



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:24 AM UTC

PDB ID : 5FAG / pdb\_00005fag  
Title : Alanine Racemase from Streptomyces coelicolor A3(2) with Bound Propionate Inhibitor  
Authors : Tassoni, R.; Pannu, N.S.  
Deposited on : 2015-12-11  
Resolution : 1.51 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2022.3.0, CSD as543be (2022)  
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

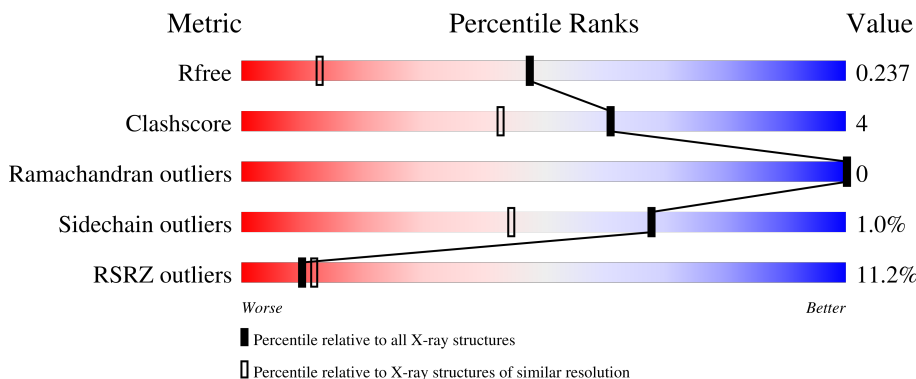
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	410	 3% 86% 9% 5%
1	B	410	 2% 87% 7% 7%
1	C	410	 9% 85% 8% 7%
1	D	410	 28% 85% 7% 7%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 12710 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
			Total	C	N	O	S			
1	A	390	Total 3047	C 1915	N 567	O 552	S 13	0	22	0
1	B	382	Total 2911	C 1829	N 536	O 534	S 12	0	13	0
1	C	382	Total 2909	C 1830	N 538	O 529	S 12	0	11	0
1	D	382	Total 2926	C 1842	N 542	O 528	S 14	0	14	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O86786
A	-17	GLY	-	expression tag	UNP O86786
A	-16	SER	-	expression tag	UNP O86786
A	-15	HIS	-	expression tag	UNP O86786
A	-14	HIS	-	expression tag	UNP O86786
A	-13	HIS	-	expression tag	UNP O86786
A	-12	HIS	-	expression tag	UNP O86786
A	-11	HIS	-	expression tag	UNP O86786
A	-10	HIS	-	expression tag	UNP O86786
A	-9	SER	-	expression tag	UNP O86786
A	-8	SER	-	expression tag	UNP O86786
A	-7	GLY	-	expression tag	UNP O86786
A	-6	LEU	-	expression tag	UNP O86786
A	-5	VAL	-	expression tag	UNP O86786
A	-4	PRO	-	expression tag	UNP O86786
A	-3	ARG	-	expression tag	UNP O86786
A	-2	GLY	-	expression tag	UNP O86786
A	-1	SER	-	expression tag	UNP O86786
A	0	HIS	-	expression tag	UNP O86786
B	-18	MET	-	initiating methionine	UNP O86786
B	-17	GLY	-	expression tag	UNP O86786

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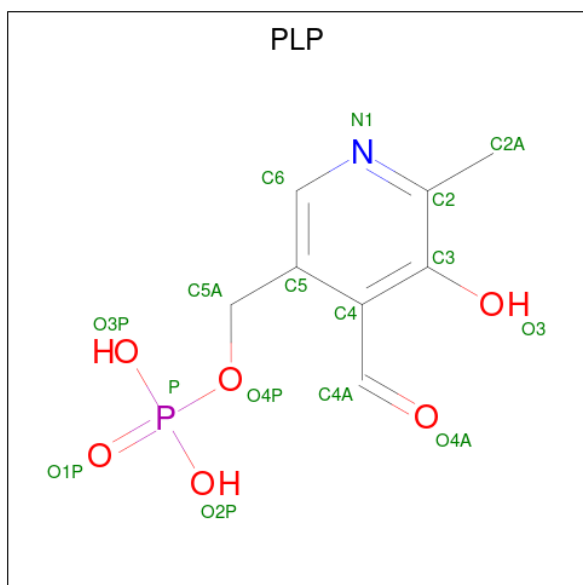
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O86786
B	-15	HIS	-	expression tag	UNP O86786
B	-14	HIS	-	expression tag	UNP O86786
B	-13	HIS	-	expression tag	UNP O86786
B	-12	HIS	-	expression tag	UNP O86786
B	-11	HIS	-	expression tag	UNP O86786
B	-10	HIS	-	expression tag	UNP O86786
B	-9	SER	-	expression tag	UNP O86786
B	-8	SER	-	expression tag	UNP O86786
B	-7	GLY	-	expression tag	UNP O86786
B	-6	LEU	-	expression tag	UNP O86786
B	-5	VAL	-	expression tag	UNP O86786
B	-4	PRO	-	expression tag	UNP O86786
B	-3	ARG	-	expression tag	UNP O86786
B	-2	GLY	-	expression tag	UNP O86786
B	-1	SER	-	expression tag	UNP O86786
B	0	HIS	-	expression tag	UNP O86786
C	-18	MET	-	initiating methionine	UNP O86786
C	-17	GLY	-	expression tag	UNP O86786
C	-16	SER	-	expression tag	UNP O86786
C	-15	HIS	-	expression tag	UNP O86786
C	-14	HIS	-	expression tag	UNP O86786
C	-13	HIS	-	expression tag	UNP O86786
C	-12	HIS	-	expression tag	UNP O86786
C	-11	HIS	-	expression tag	UNP O86786
C	-10	HIS	-	expression tag	UNP O86786
C	-9	SER	-	expression tag	UNP O86786
C	-8	SER	-	expression tag	UNP O86786
C	-7	GLY	-	expression tag	UNP O86786
C	-6	LEU	-	expression tag	UNP O86786
C	-5	VAL	-	expression tag	UNP O86786
C	-4	PRO	-	expression tag	UNP O86786
C	-3	ARG	-	expression tag	UNP O86786
C	-2	GLY	-	expression tag	UNP O86786
C	-1	SER	-	expression tag	UNP O86786
C	0	HIS	-	expression tag	UNP O86786
D	-18	MET	-	initiating methionine	UNP O86786
D	-17	GLY	-	expression tag	UNP O86786
D	-16	SER	-	expression tag	UNP O86786
D	-15	HIS	-	expression tag	UNP O86786
D	-14	HIS	-	expression tag	UNP O86786
D	-13	HIS	-	expression tag	UNP O86786

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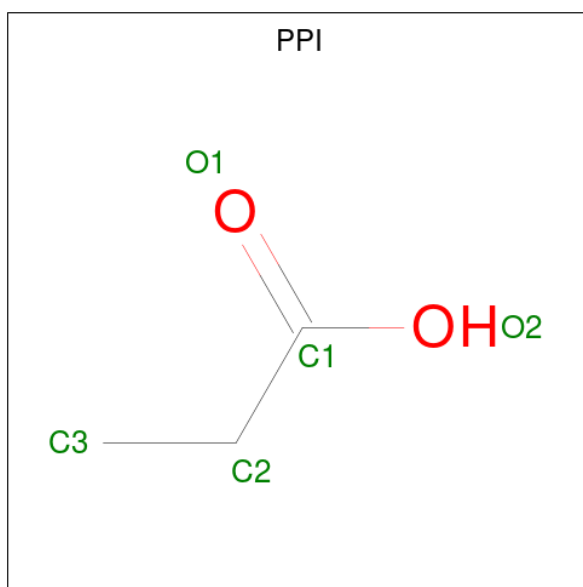
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP O86786
D	-11	HIS	-	expression tag	UNP O86786
D	-10	HIS	-	expression tag	UNP O86786
D	-9	SER	-	expression tag	UNP O86786
D	-8	SER	-	expression tag	UNP O86786
D	-7	GLY	-	expression tag	UNP O86786
D	-6	LEU	-	expression tag	UNP O86786
D	-5	VAL	-	expression tag	UNP O86786
D	-4	PRO	-	expression tag	UNP O86786
D	-3	ARG	-	expression tag	UNP O86786
D	-2	GLY	-	expression tag	UNP O86786
D	-1	SER	-	expression tag	UNP O86786
D	0	HIS	-	expression tag	UNP O86786

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PROPANOIC ACID (CCD ID: PPI) (formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>).

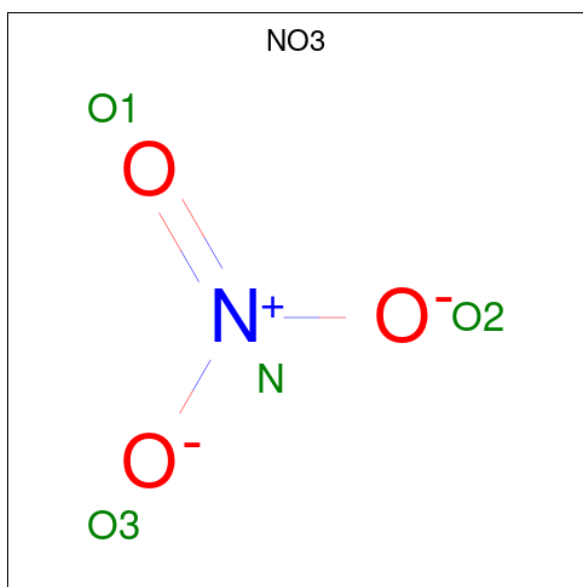


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	C	1	Total C O 5 3 2	0	0
3	D	1	Total C O 5 3 2	0	0
3	D	1	Total C O 5 3 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is NITRATE ION (CCD ID: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		

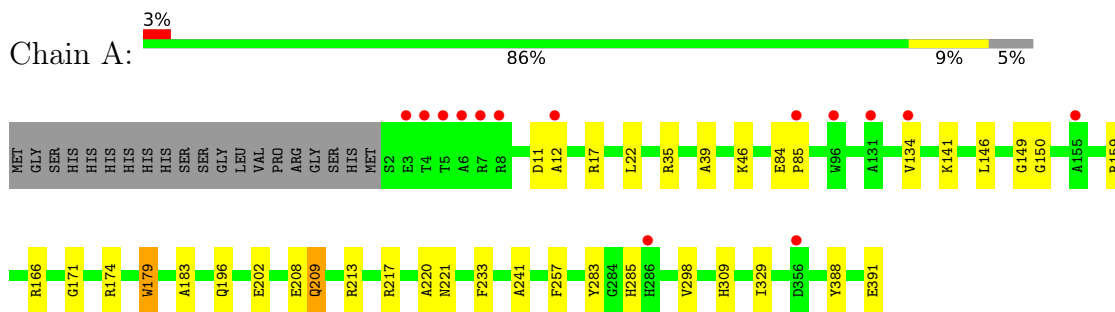
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	237	Total	O	0	0
			237	237		
6	B	239	Total	O	0	0
			239	239		
6	C	167	Total	O	0	0
			167	167		
6	D	161	Total	O	0	0
			161	161		

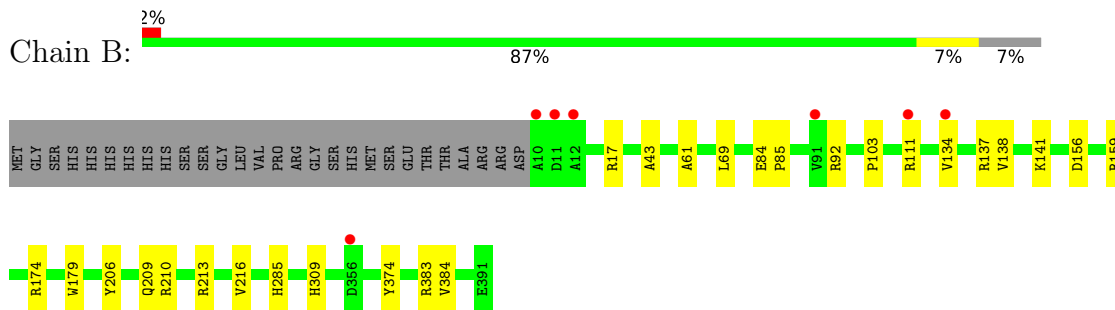
### 3 Residue-property plots [i](#)

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.

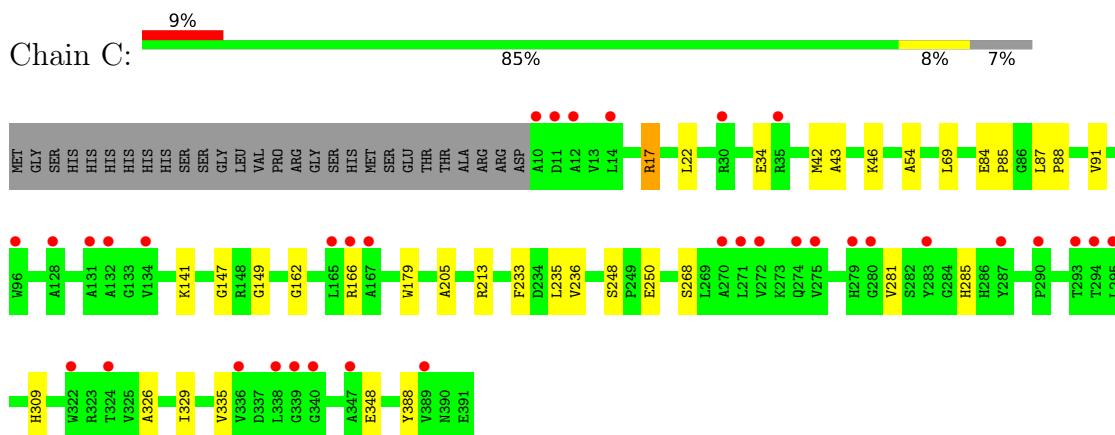
- Molecule 1: Alanine racemase



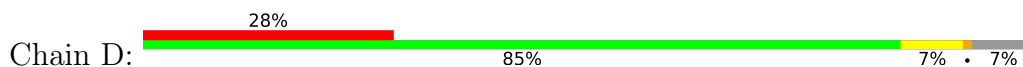
- Molecule 1: Alanine racemase

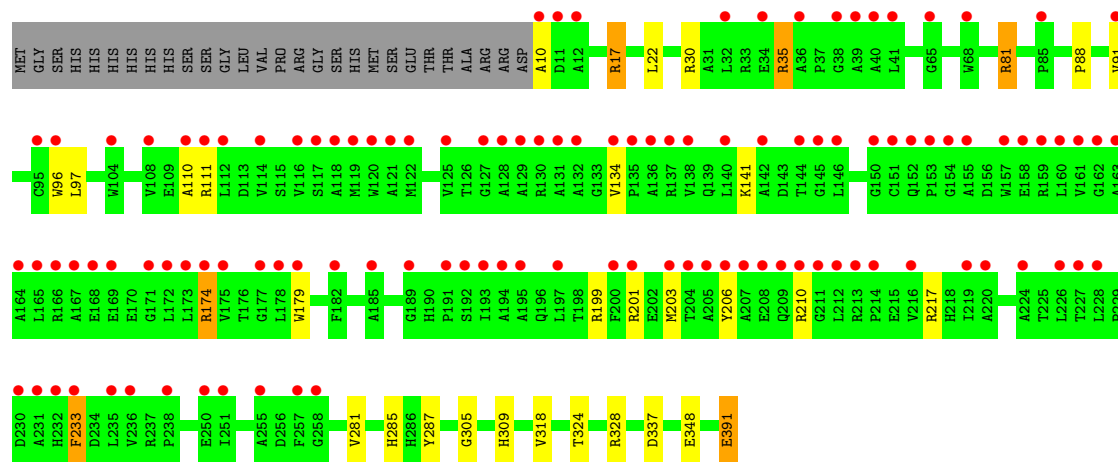


- Molecule 1: Alanine racemase



- Molecule 1: Alanine racemase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.95Å 88.58Å 108.88Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	48.06 – 1.51 48.06 – 1.51	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.06-1.51) 96.6 (48.06-1.51)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.199 , 0.225 0.212 , 0.237	Depositor DCC
$R_{free}$ test set	11051 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1838e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, PLP, PPI, NO3, NA

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	1.33	13/3174 (0.4%)	1.13	7/4321 (0.2%)
1	B	1.33	5/3003 (0.2%)	1.11	5/4098 (0.1%)
1	C	1.23	3/3001 (0.1%)	1.07	7/4093 (0.2%)
1	D	1.23	4/3027 (0.1%)	1.06	3/4127 (0.1%)
All	All	1.28	25/12205 (0.2%)	1.09	22/16639 (0.1%)

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	233	PHE	C-O	-7.12	1.17	1.24
1	A	217[A]	ARG	CA-C	6.95	1.61	1.52
1	A	217[B]	ARG	CA-C	6.95	1.61	1.52
1	A	196	GLN	CA-C	-6.81	1.44	1.52
1	A	298	VAL	CA-C	6.01	1.57	1.53

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLY	N-CA-C	8.96	127.06	115.32
1	A	220	ALA	N-CA-C	8.22	121.83	109.25
1	A	39	ALA	N-CA-C	7.43	121.59	109.85
1	C	213	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	213	ARG	NE-CZ-NH2	6.31	124.88	119.20

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	3047	0	3086	21	0
1	B	2911	0	2904	15	0
1	C	2909	0	2913	21	0
1	D	2926	0	2943	37	0
2	A	15	0	6	5	0
2	B	15	0	6	2	0
2	C	15	0	7	5	0
2	D	15	0	6	3	0
3	A	5	0	5	2	0
3	B	20	0	20	2	0
3	C	5	0	5	2	0
3	D	10	0	10	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	237	0	0	5	0
6	B	239	0	0	9	0
6	C	167	0	0	5	0
6	D	161	0	0	6	0
All	All	12710	0	11911	100	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 4.

The worst 5 of 100 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)
3:C:402:PPI:O1	6:C:501:HOH:O	1.60	1.19
1:B:137:ARG:HD3	6:B:601:HOH:O	1.40	1.17
1:D:35[A]:ARG:HH11	1:D:35[A]:ARG:HG3	1.15	1.07
1:B:92:ARG:NH1	6:B:601:HOH:O	1.88	1.05
6:A:586:HOH:O	1:B:383[B]:ARG:HD3	1.58	1.00

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	411/410 (100%)	400 (97%)	11 (3%)	0	100	100
1	B	392/410 (96%)	381 (97%)	11 (3%)	0	100	100
1	C	391/410 (95%)	377 (96%)	14 (4%)	0	100	100
1	D	394/410 (96%)	382 (97%)	12 (3%)	0	100	100
All	All	1588/1640 (97%)	1540 (97%)	48 (3%)	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	304/297 (102%)	300 (99%)	4 (1%)	61	34
1	B	286/297 (96%)	284 (99%)	2 (1%)	76	57
1	C	285/297 (96%)	283 (99%)	2 (1%)	76	57
1	D	288/297 (97%)	279 (97%)	9 (3%)	35	8
All	All	1163/1188 (98%)	1146 (98%)	17 (2%)	68	29

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	134	VAL
1	D	391	GLU
1	C	17[B]	ARG
1	D	17[A]	ARG
1	D	17[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	390	ASN
1	D	152	GLN
1	D	309	HIS
1	D	285	HIS
1	B	285	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 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	141	1	10,11,12	2.67	2 (20%)	6,12,14	2.03	2 (33%)
1	KCX	A	141	1	10,11,12	1.35	2 (20%)	6,12,14	1.30	1 (16%)
1	KCX	C	141	1	10,11,12	2.80	2 (20%)	6,12,14	2.10	2 (33%)
1	KCX	D	141	1	10,11,12	0.84	0	6,12,14	1.33	1 (16%)

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	141	1	-	1/9/10/12	-
1	KCX	A	141	1	-	1/9/10/12	-
1	KCX	C	141	1	-	1/9/10/12	-
1	KCX	D	141	1	-	1/9/10/12	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	KCX	OQ1-CX	7.86	1.36	1.21
1	C	141	KCX	OQ1-CX	7.85	1.36	1.21
1	A	141	KCX	CB-CA	2.80	1.57	1.53
1	C	141	KCX	CB-CA	2.70	1.57	1.53
1	A	141	KCX	CA-N	-2.56	1.40	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	KCX	OQ1-CX-NZ	-3.70	119.30	124.92
1	B	141	KCX	OQ1-CX-NZ	-3.62	119.42	124.92
1	C	141	KCX	CE-NZ-CX	3.42	127.78	121.98
1	B	141	KCX	CE-NZ-CX	3.26	127.51	121.98
1	D	141	KCX	CE-NZ-CX	2.98	127.03	121.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	141	KCX	CG-CD-CE-NZ
1	D	141	KCX	CG-CD-CE-NZ
1	C	141	KCX	CG-CD-CE-NZ
1	B	141	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 for Mogul analysis.

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
3	PPI	B	506	-	4,4,4	0.95	0	4,4,4	0.97	0
3	PPI	B	507	-	4,4,4	0.86	0	4,4,4	1.52	1 (25%)
2	PLP	A	401	1	15,15,16	3.02	4 (26%)	21,22,23	2.21	7 (33%)
2	PLP	C	401	1	15,15,16	2.63	3 (20%)	21,22,23	2.70	8 (38%)
3	PPI	B	501	-	4,4,4	1.60	1 (25%)	4,4,4	0.96	0
3	PPI	B	505	-	4,4,4	1.12	0	4,4,4	0.90	0
3	PPI	C	402	-	4,4,4	1.21	1 (25%)	4,4,4	1.17	0
3	PPI	D	501	-	4,4,4	1.56	1 (25%)	4,4,4	1.05	0
5	NO3	A	405	-	1,3,3	0.68	0	0,3,3	-	-
5	NO3	B	508	-	1,3,3	0.70	0	0,3,3	-	-
3	PPI	A	402	-	4,4,4	0.62	0	4,4,4	1.64	1 (25%)
2	PLP	B	502	1	15,15,16	3.43	7 (46%)	21,22,23	3.32	10 (47%)
2	PLP	D	502	1	15,15,16	3.06	5 (33%)	21,22,23	2.40	8 (38%)
3	PPI	D	503	-	4,4,4	1.11	0	4,4,4	1.20	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
3	PPI	B	506	-	-	2/2/2/2	-
3	PPI	B	507	-	-	0/2/2/2	-
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
3	PPI	B	501	-	-	2/2/2/2	-
3	PPI	B	505	-	-	2/2/2/2	-
3	PPI	C	402	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PPI	D	501	-	-	1/2/2/2	-
3	PPI	A	402	-	-	1/2/2/2	-
2	PLP	B	502	1	-	0/6/6/8	0/1/1/1
2	PLP	D	502	1	-	0/6/6/8	0/1/1/1
3	PPI	D	503	-	-	2/2/2/2	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PLP	C5-C4	10.88	1.52	1.40
2	A	401	PLP	C5-C4	10.25	1.52	1.40
2	C	401	PLP	C5-C4	8.44	1.50	1.40
2	D	502	PLP	C5-C4	8.22	1.49	1.40
2	D	502	PLP	C3-C2	5.72	1.46	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	PLP	C4A-C4-C5	10.21	131.46	120.94
2	C	401	PLP	C2A-C2-C3	-6.75	112.90	120.80
2	B	502	PLP	C2A-C2-C3	-5.87	113.93	120.80
2	C	401	PLP	C4A-C4-C5	5.64	126.75	120.94
2	A	401	PLP	C4A-C4-C5	5.61	126.72	120.94

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	506	PPI	O1-C1-C2-C3
3	C	402	PPI	O1-C1-C2-C3
3	C	402	PPI	O2-C1-C2-C3
3	D	503	PPI	O1-C1-C2-C3
3	D	503	PPI	O2-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	5	0
2	C	401	PLP	5	0
3	B	501	PPI	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	PPI	1	0
3	C	402	PPI	2	0
3	D	501	PPI	2	0
3	A	402	PPI	2	0
2	B	502	PLP	2	0
2	D	502	PLP	3	0
3	D	503	PPI	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	389/410 (94%)	0.46	14 (3%) 46 53	12, 26, 44, 83	22 (5%)
1	B	381/410 (92%)	0.28	7 (1%) 67 73	11, 25, 38, 71	13 (3%)
1	C	381/410 (92%)	0.83	35 (9%) 14 17	14, 31, 54, 74	11 (2%)
1	D	381/410 (92%)	1.34	115 (30%) 1 1	13, 34, 66, 90	14 (3%)
All	All	1532/1640 (93%)	0.73	171 (11%) 10 12	11, 28, 54, 90	60 (3%)

The worst 5 of 171 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	167	ALA	6.0
1	C	10	ALA	5.9
1	D	157	TRP	5.5
1	B	10	ALA	5.4
1	D	160	LEU	5.3

### 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	141	12/13	0.82	0.17	42,44,79,91	0
1	KCX	A	141	12/13	0.92	0.12	21,24,65,67	0
1	KCX	B	141	12/13	0.93	0.12	19,29,71,71	0
1	KCX	C	141	12/13	0.94	0.10	23,28,64,64	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
3	PPI	B	507	5/5	0.57	0.27	47,47,57,68	0
3	PPI	B	505	5/5	0.76	0.14	40,48,59,62	0
3	PPI	B	501	5/5	0.76	0.19	30,49,51,55	0
3	PPI	B	506	5/5	0.77	0.18	56,61,64,67	0
3	PPI	A	402	5/5	0.77	0.18	33,46,51,54	0
3	PPI	C	402	5/5	0.82	0.14	44,53,59,69	0
3	PPI	D	501	5/5	0.82	0.17	31,50,54,58	0
3	PPI	D	503	5/5	0.82	0.13	28,38,40,43	0
5	NO3	A	405	4/4	0.89	0.10	43,46,47,49	0
5	NO3	B	508	4/4	0.91	0.09	32,38,39,45	0
2	PLP	D	502	15/16	0.93	0.12	30,48,58,62	0
4	NA	A	404	1/1	0.96	0.10	31,31,31,31	0
4	NA	B	504	1/1	0.96	0.12	29,29,29,29	0
2	PLP	B	502	15/16	0.96	0.10	21,31,46,51	0
2	PLP	A	401	15/16	0.96	0.11	21,36,47,51	0
4	NA	A	403	1/1	0.97	0.11	31,31,31,31	0
2	PLP	C	401	15/16	0.97	0.09	22,38,50,56	0
4	NA	B	503	1/1	0.97	0.08	33,33,33,33	0
4	NA	C	403	1/1	0.98	0.05	35,35,35,35	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.