wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 12:02 am GMT

PDB ID	:	5FAG
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*
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.

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

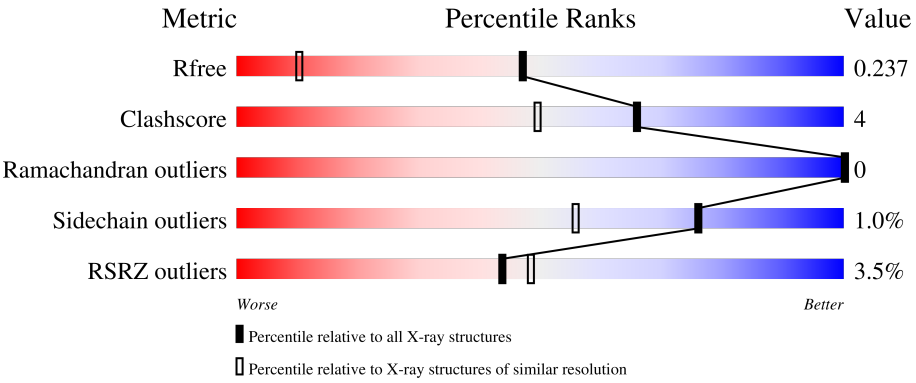
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (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 >=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	410	2% 87% 8% 5%
1	B	410	87% 6% 7%
1	C	410	2% 85% 8% 7%
1	D	410	9% 85% 6% • 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
1	A	390	Total	C	N	O	S	0	22	0
			3047	1915	567	552	13			
1	B	382	Total	C	N	O	S	0	13	0
			2911	1829	536	534	12			
1	C	382	Total	C	N	O	S	0	11	0
			2909	1830	538	529	12			
1	D	382	Total	C	N	O	S	0	14	0
			2926	1842	542	528	14			

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

Continued on next page...

Continued from previous page...

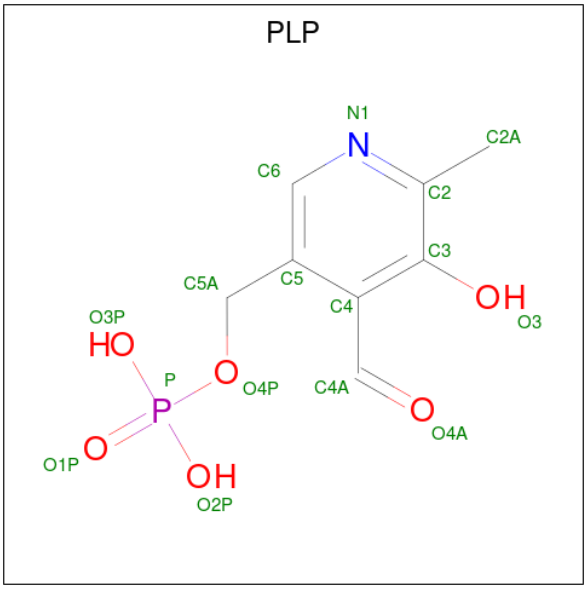
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP O86786
B	-15	HIS	-	expression tag	UNP O86786
B	-14	HIS	-	expression tag	UNP O86786
B	-13	HIS	-	expression tag	UNP O86786
B	-12	HIS	-	expression tag	UNP O86786
B	-11	HIS	-	expression tag	UNP O86786
B	-10	HIS	-	expression tag	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

Continued on next page...

Continued from previous page...

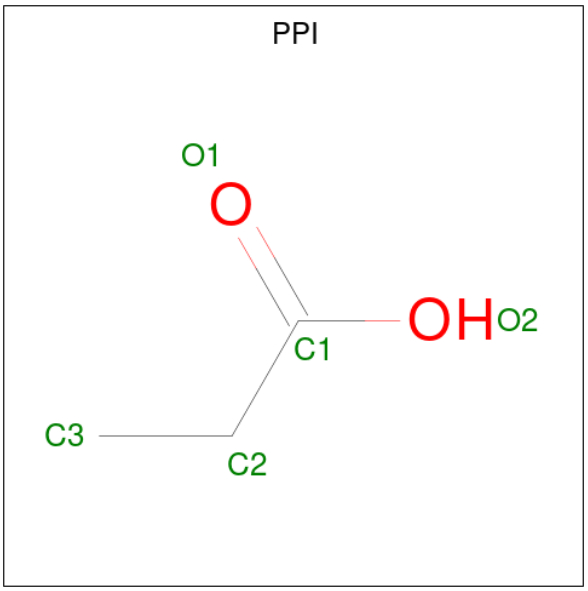
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP O86786
D	-11	HIS	-	expression tag	UNP O86786
D	-10	HIS	-	expression tag	UNP O86786
D	-9	SER	-	expression tag	UNP O86786
D	-8	SER	-	expression tag	UNP O86786
D	-7	GLY	-	expression tag	UNP O86786
D	-6	LEU	-	expression tag	UNP 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 (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (three-letter code: PPI) (formula: $C_3H_6O_2$).

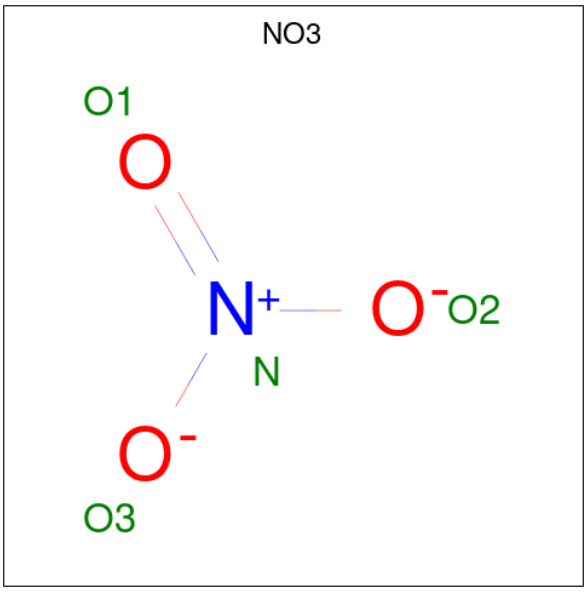


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	B	1	Total C O 5 3 2	0	0
3	C	1	Total C O 5 3 2	0	0
3	D	1	Total C O 5 3 2	0	0
3	D	1	Total C O 5 3 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: 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 (three-letter code: NO3) (formula: NO_3).



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

- Molecule 6 is water.

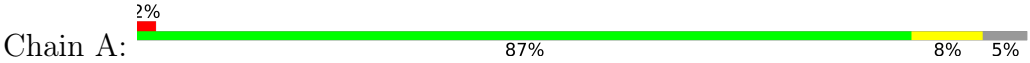
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	237	Total O 237 237	0	0
6	B	239	Total O 239 239	0	0
6	C	167	Total O 167 167	0	0
6	D	161	Total O 161 161	0	0

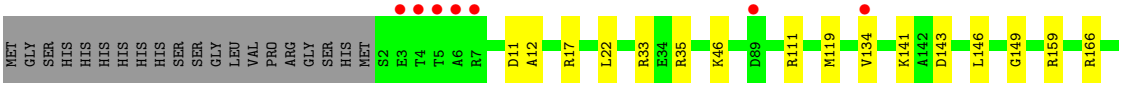
3 Residue-property plots (i)

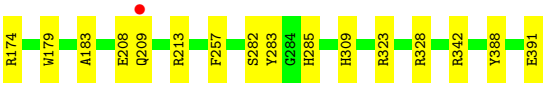
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:

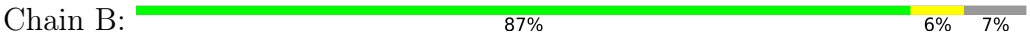


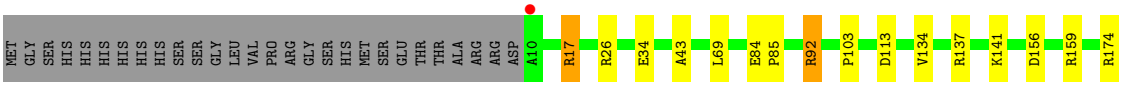




• Molecule 1: Alanine racemase

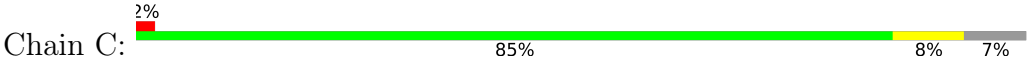
Chain B:

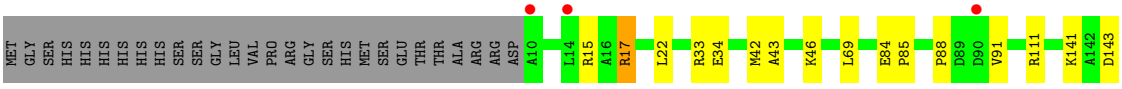


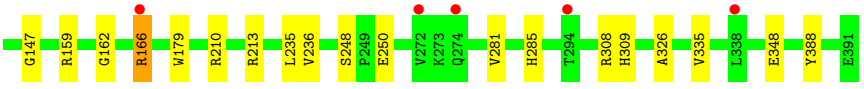


• Molecule 1: Alanine racemase

Chain C:

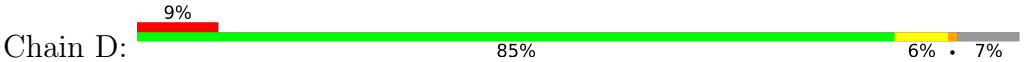


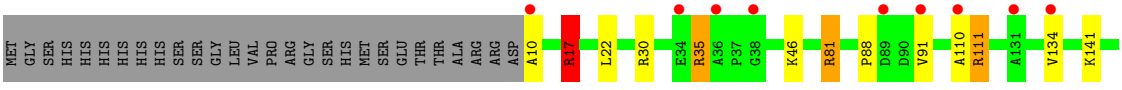


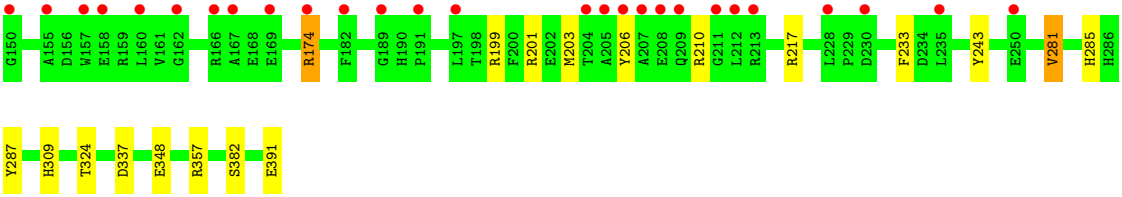


• Molecule 1: Alanine racemase

Chain D:






G150
A155
D156
W157
E158
R159
L160
V161
G162
R166
A167
E168
E169
R174
F182
G189
H190
P191
L197
T198
R199
F200
R201
E202
M203
T204
A205
Y206
A207
E208
Q209
R210
G211
L212
R213
R217
L228
P229
D230
F233
D234
L235
Y243
E250
V281
H285
H286

Y287
H309
T324
D337
E348
R357
S382
E391

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.28 (at 1.51Å)	Xtriage
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 (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12710	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, PPI, KCX, PLP, NO3

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	1.02	1/3174 (0.0%)	1.02	12/4321 (0.3%)
1	B	1.02	2/3003 (0.1%)	1.17	19/4098 (0.5%)
1	C	0.93	0/3001	1.00	10/4093 (0.2%)
1	D	0.94	2/3027 (0.1%)	0.99	12/4127 (0.3%)
All	All	0.98	5/12205 (0.0%)	1.05	53/16639 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	SER	CB-OG	5.94	1.50	1.42
1	D	382	SER	CB-OG	-5.38	1.35	1.42
1	B	34	GLU	CD-OE2	5.31	1.31	1.25
1	D	243	TYR	CE1-CZ	5.27	1.45	1.38
1	B	344	GLU	CD-OE1	-5.19	1.20	1.25

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	17[A]	ARG	NE-CZ-NH2	16.87	128.74	120.30
1	B	17[B]	ARG	NE-CZ-NH2	16.87	128.74	120.30
1	B	17[A]	ARG	NE-CZ-NH1	-14.19	113.21	120.30
1	B	17[B]	ARG	NE-CZ-NH1	-14.19	113.21	120.30
1	C	213	ARG	NE-CZ-NH2	10.00	125.30	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3085	20	0
1	B	2911	0	2903	15	0
1	C	2909	0	2912	20	0
1	D	2926	0	2942	34	0
2	A	15	0	6	5	0
2	B	15	0	6	3	0
2	C	15	0	7	4	0
2	D	15	0	6	1	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	11907	95	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 95 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%)	69	43
1	B	286/297 (96%)	283 (99%)	3 (1%)	76	56
1	C	285/297 (96%)	281 (99%)	4 (1%)	67	41
1	D	288/297 (97%)	281 (98%)	7 (2%)	49	19
All	All	1163/1188 (98%)	1145 (98%)	18 (2%)	76	38

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	35[C]	ARG
1	D	174	ARG
1	D	134	VAL
1	C	17[B]	ARG
1	D	35[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	286	HIS
1	D	285	HIS
1	B	390	ASN
1	D	152	GLN
1	B	309	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	C	141	1	9,11,12	2.92	2 (22%)	5,12,14	2.34	2 (40%)
1	KCX	A	141	1	9,11,12	1.48	2 (22%)	5,12,14	1.47	1 (20%)
1	KCX	B	141	1	9,11,12	2.78	2 (22%)	5,12,14	2.27	2 (40%)
1	KCX	D	141	1	9,11,12	0.86	0	5,12,14	1.52	1 (20%)

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	C	141	1	-	1/9/10/12	-
1	KCX	A	141	1	-	1/9/10/12	-
1	KCX	B	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	7.79	1.36	1.21
1	C	141	KCX	OQ1-CX	7.78	1.36	1.21
1	A	141	KCX	CB-CA	3.19	1.57	1.53
1	C	141	KCX	CB-CA	3.08	1.57	1.53
1	B	141	KCX	CB-CA	2.68	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	KCX	CE-NZ-CX	3.67	127.78	121.89
1	C	141	KCX	OQ1-CX-NZ	-3.65	119.30	124.96
1	B	141	KCX	OQ1-CX-NZ	-3.57	119.42	124.96
1	B	141	KCX	CE-NZ-CX	3.50	127.51	121.89
1	D	141	KCX	CE-NZ-CX	3.21	127.03	121.89

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	402	-	4,4,4	0.60	0	4,4,4	1.60	1 (25%)
3	PPI	D	503	-	4,4,4	1.09	0	4,4,4	1.19	0
5	NO3	B	508	-	1,3,3	0.68	0	0,3,3	-	-
3	PPI	C	402	-	4,4,4	1.18	1 (25%)	4,4,4	1.14	0
3	PPI	B	506	-	4,4,4	0.92	0	4,4,4	0.97	0
5	NO3	A	405	-	1,3,3	0.66	0	0,3,3	-	-
3	PPI	B	505	-	4,4,4	1.08	0	4,4,4	0.89	0
2	PLP	C	401	1	15,15,16	2.65	3 (20%)	20,22,23	2.72	8 (40%)
2	PLP	B	502	1	15,15,16	3.45	6 (40%)	20,22,23	3.37	10 (50%)
2	PLP	D	502	1	15,15,16	3.07	5 (33%)	20,22,23	2.41	8 (40%)
2	PLP	A	401	1	15,15,16	3.06	4 (26%)	20,22,23	2.24	7 (35%)
3	PPI	B	501	-	4,4,4	1.56	1 (25%)	4,4,4	0.91	0
3	PPI	B	507	-	4,4,4	0.83	0	4,4,4	1.54	1 (25%)
3	PPI	D	501	-	4,4,4	1.52	1 (25%)	4,4,4	1.00	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	A	402	-	-	0/2/2/2	-
3	PPI	D	503	-	-	2/2/2/2	-
3	PPI	C	402	-	-	2/2/2/2	-
3	PPI	B	506	-	-	2/2/2/2	-
3	PPI	B	505	-	-	0/2/2/2	-
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
3	PPI	B	501	-	-	0/2/2/2	-
3	PPI	B	507	-	-	0/2/2/2	-
3	PPI	D	501	-	-	0/2/2/2	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PLP	C5-C4	11.12	1.52	1.40
2	A	401	PLP	C5-C4	10.48	1.52	1.40
2	C	401	PLP	C5-C4	8.63	1.50	1.40
2	D	502	PLP	C5-C4	8.40	1.49	1.40
2	D	502	PLP	C3-C2	6.00	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	PLP	C4A-C4-C5	10.22	131.46	120.94
2	C	401	PLP	C2A-C2-C3	-6.47	112.90	120.89
2	C	401	PLP	C4A-C4-C5	5.65	126.75	120.94
2	B	502	PLP	C2A-C2-C3	-5.63	113.93	120.89
2	A	401	PLP	C4A-C4-C5	5.62	126.72	120.94

There are no chirality outliers.

5 of 6 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 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	PPI	2	0
3	D	503	PPI	3	0
3	C	402	PPI	2	0
3	B	505	PPI	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PLP	4	0
2	B	502	PLP	3	0
2	D	502	PLP	1	0
2	A	401	PLP	5	0
3	B	501	PPI	1	0
3	D	501	PPI	2	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	389/410 (94%)	-0.10	8 (2%) 63 68	17, 27, 45, 83	0
1	B	381/410 (92%)	-0.12	1 (0%) 94 95	17, 25, 39, 71	0
1	C	381/410 (92%)	0.05	8 (2%) 63 68	20, 32, 54, 74	0
1	D	381/410 (92%)	0.46	36 (9%) 8 8	18, 35, 66, 90	0
All	All	1532/1640 (93%)	0.07	53 (3%) 44 48	17, 29, 54, 90	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	160	LEU	5.8
1	C	10	ALA	4.9
1	B	10	ALA	4.9
1	D	189	GLY	4.7
1	D	212	LEU	4.7

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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
1	KCX	D	141	12/13	0.82	0.13	42,44,79,91	0
1	KCX	B	141	12/13	0.92	0.10	19,29,71,71	0
1	KCX	A	141	12/13	0.92	0.09	21,24,65,67	0
1	KCX	C	141	12/13	0.94	0.09	23,28,64,64	0

6.3 Carbohydrates (i)

There are no monosaccharides 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^{th} 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	PPI	B	507	5/5	0.57	0.25	47,47,57,68	0
3	PPI	D	503	5/5	0.69	0.13	28,38,40,43	0
3	PPI	B	505	5/5	0.74	0.15	40,48,59,62	0
3	PPI	A	402	5/5	0.80	0.18	33,46,51,54	0
3	PPI	B	501	5/5	0.82	0.18	30,49,51,55	0
3	PPI	C	402	5/5	0.84	0.18	44,53,59,69	0
3	PPI	B	506	5/5	0.84	0.12	56,61,64,67	0
3	PPI	D	501	5/5	0.88	0.22	31,50,54,58	0
5	NO3	A	405	4/4	0.95	0.20	43,46,47,49	0
5	NO3	B	508	4/4	0.95	0.11	32,38,39,45	0
4	NA	B	504	1/1	0.96	0.05	29,29,29,29	0
4	NA	C	403	1/1	0.97	0.06	35,35,35,35	0
2	PLP	D	502	15/16	0.97	0.15	30,48,58,62	0
2	PLP	A	401	15/16	0.97	0.14	21,36,47,51	0
2	PLP	C	401	15/16	0.98	0.11	22,38,50,56	0
2	PLP	B	502	15/16	0.98	0.10	21,31,46,51	0
4	NA	A	403	1/1	0.98	0.08	31,31,31,31	0
4	NA	A	404	1/1	0.98	0.05	31,31,31,31	0
4	NA	B	503	1/1	0.99	0.06	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.