



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:23 am GMT

PDB ID : 4S1F
Title : Fructose-6-phosphate aldolase A from E.coli soaked in acetylacetone
Authors : Stellmacher, L.; Sandalova, T.; Leptihn, S.; Schneider, G.; Sprenger, G.A.; Samland, A.K.
Deposited on : 2015-01-13
Resolution : 2.24 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

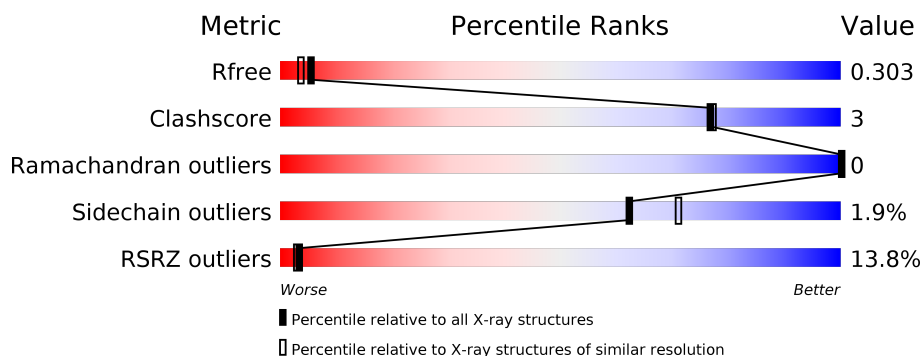
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	100719	1804 (2.26-2.22)
Clashscore	112137	1957 (2.26-2.22)
Ramachandran outliers	110173	1916 (2.26-2.22)
Sidechain outliers	110143	1917 (2.26-2.22)
RSRZ outliers	101464	1809 (2.26-2.22)

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. 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	226	<div> <div>6%</div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	B	226	<div> <div>9%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
1	C	226	<div> <div>10%</div> <div>92%</div> <div>5%</div> <div>• •</div> </div>
1	D	226	<div> <div>7%</div> <div>91%</div> <div>5%</div> <div>• •</div> </div>
1	E	226	<div> <div>4%</div> <div>90%</div> <div>7%</div> <div>• •</div> </div>
1	F	226	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	226	
1	H	226	
1	I	226	
1	J	226	
1	K	226	
1	L	226	
1	M	226	
1	N	226	
1	O	226	
1	P	226	
1	Q	226	
1	R	226	
1	S	226	
1	T	226	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P2D	B	301	-	-	X	X
2	P2D	G	301	-	-	X	X
2	P2D	H	301	-	-	X	X
2	P2D	K	301	-	-	X	-
2	P2D	P	301	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33075 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 Fructose-6-phosphate aldolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	B	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	C	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	D	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	E	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	F	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	G	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	H	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	I	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	J	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	K	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	L	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	M	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	N	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	O	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	P	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	R	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	S	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			
1	T	220	Total	C	N	O	S	0	0	0
			1615	1030	274	303	8			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP P78055
A	-4	HIS	-	EXPRESSION TAG	UNP P78055
A	-3	HIS	-	EXPRESSION TAG	UNP P78055
A	-2	HIS	-	EXPRESSION TAG	UNP P78055
A	-1	HIS	-	EXPRESSION TAG	UNP P78055
A	0	HIS	-	EXPRESSION TAG	UNP P78055
A	1	HIS	-	EXPRESSION TAG	UNP P78055
B	-5	MET	-	EXPRESSION TAG	UNP P78055
B	-4	HIS	-	EXPRESSION TAG	UNP P78055
B	-3	HIS	-	EXPRESSION TAG	UNP P78055
B	-2	HIS	-	EXPRESSION TAG	UNP P78055
B	-1	HIS	-	EXPRESSION TAG	UNP P78055
B	0	HIS	-	EXPRESSION TAG	UNP P78055
B	1	HIS	-	EXPRESSION TAG	UNP P78055
C	-5	MET	-	EXPRESSION TAG	UNP P78055
C	-4	HIS	-	EXPRESSION TAG	UNP P78055
C	-3	HIS	-	EXPRESSION TAG	UNP P78055
C	-2	HIS	-	EXPRESSION TAG	UNP P78055
C	-1	HIS	-	EXPRESSION TAG	UNP P78055
C	0	HIS	-	EXPRESSION TAG	UNP P78055
C	1	HIS	-	EXPRESSION TAG	UNP P78055
D	-5	MET	-	EXPRESSION TAG	UNP P78055
D	-4	HIS	-	EXPRESSION TAG	UNP P78055
D	-3	HIS	-	EXPRESSION TAG	UNP P78055
D	-2	HIS	-	EXPRESSION TAG	UNP P78055
D	-1	HIS	-	EXPRESSION TAG	UNP P78055
D	0	HIS	-	EXPRESSION TAG	UNP P78055
D	1	HIS	-	EXPRESSION TAG	UNP P78055
E	-5	MET	-	EXPRESSION TAG	UNP P78055
E	-4	HIS	-	EXPRESSION TAG	UNP P78055
E	-3	HIS	-	EXPRESSION TAG	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	HIS	-	EXPRESSION TAG	UNP P78055
E	-1	HIS	-	EXPRESSION TAG	UNP P78055
E	0	HIS	-	EXPRESSION TAG	UNP P78055
E	1	HIS	-	EXPRESSION TAG	UNP P78055
F	-5	MET	-	EXPRESSION TAG	UNP P78055
F	-4	HIS	-	EXPRESSION TAG	UNP P78055
F	-3	HIS	-	EXPRESSION TAG	UNP P78055
F	-2	HIS	-	EXPRESSION TAG	UNP P78055
F	-1	HIS	-	EXPRESSION TAG	UNP P78055
F	0	HIS	-	EXPRESSION TAG	UNP P78055
F	1	HIS	-	EXPRESSION TAG	UNP P78055
G	-5	MET	-	EXPRESSION TAG	UNP P78055
G	-4	HIS	-	EXPRESSION TAG	UNP P78055
G	-3	HIS	-	EXPRESSION TAG	UNP P78055
G	-2	HIS	-	EXPRESSION TAG	UNP P78055
G	-1	HIS	-	EXPRESSION TAG	UNP P78055
G	0	HIS	-	EXPRESSION TAG	UNP P78055
G	1	HIS	-	EXPRESSION TAG	UNP P78055
H	-5	MET	-	EXPRESSION TAG	UNP P78055
H	-4	HIS	-	EXPRESSION TAG	UNP P78055
H	-3	HIS	-	EXPRESSION TAG	UNP P78055
H	-2	HIS	-	EXPRESSION TAG	UNP P78055
H	-1	HIS	-	EXPRESSION TAG	UNP P78055
H	0	HIS	-	EXPRESSION TAG	UNP P78055
H	1	HIS	-	EXPRESSION TAG	UNP P78055
I	-5	MET	-	EXPRESSION TAG	UNP P78055
I	-4	HIS	-	EXPRESSION TAG	UNP P78055
I	-3	HIS	-	EXPRESSION TAG	UNP P78055
I	-2	HIS	-	EXPRESSION TAG	UNP P78055
I	-1	HIS	-	EXPRESSION TAG	UNP P78055
I	0	HIS	-	EXPRESSION TAG	UNP P78055
I	1	HIS	-	EXPRESSION TAG	UNP P78055
J	-5	MET	-	EXPRESSION TAG	UNP P78055
J	-4	HIS	-	EXPRESSION TAG	UNP P78055
J	-3	HIS	-	EXPRESSION TAG	UNP P78055
J	-2	HIS	-	EXPRESSION TAG	UNP P78055
J	-1	HIS	-	EXPRESSION TAG	UNP P78055
J	0	HIS	-	EXPRESSION TAG	UNP P78055
J	1	HIS	-	EXPRESSION TAG	UNP P78055
K	-5	MET	-	EXPRESSION TAG	UNP P78055
K	-4	HIS	-	EXPRESSION TAG	UNP P78055
K	-3	HIS	-	EXPRESSION TAG	UNP P78055

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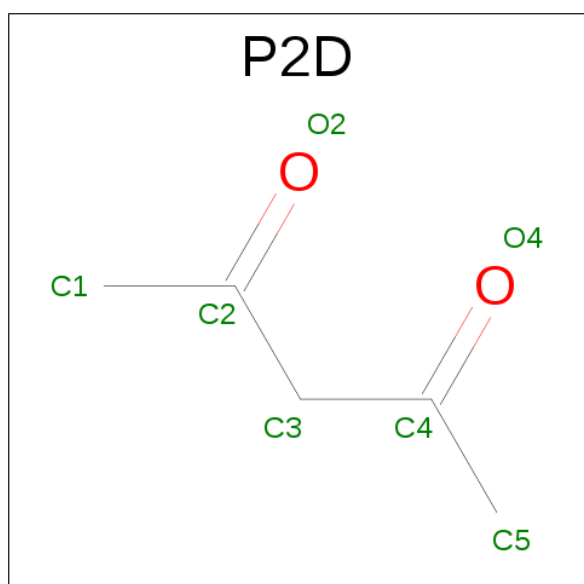
Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	HIS	-	EXPRESSION TAG	UNP P78055
K	-1	HIS	-	EXPRESSION TAG	UNP P78055
K	0	HIS	-	EXPRESSION TAG	UNP P78055
K	1	HIS	-	EXPRESSION TAG	UNP P78055
L	-5	MET	-	EXPRESSION TAG	UNP P78055
L	-4	HIS	-	EXPRESSION TAG	UNP P78055
L	-3	HIS	-	EXPRESSION TAG	UNP P78055
L	-2	HIS	-	EXPRESSION TAG	UNP P78055
L	-1	HIS	-	EXPRESSION TAG	UNP P78055
L	0	HIS	-	EXPRESSION TAG	UNP P78055
L	1	HIS	-	EXPRESSION TAG	UNP P78055
M	-5	MET	-	EXPRESSION TAG	UNP P78055
M	-4	HIS	-	EXPRESSION TAG	UNP P78055
M	-3	HIS	-	EXPRESSION TAG	UNP P78055
M	-2	HIS	-	EXPRESSION TAG	UNP P78055
M	-1	HIS	-	EXPRESSION TAG	UNP P78055
M	0	HIS	-	EXPRESSION TAG	UNP P78055
M	1	HIS	-	EXPRESSION TAG	UNP P78055
N	-5	MET	-	EXPRESSION TAG	UNP P78055
N	-4	HIS	-	EXPRESSION TAG	UNP P78055
N	-3	HIS	-	EXPRESSION TAG	UNP P78055
N	-2	HIS	-	EXPRESSION TAG	UNP P78055
N	-1	HIS	-	EXPRESSION TAG	UNP P78055
N	0	HIS	-	EXPRESSION TAG	UNP P78055
N	1	HIS	-	EXPRESSION TAG	UNP P78055
O	-5	MET	-	EXPRESSION TAG	UNP P78055
O	-4	HIS	-	EXPRESSION TAG	UNP P78055
O	-3	HIS	-	EXPRESSION TAG	UNP P78055
O	-2	HIS	-	EXPRESSION TAG	UNP P78055
O	-1	HIS	-	EXPRESSION TAG	UNP P78055
O	0	HIS	-	EXPRESSION TAG	UNP P78055
O	1	HIS	-	EXPRESSION TAG	UNP P78055
P	-5	MET	-	EXPRESSION TAG	UNP P78055
P	-4	HIS	-	EXPRESSION TAG	UNP P78055
P	-3	HIS	-	EXPRESSION TAG	UNP P78055
P	-2	HIS	-	EXPRESSION TAG	UNP P78055
P	-1	HIS	-	EXPRESSION TAG	UNP P78055
P	0	HIS	-	EXPRESSION TAG	UNP P78055
P	1	HIS	-	EXPRESSION TAG	UNP P78055
Q	-5	MET	-	EXPRESSION TAG	UNP P78055
Q	-4	HIS	-	EXPRESSION TAG	UNP P78055
Q	-3	HIS	-	EXPRESSION TAG	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-2	HIS	-	EXPRESSION TAG	UNP P78055
Q	-1	HIS	-	EXPRESSION TAG	UNP P78055
Q	0	HIS	-	EXPRESSION TAG	UNP P78055
Q	1	HIS	-	EXPRESSION TAG	UNP P78055
R	-5	MET	-	EXPRESSION TAG	UNP P78055
R	-4	HIS	-	EXPRESSION TAG	UNP P78055
R	-3	HIS	-	EXPRESSION TAG	UNP P78055
R	-2	HIS	-	EXPRESSION TAG	UNP P78055
R	-1	HIS	-	EXPRESSION TAG	UNP P78055
R	0	HIS	-	EXPRESSION TAG	UNP P78055
R	1	HIS	-	EXPRESSION TAG	UNP P78055
S	-5	MET	-	EXPRESSION TAG	UNP P78055
S	-4	HIS	-	EXPRESSION TAG	UNP P78055
S	-3	HIS	-	EXPRESSION TAG	UNP P78055
S	-2	HIS	-	EXPRESSION TAG	UNP P78055
S	-1	HIS	-	EXPRESSION TAG	UNP P78055
S	0	HIS	-	EXPRESSION TAG	UNP P78055
S	1	HIS	-	EXPRESSION TAG	UNP P78055
T	-5	MET	-	EXPRESSION TAG	UNP P78055
T	-4	HIS	-	EXPRESSION TAG	UNP P78055
T	-3	HIS	-	EXPRESSION TAG	UNP P78055
T	-2	HIS	-	EXPRESSION TAG	UNP P78055
T	-1	HIS	-	EXPRESSION TAG	UNP P78055
T	0	HIS	-	EXPRESSION TAG	UNP P78055
T	1	HIS	-	EXPRESSION TAG	UNP P78055

- Molecule 2 is PENTANE-2,4-DIONE (three-letter code: P2D) (formula: C₅H₈O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 6 5 1	0	0
2	G	1	Total C O 6 5 1	0	0
2	H	1	Total C O 6 5 1	0	0
2	K	1	Total C O 6 5 1	0	0
2	P	1	Total C O 6 5 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	67	Total O 67 67	0	0
3	B	67	Total O 67 67	0	0
3	C	52	Total O 52 52	0	0
3	D	51	Total O 51 51	0	0
3	E	63	Total O 63 63	0	0
3	F	90	Total O 90 90	0	0
3	G	78	Total O 78 78	0	0
3	H	54	Total O 54 54	0	0
3	I	55	Total O 55 55	0	0
3	J	72	Total O 72 72	0	0
3	O	1	Total O 1 1	0	0
3	P	40	Total O 40 40	0	0
3	Q	4	Total O 4 4	0	0
3	R	13	Total O 13 13	0	0
3	S	5	Total O 5 5	0	0

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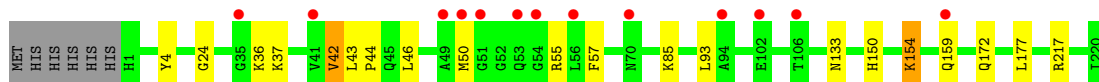
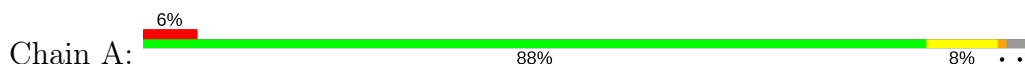
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	33	Total	O	0	0
			33	33		

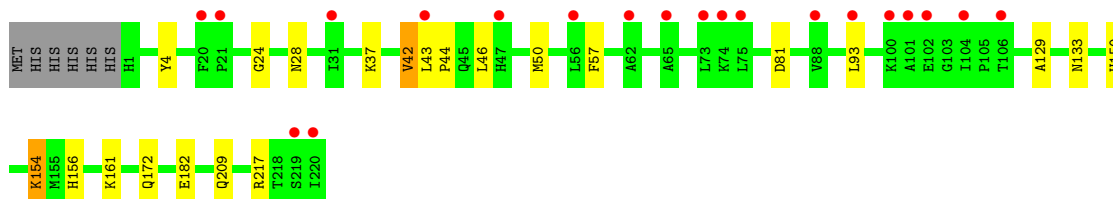
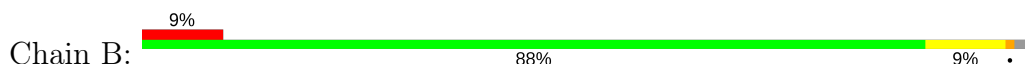
3 Residue-property plots [i](#)

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.

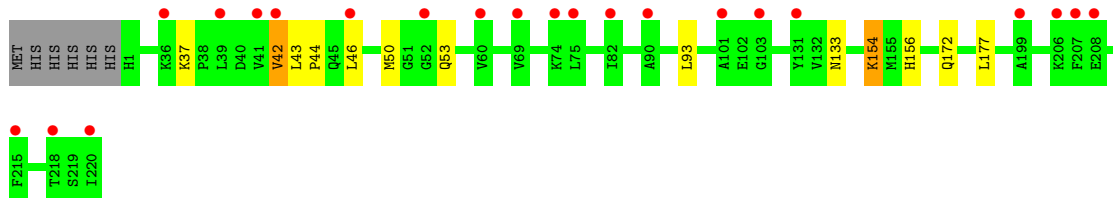
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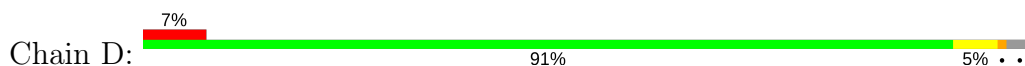
• Molecule 1: Fructose-6-phosphate aldolase 1



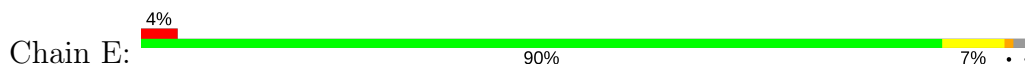
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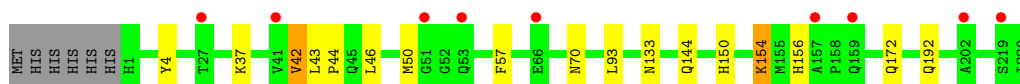


• Molecule 1: Fructose-6-phosphate aldolase 1

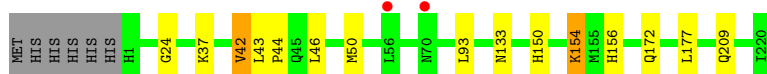
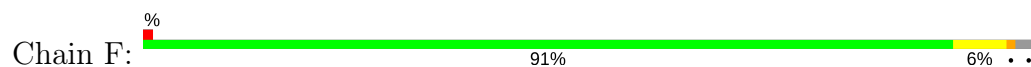


• Molecule 1: Fructose-6-phosphate aldolase 1

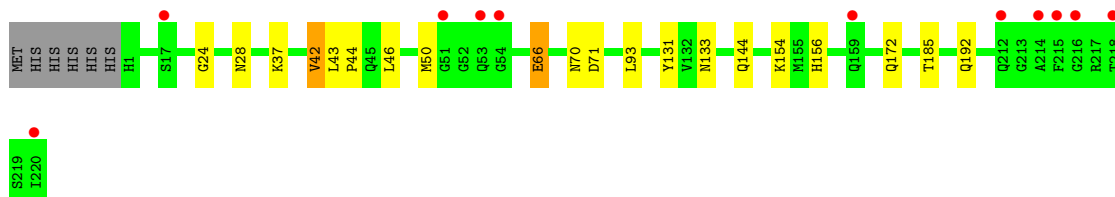
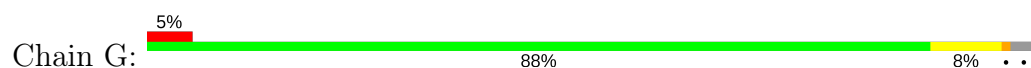




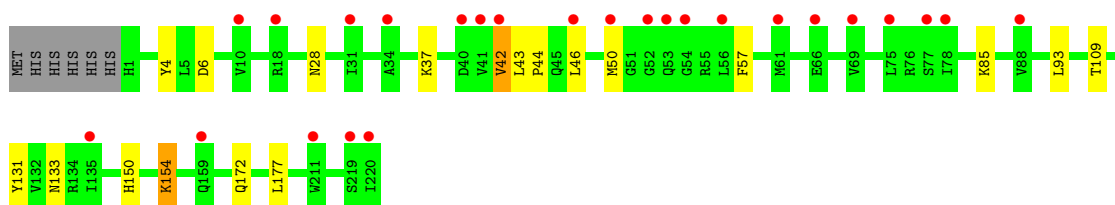
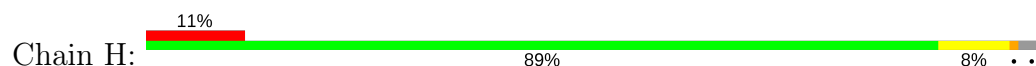
- Molecule 1: Fructose-6-phosphate aldolase 1



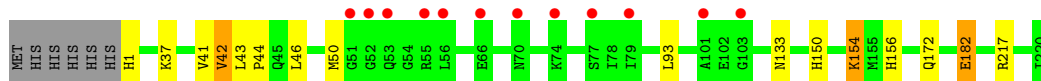
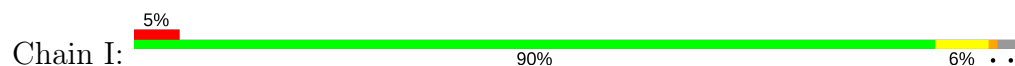
- Molecule 1: Fructose-6-phosphate aldolase 1



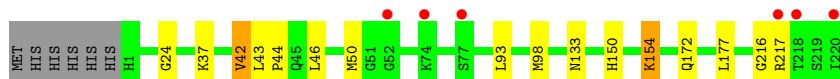
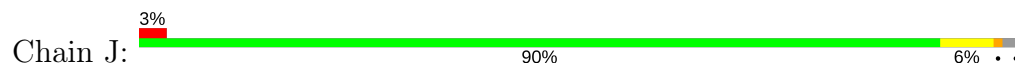
- Molecule 1: Fructose-6-phosphate aldolase 1



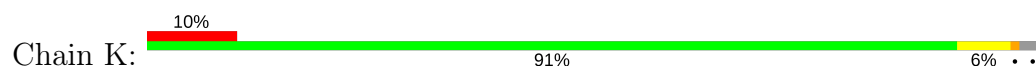
- Molecule 1: Fructose-6-phosphate aldolase 1

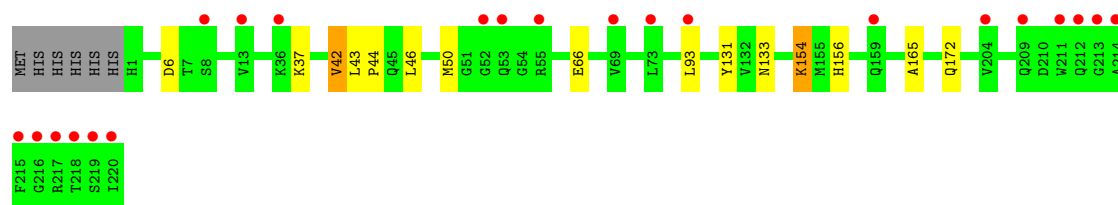


- Molecule 1: Fructose-6-phosphate aldolase 1

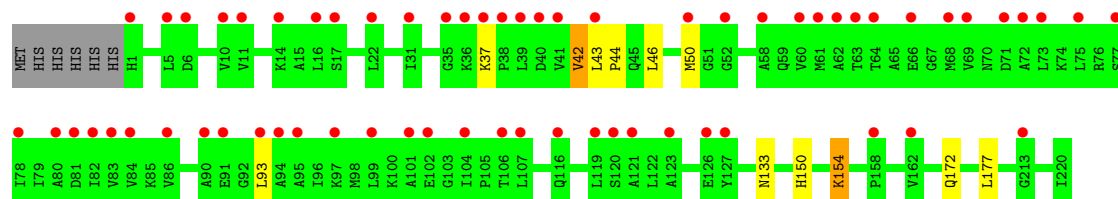
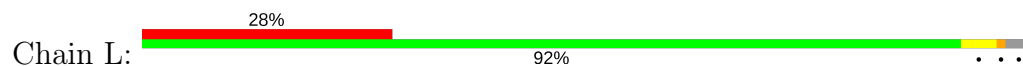


- Molecule 1: Fructose-6-phosphate aldolase 1

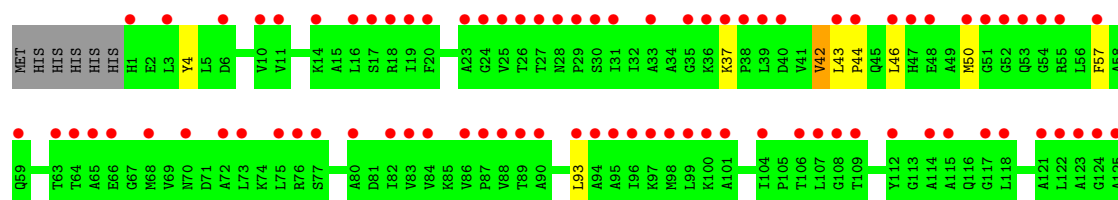
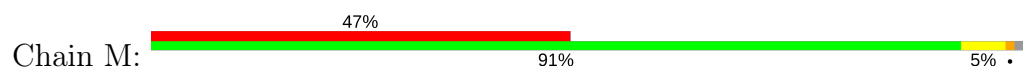




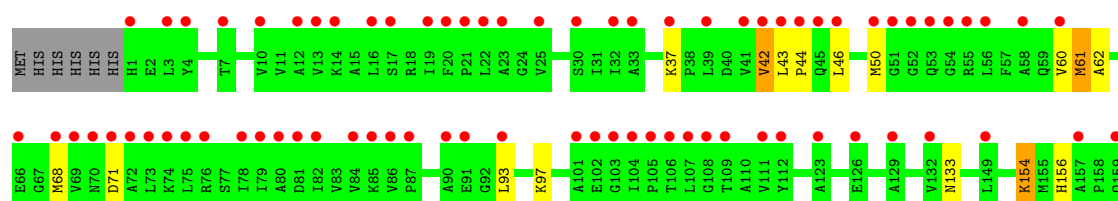
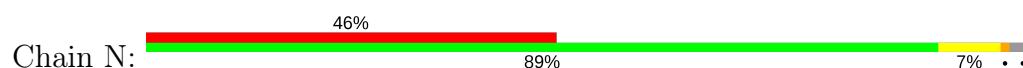
- Molecule 1: Fructose-6-phosphate aldolase 1



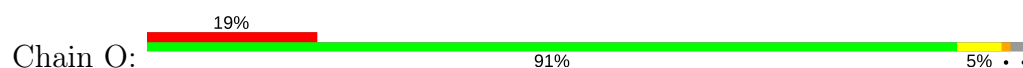
- Molecule 1: Fructose-6-phosphate aldolase 1

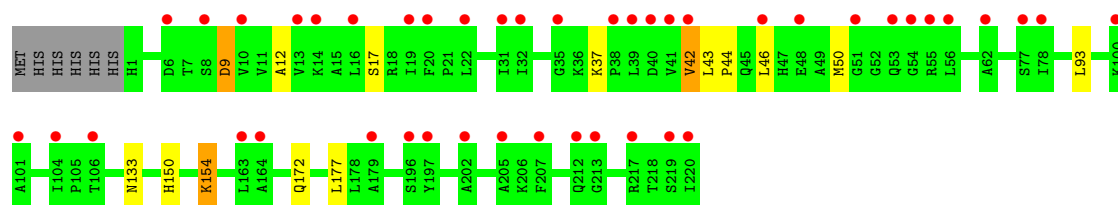


- Molecule 1: Fructose-6-phosphate aldolase 1

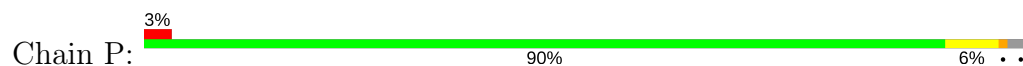


- Molecule 1: Fructose-6-phosphate aldolase 1





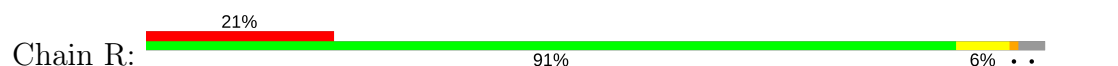
• Molecule 1: Fructose-6-phosphate aldolase 1



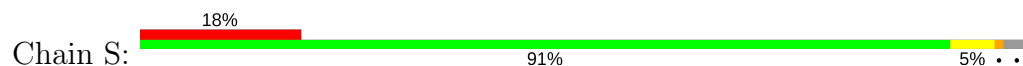
• Molecule 1: Fructose-6-phosphate aldolase 1



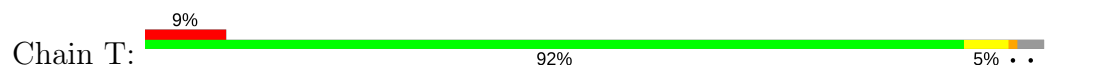
• Molecule 1: Fructose-6-phosphate aldolase 1

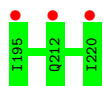


• Molecule 1: Fructose-6-phosphate aldolase 1



• Molecule 1: Fructose-6-phosphate aldolase 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.48Å 130.71Å 355.18Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	48.39 – 2.24 48.39 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.39-2.24) 99.1 (48.39-2.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.232 , 0.251 0.281 , 0.303	Depositor DCC
R_{free} test set	11025 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-l	Xtriage
Reported twinning fraction	0.750 for H, K, L 0.250 for H, -K, -L	Depositor
Outliers	1 of 217690 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33075	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: P2D

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	0.51	0/1641	0.60	0/2232
1	B	0.56	0/1641	0.63	1/2232 (0.0%)
1	C	0.48	0/1641	0.59	0/2232
1	D	0.54	0/1641	0.62	1/2232 (0.0%)
1	E	0.51	0/1641	0.63	1/2232 (0.0%)
1	F	0.63	0/1641	0.62	0/2232
1	G	0.56	0/1641	0.61	0/2232
1	H	0.47	0/1641	0.59	0/2232
1	I	0.57	2/1641 (0.1%)	0.62	1/2232 (0.0%)
1	J	0.59	0/1641	0.61	0/2232
1	K	0.53	0/1641	0.59	0/2232
1	L	0.41	0/1641	0.57	0/2232
1	M	0.37	0/1641	0.57	0/2232
1	N	0.38	0/1641	0.60	1/2232 (0.0%)
1	O	0.44	0/1641	0.58	1/2232 (0.0%)
1	P	0.57	0/1641	0.63	0/2232
1	Q	0.55	0/1641	0.60	0/2232
1	R	0.41	0/1641	0.58	0/2232
1	S	0.45	1/1641 (0.1%)	0.60	1/2232 (0.0%)
1	T	0.45	0/1641	0.59	0/2232
All	All	0.50	3/32820 (0.0%)	0.60	7/44640 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	182	GLU	CD-OE1	7.72	1.34	1.25
1	I	182	GLU	CD-OE2	6.68	1.33	1.25
1	S	40	ASP	CB-CG	-6.18	1.38	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	LYS	CD-CE-NZ	8.49	131.22	111.70
1	I	182	GLU	OE1-CD-OE2	7.21	131.95	123.30
1	E	192	GLN	CB-CG-CD	6.63	128.85	111.60
1	N	61	MET	CG-SD-CE	6.52	110.63	100.20
1	D	66	GLU	CB-CA-C	6.39	123.18	110.40
1	S	40	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	O	9	ASP	CB-CG-OD2	5.36	123.12	118.30

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	1615	0	1674	19	0
1	B	1615	0	1671	19	0
1	C	1615	0	1674	8	0
1	D	1615	0	1674	8	0
1	E	1615	0	1674	11	0
1	F	1615	0	1674	10	0
1	G	1615	0	1672	22	0
1	H	1615	0	1672	15	0
1	I	1615	0	1674	12	0
1	J	1615	0	1674	10	0
1	K	1615	0	1671	14	0
1	L	1615	0	1674	7	0
1	M	1615	0	1674	9	0
1	N	1615	0	1674	19	0
1	O	1615	0	1674	8	0
1	P	1615	0	1672	20	0
1	Q	1615	0	1674	8	0
1	R	1615	0	1674	16	0
1	S	1615	0	1674	8	0
1	T	1615	0	1674	7	0
2	B	6	0	8	4	0
2	G	6	0	8	10	0
2	H	6	0	8	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	6	0	6	8	0
2	P	6	0	8	9	0
3	A	67	0	0	4	0
3	B	67	0	0	3	0
3	C	52	0	0	1	0
3	D	51	0	0	0	0
3	E	63	0	0	2	0
3	F	90	0	0	1	0
3	G	78	0	0	3	0
3	H	54	0	0	1	0
3	I	55	0	0	3	0
3	J	72	0	0	2	0
3	O	1	0	0	0	0
3	P	40	0	0	2	0
3	Q	4	0	0	0	0
3	R	13	0	0	0	0
3	S	5	0	0	0	0
3	T	33	0	0	1	0
All	All	33075	0	33506	228	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 3.

All (228) 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:K:131:TYR:CE1	2:K:301:P2D:H6	2.07	0.90
1:P:131:TYR:CE1	2:P:301:P2D:H8	2.15	0.80
1:A:217:ARG:CZ	1:R:53:GLN:NE2	2.47	0.78
1:G:66:GLU:OE1	1:G:66:GLU:O	2.07	0.72
1:P:165:ALA:CB	2:P:301:P2D:H7	2.19	0.71
1:K:131:TYR:HE1	2:K:301:P2D:O4	1.74	0.71
1:P:131:TYR:HE1	2:P:301:P2D:H8	1.55	0.71
1:M:156:HIS:HE1	1:N:177:LEU:O	1.75	0.70
1:A:217:ARG:NH2	1:R:53:GLN:NE2	2.38	0.70
1:K:6:ASP:OD1	2:K:301:P2D:H2	1.92	0.69
1:K:131:TYR:CD1	2:K:301:P2D:H6	2.28	0.67
1:P:50:MET:HE1	3:P:430:HOH:O	1.95	0.67
1:F:209:GLN:HG2	3:F:343:HOH:O	1.93	0.67
1:H:6:ASP:OD2	2:H:301:P2D:O4	2.13	0.66
1:N:60:VAL:HG23	1:N:71:ASP:OD2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ASN:ND2	2:G:301:P2D:H7	2.13	0.64
1:B:154:LYS:HE2	1:B:182:GLU:OE2	1.98	0.64
1:G:131:TYR:CE1	2:G:301:P2D:H8	2.33	0.63
1:K:131:TYR:CE1	2:K:301:P2D:C5	2.81	0.63
1:I:154:LYS:HE2	1:I:182:GLU:OE2	1.99	0.63
1:N:60:VAL:HG22	1:N:61:MET:N	2.14	0.62
1:N:60:VAL:HG23	1:N:71:ASP:CB	2.30	0.61
1:B:150:HIS:CE1	1:B:154:LYS:HD3	2.36	0.61
1:G:131:TYR:OH	2:G:301:P2D:H6	2.01	0.61
1:G:66:GLU:C	1:G:66:GLU:OE1	2.39	0.60
1:B:133:ASN:HD22	1:B:172:GLN:HE22	1.50	0.60
1:D:150:HIS:CE1	1:D:154:LYS:HD3	2.36	0.59
1:N:60:VAL:HG22	1:N:62:ALA:H	1.68	0.59
1:I:133:ASN:HD22	1:I:172:GLN:HE22	1.51	0.58
1:A:36:LYS:NZ	3:A:328:HOH:O	2.38	0.57
1:E:133:ASN:HD22	1:E:172:GLN:HE22	1.52	0.57
1:J:133:ASN:HD22	1:J:172:GLN:HE22	1.50	0.57
1:F:177:LEU:O	1:G:156:HIS:HE1	1.88	0.57
1:A:55:ARG:HD2	3:A:322:HOH:O	2.05	0.57
1:R:177:LEU:O	1:S:156:HIS:HE1	1.86	0.57
1:F:133:ASN:HD22	1:F:172:GLN:HE22	1.53	0.57
1:G:131:TYR:CZ	2:G:301:P2D:C5	2.87	0.57
1:A:133:ASN:HD22	1:A:172:GLN:HE22	1.52	0.57
1:D:133:ASN:HD22	1:D:172:GLN:HE22	1.52	0.57
1:E:144:GLN:NE2	3:E:345:HOH:O	2.39	0.56
1:B:154:LYS:NZ	1:B:182:GLU:OE2	2.37	0.56
1:I:154:LYS:NZ	1:I:182:GLU:OE2	2.37	0.56
1:J:150:HIS:CE1	1:J:154:LYS:HD3	2.41	0.56
1:N:60:VAL:HG21	1:N:68:MET:HA	1.86	0.56
1:G:133:ASN:HD22	1:G:172:GLN:HE22	1.54	0.55
1:Q:133:ASN:HD22	1:Q:172:GLN:HE22	1.52	0.55
1:T:133:ASN:HD22	1:T:172:GLN:HE22	1.54	0.55
1:R:133:ASN:HD22	1:R:172:GLN:HE22	1.55	0.55
1:N:60:VAL:HG21	1:N:68:MET:HG2	1.87	0.55
1:L:133:ASN:HD22	1:L:172:GLN:HE22	1.53	0.55
1:N:133:ASN:HD22	1:N:172:GLN:HE22	1.55	0.55
1:H:133:ASN:HD22	1:H:172:GLN:HE22	1.54	0.54
1:H:177:LEU:O	1:I:156:HIS:HE1	1.91	0.54
1:M:133:ASN:HD22	1:M:172:GLN:HE22	1.55	0.54
1:O:46:LEU:O	1:O:50:MET:HG3	2.07	0.54
1:S:133:ASN:HD22	1:S:172:GLN:HE22	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:CE	1:B:182:GLU:OE2	2.56	0.54
1:C:46:LEU:O	1:C:50:MET:HG3	2.08	0.54
1:R:46:LEU:O	1:R:50:MET:HG3	2.07	0.54
1:H:46:LEU:O	1:H:50:MET:HG3	2.08	0.54
1:K:133:ASN:HD22	1:K:172:GLN:HE22	1.53	0.54
1:K:131:TYR:CE1	2:K:301:P2D:O4	2.59	0.54
1:L:46:LEU:O	1:L:50:MET:HG3	2.07	0.54
1:M:46:LEU:O	1:M:50:MET:HG3	2.08	0.54
1:I:46:LEU:O	1:I:50:MET:HG3	2.08	0.54
1:N:46:LEU:O	1:N:50:MET:HG3	2.07	0.54
1:T:46:LEU:O	1:T:50:MET:HG3	2.08	0.54
1:N:60:VAL:HG23	1:N:71:ASP:HB2	1.90	0.54
1:Q:46:LEU:O	1:Q:50:MET:HG3	2.08	0.54
1:B:46:LEU:O	1:B:50:MET:HG3	2.08	0.54
1:F:46:LEU:O	1:F:50:MET:HG3	2.08	0.54
1:G:28:ASN:HD22	2:G:301:P2D:H7	1.70	0.53
1:I:154:LYS:CE	1:I:182:GLU:OE2	2.56	0.53
1:P:133:ASN:HD22	1:P:172:GLN:HE22	1.54	0.53
1:C:133:ASN:HD22	1:C:172:GLN:HE22	1.55	0.53
1:E:46:LEU:O	1:E:50:MET:HG3	2.08	0.53
1:G:46:LEU:O	1:G:50:MET:HG3	2.07	0.53
1:K:46:LEU:O	1:K:50:MET:HG3	2.08	0.53
1:P:131:TYR:CE1	2:P:301:P2D:C5	2.88	0.53
1:A:46:LEU:O	1:A:50:MET:HG3	2.08	0.53
1:J:46:LEU:O	1:J:50:MET:HG3	2.08	0.53
1:A:217:ARG:NH1	1:R:53:GLN:HE22	2.07	0.53
1:C:53:GLN:HG2	3:C:348:HOH:O	2.08	0.53
1:P:46:LEU:O	1:P:50:MET:HG3	2.08	0.53
1:D:46:LEU:O	1:D:50:MET:HG3	2.08	0.53
1:O:133:ASN:HD22	1:O:172:GLN:HE22	1.55	0.53
1:S:46:LEU:O	1:S:50:MET:HG3	2.08	0.53
1:B:156:HIS:HE1	1:C:177:LEU:O	1.92	0.52
1:B:28:ASN:HB3	2:B:301:P2D:H7	1.91	0.52
1:I:37:LYS:HB2	1:I:42:VAL:HG13	1.92	0.52
1:J:37:LYS:HB2	1:J:42:VAL:HG13	1.91	0.52
1:T:37:LYS:HB2	1:T:42:VAL:HG13	1.92	0.52
1:F:37:LYS:HB2	1:F:42:VAL:HG13	1.92	0.52
1:H:37:LYS:HB2	1:H:42:VAL:HG13	1.92	0.52
1:A:37:LYS:HB2	1:A:42:VAL:HG13	1.92	0.51
1:B:37:LYS:HB2	1:B:42:VAL:HG13	1.93	0.51
1:C:37:LYS:HB2	1:C:42:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:LYS:HB2	1:G:42:VAL:HG13	1.92	0.51
1:N:37:LYS:HB2	1:N:42:VAL:HG13	1.92	0.51
1:Q:37:LYS:HB2	1:Q:42:VAL:HG13	1.92	0.51
1:R:37:LYS:HB2	1:R:42:VAL:HG13	1.93	0.51
1:E:37:LYS:HB2	1:E:42:VAL:HG13	1.93	0.51
1:P:177:LEU:O	1:Q:156:HIS:HE1	1.94	0.51
1:S:37:LYS:HB2	1:S:42:VAL:HG13	1.92	0.51
1:L:37:LYS:HB2	1:L:42:VAL:HG13	1.92	0.51
1:M:37:LYS:HB2	1:M:42:VAL:HG13	1.92	0.50
2:P:301:P2D:C1	2:P:301:P2D:C5	2.89	0.50
1:G:131:TYR:OH	2:G:301:P2D:C5	2.60	0.50
1:D:37:LYS:HB2	1:D:42:VAL:HG13	1.93	0.50
1:K:165:ALA:HB1	2:K:301:P2D:H8	1.94	0.50
1:B:129:ALA:CB	2:B:301:P2D:C1	2.90	0.50
1:K:37:LYS:HB2	1:K:42:VAL:HG13	1.94	0.50
1:T:28:ASN:HA	3:T:324:HOH:O	2.11	0.50
1:G:185:THR:HG21	2:G:301:P2D:C1	2.42	0.49
1:B:209:GLN:NE2	3:B:424:HOH:O	2.41	0.49
1:C:156:HIS:HE1	1:D:177:LEU:O	1.93	0.49
1:O:37:LYS:HB2	1:O:42:VAL:HG13	1.93	0.49
1:P:24:GLY:HA2	1:P:50:MET:HE1	1.93	0.49
1:E:70:ASN:HD21	1:R:80:ALA:HB1	1.76	0.49
1:N:60:VAL:CG2	1:N:61:MET:N	2.76	0.49
1:A:177:LEU:O	1:E:156:HIS:HE1	1.96	0.49
1:B:28:ASN:HD22	2:B:301:P2D:C4	2.26	0.48
1:P:37:LYS:HB2	1:P:42:VAL:HG13	1.95	0.48
1:J:43:LEU:HB2	1:J:44:PRO:HD3	1.96	0.48
1:E:70:ASN:ND2	1:R:80:ALA:HB1	2.29	0.48
1:A:159:GLN:HG3	3:A:325:HOH:O	2.13	0.48
1:J:216:GLY:HA3	1:Q:158:PRO:O	2.14	0.48
1:A:217:ARG:CZ	1:R:53:GLN:HE22	2.23	0.47
1:A:217:ARG:NH1	1:R:53:GLN:NE2	2.61	0.47
1:H:28:ASN:HD22	2:H:301:P2D:C4	2.27	0.47
1:G:131:TYR:CZ	2:G:301:P2D:H6	2.49	0.47
1:H:85:LYS:HE2	2:H:301:P2D:H1	1.57	0.47
1:P:165:ALA:HB1	2:P:301:P2D:H7	1.94	0.47
1:K:131:TYR:CE1	2:K:301:P2D:C4	2.98	0.47
1:G:131:TYR:CZ	2:G:301:P2D:H8	2.50	0.47
1:K:43:LEU:HB2	1:K:44:PRO:HD3	1.96	0.47
1:G:71:ASP:OD1	3:G:404:HOH:O	2.21	0.46
1:N:60:VAL:HG22	1:N:62:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:MET:HE3	3:J:351:HOH:O	2.15	0.46
1:I:1:HIS:N	3:I:347:HOH:O	2.47	0.46
1:L:43:LEU:HB2	1:L:44:PRO:HD3	1.99	0.45
1:A:43:LEU:HB2	1:A:44:PRO:HD3	1.98	0.45
1:B:43:LEU:HB2	1:B:44:PRO:HD3	1.98	0.45
1:Q:177:LEU:O	1:R:156:HIS:HE1	1.99	0.45
1:C:154:LYS:HD2	1:C:154:LYS:N	2.30	0.45
1:H:150:HIS:NE2	1:H:154:LYS:HD3	2.32	0.45
1:Q:43:LEU:HB2	1:Q:44:PRO:HD3	1.99	0.45
1:I:43:LEU:HB2	1:I:44:PRO:HD3	1.98	0.45
1:S:43:LEU:HB2	1:S:44:PRO:HD3	1.98	0.45
1:T:150:HIS:NE2	1:T:154:LYS:HD3	2.32	0.45
1:G:43:LEU:HB2	1:G:44:PRO:HD3	1.98	0.45
1:H:43:LEU:HB2	1:H:44:PRO:HD3	1.99	0.45
1:P:50:MET:CE	3:P:430:HOH:O	2.58	0.45
1:E:43:LEU:HB2	1:E:44:PRO:HD3	1.98	0.45
1:H:109:THR:OG1	2:H:301:P2D:H1	2.16	0.45
1:K:156:HIS:HE1	1:L:177:LEU:O	2.00	0.45
1:P:154:LYS:N	1:P:154:LYS:HD2	2.31	0.45
1:R:43:LEU:HB2	1:R:44:PRO:HD3	1.98	0.45
1:E:150:HIS:NE2	1:E:154:LYS:HD3	2.32	0.45
1:G:192:GLN:HG3	3:G:439:HOH:O	2.16	0.45
1:I:41:VAL:HA	3:I:334:HOH:O	2.17	0.45
1:B:217:ARG:NH1	3:B:434:HOH:O	2.50	0.44
1:F:24:GLY:HA2	1:F:50:MET:CE	2.47	0.44
1:G:144:GLN:NE2	3:G:446:HOH:O	2.50	0.44
1:B:81:ASP:O	3:B:422:HOH:O	2.21	0.44
1:H:4:TYR:CE2	1:H:57:PHE:HE1	2.35	0.44
1:M:43:LEU:HB2	1:M:44:PRO:HD3	1.99	0.44
1:E:4:TYR:CE2	1:E:57:PHE:HE1	2.36	0.44
1:F:154:LYS:N	1:F:154:LYS:HD2	2.31	0.44
1:P:165:ALA:HB1	2:P:301:P2D:C5	2.47	0.44
1:F:43:LEU:HB2	1:F:44:PRO:HD3	1.99	0.44
1:C:43:LEU:HB2	1:C:44:PRO:HD3	1.99	0.44
1:F:156:HIS:HE1	1:J:177:LEU:O	2.00	0.44
1:D:43:LEU:HB2	1:D:44:PRO:HD3	1.98	0.44
1:H:154:LYS:HD2	1:H:154:LYS:N	2.33	0.44
1:A:150:HIS:NE2	1:A:154:LYS:HD3	2.32	0.44
1:F:150:HIS:NE2	1:F:154:LYS:HD3	2.33	0.44
1:H:172:GLN:HA	3:H:438:HOH:O	2.17	0.44
1:S:154:LYS:HD2	1:S:154:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:165:ALA:CB	2:P:301:P2D:C5	2.94	0.44
1:R:154:LYS:HD2	1:R:154:LYS:N	2.33	0.44
1:P:156:HIS:HE1	1:T:177:LEU:O	2.00	0.44
1:A:217:ARG:CZ	1:R:53:GLN:CD	2.85	0.43
1:E:154:LYS:HD2	1:E:154:LYS:N	2.33	0.43
1:P:165:ALA:HB3	2:P:301:P2D:H7	1.98	0.43
1:Q:150:HIS:NE2	1:Q:154:LYS:HD3	2.33	0.43
1:T:43:LEU:HB2	1:T:44:PRO:HD3	1.99	0.43
1:O:43:LEU:HB2	1:O:44:PRO:HD3	2.00	0.43
1:N:156:HIS:HE1	1:O:177:LEU:O	2.01	0.43
1:N:97:LYS:NZ	1:O:17:SER:O	2.46	0.43
1:M:4:TYR:CE2	1:M:57:PHE:HE1	2.36	0.43
1:K:154:LYS:HD2	1:K:154:LYS:N	2.33	0.43
1:N:43:LEU:HB2	1:N:44:PRO:HD3	2.00	0.43
1:A:4:TYR:CE2	1:A:57:PHE:HE1	2.37	0.43
1:N:60:VAL:CG2	1:N:71:ASP:OD2	2.64	0.43
1:P:43:LEU:HB2	1:P:44:PRO:HD3	2.01	0.43
1:B:154:LYS:N	1:B:154:LYS:HD2	2.34	0.43
1:H:131:TYR:CE1	2:H:301:P2D:H7	2.54	0.43
1:G:66:GLU:OE1	1:G:70:ASN:ND2	2.51	0.42
1:J:24:GLY:HA2	1:J:50:MET:CE	2.49	0.42
1:P:150:HIS:NE2	1:P:154:LYS:HD3	2.34	0.42
1:S:150:HIS:NE2	1:S:154:LYS:HD3	2.35	0.42
1:D:113:GLY:HA3	3:E:316:HOH:O	2.18	0.42
1:G:131:TYR:CE1	2:G:301:P2D:C5	3.03	0.42
1:N:154:LYS:N	1:N:154:LYS:HD2	2.35	0.41
1:B:4:TYR:CE2	1:B:57:PHE:HE1	2.38	0.41
1:A:85:LYS:HE2	3:A:347:HOH:O	2.20	0.41
1:L:154:LYS:N	1:L:154:LYS:HD2	2.35	0.41
1:A:154:LYS:HD2	1:A:154:LYS:N	2.35	0.41
1:A:24:GLY:HA2	1:A:50:MET:CE	2.50	0.41
1:I:150:HIS:NE2	1:I:154:LYS:HD3	2.35	0.41
1:L:150:HIS:NE2	1:L:154:LYS:HD3	2.36	0.41
1:M:150:HIS:NE2	1:M:154:LYS:HD3	2.35	0.41
1:J:217:ARG:NH2	3:J:311:HOH:O	2.53	0.41
1:B:24:GLY:HA2	1:B:50:MET:CE	2.51	0.41
1:P:24:GLY:HA2	1:P:50:MET:CE	2.51	0.41
1:O:150:HIS:NE2	1:O:154:LYS:HD3	2.36	0.41
1:S:24:GLY:HA2	1:S:50:MET:CE	2.51	0.41
1:M:154:LYS:N	1:M:154:LYS:HD2	2.35	0.41
1:M:156:HIS:CE1	1:N:177:LEU:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:LYS:HD2	1:D:154:LYS:N	2.36	0.40
1:O:9:ASP:OD2	1:O:12:ALA:HB2	2.21	0.40
1:G:24:GLY:HA2	1:G:50:MET:CE	2.51	0.40
1:H:109:THR:OG1	2:H:301:P2D:C1	2.69	0.40
1:I:217:ARG:HB2	3:I:327:HOH:O	2.21	0.40
1:R:150:HIS:NE2	1:R:154:LYS:HD3	2.37	0.40
2:H:301:P2D:C1	2:H:301:P2D:C5	2.99	0.40
1:B:129:ALA:HB1	2:B:301:P2D:H3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	B	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	C	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	D	218/226 (96%)	215 (99%)	3 (1%)	0	100	100
1	E	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	F	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	G	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	H	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	I	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	J	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	K	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	L	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	M	218/226 (96%)	216 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	O	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	P	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	Q	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	R	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	S	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
1	T	218/226 (96%)	216 (99%)	2 (1%)	0	100	100
All	All	4360/4520 (96%)	4319 (99%)	41 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	B	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	C	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	D	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	E	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	F	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	G	167/173 (96%)	163 (98%)	4 (2%)	54	63
1	H	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	I	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	J	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	K	167/173 (96%)	163 (98%)	4 (2%)	54	63
1	L	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	M	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	N	167/173 (96%)	164 (98%)	3 (2%)	64	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	P	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	Q	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	R	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	S	167/173 (96%)	164 (98%)	3 (2%)	64	73
1	T	167/173 (96%)	164 (98%)	3 (2%)	64	73
All	All	3340/3460 (96%)	3278 (98%)	62 (2%)	62	71

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	93	LEU
1	A	154	LYS
1	B	42	VAL
1	B	93	LEU
1	B	154	LYS
1	C	42	VAL
1	C	93	LEU
1	C	154	LYS
1	D	42	VAL
1	D	93	LEU
1	D	154	LYS
1	E	42	VAL
1	E	93	LEU
1	E	154	LYS
1	F	42	VAL
1	F	93	LEU
1	F	154	LYS
1	G	42	VAL
1	G	66	GLU
1	G	93	LEU
1	G	154	LYS
1	H	42	VAL
1	H	93	LEU
1	H	154	LYS
1	I	42	VAL
1	I	93	LEU
1	I	154	LYS
1	J	42	VAL

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Mol	Chain	Res	Type
1	J	93	LEU
1	J	154	LYS
1	K	42	VAL
1	K	66	GLU
1	K	93	LEU
1	K	154	LYS
1	L	42	VAL
1	L	93	LEU
1	L	154	LYS
1	M	42	VAL
1	M	93	LEU
1	M	154	LYS
1	N	42	VAL
1	N	93	LEU
1	N	154	LYS
1	O	42	VAL
1	O	93	LEU
1	O	154	LYS
1	P	42	VAL
1	P	93	LEU
1	P	154	LYS
1	Q	42	VAL
1	Q	93	LEU
1	Q	154	LYS
1	R	42	VAL
1	R	93	LEU
1	R	154	LYS
1	S	42	VAL
1	S	93	LEU
1	S	154	LYS
1	T	42	VAL
1	T	93	LEU
1	T	154	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	144	GLN
1	A	156	HIS
1	A	212	GLN
1	B	1	HIS

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Mol	Chain	Res	Type
1	B	133	ASN
1	B	144	GLN
1	B	150	HIS
1	B	156	HIS
1	C	133	ASN
1	C	156	HIS
1	C	212	GLN
1	D	133	ASN
1	D	144	GLN
1	D	212	GLN
1	E	70	ASN
1	E	133	ASN
1	E	144	GLN
1	E	150	HIS
1	E	156	HIS
1	E	212	GLN
1	F	133	ASN
1	F	156	HIS
1	F	212	GLN
1	G	133	ASN
1	G	144	GLN
1	G	156	HIS
1	G	212	GLN
1	H	133	ASN
1	H	144	GLN
1	H	212	GLN
1	I	133	ASN
1	I	144	GLN
1	I	156	HIS
1	I	212	GLN
1	J	133	ASN
1	J	144	GLN
1	J	156	HIS
1	J	212	GLN
1	K	133	ASN
1	K	144	GLN
1	K	156	HIS
1	K	212	GLN
1	L	133	ASN
1	L	144	GLN
1	L	156	HIS
1	L	212	GLN

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Mol	Chain	Res	Type
1	M	133	ASN
1	M	144	GLN
1	M	156	HIS
1	M	212	GLN
1	N	133	ASN
1	N	144	GLN
1	N	156	HIS
1	N	212	GLN
1	O	1	HIS
1	O	133	ASN
1	O	144	GLN
1	O	156	HIS
1	O	212	GLN
1	P	133	ASN
1	P	144	GLN
1	P	156	HIS
1	P	212	GLN
1	Q	133	ASN
1	Q	144	GLN
1	Q	156	HIS
1	Q	212	GLN
1	R	53	GLN
1	R	133	ASN
1	R	144	GLN
1	R	156	HIS
1	R	212	GLN
1	S	133	ASN
1	S	144	GLN
1	S	156	HIS
1	S	212	GLN
1	T	133	ASN
1	T	144	GLN
1	T	156	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

5 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	P2D	B	301	1	5,5,6	1.83	2 (40%)	4,5,7	1.79	2 (50%)
2	P2D	G	301	1	5,5,6	1.63	1 (20%)	4,5,7	2.29	2 (50%)
2	P2D	H	301	1	5,5,6	1.48	1 (20%)	4,5,7	2.75	3 (75%)
2	P2D	K	301	1	5,5,6	1.86	2 (40%)	4,5,7	1.68	1 (25%)
2	P2D	P	301	1	5,5,6	1.45	1 (20%)	4,5,7	2.34	2 (50%)

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
2	P2D	B	301	1	-	0/3/3/4	0/0/0/0
2	P2D	G	301	1	-	0/3/3/4	0/0/0/0
2	P2D	H	301	1	-	0/3/3/4	0/0/0/0
2	P2D	K	301	1	-	0/3/3/4	0/0/0/0
2	P2D	P	301	1	-	0/3/3/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	P2D	C2-C3	-3.54	1.32	1.51
2	K	301	P2D	C2-C3	-3.47	1.32	1.51
2	G	301	P2D	C2-C3	-3.32	1.33	1.51
2	H	301	P2D	C2-C3	-3.26	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	301	P2D	C2-C3	-2.79	1.36	1.51
2	K	301	P2D	C3-C4	-2.23	1.44	1.50
2	B	301	P2D	C3-C4	-2.03	1.45	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	P2D	C5-C4-C3	-3.63	107.70	116.87
2	B	301	P2D	O4-C4-C3	-2.64	115.56	121.54
2	P	301	P2D	O4-C4-C5	-2.23	115.66	121.37
2	K	301	P2D	C5-C4-C3	-2.19	111.33	116.87
2	H	301	P2D	O4-C4-C5	-2.17	115.82	121.37
2	G	301	P2D	O4-C4-C3	2.26	126.66	121.54
2	B	301	P2D	C5-C4-C3	2.36	122.83	116.87
2	H	301	P2D	C1-C2-C3	2.90	125.08	112.67
2	P	301	P2D	C1-C2-C3	3.74	128.68	112.67
2	H	301	P2D	C5-C4-C3	3.79	126.44	116.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	P2D	4	0
2	G	301	P2D	10	0
2	H	301	P2D	7	0
2	K	301	P2D	8	0
2	P	301	P2D	9	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	220/226 (97%)	0.61	13 (5%) 23 23	18, 34, 60, 87	0
1	B	220/226 (97%)	0.66	20 (9%) 10 10	17, 36, 57, 79	0
1	C	220/226 (97%)	0.89	22 (10%) 8 7	21, 41, 69, 92	0
1	D	220/226 (97%)	0.53	15 (6%) 18 18	18, 31, 66, 86	0
1	E	220/226 (97%)	0.42	9 (4%) 38 38	16, 32, 52, 82	0
1	F	220/226 (97%)	0.18	2 (0%) 84 84	15, 26, 46, 65	0
1	G	220/226 (97%)	0.45	11 (5%) 30 30	16, 31, 63, 84	0
1	H	220/226 (97%)	0.86	25 (11%) 6 5	21, 42, 68, 96	0
1	I	220/226 (97%)	0.60	12 (5%) 26 26	19, 37, 60, 82	0
1	J	220/226 (97%)	0.32	6 (2%) 55 56	14, 27, 51, 59	0
1	K	220/226 (97%)	0.78	22 (10%) 8 7	19, 39, 64, 89	0
1	L	220/226 (97%)	1.57	63 (28%) 1 0	26, 54, 95, 119	0
1	M	220/226 (97%)	2.33	107 (48%) 0 0	38, 70, 102, 115	0
1	N	220/226 (97%)	2.35	105 (47%) 0 0	37, 68, 100, 119	0
1	O	220/226 (97%)	1.22	44 (20%) 1 1	27, 49, 87, 109	0
1	P	220/226 (97%)	0.36	6 (2%) 55 56	19, 28, 48, 55	0
1	Q	220/226 (97%)	0.49	16 (7%) 16 15	15, 33, 69, 104	0
1	R	220/226 (97%)	1.20	48 (21%) 1 1	26, 52, 73, 91	0
1	S	220/226 (97%)	1.26	41 (18%) 1 1	29, 48, 71, 96	0
1	T	220/226 (97%)	0.78	21 (9%) 9 8	25, 43, 73, 93	0
All	All	4400/4520 (97%)	0.89	608 (13%) 3 3	14, 40, 80, 119	0

All (608) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	83	VAL	14.6
1	N	51	GLY	10.7
1	M	19	ILE	9.6
1	Q	218	THR	9.6
1	I	51	GLY	9.4
1	M	53	GLN	8.9
1	N	103	GLY	8.7
1	N	54	GLY	8.6
1	M	72	ALA	8.5
1	N	23	ALA	8.3
1	N	46	LEU	8.2
1	O	219	SER	8.2
1	D	216	GLY	8.1
1	N	50	MET	8.1
1	N	1	HIS	8.1
1	N	79	ILE	7.7
1	M	88	VAL	7.6
1	O	51	GLY	7.6
1	N	195	ILE	7.3
1	M	44	PRO	7.2
1	M	84	VAL	6.9
1	M	215	PHE	6.9
1	O	101	ALA	6.8
1	R	62	ALA	6.7
1	M	16	LEU	6.6
1	K	219	SER	6.6
1	L	101	ALA	6.5
1	O	202	ALA	6.4
1	N	80	ALA	6.4
1	M	82	ILE	6.4
1	N	33	ALA	6.4
1	N	220	ILE	6.3
1	M	10	VAL	6.2
1	I	101	ALA	6.1
1	N	167	PHE	6.1
1	M	131	TYR	6.1
1	M	80	ALA	6.1
1	H	77	SER	6.1
1	T	44	PRO	6.1
1	N	81	ASP	6.1
1	D	215	PHE	6.0
1	M	159	GLN	5.8
1	L	127	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
1	N	109	THR	5.8
1	L	75	LEU	5.8
1	S	50	MET	5.7
1	L	84	VAL	5.7
1	N	159	GLN	5.6
1	Q	220	ILE	5.6
1	C	39	LEU	5.6
1	R	220	ILE	5.6
1	M	52	GLY	5.6
1	A	51	GLY	5.5
1	N	200	VAL	5.5
1	N	165	ALA	5.5
1	N	91	GLU	5.3
1	Q	51	GLY	5.3
1	K	216	GLY	5.3
1	N	72	ALA	5.2
1	D	54	GLY	5.2
1	C	220	ILE	5.1
1	K	220	ILE	5.1
1	L	99	LEU	5.1
1	M	77	SER	5.1
1	N	203	ALA	5.1
1	L	68	MET	5.0
1	M	211	TRP	5.0
1	O	207	PHE	5.0
1	N	19	ILE	5.0
1	D	52	GLY	4.9
1	R	215	PHE	4.9
1	K	215	PHE	4.9
1	L	104	ILE	4.8
1	M	43	LEU	4.8
1	S	53	GLN	4.8
1	S	63	THR	4.8
1	L	80	ALA	4.8
1	M	107	LEU	4.8
1	N	82	ILE	4.8
1	M	93	LEU	4.8
1	S	20	PHE	4.7
1	M	87	PRO	4.7
1	N	106	THR	4.7
1	L	22	LEU	4.7
1	M	73	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	101	ALA	4.5
1	M	28	ASN	4.5
1	L	69	VAL	4.5
1	N	211	TRP	4.5
1	L	119	LEU	4.5
1	A	94	ALA	4.5
1	N	16	LEU	4.5
1	H	53	GLN	4.5
1	Q	219	SER	4.4
1	L	83	VAL	4.4
1	N	41	VAL	4.4
1	N	56	LEU	4.4
1	O	55	ARG	4.4
1	Q	212	GLN	4.4
1	M	101	ALA	4.4
1	O	39	LEU	4.4
1	S	207	PHE	4.4
1	K	218	THR	4.3
1	L	63	THR	4.3
1	G	215	PHE	4.3
1	N	108	GLY	4.2
1	R	211	TRP	4.2
1	N	74	LYS	4.2
1	L	82	ILE	4.2
1	M	31	ILE	4.2
1	M	18	ARG	4.2
1	O	41	VAL	4.2
1	M	14	LYS	4.2
1	M	40	ASP	4.2
1	A	106	THR	4.1
1	D	214	ALA	4.1
1	L	78	ILE	4.1
1	L	73	LEU	4.1
1	L	72	ALA	4.1
1	R	10	VAL	4.1
1	S	17	SER	4.1
1	S	74	LYS	4.1
1	N	17	SER	4.1
1	N	66	GLU	4.1
1	N	212	GLN	4.1
1	O	205	ALA	4.1
1	O	13	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	Q	216	GLY	4.1
1	O	46	LEU	4.1
1	L	10	VAL	4.0
1	R	195	ILE	4.0
1	L	123	ALA	4.0
1	N	42	VAL	4.0
1	R	41	VAL	4.0
1	G	51	GLY	3.9
1	M	39	LEU	3.9
1	C	60	VAL	3.9
1	O	8	SER	3.9
1	Q	217	ARG	3.9
1	M	26	THR	3.9
1	N	43	LEU	3.9
1	N	4	TYR	3.9
1	K	213	GLY	3.9
1	M	68	MET	3.9
1	B	101	ALA	3.8
1	L	97	LYS	3.8
1	B	31	ILE	3.8
1	M	11	VAL	3.8
1	N	39	LEU	3.8
1	Q	213	GLY	3.8
1	K	212	GLN	3.8
1	R	53	GLN	3.8
1	N	123	ALA	3.8
1	L	5	LEU	3.8
1	A	53	GLN	3.8
1	L	37	LYS	3.8
1	L	93	LEU	3.8
1	M	27	THR	3.7
1	N	60	VAL	3.7
1	M	57	PHE	3.7
1	B	62	ALA	3.7
1	M	63	THR	3.7
1	S	93	LEU	3.7
1	M	51	GLY	3.7
1	N	75	LEU	3.7
1	M	70	ASN	3.7
1	L	102	GLU	3.7
1	L	126	GLU	3.7
1	G	216	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	159	GLN	3.7
1	N	194	MET	3.7
1	R	39	LEU	3.6
1	L	17	SER	3.6
1	M	17	SER	3.6
1	N	84	VAL	3.6
1	N	101	ALA	3.6
1	M	76	ARG	3.6
1	O	212	GLN	3.6
1	T	72	ALA	3.6
1	R	192	GLN	3.6
1	M	96	ILE	3.6
1	S	51	GLY	3.6
1	B	75	LEU	3.5
1	N	214	ALA	3.5
1	O	62	ALA	3.5
1	A	56	LEU	3.5
1	S	75	LEU	3.5
1	Q	211	TRP	3.5
1	S	214	ALA	3.5
1	D	212	GLN	3.5
1	L	116	GLN	3.5
1	L	107	LEU	3.5
1	C	74	LYS	3.5
1	R	46	LEU	3.5
1	M	94	ALA	3.5
1	C	46	LEU	3.4
1	L	43	LEU	3.4
1	T	79	ILE	3.4
1	I	77	SER	3.4
1	M	100	LYS	3.4
1	T	36	LYS	3.4
1	H	40	ASP	3.4
1	L	50	MET	3.4
1	M	24	GLY	3.4
1	M	130	PRO	3.4
1	M	64	THR	3.4
1	M	95	ALA	3.4
1	O	78	ILE	3.4
1	H	54	GLY	3.4
1	N	207	PHE	3.4
1	T	78	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	216	GLY	3.4
1	O	220	ILE	3.4
1	S	219	SER	3.3
1	C	131	TYR	3.3
1	C	52	GLY	3.3
1	G	218	THR	3.3
1	N	12	ALA	3.3
1	N	53	GLN	3.3
1	N	209	GLN	3.3
1	S	104	ILE	3.3
1	S	217	ARG	3.3
1	R	35	GLY	3.3
1	M	46	LEU	3.3
1	N	3	LEU	3.3
1	N	87	PRO	3.3
1	R	87	PRO	3.3
1	T	220	ILE	3.3
1	M	50	MET	3.2
1	N	20	PHE	3.2
1	H	42	VAL	3.2
1	H	34	ALA	3.2
1	O	38	PRO	3.2
1	S	61	MET	3.2
1	N	215	PHE	3.2
1	R	22	LEU	3.2
1	N	25	VAL	3.2
1	O	10	VAL	3.2
1	L	14	LYS	3.2
1	T	101	ALA	3.2
1	D	22	LEU	3.2
1	M	186	LEU	3.2
1	G	54	GLY	3.2
1	N	55	ARG	3.2
1	L	90	ALA	3.1
1	C	36	LYS	3.1
1	N	22	LEU	3.1
1	M	65	ALA	3.1
1	B	102	GLU	3.1
1	I	53	GLN	3.1
1	N	196	SER	3.1
1	C	207	PHE	3.1
1	M	35	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	3.1
1	B	104	ILE	3.1
1	L	62	ALA	3.1
1	G	159	GLN	3.1
1	K	53	GLN	3.1
1	R	185	THR	3.1
1	N	105	PRO	3.1
1	R	139	GLY	3.1
1	H	66	GLU	3.1
1	M	1	HIS	3.1
1	G	53	GLN	3.1
1	T	8	SER	3.1
1	R	165	ALA	3.1
1	N	70	ASN	3.0
1	M	98	MET	3.0
1	L	95	ALA	3.0
1	N	102	GLU	3.0
1	L	61	MET	3.0
1	L	158	PRO	3.0
1	M	123	ALA	3.0
1	H	50	MET	3.0
1	N	73	LEU	3.0
1	L	31	ILE	3.0
1	K	217	ARG	3.0
1	L	77	SER	3.0
1	C	218	THR	3.0
1	M	158	PRO	3.0
1	N	186	LEU	3.0
1	G	17	SER	3.0
1	S	135	ILE	3.0
1	L	162	VAL	3.0
1	M	38	PRO	3.0
1	O	22	LEU	3.0
1	D	74	LYS	3.0
1	N	7	THR	3.0
1	J	217	ARG	3.0
1	H	56	LEU	2.9
1	N	93	LEU	2.9
1	O	56	LEU	2.9
1	N	45	GLN	2.9
1	L	6	ASP	2.9
1	I	52	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	S	60	VAL	2.9
1	J	218	THR	2.9
1	N	14	LYS	2.9
1	L	38	PRO	2.9
1	N	111	VAL	2.9
1	N	107	LEU	2.9
1	R	74	LYS	2.9
1	C	90	ALA	2.9
1	R	31	ILE	2.9
1	S	44	PRO	2.9
1	A	50	MET	2.9
1	Q	202	ALA	2.9
1	R	70	ASN	2.9
1	H	135	ILE	2.9
1	N	104	ILE	2.9
1	D	41	VAL	2.9
1	D	213	GLY	2.9
1	L	60	VAL	2.9
1	S	88	VAL	2.9
1	O	40	ASP	2.8
1	J	77	SER	2.8
1	O	31	ILE	2.8
1	L	86	VAL	2.8
1	L	121	ALA	2.8
1	M	75	LEU	2.8
1	S	98	MET	2.8
1	M	54	GLY	2.8
1	A	41	VAL	2.8
1	R	218	THR	2.8
1	O	53	GLN	2.8
1	S	7	THR	2.8
1	B	220	ILE	2.8
1	H	220	ILE	2.8
1	L	36	LYS	2.8
1	M	20	PHE	2.7
1	N	126	GLU	2.8
1	R	61	MET	2.7
1	S	188	LEU	2.7
1	B	65	ALA	2.7
1	K	211	TRP	2.7
1	L	94	ALA	2.7
1	N	188	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	37	LYS	2.7
1	N	175	ASP	2.7
1	L	35	GLY	2.7
1	M	219	SER	2.7
1	O	164	ALA	2.7
1	S	212	GLN	2.7
1	S	39	LEU	2.7
1	N	30	SER	2.7
1	R	58	ALA	2.7
1	T	39	LEU	2.7
1	M	194	MET	2.7
1	R	63	THR	2.7
1	E	41	VAL	2.7
1	M	86	VAL	2.7
1	M	118	LEU	2.7
1	G	212	GLN	2.7
1	K	214	ALA	2.7
1	M	214	ALA	2.7
1	N	112	TYR	2.7
1	R	207	PHE	2.7
1	A	35	GLY	2.7
1	H	52	GLY	2.6
1	M	47	HIS	2.6
1	T	109	THR	2.6
1	O	42	VAL	2.6
1	O	163	LEU	2.6
1	R	68	MET	2.6
1	G	220	ILE	2.6
1	I	79	ILE	2.6
1	M	33	ALA	2.6
1	R	51	GLY	2.6
1	L	81	ASP	2.6
1	L	41	VAL	2.6
1	N	149	LEU	2.6
1	R	217	ARG	2.6
1	M	121	ALA	2.6
1	D	195	ILE	2.6
1	Q	209	GLN	2.6
1	M	3	LEU	2.6
1	S	167	PHE	2.6
1	A	102	GLU	2.6
1	S	126	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	54	GLY	2.6
1	N	32	ILE	2.6
1	K	204	VAL	2.6
1	J	52	GLY	2.6
1	N	157	ALA	2.6
1	N	202	ALA	2.6
1	T	108	GLY	2.6
1	O	16	LEU	2.5
1	Q	41	VAL	2.5
1	L	71	ASP	2.5
1	T	53	GLN	2.5
1	N	166	SER	2.5
1	M	193	GLN	2.5
1	M	99	LEU	2.5
1	O	6	ASP	2.5
1	S	118	LEU	2.5
1	M	25	VAL	2.5
1	R	196	SER	2.5
1	R	219	SER	2.5
1	M	106	THR	2.5
1	H	159	GLN	2.5
1	R	198	PRO	2.5
1	I	74	LYS	2.5
1	B	43	LEU	2.5
1	P	73	LEU	2.5
1	S	52	GLY	2.5
1	S	67	GLY	2.5
1	O	179	ALA	2.5
1	L	91	GLU	2.5
1	L	106	THR	2.5
1	M	109	THR	2.5
1	M	117	GLY	2.5
1	T	159	GLN	2.5
1	M	112	TYR	2.5
1	M	189	ASP	2.5
1	I	55	ARG	2.5
1	B	100	LYS	2.5
1	M	122	LEU	2.5
1	L	66	GLU	2.5
1	L	52	GLY	2.5
1	R	32	ILE	2.5
1	K	8	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	199	ALA	2.4
1	D	53	GLN	2.4
1	O	19	ILE	2.4
1	K	52	GLY	2.4
1	R	1	HIS	2.4
1	N	71	ASP	2.4
1	H	75	LEU	2.4
1	N	205	ALA	2.4
1	R	191	ALA	2.4
1	S	58	ALA	2.4
1	C	208	GLU	2.4
1	M	208	GLU	2.4
1	P	159	GLN	2.4
1	R	56	LEU	2.4
1	C	103	GLY	2.4
1	M	125	ALA	2.4
1	N	129	ALA	2.4
1	C	69	VAL	2.4
1	H	18	ARG	2.4
1	R	7	THR	2.4
1	S	220	ILE	2.4
1	E	66	GLU	2.4
1	I	56	LEU	2.4
1	C	199	ALA	2.4
1	Q	210	ASP	2.4
1	S	80	ALA	2.4
1	B	20	PHE	2.4
1	I	66	GLU	2.4
1	S	59	GLN	2.4
1	D	24	GLY	2.4
1	K	73	LEU	2.4
1	R	188	LEU	2.4
1	M	115	ALA	2.4
1	N	58	ALA	2.4
1	M	207	PHE	2.4
1	Q	215	PHE	2.4
1	E	51	GLY	2.3
1	P	66	GLU	2.3
1	Q	214	ALA	2.3
1	S	16	LEU	2.3
1	S	130	PRO	2.3
1	O	106	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	219	SER	2.3
1	H	41	VAL	2.3
1	B	47	HIS	2.3
1	J	220	ILE	2.3
1	O	197	TYR	2.3
1	B	56	LEU	2.3
1	E	157	ALA	2.3
1	M	149	LEU	2.3
1	N	160	ALA	2.3
1	N	177	LEU	2.3
1	O	100	LYS	2.3
1	O	217	ARG	2.3
1	C	41	VAL	2.3
1	C	42	VAL	2.3
1	M	156	HIS	2.3
1	N	90	ALA	2.3
1	S	129	ALA	2.3
1	N	183	SER	2.3
1	T	60	VAL	2.3
1	R	193	GLN	2.3
1	H	31	ILE	2.3
1	O	48	GLU	2.3
1	T	33	ALA	2.3
1	T	50	MET	2.3
1	H	10	VAL	2.3
1	M	132	VAL	2.3
1	N	204	VAL	2.3
1	O	20	PHE	2.3
1	B	106	THR	2.3
1	R	146	VAL	2.3
1	B	74	LYS	2.3
1	B	219	SER	2.3
1	L	120	SER	2.3
1	M	104	ILE	2.3
1	A	70	ASN	2.2
1	N	85	LYS	2.2
1	N	76	ARG	2.2
1	D	51	GLY	2.2
1	L	16	LEU	2.2
1	N	68	MET	2.2
1	K	13	VAL	2.2
1	M	204	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	44	PRO	2.2
1	M	218	THR	2.2
1	R	104	ILE	2.2
1	M	212	GLN	2.2
1	N	86	VAL	2.2
1	O	14	LYS	2.2
1	H	219	SER	2.2
1	M	30	SER	2.2
1	O	213	GLY	2.2
1	E	27	THR	2.2
1	L	40	ASP	2.2
1	E	159	GLN	2.2
1	M	192	GLN	2.2
1	M	36	LYS	2.2
1	M	37	LYS	2.2
1	H	88	VAL	2.2
1	N	13	VAL	2.2
1	R	42	VAL	2.2
1	L	64	THR	2.2
1	H	211	TRP	2.2
1	N	78	ILE	2.2
1	H	61	MET	2.2
1	R	131	TYR	2.2
1	M	124	GLY	2.2
1	S	216	GLY	2.2
1	I	70	ASN	2.2
1	M	90	ALA	2.2
1	T	74	LYS	2.2
1	F	56	LEU	2.2
1	H	46	LEU	2.2
1	K	93	LEU	2.2
1	C	206	LYS	2.1
1	P	213	GLY	2.2
1	M	23	ALA	2.1
1	R	205	ALA	2.1
1	O	32	ILE	2.1
1	R	78	ILE	2.1
1	K	36	LYS	2.1
1	P	38	PRO	2.1
1	T	55	ARG	2.1
1	N	10	VAL	2.1
1	M	97	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	59	GLN	2.1
1	F	70	ASN	2.1
1	G	214	ALA	2.1
1	H	69	VAL	2.1
1	C	215	PHE	2.1
1	E	53	GLN	2.1
1	K	159	GLN	2.1
1	B	73	LEU	2.1
1	L	213	GLY	2.1
1	N	21	PRO	2.1
1	O	35	GLY	2.1
1	O	196	SER	2.1
1	T	195	ILE	2.1
1	T	212	GLN	2.1
1	D	218	THR	2.1
1	M	55	ARG	2.1
1	N	197	TYR	2.1
1	T	41	VAL	2.1
1	B	21	PRO	2.1
1	I	103	GLY	2.1
1	N	182	GLU	2.1
1	A	49	ALA	2.1
1	M	89	THR	2.1
1	N	132	VAL	2.1
1	O	77	SER	2.1
1	S	35	GLY	2.1
1	S	112	TYR	2.1
1	R	23	ALA	2.1
1	K	69	VAL	2.1
1	R	8	SER	2.1
1	R	67	GLY	2.1
1	S	77	SER	2.1
1	N	193	GLN	2.0
1	B	93	LEU	2.0
1	K	55	ARG	2.0
1	L	39	LEU	2.0
1	O	54	GLY	2.0
1	M	48	GLU	2.0
1	B	88	VAL	2.0
1	M	6	ASP	2.0
1	C	82	ILE	2.0
1	O	104	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	66	GLU	2.0
1	N	52	GLY	2.0
1	E	202	ALA	2.0
1	K	209	GLN	2.0
1	L	58	ALA	2.0
1	N	219	SER	2.0
1	P	80	ALA	2.0
1	M	29	PRO	2.0
1	L	1	HIS	2.0
1	L	11	VAL	2.0
1	N	69	VAL	2.0
1	Q	42	VAL	2.0
1	H	78	ILE	2.0
1	M	177	LEU	2.0
1	R	79	ILE	2.0
1	S	91	GLU	2.0
1	M	108	GLY	2.0
1	J	74	LYS	2.0
1	M	114	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	P2D	G	301	6/7	0.86	0.32	8.74	39,50,54,58	0
2	P2D	P	301	6/7	0.80	0.37	8.39	41,42,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	P2D	H	301	6/7	0.82	0.30	3.59	56,60,62,66	0
2	P2D	B	301	6/7	0.73	0.34	2.83	43,46,51,55	0
2	P2D	K	301	6/7	0.89	0.21	1.69	41,43,53,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.