 (95%)	13 (5%)	27	60
All	All	1124/1128 (100%)	1077 (96%)	47 (4%)	30	63

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	11	GLN
1	A	24	THR

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Mol	Chain	Res	Type
1	A	27	LYS
1	A	37	TYR
1	A	72	ARG
1	A	123	LEU
1	A	149	ASN
1	A	166	ASP
1	A	185	THR
1	A	201	ARG
1	B	5	ARG
1	B	11	GLN
1	B	24	THR
1	B	27	LYS
1	B	72	ARG
1	B	112	ARG
1	B	123	LEU
1	B	149	ASN
1	B	166	ASP
1	B	201	ARG
1	B	223	GLN
1	C	5	ARG
1	C	11	GLN
1	C	24	THR
1	C	27	LYS
1	C	37	TYR
1	C	72	ARG
1	C	112	ARG
1	C	113	LEU
1	C	123	LEU
1	C	166	ASP
1	C	201	ARG
1	C	223	GLN
1	D	5	ARG
1	D	11	GLN
1	D	24	THR
1	D	27	LYS
1	D	72	ARG
1	D	112	ARG
1	D	123	LEU
1	D	149	ASN
1	D	166	ASP
1	D	181	ARG
1	D	201	ARG

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Mol	Chain	Res	Type
1	D	223	GLN
1	D	313	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	149	ASN
1	A	158	HIS
1	A	223	GLN
1	A	294	GLN
1	B	100	HIS
1	B	158	HIS
1	B	223	GLN
1	B	294	GLN
1	C	100	HIS
1	C	149	ASN
1	C	158	HIS
1	C	223	GLN
1	D	100	HIS
1	D	149	ASN
1	D	158	HIS
1	D	223	GLN
1	D	313	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	KCX	B	122	1	7,11,12	0.88	1 (14%)	4,12,14	0.65	0
1	LLP	A	33	1	23,24,25	2.76	4 (17%)	25,32,34	1.50	3 (12%)
1	KCX	D	122	1	7,11,12	0.73	0	4,12,14	0.71	0
1	LLP	C	33	1	23,24,25	2.76	4 (17%)	25,32,34	1.46	3 (12%)
1	LLP	D	33	1	23,24,25	2.74	4 (17%)	25,32,34	1.49	3 (12%)
1	KCX	C	122	1	7,11,12	0.85	0	4,12,14	0.64	0
1	LLP	B	33	1	23,24,25	2.78	4 (17%)	25,32,34	1.48	3 (12%)
1	KCX	A	122	1	7,11,12	0.77	0	4,12,14	0.73	0

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
1	KCX	B	122	1	-	0/7/10/12	-
1	LLP	A	33	1	-	5/16/17/19	0/1/1/1
1	KCX	D	122	1	-	1/7/10/12	-
1	LLP	C	33	1	-	4/16/17/19	0/1/1/1
1	LLP	D	33	1	-	4/16/17/19	0/1/1/1
1	KCX	C	122	1	-	1/7/10/12	-
1	LLP	B	33	1	-	5/16/17/19	0/1/1/1
1	KCX	A	122	1	-	1/7/10/12	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	LLP	C3-C2	8.42	1.49	1.40
1	B	33	LLP	C3-C2	8.40	1.49	1.40
1	C	33	LLP	C3-C2	8.35	1.49	1.40
1	D	33	LLP	C3-C2	8.28	1.49	1.40
1	D	33	LLP	O-C	6.02	1.44	1.19
1	B	33	LLP	O-C	6.02	1.44	1.19
1	C	33	LLP	O-C	5.98	1.43	1.19
1	A	33	LLP	O-C	5.98	1.43	1.19
1	B	33	LLP	C4-C5	5.98	1.49	1.42
1	A	33	LLP	C4-C5	5.90	1.49	1.42
1	C	33	LLP	C4-C5	5.84	1.49	1.42
1	D	33	LLP	C4-C5	5.80	1.49	1.42
1	C	33	LLP	C4-C3	5.37	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	33	LLP	C4-C3	5.29	1.48	1.40
1	D	33	LLP	C4-C3	5.24	1.48	1.40
1	A	33	LLP	C4-C3	5.21	1.48	1.40
1	B	122	KCX	CE-NZ	2.02	1.50	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	LLP	C4-C3-C2	-4.73	117.26	120.19
1	C	33	LLP	C4-C3-C2	-4.72	117.26	120.19
1	D	33	LLP	C4-C3-C2	-4.46	117.43	120.19
1	A	33	LLP	C4-C3-C2	-4.29	117.53	120.19
1	A	33	LLP	CD-CE-NZ	-3.20	103.09	110.93
1	D	33	LLP	CD-CE-NZ	-2.95	103.69	110.93
1	B	33	LLP	CD-CE-NZ	-2.87	103.89	110.93
1	C	33	LLP	CD-CE-NZ	-2.65	104.44	110.93
1	B	33	LLP	C6-N1-C2	2.45	123.71	119.17
1	D	33	LLP	C6-N1-C2	2.39	123.59	119.17
1	A	33	LLP	C6-N1-C2	2.35	123.52	119.17
1	C	33	LLP	C6-N1-C2	2.33	123.48	119.17

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	33	LLP	CG-CD-CE-NZ
1	D	33	LLP	C5-C4-C4'-NZ
1	D	33	LLP	CG-CD-CE-NZ
1	B	33	LLP	CG-CD-CE-NZ
1	A	33	LLP	CG-CD-CE-NZ
1	D	33	LLP	C3-C4-C4'-NZ
1	B	33	LLP	C3-C4-C4'-NZ
1	A	33	LLP	C3-C4-C4'-NZ
1	C	33	LLP	C3-C4-C4'-NZ
1	D	33	LLP	CD-CE-NZ-C4'
1	B	33	LLP	CD-CE-NZ-C4'
1	A	33	LLP	C4-C5-C5'-OP4
1	B	33	LLP	C5-C4-C4'-NZ
1	C	33	LLP	CD-CE-NZ-C4'
1	B	33	LLP	C5'-OP4-P-OP1
1	A	122	KCX	CG-CD-CE-NZ
1	A	33	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	D	122	KCX	CG-CD-CE-NZ
1	C	122	KCX	CG-CD-CE-NZ
1	A	33	LLP	C5-C4-C4'-NZ
1	C	33	LLP	C5-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	33	LLP	1	0
1	C	33	LLP	1	0
1	D	33	LLP	1	0
1	B	33	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z  > 2$
2	ACT	A	1400	-	1,3,3	1.32	0	0,3,3	0.00	-
2	ACT	B	400	-	1,3,3	1.34	0	0,3,3	0.00	-
2	ACT	C	3400	-	1,3,3	1.29	0	0,3,3	0.00	-
2	ACT	D	2400	-	1,3,3	1.28	0	0,3,3	0.00	-

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1400	ACT	1	0
2	C	3400	ACT	1	0
2	D	2400	ACT	1	0

## 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	354/357 (99%)	-0.09	2 (0%) 89 86	40, 49, 60, 64	0
1	B	354/357 (99%)	-0.01	5 (1%) 75 70	43, 51, 63, 68	0
1	C	354/357 (99%)	-0.00	9 (2%) 57 47	44, 54, 67, 70	0
1	D	354/357 (99%)	0.07	7 (1%) 65 56	44, 55, 69, 72	0
All	All	1416/1428 (99%)	-0.01	23 (1%) 72 66	40, 52, 65, 72	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	GLY	9.8
1	A	356	GLY	5.5
1	D	313	GLN	4.7
1	C	182	ALA	3.8
1	D	355	SER	3.7
1	C	356	GLY	3.7
1	C	183	ASP	3.6
1	C	355	SER	3.5
1	C	313	GLN	3.5
1	D	183	ASP	3.0
1	D	356	GLY	2.9
1	C	185	THR	2.8
1	B	11	GLN	2.5
1	D	138	LYS	2.5
1	A	112	ARG	2.4
1	D	182	ALA	2.3
1	B	265	ILE	2.2
1	B	110	GLN	2.2
1	C	144	LEU	2.1
1	B	355	SER	2.1
1	D	312	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	112	ARG	2.1
1	C	147	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	D	122	12/13	0.91	0.15	57,57,57,58	0
1	KCX	A	122	12/13	0.92	0.18	44,46,47,47	0
1	LLP	D	33	24/25	0.94	0.23	45,45,48,48	0
1	KCX	C	122	12/13	0.95	0.17	54,55,55,55	0
1	KCX	B	122	12/13	0.95	0.19	49,50,50,50	0
1	LLP	B	33	24/25	0.96	0.16	39,40,44,45	0
1	LLP	A	33	24/25	0.97	0.16	34,35,39,39	0
1	LLP	C	33	24/25	0.97	0.17	42,43,45,45	0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ACT	D	2400	4/4	0.92	0.21	52,52,52,52	0
2	ACT	A	1400	4/4	0.94	0.21	49,49,49,49	0
2	ACT	C	3400	4/4	0.96	0.25	55,55,55,55	0
2	ACT	B	400	4/4	0.97	0.18	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.