



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 08:53 PM EST

PDB ID : 3OVG
Title : The crystal structure of an amidohydrolase from Mycoplasma synoviae with Zn ion bound
Authors : Zhang, Z.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-09-16
Resolution : 2.06 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	:	2.16
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)	:	2.16

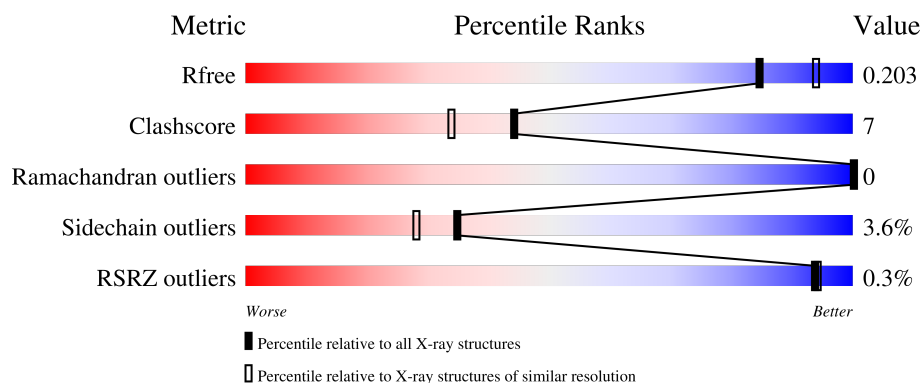
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 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 $\leq 5\%$. 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	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	

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Mol	Chain	Length	Quality of chain
1	F	363	<div><div></div><div>82%</div><div>13% ..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17874 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 amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	Se	0	1	0
			2775	1783	467	515	4	6			
1	B	351	Total	C	N	O	S	Se	0	0	0
			2767	1779	465	513	4	6			
1	C	351	Total	C	N	O	S	Se	0	2	0
			2780	1786	468	516	4	6			
1	D	351	Total	C	N	O	S	Se	0	1	0
			2775	1783	467	515	4	6			
1	E	351	Total	C	N	O	S	Se	0	1	0
			2775	1783	467	515	4	6			
1	F	351	Total	C	N	O	S	Se	0	1	0
			2775	1783	467	515	4	6			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q4A724
A	0	SER	-	expression tag	UNP Q4A724
A	1	LEU	-	expression tag	UNP Q4A724
A	354	GLU	-	expression tag	UNP Q4A724
A	355	GLY	-	expression tag	UNP Q4A724
A	356	HIS	-	expression tag	UNP Q4A724
A	357	HIS	-	expression tag	UNP Q4A724
A	358	HIS	-	expression tag	UNP Q4A724
A	359	HIS	-	expression tag	UNP Q4A724
A	360	HIS	-	expression tag	UNP Q4A724
A	361	HIS	-	expression tag	UNP Q4A724
B	-1	MSE	-	expression tag	UNP Q4A724
B	0	SER	-	expression tag	UNP Q4A724
B	1	LEU	-	expression tag	UNP Q4A724
B	354	GLU	-	expression tag	UNP Q4A724
B	355	GLY	-	expression tag	UNP Q4A724
B	356	HIS	-	expression tag	UNP Q4A724

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Chain	Residue	Modelled	Actual	Comment	Reference
B	357	HIS	-	expression tag	UNP Q4A724
B	358	HIS	-	expression tag	UNP Q4A724
B	359	HIS	-	expression tag	UNP Q4A724
B	360	HIS	-	expression tag	UNP Q4A724
B	361	HIS	-	expression tag	UNP Q4A724
C	-1	MSE	-	expression tag	UNP Q4A724
C	0	SER	-	expression tag	UNP Q4A724
C	1	LEU	-	expression tag	UNP Q4A724
C	354	GLU	-	expression tag	UNP Q4A724
C	355	GLY	-	expression tag	UNP Q4A724
C	356	HIS	-	expression tag	UNP Q4A724
C	357	HIS	-	expression tag	UNP Q4A724
C	358	HIS	-	expression tag	UNP Q4A724
C	359	HIS	-	expression tag	UNP Q4A724
C	360	HIS	-	expression tag	UNP Q4A724
C	361	HIS	-	expression tag	UNP Q4A724
D	-1	MSE	-	expression tag	UNP Q4A724
D	0	SER	-	expression tag	UNP Q4A724
D	1	LEU	-	expression tag	UNP Q4A724
D	354	GLU	-	expression tag	UNP Q4A724
D	355	GLY	-	expression tag	UNP Q4A724
D	356	HIS	-	expression tag	UNP Q4A724
D	357	HIS	-	expression tag	UNP Q4A724
D	358	HIS	-	expression tag	UNP Q4A724
D	359	HIS	-	expression tag	UNP Q4A724
D	360	HIS	-	expression tag	UNP Q4A724
D	361	HIS	-	expression tag	UNP Q4A724
E	-1	MSE	-	expression tag	UNP Q4A724
E	0	SER	-	expression tag	UNP Q4A724
E	1	LEU	-	expression tag	UNP Q4A724
E	354	GLU	-	expression tag	UNP Q4A724
E	355	GLY	-	expression tag	UNP Q4A724
E	356	HIS	-	expression tag	UNP Q4A724
E	357	HIS	-	expression tag	UNP Q4A724
E	358	HIS	-	expression tag	UNP Q4A724
E	359	HIS	-	expression tag	UNP Q4A724
E	360	HIS	-	expression tag	UNP Q4A724
E	361	HIS	-	expression tag	UNP Q4A724
F	-1	MSE	-	expression tag	UNP Q4A724
F	0	SER	-	expression tag	UNP Q4A724
F	1	LEU	-	expression tag	UNP Q4A724
F	354	GLU	-	expression tag	UNP Q4A724

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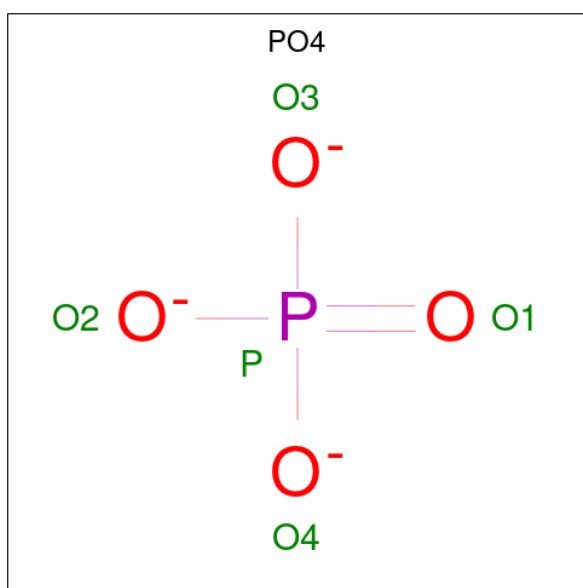
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Chain	Residue	Modelled	Actual	Comment	Reference
F	355	GLY	-	expression tag	UNP Q4A724
F	356	HIS	-	expression tag	UNP Q4A724
F	357	HIS	-	expression tag	UNP Q4A724
F	358	HIS	-	expression tag	UNP Q4A724
F	359	HIS	-	expression tag	UNP Q4A724
F	360	HIS	-	expression tag	UNP Q4A724
F	361	HIS	-	expression tag	UNP Q4A724

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

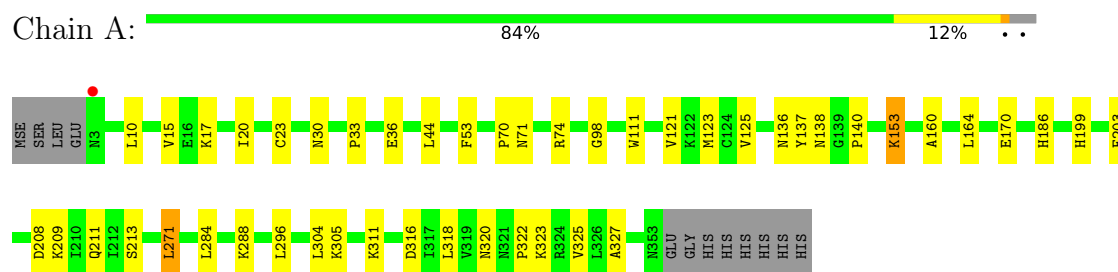
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	199	Total O 199 199	0	0
4	B	200	Total O 200 200	0	0
4	C	195	Total O 195 195	0	0
4	D	197	Total O 197 197	0	0
4	E	198	Total O 198 198	0	0
4	F	196	Total O 196 196	0	0

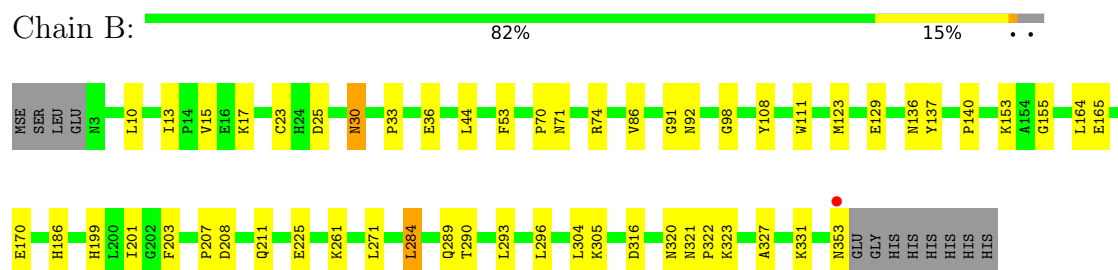
3 Residue-property plots

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.

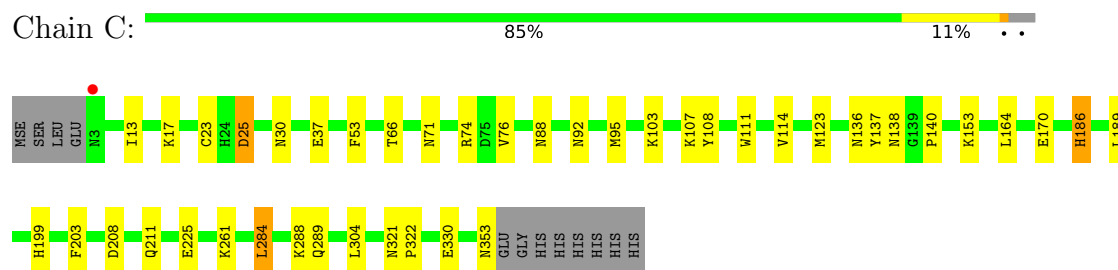
• Molecule 1: amidohydrolase



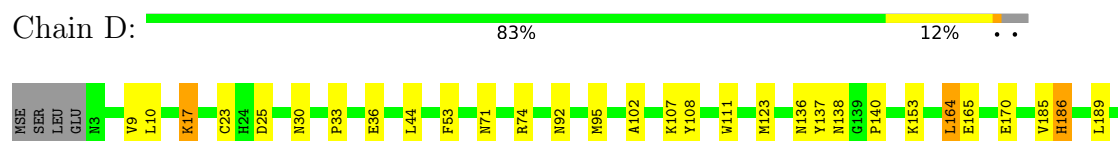
• Molecule 1: amidohydrolase



• Molecule 1: amidohydrolase



• Molecule 1: amidohydrolase





- Molecule 1: amidohydrolase

Chain E: 83% 12% ..



- Molecule 1: amidohydrolase

Chain F: 82% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.26Å 89.19Å 96.06Å 98.95° 92.89° 119.86°	Depositor
Resolution (Å)	43.75 – 2.06 43.75 – 2.06	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.75-2.06) 97.8 (43.75-2.06)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.172 , 0.210 0.167 , 0.203	Depositor DCC
R_{free} test set	7631 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17874	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.69% 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: ZN, PO4, KCX

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	0.64	0/2808	0.68	0/3779
1	B	0.66	0/2800	0.68	0/3768
1	C	0.67	0/2816	0.68	0/3790
1	D	0.62	0/2808	0.66	0/3779
1	E	0.64	0/2808	0.67	0/3779
1	F	0.66	0/2808	0.68	0/3779
All	All	0.65	0/16848	0.68	0/22674

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 [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	2775	0	2837	33	0
1	B	2767	0	2831	45	0
1	C	2780	0	2842	45	0
1	D	2775	0	2836	46	0
1	E	2775	0	2837	41	0
1	F	2775	0	2836	41	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	199	0	0	0	0
4	B	200	0	0	4	0
4	C	195	0	0	3	0
4	D	197	0	0	5	0
4	E	198	0	0	7	0
4	F	196	0	0	4	0
All	All	17874	0	17019	223	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 7.

All (223) 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:D:17:LYS:HE3	1:D:92:ASN:HD21	1.02	1.18
1:B:123:MSE:HE2	1:C:140:PRO:HB2	1.10	1.08
1:F:123:MSE:HE3	1:F:137:TYR:CZ	1.90	1.07
1:D:123:MSE:HE3	1:D:137:TYR:CZ	1.90	1.05
1:C:123:MSE:HE3	1:C:137:TYR:CZ	1.92	1.04
1:B:123:MSE:HE2	1:C:140:PRO:CB	1.87	1.04
1:B:123:MSE:HE3	1:B:137:TYR:CE1	1.92	1.03
1:A:123:MSE:HE3	1:A:137:TYR:CZ	1.94	1.02
1:E:123:MSE:HE3	1:E:137:TYR:CZ	1.97	0.99
1:D:17:LYS:HE3	1:D:92:ASN:ND2	1.80	0.96
1:C:123:MSE:HE3	1:C:137:TYR:CE1	2.04	0.93
1:C:88[B]:ASN:H	1:C:88[B]:ASN:HD22	1.14	0.92
1:F:123:MSE:CE	1:F:137:TYR:CE1	2.54	0.91
1:E:123:MSE:CE	1:E:137:TYR:CE1	2.55	0.90
1:B:123:MSE:CE	1:C:140:PRO:HB2	2.02	0.89
1:A:123:MSE:HE2	1:F:140:PRO:HB2	1.53	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:PRO:HB2	1:C:123:MSE:HE2	1.56	0.87
1:F:123:MSE:HE3	1:F:137:TYR:CE1	2.09	0.86
1:C:123:MSE:CE	1:C:137:TYR:CE1	2.60	0.85
1:E:123:MSE:HE3	1:E:137:TYR:CE1	2.11	0.85
1:C:88[B]:ASN:H	1:C:88[B]:ASN:ND2	1.72	0.82
1:E:305:LYS:HG2	4:E:1083:HOH:O	1.79	0.82
1:C:37:GLU:OE2	1:C:103:LYS:HE2	1.80	0.81
1:A:123:MSE:HE3	1:A:137:TYR:CE1	2.16	0.81
1:D:123:MSE:CE	1:D:137:TYR:CE1	2.64	0.79
1:F:71:ASN:HD21	1:F:111:TRP:HE1	1.31	0.78
1:C:17:LYS:NZ	1:C:92:ASN:HD21	1.83	0.77
1:E:123:MSE:HE3	1:E:137:TYR:OH	1.85	0.76
1:B:123:MSE:HE3	1:B:137:TYR:CZ	2.20	0.76
1:D:17:LYS:CE	1:D:92:ASN:HD21	1.91	0.76
1:B:140:PRO:CB	1:C:123:MSE:HE2	2.15	0.75
1:A:123:MSE:HE2	1:F:140:PRO:CB	2.17	0.75
1:E:301:LEU:O	1:E:305:LYS:HE3	1.87	0.75
1:D:123:MSE:HE3	1:D:137:TYR:OH	1.88	0.73
1:A:123:MSE:CE	1:A:137:TYR:CE1	2.72	0.73
1:D:123:MSE:CE	1:D:137:TYR:CZ	2.72	0.72
1:C:13:ILE:HB	1:C:17:LYS:HD3	1.70	0.71
1:C:288:LYS:HE3	4:C:956:HOH:O	1.90	0.71
1:B:305:LYS:HG2	4:B:964:HOH:O	1.89	0.71
1:F:17:LYS:NZ	1:F:92:ASN:HD21	1.90	0.70
1:E:9:VAL:HG23	1:E:10:LEU:HD13	1.74	0.70
1:D:30:ASN:HD22	1:D:44:LEU:HD21	1.57	0.70
1:D:123:MSE:HE2	1:E:140:PRO:HB2	1.72	0.69
1:F:123:MSE:HE3	1:F:137:TYR:OH	1.92	0.69
1:D:123:MSE:HE3	1:D:137:TYR:CE1	2.26	0.69
1:E:17:LYS:NZ	1:E:92:ASN:HD21	1.89	0.69
1:B:170:GLU:HB2	1:B:203:PHE:CZ	2.29	0.68
1:B:123:MSE:CE	1:B:137:TYR:CE1	2.73	0.68
1:D:123:MSE:HE2	1:E:140:PRO:CB	2.24	0.68
1:A:140:PRO:CB	1:F:123:MSE:HE2	2.24	0.67
1:E:208:ASP:HB3	4:E:959:HOH:O	1.93	0.67
1:B:17:LYS:NZ	1:B:92:ASN:HD21	1.92	0.67
1:B:74:ARG:HE	1:B:136:ASN:ND2	1.93	0.66
1:C:71:ASN:HD21	1:C:111:TRP:HE1	1.44	0.66
1:A:271:LEU:HD21	1:A:296:LEU:HB2	1.78	0.66
1:F:74:ARG:HE	1:F:136:ASN:ND2	1.95	0.65
1:B:108:TYR:HB3	1:C:30:ASN:ND2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASN:HD21	1:B:111:TRP:HE1	1.45	0.64
1:B:74:ARG:HE	1:B:136:ASN:HD22	1.44	0.64
1:A:140:PRO:HB2	1:F:123:MSE:HE2	1.78	0.64
1:C:17:LYS:HZ2	1:C:92:ASN:HD21	1.46	0.64
1:B:30:ASN:ND2	1:C:108:TYR:HB3	2.14	0.63
1:F:74:ARG:HE	1:F:136:ASN:HD22	1.47	0.63
1:E:30:ASN:HD22	1:E:44:LEU:HD21	1.63	0.62
1:A:123:MSE:HE3	1:A:137:TYR:OH	1.99	0.62
1:D:209:LYS:HE3	1:D:209:LYS:HA	1.81	0.62
1:A:316:ASP:HA	1:A:320:ASN:HB2	1.80	0.62
1:D:71:ASN:HD21	1:D:111:TRP:HE1	1.45	0.62
1:E:74:ARG:HE	1:E:136:ASN:HD22	1.46	0.61
1:C:74:ARG:HE	1:C:136:ASN:ND2	1.99	0.61
1:A:33:PRO:O	1:A:36:GLU:HB2	2.02	0.60
1:D:288:LYS:HE3	4:D:1005:HOH:O	2.00	0.60
1:F:217:LYS:HE3	4:F:961:HOH:O	2.01	0.60
1:C:199:HIS:HD2	4:C:667:HOH:O	1.85	0.60
1:E:217:LYS:HE3	4:E:958:HOH:O	2.01	0.60
1:C:74:ARG:HE	1:C:136:ASN:HD22	1.50	0.60
1:B:108:TYR:HB3	1:C:30:ASN:HD21	1.67	0.59
1:E:13:ILE:HG21	1:E:17:LYS:HE3	1.85	0.59
1:D:74:ARG:HE	1:D:136:ASN:HD22	1.49	0.58
1:F:30:ASN:HD22	1:F:44:LEU:HD21	1.66	0.58
1:E:74:ARG:HE	1:E:136:ASN:ND2	2.00	0.58
1:D:353:ASN:ND2	4:D:411:HOH:O	2.33	0.58
1:F:17:LYS:HZ2	1:F:92:ASN:HD21	1.53	0.57
1:C:186:HIS:CD2	1:C:186:HIS:C	2.77	0.57
1:F:71:ASN:ND2	1:F:111:TRP:HE1	2.02	0.57
1:E:321:ASN:HB2	1:E:322:PRO:HD3	1.87	0.57
1:D:30:ASN:HD22	1:D:44:LEU:CD2	2.17	0.56
1:E:71:ASN:HD21	1:E:111:TRP:HE1	1.53	0.56
1:E:288:LYS:HE3	4:E:880:HOH:O	2.05	0.56
1:A:209:LYS:NZ	1:A:327:ALA:O	2.38	0.56
1:D:74:ARG:HE	1:D:136:ASN:ND2	2.03	0.56
1:E:123:MSE:HE2	1:E:137:TYR:CE1	2.39	0.56
1:F:186:HIS:C	1:F:186:HIS:CD2	2.79	0.56
1:D:17:LYS:O	1:D:17:LYS:HG2	2.06	0.55
1:F:30:ASN:ND2	1:F:44:LEU:HD21	2.22	0.55
1:C:123:MSE:HE3	1:C:137:TYR:OH	2.05	0.55
1:D:289:GLN:OE1	1:F:199:HIS:HE1	1.90	0.55
1:A:74:ARG:HE	1:A:136:ASN:HD22	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASN:ND2	1:C:111:TRP:HE1	2.03	0.54
1:B:71:ASN:ND2	1:B:111:TRP:HE1	2.04	0.54
1:E:17:LYS:HZ1	1:E:92:ASN:HD21	1.56	0.53
1:B:17:LYS:HZ2	1:B:92:ASN:HD21	1.55	0.53
1:A:71:ASN:HD21	1:A:111:TRP:HE1	1.55	0.53
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.91	0.53
1:F:199:HIS:HD2	4:F:703:HOH:O	1.91	0.53
1:C:199:HIS:HE1	1:F:289:GLN:OE1	1.91	0.53
1:C:17:LYS:HZ1	1:C:92:ASN:HD21	1.57	0.53
1:D:33:PRO:O	1:D:36:GLU:HB2	2.09	0.53
1:C:76:VAL:HA	1:C:95:MSE:HE1	1.89	0.52
1:D:170:GLU:HB2	1:D:203:PHE:CZ	2.44	0.52
1:B:316:ASP:HA	1:B:320:ASN:HB2	1.92	0.52
1:C:23:CYS:HB3	1:C:211:GLN:HE22	1.74	0.52
1:A:140:PRO:CG	1:F:123:MSE:HE2	2.39	0.52
1:B:199:HIS:HE1	1:E:289:GLN:OE1	1.92	0.51
1:A:288:LYS:HE3	4:E:944:HOH:O	2.10	0.51
1:D:324:ARG:NH1	1:D:325:VAL:HG12	2.25	0.51
1:B:199:HIS:HD2	4:B:425:HOH:O	1.92	0.51
1:E:316:ASP:HA	1:E:320:ASN:HB2	1.93	0.51
1:F:316:ASP:HA	1:F:320:ASN:HB2	1.93	0.51
1:D:199:HIS:HD2	4:D:829:HOH:O	1.94	0.50
1:F:25:ASP:OD2	1:F:293:LEU:HD11	2.12	0.50
1:A:71:ASN:ND2	1:A:111:TRP:HE1	2.10	0.50
1:F:153:KCX:OQ2	1:F:186:HIS:HB2	2.12	0.49
1:B:271:LEU:HD21	1:B:296:LEU:HB2	1.94	0.49
1:D:140:PRO:HB2	1:E:123:MSE:HE2	1.93	0.49
1:E:123:MSE:CE	1:E:137:TYR:CZ	2.80	0.48
1:F:121:VAL:O	1:F:125:VAL:HG23	2.13	0.48
1:A:305:LYS:HE3	1:A:311:LYS:HG2	1.94	0.48
1:A:74:ARG:HE	1:A:136:ASN:ND2	2.12	0.48
1:F:155:GLY:O	1:F:165:GLU:HG2	2.14	0.48
1:A:70:PRO:HD2	1:A:98:GLY:O	2.13	0.48
1:A:160:ALA:HB2	1:B:290:THR:HG22	1.96	0.48
1:B:201:ILE:HG12	1:B:207:PRO:HG3	1.95	0.47
1:A:23:CYS:HB3	1:A:211:GLN:HE22	1.78	0.47
1:E:76:VAL:HA	1:E:95:MSE:HE1	1.96	0.47
1:B:140:PRO:HB2	1:C:123:MSE:CE	2.38	0.47
1:C:107:LYS:HE3	1:C:108:TYR:CZ	2.49	0.47
1:E:301:LEU:C	1:E:305:LYS:HE3	2.35	0.47
1:E:17:LYS:HZ2	1:E:92:ASN:HD21	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:ILE:HB	1:F:61:GLY:HA2	1.96	0.47
1:C:289:GLN:OE1	1:D:199:HIS:HE1	1.98	0.46
1:D:107:LYS:HE3	1:D:108:TYR:CZ	2.50	0.46
1:B:70:PRO:HD2	1:B:98:GLY:O	2.16	0.46
1:A:170:GLU:HB2	1:A:203:PHE:CZ	2.51	0.46
1:A:288:LYS:CE	4:E:944:HOH:O	2.63	0.46
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.98	0.46
1:A:322:PRO:HA	1:A:325:VAL:HG22	1.98	0.46
1:B:23:CYS:HB3	1:B:211:GLN:HE22	1.81	0.45
1:B:123:MSE:HE2	1:C:140:PRO:CG	2.44	0.45
1:D:71:ASN:HA	1:D:138[A]:ASN:HD21	1.82	0.45
1:F:123:MSE:HE2	1:F:137:TYR:CE1	2.46	0.45
1:D:23:CYS:HB3	1:D:211:GLN:HE22	1.81	0.45
1:D:324:ARG:HG2	1:D:324:ARG:HH11	1.81	0.45
1:F:34:GLU:HB2	4:F:416:HOH:O	2.16	0.45
1:B:186:HIS:C	1:B:186:HIS:CD2	2.90	0.45
1:B:15:VAL:HG11	1:B:327:ALA:HB2	1.99	0.45
1:A:20:ILE:HG23	1:A:318:LEU:HB3	1.98	0.44
1:C:284:LEU:HD13	4:C:437:HOH:O	2.16	0.44
1:C:25:ASP:O	1:C:66:THR:HA	2.18	0.44
1:A:30:ASN:HD22	1:A:44:LEU:HD21	1.82	0.44
1:B:74:ARG:NE	1:B:136:ASN:HD22	2.13	0.44
1:A:15:VAL:HB	1:A:323:LYS:HG3	2.00	0.44
1:D:71:ASN:ND2	1:D:111:TRP:HE1	2.15	0.44
1:D:140:PRO:CB	1:E:123:MSE:HE2	2.47	0.44
1:E:52:GLU:OE2	1:E:292:GLY:HA3	2.18	0.44
1:C:170:GLU:HB2	1:C:203:PHE:CZ	2.53	0.44
1:D:305:LYS:HG2	4:D:1176:HOH:O	2.17	0.44
1:F:74:ARG:NE	1:F:136:ASN:HD22	2.13	0.44
1:A:71:ASN:HA	1:A:138[A]:ASN:HD21	1.83	0.44
1:D:324:ARG:HH12	1:D:325:VAL:HG12	1.82	0.44
1:D:102:ALA:HB2	1:D:165:GLU:HG3	1.99	0.44
1:D:265:LYS:HA	1:D:321:ASN:HD21	1.82	0.44
1:E:189:LEU:O	1:E:218:ASN:HB2	2.17	0.44
4:B:1181:HOH:O	1:C:114:VAL:HG11	2.17	0.43
1:E:71:ASN:ND2	1:E:111:TRP:HE1	2.15	0.43
1:B:140:PRO:CG	1:C:123:MSE:HE2	2.47	0.43
1:E:288:LYS:CE	4:E:880:HOH:O	2.64	0.43
1:F:164:LEU:HD22	4:F:494:HOH:O	2.19	0.43
1:B:321:ASN:HB2	1:B:322:PRO:HD3	2.00	0.43
1:B:225:GLU:OE2	1:B:261:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:HIS:CD2	1:D:186:HIS:C	2.92	0.43
1:E:186:HIS:C	1:E:186:HIS:CD2	2.91	0.43
1:D:209:LYS:HE3	1:D:209:LYS:CA	2.47	0.43
1:D:9:VAL:HG11	1:D:95:MSE:HG3	2.01	0.43
1:E:65:VAL:HG12	1:E:67:MSE:SE	2.69	0.43
1:C:186:HIS:CD2	1:C:186:HIS:O	2.72	0.42
1:E:15:VAL:HB	1:E:323:LYS:HG3	2.01	0.42
1:A:153:KCX:OQ1	1:A:186:HIS:HB2	2.19	0.42
1:D:140:PRO:HG3	1:E:137:TYR:CD1	2.54	0.42
1:F:23:CYS:HB3	1:F:211:GLN:HE22	1.85	0.42
1:E:13:ILE:CG2	1:E:17:LYS:HE3	2.49	0.42
1:A:121:VAL:O	1:A:125:VAL:HG23	2.19	0.42
1:F:215:LEU:HG	1:F:235:LEU:HD22	2.02	0.42
1:B:13:ILE:HG21	1:B:17:LYS:HE3	2.02	0.41
1:F:189:LEU:O	1:F:218:ASN:HB2	2.20	0.41
1:F:321:ASN:HB2	1:F:322:PRO:HD3	2.02	0.41
1:C:71:ASN:HA	1:C:138[A]:ASN:HD21	1.84	0.41
1:E:33:PRO:O	1:E:36:GLU:HB2	2.20	0.41
1:D:185:VAL:HG11	1:D:196:VAL:HG11	2.02	0.41
1:D:9:VAL:CG1	1:D:95:MSE:HG3	2.51	0.41
1:E:80:LEU:HD23	1:E:80:LEU:HA	1.95	0.41
1:A:30:ASN:ND2	1:F:108:TYR:HB3	2.35	0.41
1:B:86:VAL:HG23	1:B:91:GLY:HA3	2.02	0.41
1:B:15:VAL:HB	1:B:323:LYS:HG3	2.02	0.41
1:B:33:PRO:O	1:B:36:GLU:HB2	2.19	0.41
1:C:74:ARG:NE	1:C:136:ASN:HD22	2.17	0.41
1:D:261:LYS:HD2	1:D:261:LYS:HA	1.88	0.41
1:E:71:ASN:HA	1:E:138[A]:ASN:HD21	1.86	0.41
1:B:284:LEU:HD13	4:B:438:HOH:O	2.21	0.41
1:F:271:LEU:HD21	1:F:296:LEU:HB2	2.03	0.41
1:A:199:HIS:HE1	1:B:289:GLN:OE1	2.04	0.40
1:B:129:GLU:OE2	1:B:331:LYS:HE2	2.21	0.40
1:D:164:LEU:HD22	4:D:1151:HOH:O	2.20	0.40
1:D:324:ARG:HG2	1:D:324:ARG:NH1	2.35	0.40
1:F:9:VAL:CG1	1:F:95:MSE:HG3	2.50	0.40
1:B:17:LYS:HZ1	1:B:92:ASN:HD21	1.68	0.40
1:F:177:ILE:HD11	1:F:204:GLY:C	2.42	0.40
1:B:44:LEU:HD23	1:B:44:LEU:HA	1.93	0.40
1:F:261:LYS:HA	1:F:261:LYS:HD2	1.85	0.40
1:B:155:GLY:O	1:B:165:GLU:HG2	2.22	0.40
1:C:225:GLU:OE2	1:C:261:LYS:HE2	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	349/363 (96%)	338 (97%)	11 (3%)	0	100	100
1	B	348/363 (96%)	334 (96%)	14 (4%)	0	100	100
1	C	350/363 (96%)	337 (96%)	13 (4%)	0	100	100
1	D	349/363 (96%)	336 (96%)	13 (4%)	0	100	100
1	E	349/363 (96%)	338 (97%)	11 (3%)	0	100	100
1	F	349/363 (96%)	339 (97%)	10 (3%)	0	100	100
All	All	2094/2178 (96%)	2022 (97%)	72 (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	301/304 (99%)	292 (97%)	9 (3%)	41	35
1	B	300/304 (99%)	290 (97%)	10 (3%)	38	31
1	C	302/304 (99%)	292 (97%)	10 (3%)	38	31
1	D	301/304 (99%)	290 (96%)	11 (4%)	34	27
1	E	301/304 (99%)	288 (96%)	13 (4%)	29	22
1	F	301/304 (99%)	289 (96%)	12 (4%)	31	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1806/1824 (99%)	1741 (96%)	65 (4%)	35 28

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	17	LYS
1	A	53	PHE
1	A	164	LEU
1	A	208	ASP
1	A	213	SER
1	A	271	LEU
1	A	284	LEU
1	A	304	LEU
1	B	10	LEU
1	B	25	ASP
1	B	30	ASN
1	B	53	PHE
1	B	164	LEU
1	B	208	ASP
1	B	284	LEU
1	B	293	LEU
1	B	304	LEU
1	B	353	ASN
1	C	25	ASP
1	C	53	PHE
1	C	164	LEU
1	C	186	HIS
1	C	189	LEU
1	C	208	ASP
1	C	284	LEU
1	C	304	LEU
1	C	330	GLU
1	C	353	ASN
1	D	10	LEU
1	D	17	LYS
1	D	25	ASP
1	D	53	PHE
1	D	164	LEU
1	D	186	HIS
1	D	189	LEU
1	D	209	LYS

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Mol	Chain	Res	Type
1	D	284	LEU
1	D	304	LEU
1	D	329	ASP
1	E	10	LEU
1	E	25	ASP
1	E	53	PHE
1	E	87	LYS
1	E	164	LEU
1	E	186	HIS
1	E	189	LEU
1	E	208	ASP
1	E	209	LYS
1	E	213	SER
1	E	284	LEU
1	E	293	LEU
1	E	304	LEU
1	F	10	LEU
1	F	53	PHE
1	F	164	LEU
1	F	186	HIS
1	F	189	LEU
1	F	208	ASP
1	F	209	LYS
1	F	213	SER
1	F	284	LEU
1	F	293	LEU
1	F	304	LEU
1	F	351	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	71	ASN
1	A	136	ASN
1	A	199	HIS
1	A	211	GLN
1	A	321	ASN
1	B	24	HIS
1	B	30	ASN
1	B	71	ASN
1	B	92	ASN

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Mol	Chain	Res	Type
1	B	136	ASN
1	B	138	ASN
1	B	199	HIS
1	B	211	GLN
1	B	321	ASN
1	C	30	ASN
1	C	71	ASN
1	C	92	ASN
1	C	136	ASN
1	C	186	HIS
1	C	199	HIS
1	C	211	GLN
1	C	321	ASN
1	D	30	ASN
1	D	71	ASN
1	D	92	ASN
1	D	136	ASN
1	D	199	HIS
1	D	211	GLN
1	D	321	ASN
1	E	30	ASN
1	E	71	ASN
1	E	92	ASN
1	E	136	ASN
1	E	211	GLN
1	E	289	GLN
1	E	321	ASN
1	F	30	ASN
1	F	71	ASN
1	F	92	ASN
1	F	136	ASN
1	F	199	HIS
1	F	211	GLN
1	F	321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	D	153	1,2	7,11,12	0.85	0	4,12,14	3.03	1 (25%)
1	KCX	E	153	1,2	7,11,12	0.77	0	4,12,14	3.95	1 (25%)
1	KCX	A	153	1,2	7,11,12	0.71	0	4,12,14	3.09	1 (25%)
1	KCX	C	153	1,2	7,11,12	0.74	0	4,12,14	3.40	1 (25%)
1	KCX	F	153	1,2	7,11,12	0.87	0	4,12,14	4.31	1 (25%)
1	KCX	B	153	1,2	7,11,12	0.78	0	4,12,14	3.00	1 (25%)

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	D	153	1,2	-	1/7/10/12	-
1	KCX	E	153	1,2	-	1/7/10/12	-
1	KCX	A	153	1,2	-	2/7/10/12	-
1	KCX	C	153	1,2	-	0/7/10/12	-
1	KCX	F	153	1,2	-	0/7/10/12	-
1	KCX	B	153	1,2	-	1/7/10/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	153	KCX	CE-NZ-CX	-8.52	108.52	122.95
1	E	153	KCX	CE-NZ-CX	-7.88	109.61	122.95
1	C	153	KCX	CE-NZ-CX	-6.75	111.52	122.95
1	A	153	KCX	CE-NZ-CX	-6.05	112.70	122.95
1	B	153	KCX	CE-NZ-CX	-5.89	112.98	122.95
1	D	153	KCX	CE-NZ-CX	-5.64	113.39	122.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	153	KCX	O-C-CA-CB
1	A	153	KCX	O-C-CA-CB
1	E	153	KCX	CG-CD-CE-NZ
1	B	153	KCX	CG-CD-CE-NZ
1	A	153	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	153	KCX	1	0
1	F	153	KCX	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	PO4	D	364	-	4,4,4	1.01	0	6,6,6	0.70	0
3	PO4	B	364	-	4,4,4	0.57	0	6,6,6	0.87	0
3	PO4	C	364	-	4,4,4	0.52	0	6,6,6	0.75	0
3	PO4	A	364	-	4,4,4	0.82	0	6,6,6	0.69	0
3	PO4	E	364	-	4,4,4	1.00	0	6,6,6	0.52	0
3	PO4	F	364	-	4,4,4	0.75	0	6,6,6	0.93	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	344/363 (94%)	-0.72	1 (0%) 94 94	14, 19, 30, 44	0
1	B	344/363 (94%)	-0.68	1 (0%) 94 94	13, 18, 27, 44	0
1	C	344/363 (94%)	-0.63	1 (0%) 94 94	13, 18, 28, 45	0
1	D	344/363 (94%)	-0.72	1 (0%) 94 94	14, 19, 29, 43	0
1	E	344/363 (94%)	-0.65	1 (0%) 94 94	14, 19, 29, 44	0
1	F	344/363 (94%)	-0.65	1 (0%) 94 94	14, 19, 30, 40	0
All	All	2064/2178 (94%)	-0.67	6 (0%) 94 94	13, 19, 29, 45	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	353	ASN	3.2
1	D	353	ASN	2.5
1	C	3	ASN	2.4
1	F	3	ASN	2.3
1	A	3	ASN	2.0
1	B	353	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	KCX	B	153	12/13	0.85	0.18	12,15,28,30	0
1	KCX	D	153	12/13	0.87	0.14	15,17,27,28	0
1	KCX	C	153	12/13	0.89	0.16	12,16,25,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	KCX	E	153	12/13	0.89	0.11	14,17,27,28	0
1	KCX	A	153	12/13	0.90	0.12	13,16,28,28	0
1	KCX	F	153	12/13	0.91	0.12	13,16,28,29	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, 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(\AA^2)	Q<0.9
3	PO4	E	364	5/5	0.78	0.23	25,34,41,46	0
3	PO4	A	364	5/5	0.83	0.23	27,32,40,46	0
3	PO4	D	364	5/5	0.86	0.26	26,35,42,45	0
3	PO4	F	364	5/5	0.87	0.25	24,32,41,43	0
3	PO4	C	364	5/5	0.89	0.20	27,35,37,43	0
3	PO4	B	364	5/5	0.91	0.22	30,35,42,44	0
2	ZN	A	363	1/1	0.98	0.10	46,46,46,46	0
2	ZN	D	362	1/1	0.98	0.12	49,49,49,49	0
2	ZN	E	363	1/1	0.99	0.03	34,34,34,34	0
2	ZN	F	363	1/1	0.99	0.11	46,46,46,46	0
2	ZN	E	362	1/1	0.99	0.18	55,55,55,55	0
2	ZN	B	363	1/1	0.99	0.02	33,33,33,33	0
2	ZN	B	362	1/1	0.99	0.19	50,50,50,50	0
2	ZN	A	362	1/1	0.99	0.02	34,34,34,34	0
2	ZN	C	363	1/1	0.99	0.17	51,51,51,51	0
2	ZN	C	362	1/1	0.99	0.02	33,33,33,33	0
2	ZN	D	363	1/1	0.99	0.04	35,35,35,35	0
2	ZN	F	362	1/1	1.00	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.