wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2023 – 07:25 AM EDT

PDB ID	:	3OPV
Title	:	Crystal structure of E. Coli purine nucleoside phosphorylase Arg24Ala mutant
Authors	:	Mikleusevic, G.; Stefanic, Z.; Narzyk, M.; Wielgus-Kutrowska, B.; Bzowska, A.; Luic, M.
Deposited on	:	2010-09-02
Resolution	:	2.40 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:

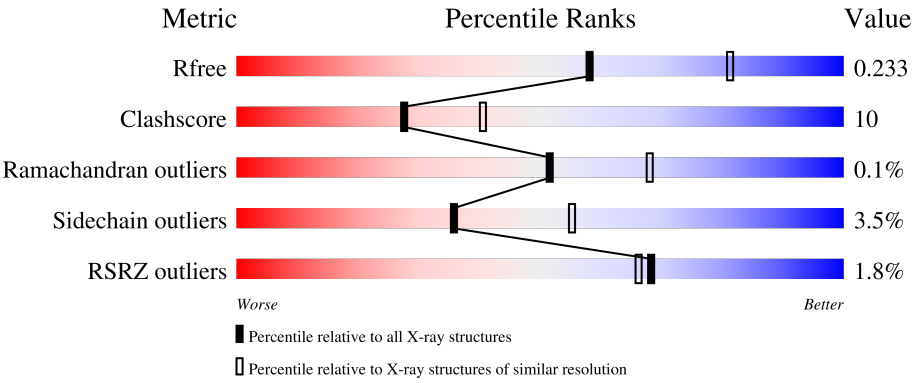
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	237	5% 82% 16% ·
1	B	237	3% 82% 16% ·
1	C	237	% 81% 17% ·
1	D	237	% 76% 24% ·
1	E	237	3% 73% 24% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	237	3% 76% 21%
1	G	237	2% 82% 16%
1	H	237	% 82% 16%
1	I	237	% 82% 16%
1	J	237	% 74% 22%
1	K	237	% 79% 20%
1	L	237	2% 76% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22982 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 Purine nucleoside phosphorylase deoD-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1788	1130	304	339	15			
1	B	237	Total	C	N	O	S	0	0	0
			1791	1132	305	339	15			
1	C	237	Total	C	N	O	S	0	1	0
			1796	1135	307	339	15			
1	D	237	Total	C	N	O	S	0	2	0
			1806	1142	310	339	15			
1	E	232	Total	C	N	O	S	0	0	0
			1749	1108	297	329	15			
1	F	237	Total	C	N	O	S	0	0	0
			1788	1130	304	339	15			
1	G	237	Total	C	N	O	S	0	0	0
			1788	1130	304	339	15			
1	H	237	Total	C	N	O	S	0	0	0
			1791	1132	305	339	15			
1	I	237	Total	C	N	O	S	0	0	0
			1791	1132	305	339	15			
1	J	233	Total	C	N	O	S	0	1	0
			1760	1115	299	331	15			
1	K	237	Total	C	N	O	S	0	0	0
			1787	1130	304	338	15			
1	L	237	Total	C	N	O	S	0	0	0
			1784	1127	303	339	15			

There are 12 discrepancies between the modelled and reference sequences:

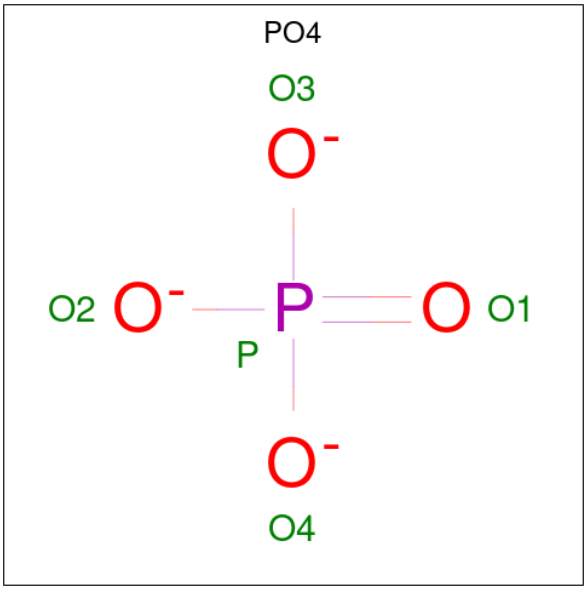
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ALA	ARG	engineered mutation	UNP C9QST6
B	24	ALA	ARG	engineered mutation	UNP C9QST6
C	24	ALA	ARG	engineered mutation	UNP C9QST6
D	24	ALA	ARG	engineered mutation	UNP C9QST6
E	24	ALA	ARG	engineered mutation	UNP C9QST6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	24	ALA	ARG	engineered mutation	UNP C9QST6
G	24	ALA	ARG	engineered mutation	UNP C9QST6
H	24	ALA	ARG	engineered mutation	UNP C9QST6
I	24	ALA	ARG	engineered mutation	UNP C9QST6
J	24	ALA	ARG	engineered mutation	UNP C9QST6
K	24	ALA	ARG	engineered mutation	UNP C9QST6
L	24	ALA	ARG	engineered mutation	UNP C9QST6

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

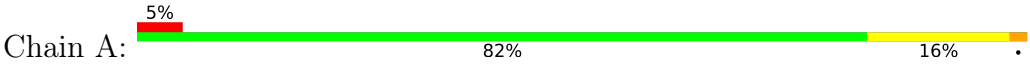
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	99	Total O 99 99	0	0
3	B	136	Total O 136 136	0	0
3	C	109	Total O 109 109	0	0
3	D	151	Total O 151 151	0	0
3	E	93	Total O 93 93	0	0
3	F	104	Total O 104 104	0	0
3	G	81	Total O 81 81	0	0
3	H	155	Total O 155 155	0	0
3	I	159	Total O 159 159	0	0
3	J	131	Total O 131 131	0	0
3	K	114	Total O 114 114	0	0
3	L	161	Total O 161 161	0	0

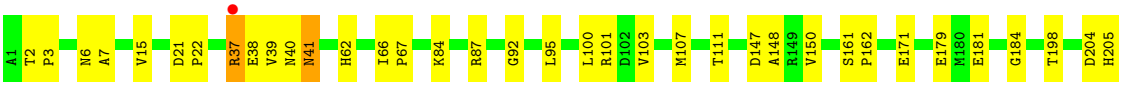
3 Residue-property plots (i)

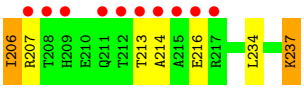
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

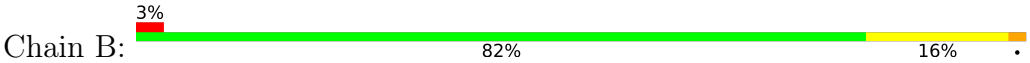


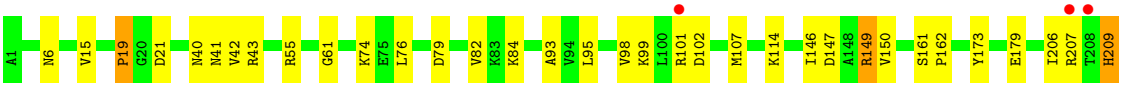


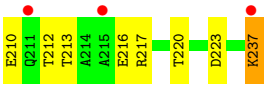


• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain B:

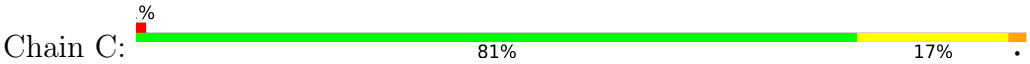


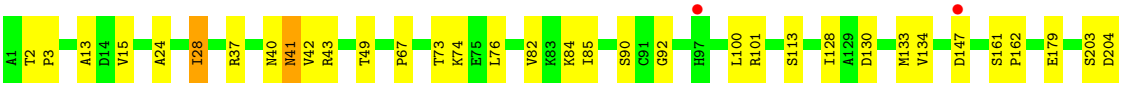


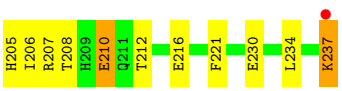


• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain C:

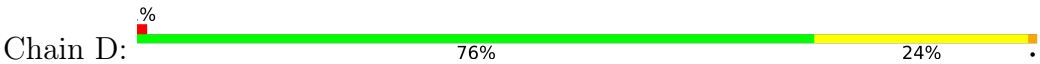


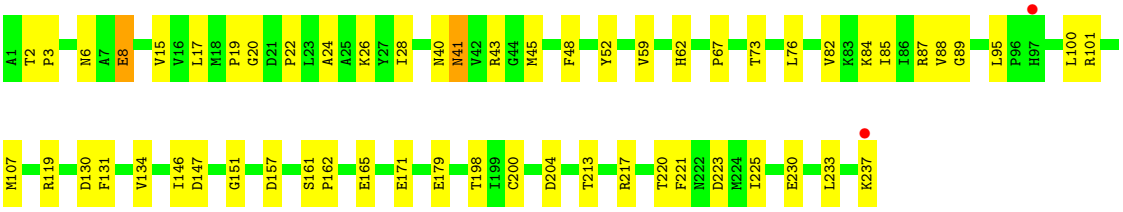




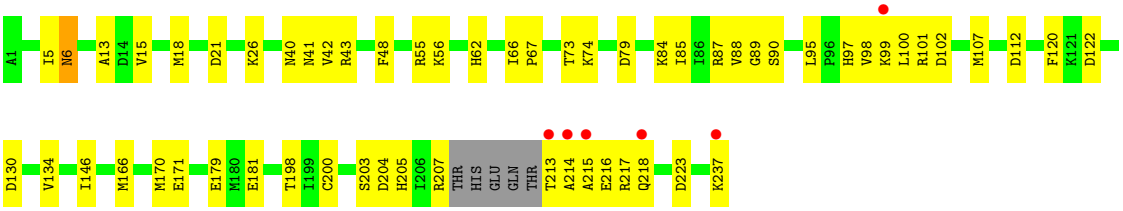
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain D:

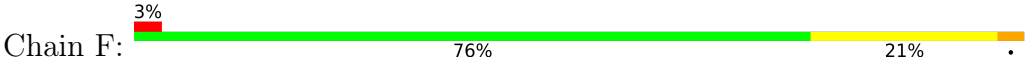


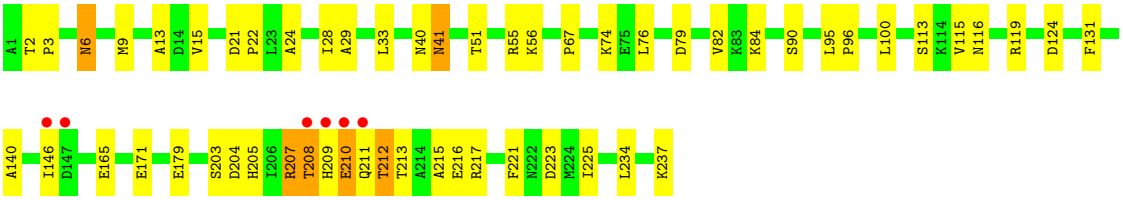


• Molecule 1: Purine nucleoside phosphorylase deoD-type

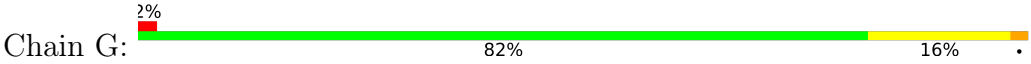


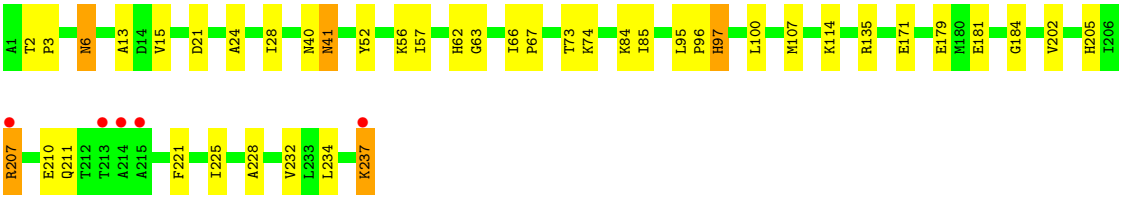
• Molecule 1: Purine nucleoside phosphorylase deoD-type



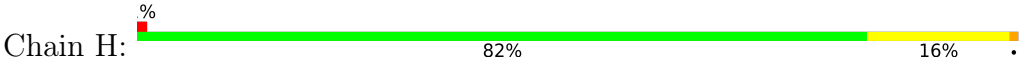


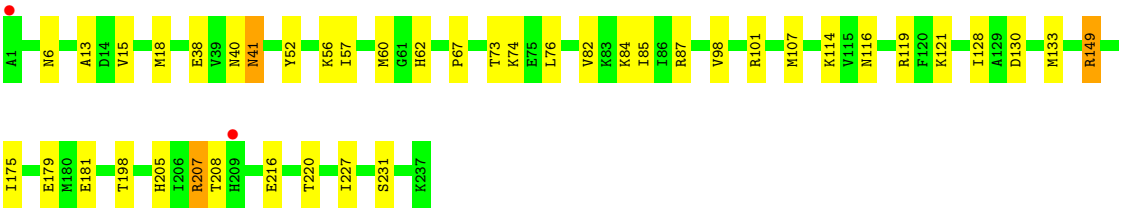
• Molecule 1: Purine nucleoside phosphorylase deoD-type





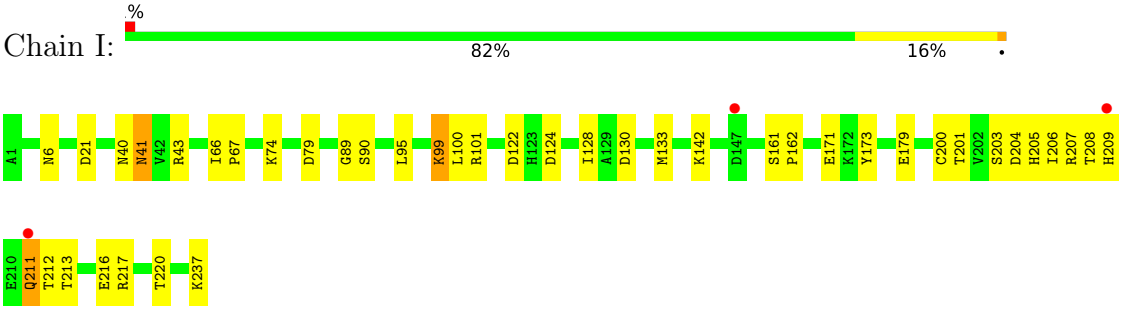
• Molecule 1: Purine nucleoside phosphorylase deoD-type





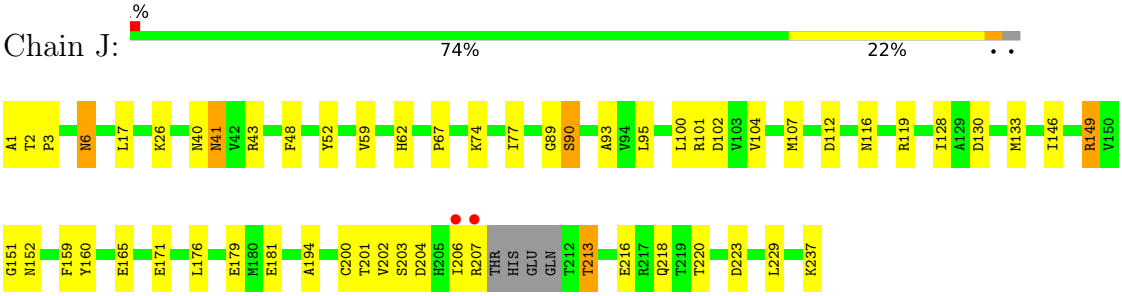
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain I:



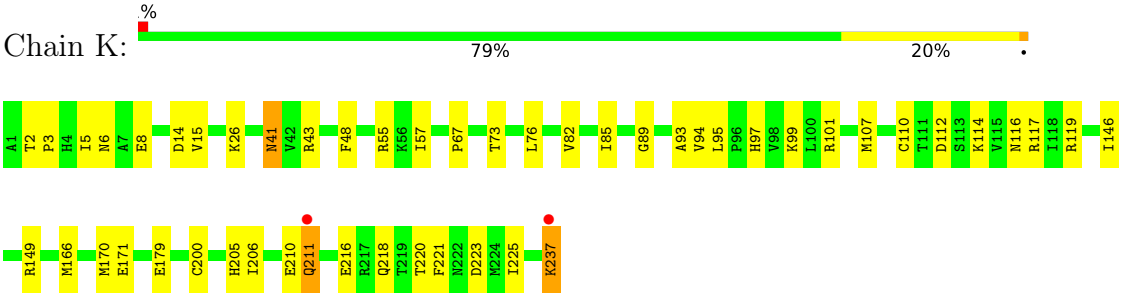
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain J:



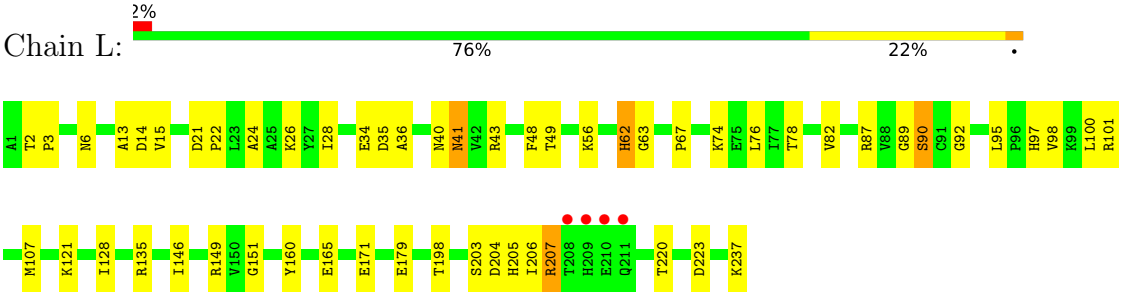
• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain K:



• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.21Å 158.78Å 122.24Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	19.10 – 2.40 19.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.10-2.40) 100.0 (19.12-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.30Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.181 , 0.238 0.177 , 0.233	Depositor DCC
R_{free} test set	2009 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22982	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 38.56 % 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 3.6178e-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: PO4

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	0.27	0/1817	0.44	0/2451
1	B	0.27	0/1820	0.44	0/2454
1	C	0.25	0/1828	0.44	0/2465
1	D	0.28	0/1842	0.44	0/2483
1	E	0.25	0/1776	0.43	0/2392
1	F	0.28	0/1817	0.47	0/2451
1	G	0.25	0/1817	0.44	0/2451
1	H	0.27	0/1820	0.44	0/2454
1	I	0.27	0/1820	0.45	0/2454
1	J	0.26	0/1791	0.44	0/2414
1	K	0.26	0/1816	0.44	0/2449
1	L	0.28	0/1813	0.45	0/2447
All	All	0.27	0/21777	0.44	0/29365

There are no bond length outliers.

There are no bond angle outliers.

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	1788	0	1785	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1791	0	1794	35	0
1	C	1796	0	1798	38	0
1	D	1806	0	1814	40	0
1	E	1749	0	1758	35	0
1	F	1788	0	1785	47	0
1	G	1788	0	1785	37	0
1	H	1791	0	1794	45	0
1	I	1791	0	1794	36	0
1	J	1760	0	1763	46	0
1	K	1787	0	1782	35	0
1	L	1784	0	1774	40	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	15	0	0	0	0
3	A	99	0	0	1	0
3	B	136	0	0	5	0
3	C	109	0	0	6	0
3	D	151	0	0	5	0
3	E	93	0	0	2	0
3	F	104	0	0	1	0
3	G	81	0	0	1	0
3	H	155	0	0	0	0
3	I	159	0	0	3	0
3	J	131	0	0	2	0
3	K	114	0	0	2	0
3	L	161	0	0	3	0
All	All	22982	0	21426	427	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 10.

The worst 5 of 427 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:G:207:ARG:HG2	1:G:207:ARG:HH11	1.22	0.99
1:C:128:ILE:HD12	1:E:107:MET:HE3	1.53	0.89
1:F:207:ARG:HG2	1:F:208:THR:N	1.86	0.87
1:J:213:THR:HG22	1:J:216:GLU:H	1.39	0.87
1:G:107:MET:HE3	1:L:128:ILE:HD12	1.56	0.86

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	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
1	B	235/237 (99%)	225 (96%)	9 (4%)	1 (0%)	34	48
1	C	236/237 (100%)	221 (94%)	15 (6%)	0	100	100
1	D	237/237 (100%)	228 (96%)	9 (4%)	0	100	100
1	E	228/237 (96%)	218 (96%)	10 (4%)	0	100	100
1	F	235/237 (99%)	220 (94%)	14 (6%)	1 (0%)	34	48
1	G	235/237 (99%)	226 (96%)	9 (4%)	0	100	100
1	H	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
1	I	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
1	J	230/237 (97%)	223 (97%)	7 (3%)	0	100	100
1	K	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
1	L	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
All	All	2811/2844 (99%)	2686 (96%)	123 (4%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	210	GLU
1	B	209	HIS

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	186/187 (100%)	181 (97%)	5 (3%)	44	65
1	B	187/187 (100%)	179 (96%)	8 (4%)	29	46
1	C	187/187 (100%)	180 (96%)	7 (4%)	34	53
1	D	189/187 (101%)	184 (97%)	5 (3%)	46	66
1	E	182/187 (97%)	174 (96%)	8 (4%)	28	45
1	F	186/187 (100%)	179 (96%)	7 (4%)	33	51
1	G	186/187 (100%)	179 (96%)	7 (4%)	33	51
1	H	187/187 (100%)	182 (97%)	5 (3%)	44	65
1	I	187/187 (100%)	181 (97%)	6 (3%)	39	59
1	J	183/187 (98%)	175 (96%)	8 (4%)	28	45
1	K	185/187 (99%)	179 (97%)	6 (3%)	39	59
1	L	185/187 (99%)	179 (97%)	6 (3%)	39	59
All	All	2230/2244 (99%)	2152 (96%)	78 (4%)	36	55

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	211	GLN
1	K	237	LYS
1	J	41	ASN
1	J	237	LYS
1	L	179	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	41	ASN
1	L	222	ASN
1	J	218	GLN
1	K	116	ASN
1	E	40	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	PO4	I	238	-	4,4,4	0.94	0	6,6,6	0.46	0
2	PO4	H	238	-	4,4,4	0.88	0	6,6,6	0.57	0
2	PO4	D	238	-	4,4,4	0.91	0	6,6,6	0.50	0
2	PO4	L	239	-	4,4,4	0.83	0	6,6,6	0.42	0
2	PO4	C	238	-	4,4,4	0.90	0	6,6,6	0.42	0
2	PO4	J	238	-	4,4,4	0.88	0	6,6,6	0.44	0
2	PO4	B	238	-	4,4,4	0.98	0	6,6,6	0.56	0
2	PO4	L	240	-	4,4,4	0.89	0	6,6,6	0.50	0
2	PO4	F	238	-	4,4,4	0.88	0	6,6,6	0.50	0
2	PO4	G	238	-	4,4,4	0.93	0	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	K	238	-	4,4,4	0.89	0	6,6,6	0.39	0
2	PO4	A	238	-	4,4,4	0.91	0	6,6,6	0.52	0
2	PO4	E	238	-	4,4,4	0.94	0	6,6,6	0.56	0
2	PO4	L	238	-	4,4,4	0.99	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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	237/237 (100%)	-0.40	11 (4%)	32	31	19, 33, 70, 109	0
1	B	237/237 (100%)	-0.66	6 (2%)	57	55	15, 26, 57, 90	0
1	C	237/237 (100%)	-0.47	3 (1%)	77	75	20, 35, 55, 69	0
1	D	237/237 (100%)	-0.70	2 (0%)	86	84	15, 27, 46, 64	0
1	E	232/237 (97%)	-0.44	6 (2%)	56	54	17, 36, 70, 108	0
1	F	237/237 (100%)	-0.50	6 (2%)	57	55	18, 32, 60, 101	0
1	G	237/237 (100%)	-0.34	5 (2%)	63	61	21, 39, 72, 95	0
1	H	237/237 (100%)	-0.66	2 (0%)	86	84	17, 30, 47, 68	0
1	I	237/237 (100%)	-0.68	3 (1%)	77	75	17, 27, 46, 72	0
1	J	233/237 (98%)	-0.63	2 (0%)	84	82	18, 32, 48, 72	0
1	K	237/237 (100%)	-0.65	2 (0%)	86	84	18, 31, 52, 77	0
1	L	237/237 (100%)	-0.69	4 (1%)	70	68	17, 29, 45, 78	0
All	All	2835/2844 (99%)	-0.57	52 (1%)	68	66	15, 31, 58, 109	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	215	ALA	6.4
1	A	211	GLN	5.0
1	E	213	THR	4.9
1	F	208	THR	4.6
1	F	209	HIS	4.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (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
2	PO4	L	239	5/5	0.92	0.32	49,56,58,67	0
2	PO4	L	240	5/5	0.97	0.13	45,52,56,66	0
2	PO4	C	238	5/5	0.98	0.06	31,39,41,44	0
2	PO4	H	238	5/5	0.98	0.07	27,30,31,36	0
2	PO4	E	238	5/5	0.99	0.08	30,30,34,35	0
2	PO4	F	238	5/5	0.99	0.06	23,31,33,33	0
2	PO4	G	238	5/5	0.99	0.10	35,37,37,38	0
2	PO4	B	238	5/5	0.99	0.08	21,22,27,32	0
2	PO4	I	238	5/5	0.99	0.06	24,25,29,31	0
2	PO4	J	238	5/5	0.99	0.06	27,30,35,40	0
2	PO4	K	238	5/5	0.99	0.06	27,32,36,37	0
2	PO4	L	238	5/5	0.99	0.06	24,28,29,29	0
2	PO4	A	238	5/5	0.99	0.08	27,33,34,37	0
2	PO4	D	238	5/5	0.99	0.05	26,28,31,34	0

6.5 Other polymers (i)

There are no such residues in this entry.