



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:26 pm BST

PDB ID : 6NBG
Title : 2.05 Angstrom Resolution Crystal Structure of Hypothetical Protein KP1_5497 from *Klebsiella pneumoniae*.
Authors : Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovska, I.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2018-12-07
Resolution : 2.05 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

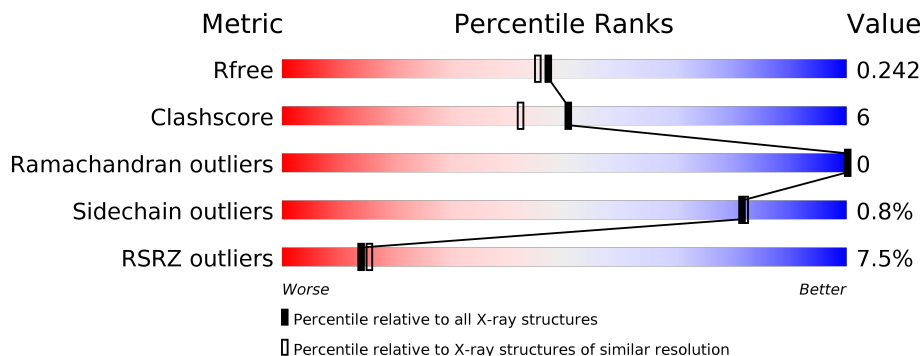
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 ≥ 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	242	 4% 88% 11% •
1	B	242	 3% 91% 7% •
1	C	242	 9% 90% 8% ••
1	D	242	 % 90% 8% •
1	E	242	 5% 89% 10% •
1	F	242	 21% 81% 17% ••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11887 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 Glucosamine-6-phosphate deaminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	242	Total 1864	C 1174	N 328	O 351	S 1	Se 10	0	2	0
1	B	241	Total 1858	C 1171	N 327	O 349	S 1	Se 10	0	2	0
1	C	240	Total 1831	C 1156	N 323	O 342	S 1	Se 9	0	0	0
1	D	239	Total 1831	C 1157	N 322	O 341	S 1	Se 10	0	1	0
1	E	240	Total 1831	C 1156	N 323	O 342	S 1	Se 9	0	0	0
1	F	240	Total 1833	C 1157	N 323	O 343	S 1	Se 9	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

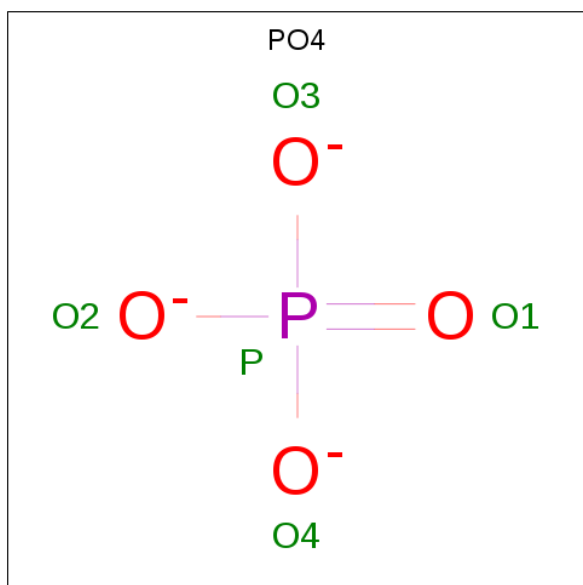
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A332QZQ2
A	-1	ASN	-	expression tag	UNP A0A332QZQ2
A	0	ALA	-	expression tag	UNP A0A332QZQ2
A	1	MSE	-	expression tag	UNP A0A332QZQ2
B	-2	SER	-	expression tag	UNP A0A332QZQ2
B	-1	ASN	-	expression tag	UNP A0A332QZQ2
B	0	ALA	-	expression tag	UNP A0A332QZQ2
B	1	MSE	-	expression tag	UNP A0A332QZQ2
C	-2	SER	-	expression tag	UNP A0A332QZQ2
C	-1	ASN	-	expression tag	UNP A0A332QZQ2
C	0	ALA	-	expression tag	UNP A0A332QZQ2
C	1	MSE	-	expression tag	UNP A0A332QZQ2
D	-2	SER	-	expression tag	UNP A0A332QZQ2
D	-1	ASN	-	expression tag	UNP A0A332QZQ2
D	0	ALA	-	expression tag	UNP A0A332QZQ2
D	1	MSE	-	expression tag	UNP A0A332QZQ2
E	-2	SER	-	expression tag	UNP A0A332QZQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP A0A332QZQ2
E	0	ALA	-	expression tag	UNP A0A332QZQ2
E	1	MSE	-	expression tag	UNP A0A332QZQ2
F	-2	SER	-	expression tag	UNP A0A332QZQ2
F	-1	ASN	-	expression tag	UNP A0A332QZQ2
F	0	ALA	-	expression tag	UNP A0A332QZQ2
F	1	MSE	-	expression tag	UNP A0A332QZQ2

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	1
2	E	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 10 8 2	0	1
2	F	1	Total O P 5 4 1	0	1

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Cl 2 2	0	1

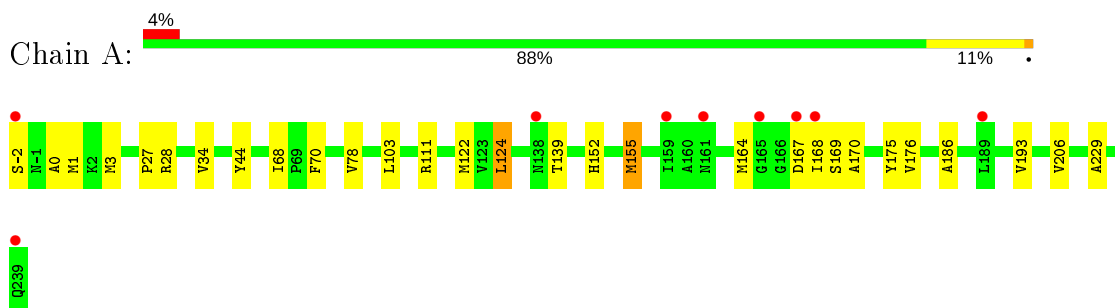
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	186	Total O 189 189	0	3
4	B	159	Total O 164 164	0	5
4	C	104	Total O 111 111	0	7
4	D	149	Total O 154 154	0	6
4	E	117	Total O 123 123	0	6
4	F	48	Total O 51 51	0	3

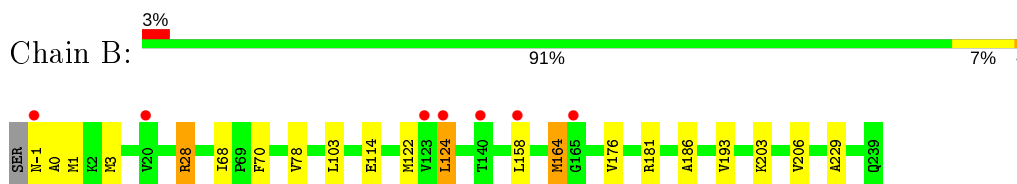
3 Residue-property plots [i](#)

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.

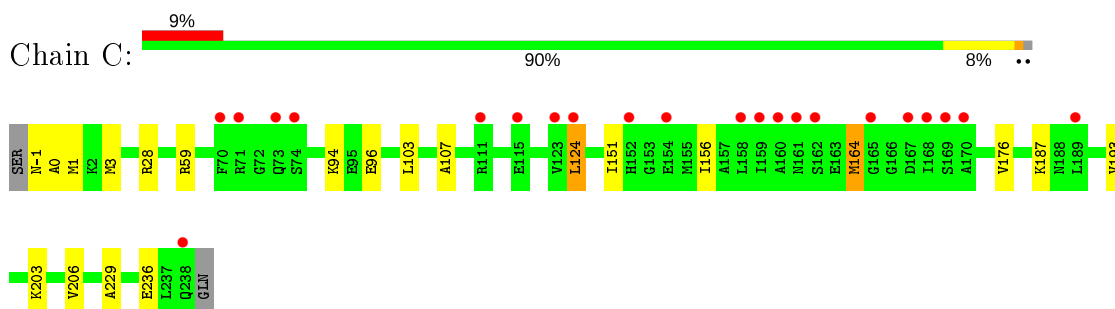
- Molecule 1: Glucosamine-6-phosphate deaminase



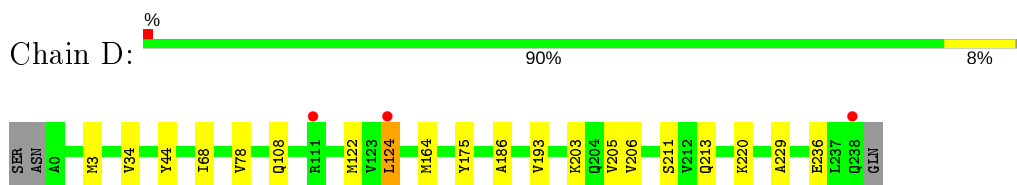
- Molecule 1: Glucosamine-6-phosphate deaminase



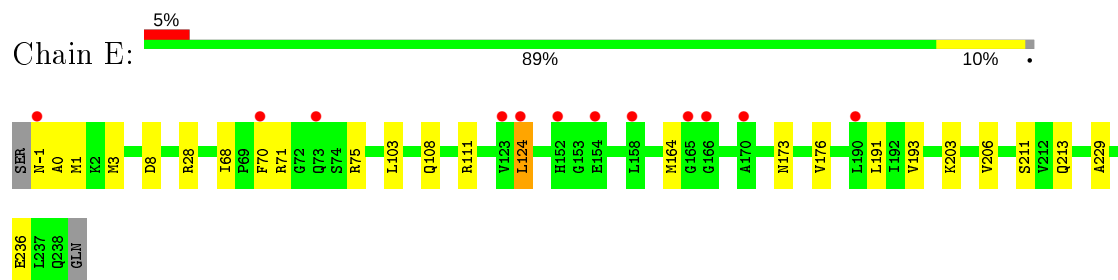
- Molecule 1: Glucosamine-6-phosphate deaminase



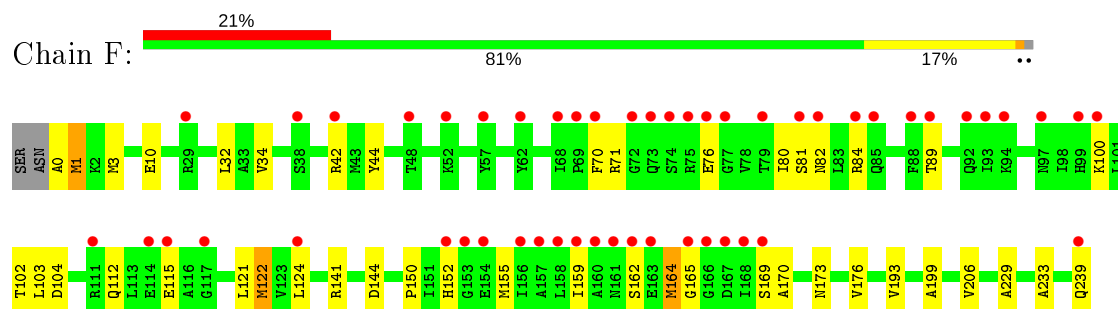
- Molecule 1: Glucosamine-6-phosphate deaminase



- Molecule 1: Glucosamine-6-phosphate deaminase



- Molecule 1: Glucosamine-6-phosphate deaminase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.48Å 123.81Å 299.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.05 29.60 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.62-2.05) 99.6 (29.60-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.04Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.201 , 0.231 0.213 , 0.242	Depositor DCC
R_{free} test set	4491 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtrriage
Anisotropy	0.298	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11887	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, CL

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	0.67	0/1890	0.83	2/2546 (0.1%)
1	B	0.66	0/1884	0.77	0/2538
1	C	0.66	0/1857	0.77	1/2504 (0.0%)
1	D	0.67	0/1857	0.79	1/2503 (0.0%)
1	E	0.68	0/1857	0.77	0/2504
1	F	0.67	0/1859	0.81	4/2505 (0.2%)
All	All	0.67	0/11204	0.79	8/15100 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	MSE	CG-SE-CE	10.07	121.05	98.90
1	F	155	MSE	CG-SE-CE	6.96	114.20	98.90
1	F	164	MSE	CG-SE-CE	6.74	113.73	98.90
1	C	164	MSE	CG-SE-CE	6.50	113.19	98.90
1	D	164	MSE	CG-SE-CE	6.37	112.91	98.90
1	A	155	MSE	CB-CG-SE	-5.66	95.73	112.70
1	F	1	MSE	CG-SE-CE	5.20	110.34	98.90
1	F	122	MSE	CG-SE-CE	5.03	109.96	98.90

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	1864	0	1869	35	0
1	B	1858	0	1864	26	0
1	C	1831	0	1843	21	0
1	D	1831	0	1845	16	0
1	E	1831	0	1843	17	0
1	F	1833	0	1845	28	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	15	0	0	0	0
3	C	2	0	0	0	0
4	A	189	0	0	0	0
4	B	164	0	0	1	0
4	C	111	0	0	1	0
4	D	154	0	0	0	0
4	E	123	0	0	1	0
4	F	51	0	0	3	0
All	All	11887	0	11109	127	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 6.

All (127) 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:A:68:ILE:HD13	1:A:175:TYR:HB2	1.57	0.87
1:D:68:ILE:HD13	1:D:175:TYR:HB2	1.60	0.83
1:A:78:VAL:HG11	1:A:164:MSE:CG	2.11	0.80
1:A:78:VAL:HG11	1:A:164:MSE:HG2	1.71	0.72
1:B:28:ARG:HD3	1:B:28:ARG:H	1.58	0.69
1:A:164:MSE:HE3	1:A:170:ALA:HB3	1.78	0.66
1:B:181:ARG:NH2	1:E:-1:ASN:HD22	1.95	0.65
1:F:84:ARG:HG2	1:F:89:THR:OG1	1.95	0.65
1:D:124:LEU:H	1:D:124:LEU:HD23	1.62	0.65
1:C:124:LEU:HD23	1:C:124:LEU:H	1.61	0.64
1:A:124:LEU:HD23	1:A:124:LEU:H	1.61	0.64
1:B:124:LEU:H	1:B:124:LEU:HD23	1.62	0.63
1:B:124:LEU:HD23	1:B:124:LEU:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:N	1:A:124:LEU:HD23	2.14	0.62
1:E:71:ARG:NH1	1:E:173:ASN:OD1	2.32	0.62
1:A:139:THR:HG21	1:A:155:MSE:HE2	1.79	0.62
1:A:27:PRO:HG3	1:B:-1:ASN:ND2	2.13	0.62
1:B:114[B]:GLU:OE2	1:C:59:ARG:NH1	2.33	0.62
1:D:124:LEU:HD23	1:D:124:LEU:N	2.14	0.61
1:C:124:LEU:N	1:C:124:LEU:HD23	2.15	0.61
1:C:107:ALA:HB1	1:D:108:GLN:HG2	1.83	0.60
1:F:71:ARG:NH2	1:F:173:ASN:OD1	2.35	0.59
1:F:150:PRO:HB2	1:F:152:HIS:NE2	2.18	0.59
1:E:108:GLN:OE1	1:E:111:ARG:NH2	2.26	0.58
1:F:100:LYS:HE2	1:F:102:THR:HG22	1.84	0.58
1:F:112:GLN:O	1:F:115:GLU:HG2	2.03	0.58
1:C:-1:ASN:HA	1:E:28:ARG:CZ	2.33	0.58
1:A:28:ARG:CZ	1:B:-1:ASN:HA	2.34	0.58
1:C:151:ILE:HG22	1:C:156:ILE:HD13	1.86	0.57
1:A:68:ILE:HD13	1:A:175:TYR:CB	2.33	0.57
1:A:78:VAL:HG11	1:A:164:MSE:HG3	1.87	0.57
1:B:114[B]:GLU:OE2	1:C:59:ARG:NH2	2.37	0.57
1:B:114[B]:GLU:C	1:B:114[B]:GLU:OE1	2.44	0.56
1:A:168:ILE:HD12	1:A:168:ILE:C	2.26	0.56
1:A:122[B]:MSE:HG3	1:A:186:ALA:CB	2.36	0.56
1:B:203:LYS:HE2	4:B:505:HOH:O	2.06	0.55
1:B:158:LEU:C	1:B:158:LEU:HD23	2.27	0.55
1:E:211:SER:OG	1:E:213:GLN:HG2	2.07	0.55
1:F:239:GLN:NE2	4:F:401:HOH:O	2.39	0.55
1:A:164:MSE:CE	1:A:170:ALA:HB3	2.38	0.54
1:D:68:ILE:CD1	1:D:175:TYR:HB2	2.35	0.54
1:D:211:SER:OG	1:D:213:GLN:HG2	2.07	0.54
1:F:10:GLU:HG2	4:F:433[A]:HOH:O	2.08	0.53
1:A:70:PHE:CZ	1:A:78:VAL:HG12	2.44	0.53
1:B:122[B]:MSE:HG3	1:B:186:ALA:CB	2.38	0.53
1:F:141:ARG:NH2	1:F:144:ASP:OD1	2.42	0.53
1:F:76:GLU:HG3	1:F:81:SER:OG	2.09	0.53
1:A:28:ARG:NH2	1:B:-1:ASN:HA	2.24	0.52
1:A:27:PRO:HG3	1:B:-1:ASN:HD22	1.75	0.52
1:A:68:ILE:CD1	1:A:175:TYR:CB	2.89	0.51
1:B:70:PHE:CZ	1:B:78:VAL:HG12	2.46	0.50
1:A:3:MSE:CE	1:A:206:VAL:HG21	2.42	0.50
1:D:122[B]:MSE:HG3	1:D:186:ALA:CB	2.43	0.49
1:A:164:MSE:HE1	1:A:170:ALA:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ALA:CB	1:D:108:GLN:HG2	2.43	0.49
1:D:68:ILE:CD1	1:D:175:TYR:CB	2.91	0.48
1:F:122:MSE:SE	1:F:124:LEU:HD21	2.63	0.48
1:E:124:LEU:HD13	1:E:191:LEU:HD13	1.94	0.48
1:F:3:MSE:HE3	1:F:206:VAL:HG21	1.95	0.48
1:A:3:MSE:HE3	1:A:206:VAL:HG21	1.95	0.48
1:B:68:ILE:HG22	1:B:164:MSE:HE1	1.94	0.48
1:A:168:ILE:HD12	1:A:169:SER:N	2.29	0.47
1:A:68:ILE:CD1	1:A:175:TYR:HB2	2.34	0.47
1:F:3:MSE:CE	1:F:206:VAL:HG21	2.43	0.47
1:C:94:LYS:HD3	1:C:96:GLU:OE2	2.14	0.47
1:B:103:LEU:HD23	1:B:176:VAL:HB	1.96	0.47
1:A:0:ALA:O	1:A:1:MSE:C	2.53	0.47
1:B:181:ARG:NH2	1:E:-1:ASN:ND2	2.62	0.46
1:F:80:ILE:HG21	1:F:100:LYS:HE3	1.96	0.46
1:A:-2:SER:HB3	1:C:187:LYS:HG2	1.98	0.46
1:F:103:LEU:HD23	1:F:176:VAL:HB	1.98	0.46
1:F:70:PHE:HE1	1:F:165:GLY:HA2	1.80	0.46
1:F:82:ASN:OD1	1:F:164:MSE:HE2	2.16	0.46
1:A:-2:SER:HB3	1:C:187:LYS:CG	2.46	0.46
1:C:-1:ASN:HA	1:E:28:ARG:NH2	2.30	0.46
1:B:3:MSE:CE	1:B:206:VAL:HG21	2.45	0.46
1:C:103:LEU:HD23	1:C:176:VAL:HB	1.97	0.46
1:A:27:PRO:CG	1:B:-1:ASN:ND2	2.80	0.45
1:B:0:ALA:O	1:B:1:MSE:C	2.54	0.45
1:B:3:MSE:HE3	1:B:206:VAL:HG21	1.98	0.45
1:E:193:VAL:O	1:E:229:ALA:HA	2.16	0.45
1:A:152:HIS:NE2	1:A:155:MSE:HE3	2.31	0.45
1:C:0:ALA:O	1:C:1:MSE:C	2.54	0.45
1:F:71:ARG:HD2	1:F:169:SER:O	2.16	0.45
1:E:68:ILE:HD11	2:E:302:PO4:O4	2.16	0.45
1:C:193:VAL:O	1:C:229:ALA:HA	2.17	0.44
1:D:193:VAL:O	1:D:229:ALA:HA	2.17	0.44
1:F:70:PHE:HD1	1:F:170:ALA:HB1	1.82	0.44
1:C:3:MSE:CE	1:C:206:VAL:HG21	2.48	0.44
1:F:159:ILE:O	1:F:162:SER:O	2.35	0.44
1:B:193:VAL:O	1:B:229:ALA:HA	2.18	0.44
1:B:158:LEU:HD23	1:B:158:LEU:O	2.17	0.44
1:F:193:VAL:O	1:F:229:ALA:HA	2.18	0.44
1:D:68:ILE:HB	1:D:78:VAL:HG12	2.00	0.44
1:A:103:LEU:HD23	1:A:176:VAL:HB	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LEU:HD23	1:E:176:VAL:HB	2.00	0.43
1:C:151:ILE:HG22	1:C:156:ILE:CD1	2.48	0.43
1:E:3:MSE:HE3	1:E:206:VAL:HG21	2.01	0.43
1:E:8:ASP:HB2	4:E:465:HOH:O	2.19	0.43
1:E:3:MSE:CE	1:E:206:VAL:HG21	2.48	0.42
1:F:104:ASP:HB2	4:F:409:HOH:O	2.19	0.42
1:E:0:ALA:O	1:E:1:MSE:C	2.56	0.42
1:A:122[B]:MSE:HG3	1:A:186:ALA:HB2	2.02	0.42
1:F:0:ALA:O	1:F:1:MSE:C	2.57	0.42
1:A:111:ARG:HE	1:A:111:ARG:HB2	1.41	0.42
1:D:3:MSE:CE	1:D:206:VAL:HG21	2.50	0.42
1:F:32:LEU:HD22	1:F:121:LEU:HB3	2.02	0.42
1:E:70:PHE:CE2	1:E:75:ARG:CZ	3.03	0.42
1:C:151:ILE:CG2	1:C:156:ILE:HD13	2.49	0.42
1:A:193:VAL:O	1:A:229:ALA:HA	2.19	0.42
1:F:112:GLN:HA	1:F:115:GLU:HG2	2.00	0.42
1:F:42:ARG:HD2	1:F:42:ARG:HA	1.93	0.42
1:E:203:LYS:HD2	1:E:236:GLU:HB3	2.01	0.41
1:B:122[B]:MSE:HG3	1:B:186:ALA:HB2	2.01	0.41
1:C:3:MSE:HE3	1:C:206:VAL:HG21	2.02	0.41
1:D:203:LYS:HD2	1:D:236:GLU:HB3	2.02	0.41
1:C:203:LYS:HD2	1:C:236:GLU:HB3	2.02	0.41
1:C:28:ARG:NH1	4:C:409:HOH:O	2.52	0.41
1:A:164:MSE:HE2	1:A:167:ASP:O	2.21	0.41
1:D:205:VAL:O	1:D:220:LYS:HE3	2.21	0.41
1:D:3:MSE:HE3	1:D:206:VAL:HG21	2.01	0.41
1:F:10:GLU:OE2	1:F:42:ARG:NE	2.54	0.41
1:F:34:VAL:HB	1:F:44:TYR:OH	2.21	0.40
1:D:34:VAL:HB	1:D:44:TYR:OH	2.20	0.40
1:A:34:VAL:HB	1:A:44:TYR:OH	2.21	0.40
1:A:27:PRO:CG	1:B:-1:ASN:HD22	2.34	0.40
1:F:199:ALA:HA	1:F:233:ALA:O	2.22	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	242/242 (100%)	234 (97%)	8 (3%)	0	100	100
1	B	241/242 (100%)	233 (97%)	8 (3%)	0	100	100
1	C	238/242 (98%)	228 (96%)	10 (4%)	0	100	100
1	D	238/242 (98%)	231 (97%)	7 (3%)	0	100	100
1	E	238/242 (98%)	231 (97%)	7 (3%)	0	100	100
1	F	238/242 (98%)	227 (95%)	11 (5%)	0	100	100
All	All	1435/1452 (99%)	1384 (96%)	51 (4%)	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	199/188 (106%)	198 (100%)	1 (0%)	88	89
1	B	198/188 (105%)	195 (98%)	3 (2%)	65	63
1	C	195/188 (104%)	193 (99%)	2 (1%)	76	75
1	D	195/188 (104%)	194 (100%)	1 (0%)	88	89
1	E	195/188 (104%)	193 (99%)	2 (1%)	76	75
1	F	195/188 (104%)	195 (100%)	0	100	100
All	All	1177/1128 (104%)	1168 (99%)	9 (1%)	81	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	B	28	ARG
1	B	124	LEU

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Mol	Chain	Res	Type
1	B	164	MSE
1	C	124	LEU
1	C	164	MSE
1	D	124	LEU
1	E	124	LEU
1	E	164	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	B	-1	ASN
1	B	109	HIS
1	B	112	GLN
1	C	138	ASN
1	C	213	GLN
1	D	18	HIS
1	E	109	HIS
1	F	18	HIS
1	F	108	GLN
1	F	109	HIS
1	F	239	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
2	PO4	F	301[B]	-	4,4,4	0.69	0	6,6,6	0.44	0
2	PO4	E	302	-	4,4,4	0.63	0	6,6,6	0.45	0
2	PO4	E	301	-	4,4,4	0.70	0	6,6,6	0.40	0
2	PO4	D	302[B]	-	4,4,4	0.65	0	6,6,6	0.43	0
2	PO4	D	301	-	4,4,4	0.73	0	6,6,6	0.40	0
2	PO4	A	301	-	4,4,4	0.68	0	6,6,6	0.43	0
2	PO4	F	302[A]	-	4,4,4	0.66	0	6,6,6	0.44	0
2	PO4	B	301	-	4,4,4	0.70	0	6,6,6	0.45	0
2	PO4	F	301[A]	-	4,4,4	0.64	0	6,6,6	0.45	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	302	PO4	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, 95th 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	233/242 (96%)	0.09	9 (3%) 39 42	22, 32, 57, 67	0
1	B	232/242 (95%)	0.07	7 (3%) 50 54	22, 32, 51, 63	0
1	C	231/242 (95%)	0.43	22 (9%) 8 9	25, 43, 91, 122	0
1	D	230/242 (95%)	0.05	3 (1%) 77 79	23, 37, 56, 93	0
1	E	231/242 (95%)	0.32	12 (5%) 27 29	26, 41, 67, 84	0
1	F	231/242 (95%)	1.03	51 (22%) 0 0	30, 62, 110, 131	0
All	All	1388/1452 (95%)	0.33	104 (7%) 14 15	22, 39, 88, 131	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	ALA	5.8
1	E	165	GLY	5.1
1	C	165	GLY	4.9
1	E	-1	ASN	4.8
1	F	97	ASN	4.8
1	F	70	PHE	4.6
1	F	161	ASN	4.6
1	F	156	ILE	4.3
1	F	152	HIS	4.3
1	F	163	GLU	4.3
1	F	89	THR	4.3
1	F	73	GLN	4.3
1	E	158	LEU	4.0
1	C	70	PHE	3.9
1	C	169	SER	3.9
1	F	159	ILE	3.9
1	F	111	ARG	3.7
1	C	167	ASP	3.6
1	A	159	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	ILE	3.5
1	F	115	GLU	3.5
1	F	160	ALA	3.4
1	F	62	TYR	3.4
1	C	152	HIS	3.3
1	C	168	ILE	3.3
1	A	-2	SER	3.2
1	C	238	GLN	3.2
1	F	93	ILE	3.2
1	F	167	ASP	3.1
1	E	73	GLN	3.1
1	C	159	ILE	3.1
1	D	238	GLN	3.0
1	B	165	GLY	3.0
1	F	158	LEU	3.0
1	C	160	ALA	3.0
1	F	165	GLY	3.0
1	F	124	LEU	3.0
1	E	170	ALA	2.9
1	E	124	LEU	2.9
1	B	123	VAL	2.8
1	A	167	ASP	2.8
1	E	166	GLY	2.8
1	F	68	ILE	2.7
1	C	158	LEU	2.7
1	F	100	LYS	2.7
1	F	77	GLY	2.7
1	C	123	VAL	2.7
1	C	161	ASN	2.7
1	F	29	ARG	2.7
1	F	92	GLN	2.7
1	F	81	SER	2.6
1	C	154	GLU	2.6
1	F	88	PHE	2.6
1	A	239	GLN	2.6
1	C	71	ARG	2.6
1	F	52	LYS	2.6
1	F	94	LYS	2.6
1	F	166	GLY	2.5
1	C	74	SER	2.5
1	E	154	GLU	2.5
1	E	70	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	38	SER	2.5
1	D	124	LEU	2.5
1	F	42	ARG	2.4
1	F	85	GLN	2.4
1	D	111	ARG	2.4
1	B	-1	ASN	2.4
1	C	124	LEU	2.4
1	F	169	SER	2.4
1	F	157	ALA	2.4
1	B	124	LEU	2.4
1	F	154	GLU	2.4
1	E	123	VAL	2.4
1	F	99	HIS	2.4
1	E	190	LEU	2.3
1	F	82	ASN	2.3
1	A	161	ASN	2.2
1	F	239	GLN	2.2
1	F	72	GLY	2.2
1	F	117	GLY	2.2
1	F	168	ILE	2.2
1	A	165	GLY	2.2
1	F	153	GLY	2.2
1	F	162	SER	2.2
1	F	76	GLU	2.2
1	B	20	VAL	2.2
1	A	189	LEU	2.2
1	F	69	PRO	2.2
1	B	158	LEU	2.2
1	C	189	LEU	2.2
1	C	111	ARG	2.1
1	F	48	THR	2.1
1	F	75	ARG	2.1
1	A	138	ASN	2.1
1	B	140	THR	2.1
1	F	74	SER	2.1
1	C	73	GLN	2.1
1	F	57	TYR	2.1
1	F	84	ARG	2.0
1	E	152	HIS	2.0
1	F	79	THR	2.0
1	F	114	GLU	2.0
1	C	162	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	115	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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, 95th 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	D	302[B]	5/5	0.81	0.28	52,55,58,59	5
2	PO4	E	302	5/5	0.82	0.19	82,88,92,93	0
2	PO4	F	302[A]	5/5	0.83	0.25	51,51,56,58	5
2	PO4	F	301[B]	5/5	0.88	0.20	64,65,68,68	5
2	PO4	F	301[A]	5/5	0.88	0.20	49,50,52,54	5
2	PO4	E	301	5/5	0.91	0.22	65,69,86,86	0
2	PO4	A	301	5/5	0.93	0.14	77,80,84,85	0
2	PO4	B	301	5/5	0.93	0.19	56,67,70,71	0
2	PO4	D	301	5/5	0.93	0.15	57,61,66,75	0
3	CL	C	301[B]	1/1	0.94	0.17	43,43,43,43	1
3	CL	C	301[A]	1/1	0.94	0.17	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.