Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2023 – 08:39 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

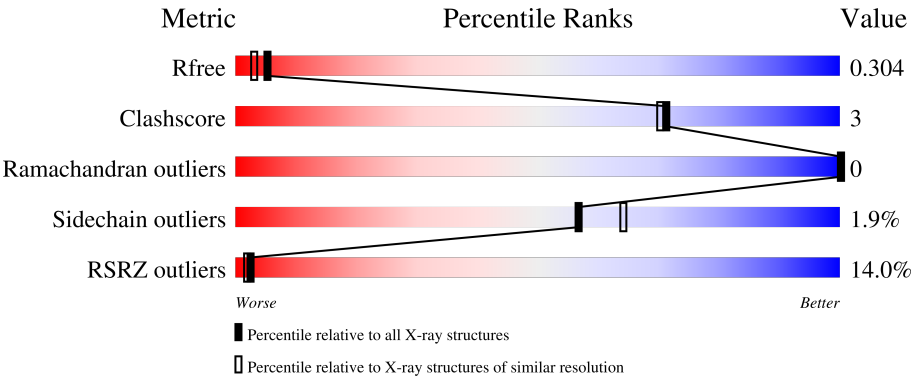
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	226	6% 88% 8%
1	B	226	10% 88% 9%
1	C	226	11% 92% 5%
1	D	226	7% 91% 5%
1	E	226	4% 90% 7%

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Mol	Chain	Length	Quality of chain
1	F	226	91% 6%
1	G	226	5% 88% 8%
1	H	226	11% 89% 8%
1	I	226	5% 90% 6%
1	J	226	2% 90% 6%
1	K	226	10% 91% 6%
1	L	226	27% 92%
1	M	226	47% 91% 5%
1	N	226	47% 89% 7%
1	O	226	20% 91% 5%
1	P	226	3% 90% 6%
1	Q	226	7% 91% 5%
1	R	226	22% 91% 6%
1	S	226	18% 91% 5%
1	T	226	9% 92% 5%

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	-
2	P2D	G	301	-	-	X	-
2	P2D	H	301	-	X	X	-
2	P2D	K	301	-	-	X	-
2	P2D	P	301	-	X	X	-

2 Entry composition (i)

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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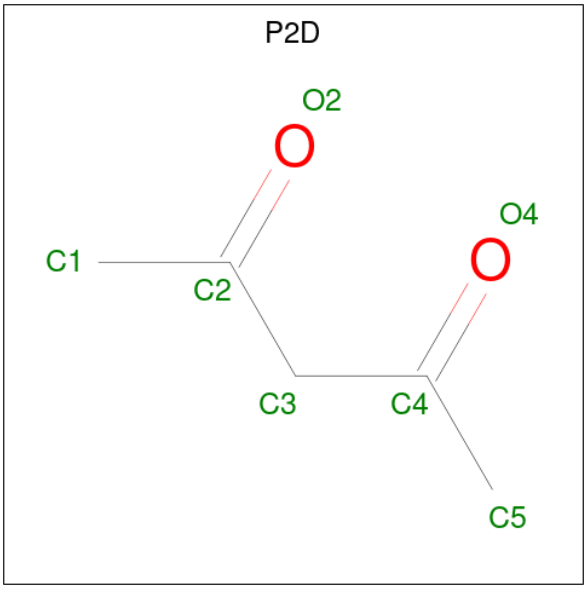
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-2	HIS	-	expression tag	UNP P78055
Q	-1	HIS	-	expression tag	UNP P78055
Q	0	HIS	-	expression tag	UNP P78055
Q	1	HIS	-	expression tag	UNP P78055
R	-5	MET	-	expression tag	UNP P78055
R	-4	HIS	-	expression tag	UNP P78055
R	-3	HIS	-	expression tag	UNP P78055
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: $C_5H_8O_2$).



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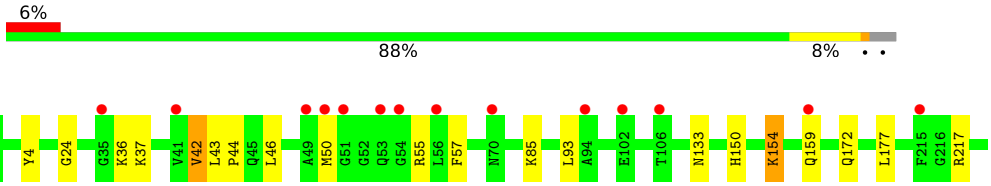
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	T	33	Total O 33 33	0	0

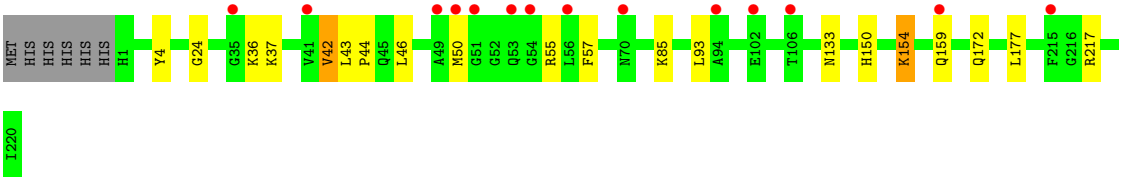
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fructose-6-phosphate aldolase 1

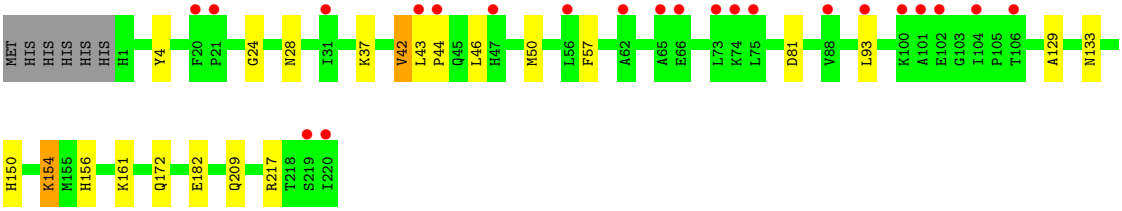
Chain A:





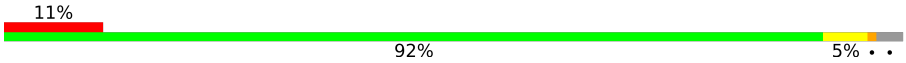
• Molecule 1: Fructose-6-phosphate aldolase 1

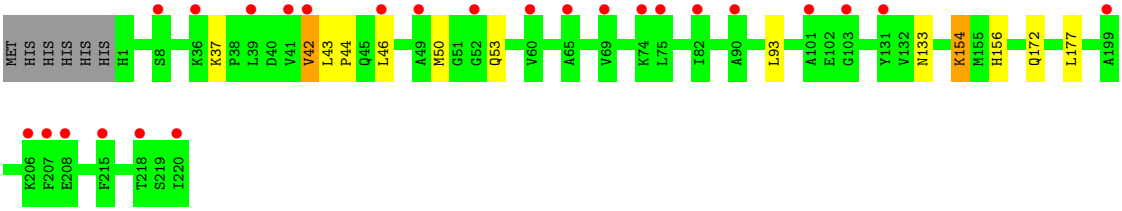
Chain B:



• Molecule 1: Fructose-6-phosphate aldolase 1

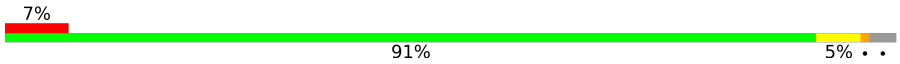
Chain C:

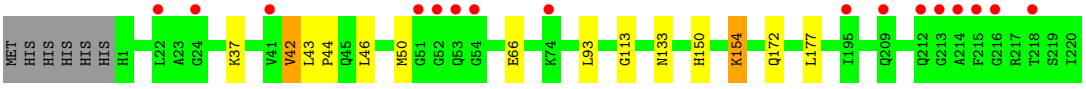




• Molecule 1: Fructose-6-phosphate aldolase 1

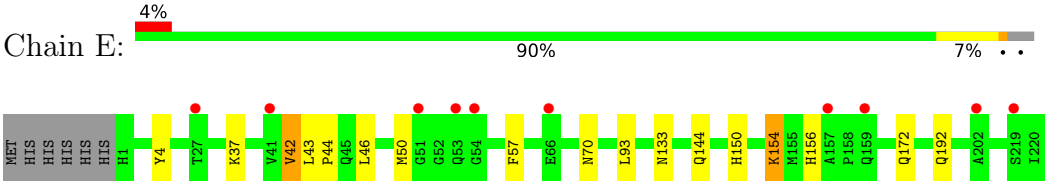
Chain D:





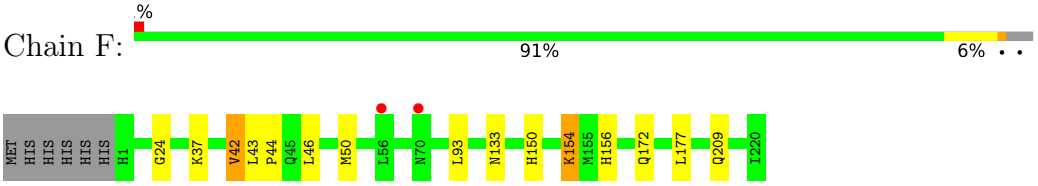
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain E:



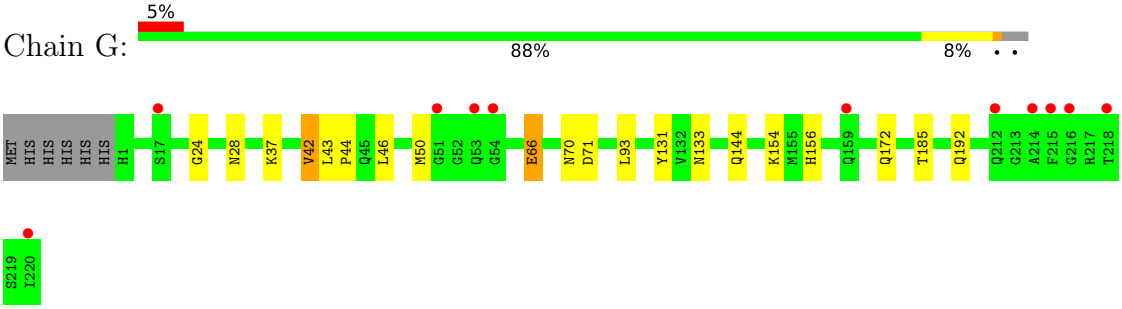
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain F:



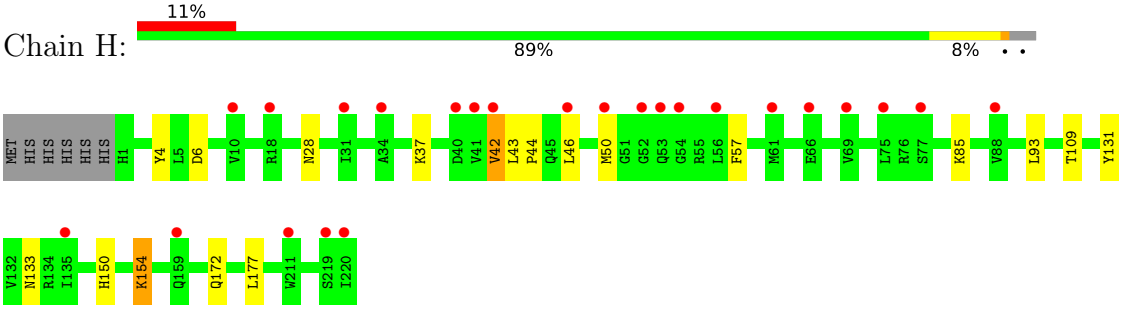
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain G:



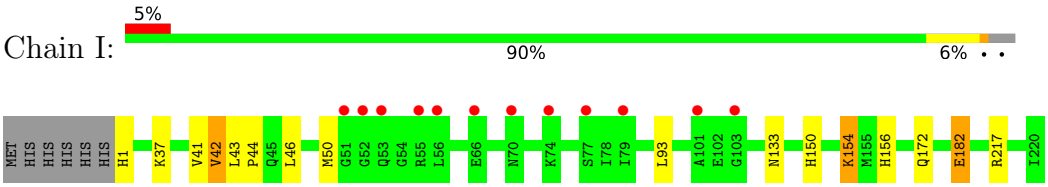
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain H:



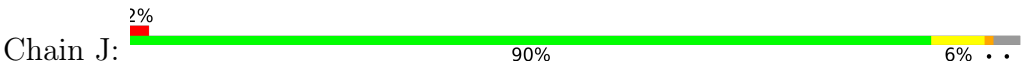
• Molecule 1: Fructose-6-phosphate aldolase 1

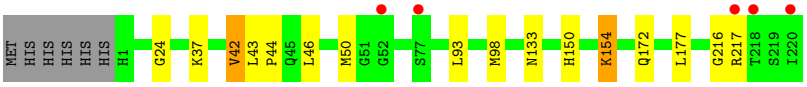
Chain I:



• Molecule 1: Fructose-6-phosphate aldolase 1

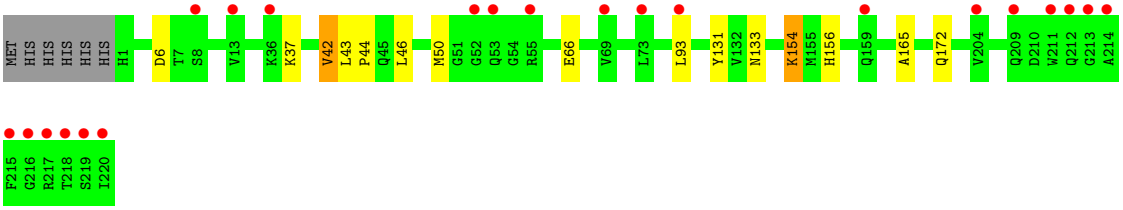
Chain J:





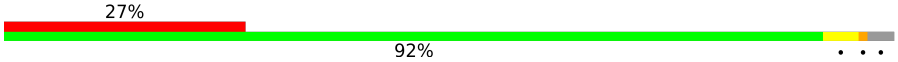
• Molecule 1: Fructose-6-phosphate aldolase 1

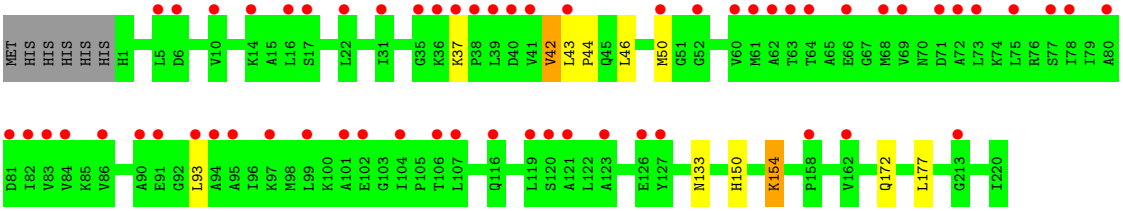
Chain K:



• Molecule 1: Fructose-6-phosphate aldolase 1

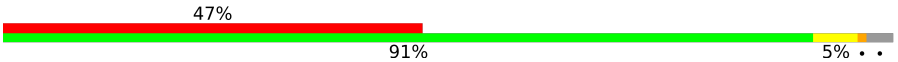
Chain L:

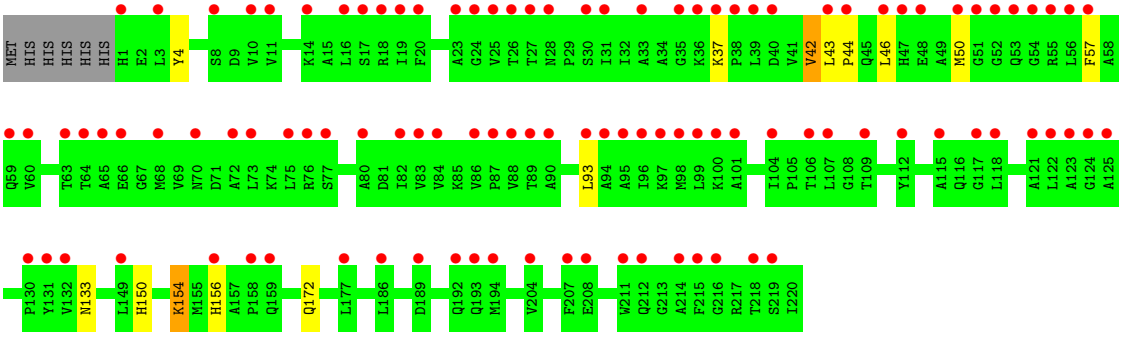




• Molecule 1: Fructose-6-phosphate aldolase 1

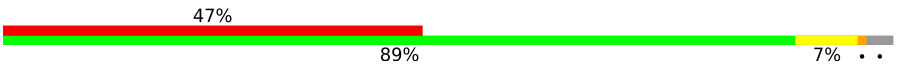
Chain M:

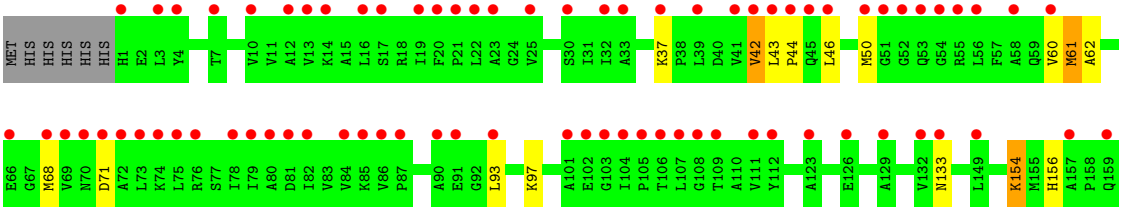


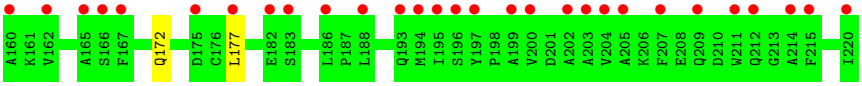


• Molecule 1: Fructose-6-phosphate aldolase 1

Chain N:

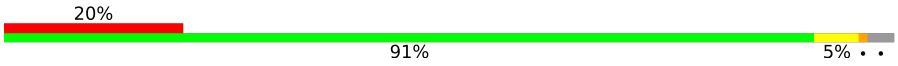


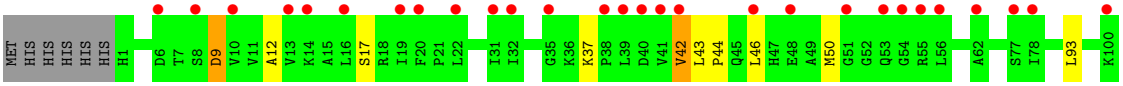


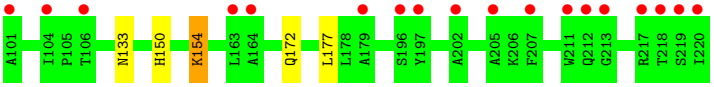


• Molecule 1: Fructose-6-phosphate aldolase 1

Chain O:

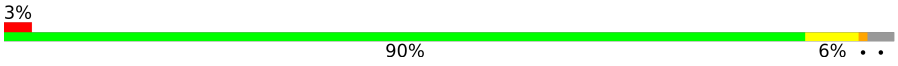


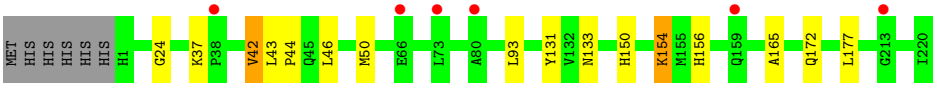




• Molecule 1: Fructose-6-phosphate aldolase 1

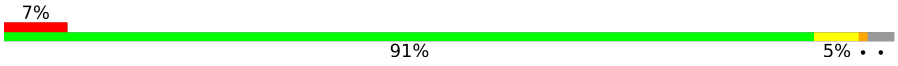
Chain P:

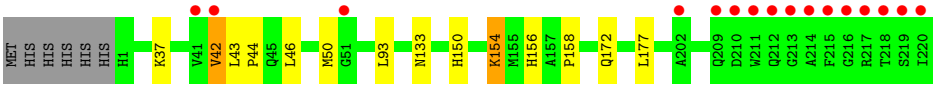




• Molecule 1: Fructose-6-phosphate aldolase 1

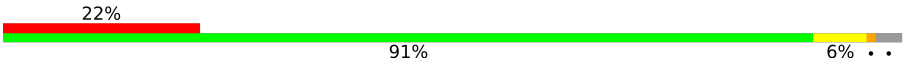
Chain Q:

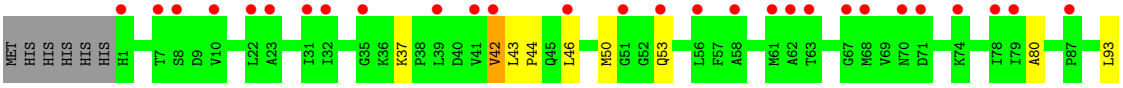


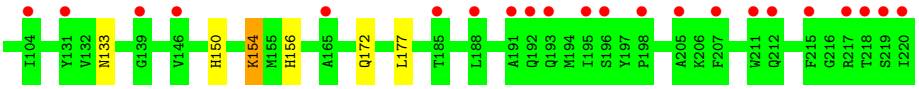


• Molecule 1: Fructose-6-phosphate aldolase 1

Chain R:

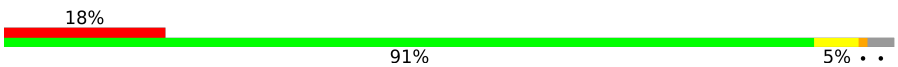


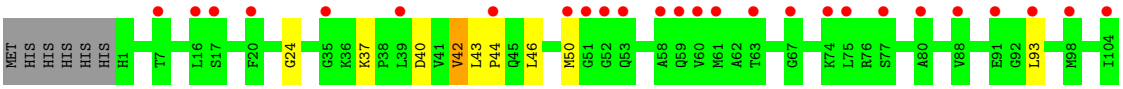


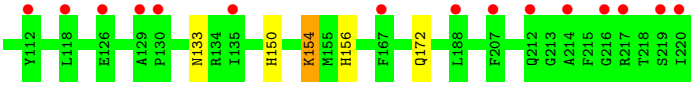


• Molecule 1: Fructose-6-phosphate aldolase 1

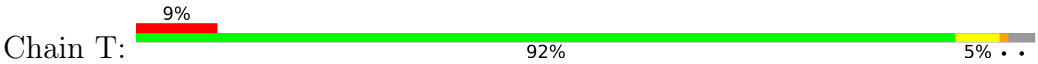
Chain S:

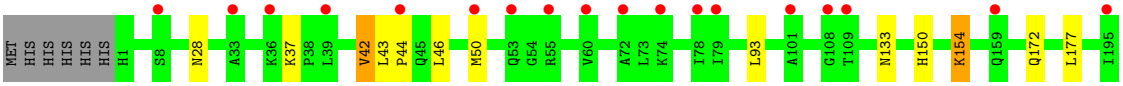






• Molecule 1: Fructose-6-phosphate aldolase 1





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.87 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.232 , 0.251 0.279 , 0.304	Depositor DCC
R_{free} test set	11038 reflections (5.07%)	wwPDB-VP
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]	$< \|L\| > = 0.54$, $< L^2 > = 0.39$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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 (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	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:OE1	1:G:66:GLU:C	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:131:TYR:CE1	2:K:301:P2D:O4	2.59	0.54
1:K:133:ASN:HD22	1:K:172:GLN:HE22	1.53	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:C5	2:P:301:P2D:C1	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:E:70:ASN:ND2	1:R:80:ALA:HB1	2.29	0.48
1:J:43:LEU:HB2	1:J:44:PRO:HD3	1.96	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:156:HIS:HE1	1:T:177:LEU:O	2.00	0.44
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:A:217:ARG:CZ	1:R:53:GLN:CD	2.85	0.43
1:E:154:LYS:N	1:E:154:LYS:HD2	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:97:LYS:NZ	1:O:17:SER:O	2.46	0.43
1:N:156:HIS:HE1	1:O:177:LEU:O	2.01	0.43
1:M:4:TYR:CE2	1:M:57:PHE:HE1	2.36	0.43
1:K:154:LYS:N	1:K:154:LYS:HD2	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:HD2	1:L:154:LYS:N	2.35	0.41
1:A:24:GLY:HA2	1:A:50:MET:CE	2.50	0.41
1:A:154:LYS:N	1:A:154:LYS:HD2	2.35	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:HD2	1:M:154:LYS:N	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:N	1:D:154:LYS:HD2	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 (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	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 (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	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	B	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	C	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	D	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	E	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	F	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	G	167/173 (96%)	163 (98%)	4 (2%)	49	55
1	H	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	I	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	J	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	K	167/173 (96%)	163 (98%)	4 (2%)	49	55
1	L	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	M	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	N	167/173 (96%)	164 (98%)	3 (2%)	59	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	P	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	Q	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	R	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	S	167/173 (96%)	164 (98%)	3 (2%)	59	66
1	T	167/173 (96%)	164 (98%)	3 (2%)	59	66
All	All	3340/3460 (96%)	3278 (98%)	62 (2%)	57	64

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

Sometimes 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 monosaccharides 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	K	301	1	5,5,6	1.81	1 (20%)	4,5,7	1.54	0
2	P2D	H	301	1	5,5,6	1.49	1 (20%)	4,5,7	2.43	3 (75%)
2	P2D	B	301	1	5,5,6	1.79	1 (20%)	4,5,7	1.37	0
2	P2D	P	301	1	5,5,6	1.44	1 (20%)	4,5,7	2.29	2 (50%)
2	P2D	G	301	1	5,5,6	1.61	1 (20%)	4,5,7	1.88	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
2	P2D	K	301	1	-	0/3/3/4	-
2	P2D	H	301	1	-	3/3/3/4	-
2	P2D	B	301	1	-	2/3/3/4	-
2	P2D	P	301	1	-	3/3/3/4	-
2	P2D	G	301	1	-	0/3/3/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	P2D	C2-C3	-3.59	1.32	1.51
2	K	301	P2D	C2-C3	-3.52	1.32	1.51
2	G	301	P2D	C2-C3	-3.36	1.33	1.51
2	H	301	P2D	C2-C3	-3.31	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	301	P2D	C2-C3	-2.83	1.36	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	301	P2D	C1-C2-C3	3.75	128.68	112.67
2	H	301	P2D	C5-C4-C3	2.96	126.44	116.94
2	H	301	P2D	C1-C2-C3	2.90	125.08	112.67
2	G	301	P2D	C5-C4-C3	-2.88	107.70	116.94
2	P	301	P2D	O4-C4-C5	-2.26	115.66	121.40
2	H	301	P2D	O4-C4-C5	-2.20	115.82	121.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	P2D	C2-C3-C4-C5
2	B	301	P2D	C2-C3-C4-O4
2	H	301	P2D	C1-C2-C3-C4
2	H	301	P2D	C2-C3-C4-C5
2	H	301	P2D	C2-C3-C4-O4
2	P	301	P2D	C1-C2-C3-C4
2	P	301	P2D	C2-C3-C4-C5
2	P	301	P2D	C2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	301	P2D	8	0
2	H	301	P2D	7	0
2	B	301	P2D	4	0
2	P	301	P2D	9	0
2	G	301	P2D	10	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	220/226 (97%)	0.62	14 (6%) 19 19	18, 34, 60, 87	0
1	B	220/226 (97%)	0.67	22 (10%) 7 6	17, 36, 57, 79	0
1	C	220/226 (97%)	0.90	25 (11%) 5 4	21, 41, 69, 92	0
1	D	220/226 (97%)	0.54	16 (7%) 15 14	18, 31, 66, 86	0
1	E	220/226 (97%)	0.43	10 (4%) 33 33	16, 32, 52, 82	0
1	F	220/226 (97%)	0.19	2 (0%) 84 84	15, 26, 46, 65	0
1	G	220/226 (97%)	0.46	11 (5%) 28 28	16, 31, 63, 84	0
1	H	220/226 (97%)	0.87	24 (10%) 5 5	21, 42, 68, 96	0
1	I	220/226 (97%)	0.61	12 (5%) 25 24	19, 37, 60, 82	0
1	J	220/226 (97%)	0.33	5 (2%) 60 61	14, 27, 50, 59	0
1	K	220/226 (97%)	0.80	22 (10%) 7 6	19, 39, 64, 89	0
1	L	220/226 (97%)	1.58	60 (27%) 0 0	26, 54, 95, 119	0
1	M	220/226 (97%)	2.34	106 (48%) 0 0	38, 70, 102, 115	0
1	N	220/226 (97%)	2.36	106 (48%) 0 0	37, 68, 100, 119	0
1	O	220/226 (97%)	1.24	46 (20%) 1 0	27, 49, 87, 109	0
1	P	220/226 (97%)	0.36	6 (2%) 54 55	19, 28, 48, 55	0
1	Q	220/226 (97%)	0.51	16 (7%) 15 14	15, 33, 69, 104	0
1	R	220/226 (97%)	1.21	50 (22%) 0 0	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	20 (9%) 9 9	25, 43, 73, 93	0
All	All	4400/4520 (97%)	0.90	614 (13%) 2 2	14, 40, 80, 119	0

All (614) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	83	VAL	14.6
1	N	51	GLY	10.7
1	Q	218	THR	10.2
1	M	19	ILE	9.7
1	I	51	GLY	9.5
1	M	53	GLN	9.1
1	N	103	GLY	8.9
1	M	72	ALA	8.8
1	N	54	GLY	8.6
1	N	46	LEU	8.5
1	O	219	SER	8.4
1	N	50	MET	8.4
1	D	216	GLY	8.2
1	N	23	ALA	8.1
1	N	1	HIS	8.0
1	N	79	ILE	7.8
1	O	51	GLY	7.6
1	M	88	VAL	7.5
1	N	195	ILE	7.2
1	M	44	PRO	7.1
1	M	215	PHE	7.0
1	M	84	VAL	7.0
1	R	62	ALA	6.8
1	O	101	ALA	6.7
1	K	219	SER	6.7
1	L	101	ALA	6.7
1	N	33	ALA	6.7
1	M	16	LEU	6.6
1	M	82	ILE	6.6
1	N	80	ALA	6.5
1	M	10	VAL	6.4
1	N	167	PHE	6.3
1	O	202	ALA	6.3
1	N	220	ILE	6.2
1	N	81	ASP	6.2
1	I	101	ALA	6.2
1	M	80	ALA	6.2
1	T	44	PRO	6.2
1	D	215	PHE	6.1
1	H	77	SER	6.0
1	M	131	TYR	6.0
1	L	127	TYR	5.9
1	S	50	MET	5.9

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Mol	Chain	Res	Type	RSRZ
1	L	84	VAL	5.8
1	L	75	LEU	5.8
1	M	159	GLN	5.8
1	M	52	GLY	5.7
1	Q	220	ILE	5.7
1	A	51	GLY	5.7
1	N	109	THR	5.6
1	R	220	ILE	5.6
1	C	39	LEU	5.5
1	N	159	GLN	5.5
1	N	165	ALA	5.5
1	N	91	GLU	5.4
1	N	200	VAL	5.4
1	K	216	GLY	5.3
1	D	54	GLY	5.3
1	L	99	LEU	5.3
1	M	77	SER	5.2
1	Q	51	GLY	5.2
1	M	211	TRP	5.2
1	N	72	ALA	5.2
1	L	68	MET	5.2
1	R	215	PHE	5.2
1	K	220	ILE	5.1
1	K	215	PHE	5.1
1	C	220	ILE	5.1
1	N	203	ALA	5.1
1	L	104	ILE	5.1
1	N	19	ILE	5.0
1	N	106	THR	5.0
1	L	80	ALA	4.9
1	S	53	GLN	4.9
1	D	52	GLY	4.9
1	M	43	LEU	4.8
1	N	82	ILE	4.8
1	Q	212	GLN	4.8
1	O	207	PHE	4.8
1	M	73	LEU	4.8
1	S	63	THR	4.8
1	M	107	LEU	4.8
1	M	93	LEU	4.8
1	L	22	LEU	4.7
1	S	20	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	L	69	VAL	4.6
1	M	87	PRO	4.6
1	R	211	TRP	4.6
1	K	218	THR	4.6
1	Q	219	SER	4.6
1	N	16	LEU	4.6
1	A	94	ALA	4.5
1	C	101	ALA	4.5
1	N	211	TRP	4.5
1	L	63	THR	4.4
1	N	56	LEU	4.4
1	O	55	ARG	4.4
1	L	83	VAL	4.4
1	H	53	GLN	4.4
1	N	41	VAL	4.4
1	G	215	PHE	4.4
1	L	119	LEU	4.4
1	O	39	LEU	4.4
1	M	101	ALA	4.4
1	M	28	ASN	4.3
1	S	207	PHE	4.3
1	L	82	ILE	4.3
1	M	14	LYS	4.3
1	N	108	GLY	4.3
1	L	78	ILE	4.2
1	A	106	THR	4.2
1	N	17	SER	4.2
1	M	18	ARG	4.2
1	O	46	LEU	4.2
1	O	13	VAL	4.2
1	M	31	ILE	4.2
1	L	73	LEU	4.2
1	R	10	VAL	4.2
1	D	214	ALA	4.2
1	L	72	ALA	4.2
1	O	8	SER	4.1
1	O	41	VAL	4.1
1	Q	216	GLY	4.1
1	N	74	LYS	4.1
1	N	42	VAL	4.1
1	S	17	SER	4.1
1	N	212	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	Q	217	ARG	4.1
1	S	74	LYS	4.1
1	N	66	GLU	4.1
1	Q	213	GLY	4.1
1	K	213	GLY	4.0
1	O	205	ALA	4.0
1	M	68	MET	4.0
1	L	10	VAL	4.0
1	M	40	ASP	4.0
1	L	123	ALA	4.0
1	L	97	LYS	4.0
1	N	43	LEU	3.9
1	B	101	ALA	3.9
1	R	195	ILE	3.9
1	K	212	GLN	3.9
1	G	51	GLY	3.9
1	C	60	VAL	3.9
1	L	102	GLU	3.9
1	M	70	ASN	3.9
1	N	123	ALA	3.9
1	O	212	GLN	3.8
1	B	31	ILE	3.8
1	R	41	VAL	3.8
1	L	93	LEU	3.8
1	M	11	VAL	3.8
1	L	37	LYS	3.8
1	L	5	LEU	3.8
1	N	4	TYR	3.8
1	M	26	THR	3.8
1	M	39	LEU	3.8
1	A	53	GLN	3.8
1	G	216	GLY	3.8
1	M	51	GLY	3.8
1	B	62	ALA	3.8
1	N	60	VAL	3.8
1	N	39	LEU	3.8
1	N	84	VAL	3.7
1	M	57	PHE	3.7
1	L	126	GLU	3.7
1	C	46	LEU	3.7
1	Q	211	TRP	3.7
1	R	53	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	17	SER	3.7
1	S	93	LEU	3.7
1	M	63	THR	3.7
1	M	76	ARG	3.7
1	R	39	LEU	3.7
1	N	214	ALA	3.7
1	N	194	MET	3.7
1	L	17	SER	3.6
1	M	27	THR	3.6
1	T	72	ALA	3.6
1	N	75	LEU	3.6
1	R	46	LEU	3.6
1	O	62	ALA	3.6
1	M	96	ILE	3.6
1	N	101	ALA	3.6
1	A	159	GLN	3.6
1	S	51	GLY	3.6
1	D	212	GLN	3.6
1	L	50	MET	3.5
1	C	74	LYS	3.5
1	R	192	GLN	3.5
1	H	54	GLY	3.5
1	S	219	SER	3.5
1	T	79	ILE	3.5
1	M	94	ALA	3.5
1	M	24	GLY	3.5
1	M	50	MET	3.5
1	A	56	LEU	3.5
1	L	116	GLN	3.5
1	I	77	SER	3.5
1	L	43	LEU	3.5
1	L	107	LEU	3.5
1	S	75	LEU	3.5
1	M	95	ALA	3.5
1	S	214	ALA	3.5
1	C	52	GLY	3.5
1	M	130	PRO	3.4
1	G	218	THR	3.4
1	M	64	THR	3.4
1	S	217	ARG	3.4
1	H	40	ASP	3.4
1	M	216	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	N	209	GLN	3.4
1	M	46	LEU	3.4
1	M	100	LYS	3.4
1	T	36	LYS	3.4
1	T	78	ILE	3.4
1	O	78	ILE	3.4
1	O	220	ILE	3.4
1	R	35	GLY	3.3
1	B	75	LEU	3.3
1	N	215	PHE	3.3
1	N	207	PHE	3.3
1	N	12	ALA	3.3
1	N	25	VAL	3.3
1	N	53	GLN	3.3
1	L	62	ALA	3.3
1	S	61	MET	3.3
1	O	10	VAL	3.3
1	L	95	ALA	3.2
1	O	38	PRO	3.2
1	C	131	TYR	3.2
1	H	42	VAL	3.2
1	N	87	PRO	3.2
1	R	87	PRO	3.2
1	S	104	ILE	3.2
1	T	220	ILE	3.2
1	C	218	THR	3.2
1	B	102	GLU	3.2
1	M	65	ALA	3.2
1	G	54	GLY	3.2
1	H	34	ALA	3.2
1	L	90	ALA	3.2
1	T	8	SER	3.2
1	T	101	ALA	3.2
1	N	105	PRO	3.2
1	R	22	LEU	3.2
1	N	20	PHE	3.2
1	N	55	ARG	3.2
1	I	53	GLN	3.2
1	L	61	MET	3.2
1	C	207	PHE	3.2
1	N	3	LEU	3.2
1	N	22	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	104	ILE	3.1
1	C	36	LYS	3.1
1	K	217	ARG	3.1
1	L	14	LYS	3.1
1	M	35	GLY	3.1
1	R	139	GLY	3.1
1	D	22	LEU	3.1
1	H	50	MET	3.1
1	S	135	ILE	3.1
1	H	66	GLU	3.1
1	J	218	THR	3.1
1	R	185	THR	3.1
1	I	52	GLY	3.1
1	C	75	LEU	3.1
1	K	53	GLN	3.1
1	M	186	LEU	3.1
1	N	7	THR	3.1
1	N	104	ILE	3.1
1	L	77	SER	3.0
1	N	196	SER	3.0
1	A	50	MET	3.0
1	H	56	LEU	3.0
1	M	98	MET	3.0
1	L	38	PRO	3.0
1	J	217	ARG	3.0
1	G	53	GLN	3.0
1	G	159	GLN	3.0
1	N	45	GLN	3.0
1	N	186	LEU	3.0
1	L	162	VAL	3.0
1	N	93	LEU	3.0
1	O	56	LEU	3.0
1	N	102	GLU	3.0
1	M	1	HIS	3.0
1	R	165	ALA	3.0
1	M	158	PRO	3.0
1	N	70	ASN	3.0
1	N	107	LEU	3.0
1	R	31	ILE	3.0
1	K	211	TRP	3.0
1	L	158	PRO	3.0
1	M	38	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	S	44	PRO	3.0
1	D	74	LYS	3.0
1	K	214	ALA	2.9
1	M	123	ALA	2.9
1	N	14	LYS	2.9
1	N	73	LEU	2.9
1	G	17	SER	2.9
1	S	98	MET	2.9
1	L	60	VAL	2.9
1	D	213	GLY	2.9
1	M	54	GLY	2.9
1	O	22	LEU	2.9
1	C	90	ALA	2.9
1	R	70	ASN	2.9
1	R	74	LYS	2.9
1	D	41	VAL	2.9
1	B	65	ALA	2.9
1	S	212	GLN	2.9
1	H	135	ILE	2.9
1	R	218	THR	2.9
1	L	86	VAL	2.9
1	N	111	VAL	2.9
1	S	60	VAL	2.9
1	Q	202	ALA	2.9
1	M	219	SER	2.8
1	A	41	VAL	2.8
1	L	94	ALA	2.8
1	M	75	LEU	2.8
1	O	31	ILE	2.8
1	R	61	MET	2.8
1	N	37	LYS	2.8
1	H	220	ILE	2.8
1	L	31	ILE	2.8
1	R	63	THR	2.8
1	L	36	LYS	2.8
1	S	88	VAL	2.8
1	L	121	ALA	2.8
1	G	212	GLN	2.8
1	Q	209	GLN	2.8
1	L	6	ASP	2.8
1	S	7	THR	2.8
1	O	164	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	S	188	LEU	2.8
1	N	126	GLU	2.8
1	M	47	HIS	2.8
1	M	214	ALA	2.7
1	O	40	ASP	2.7
1	J	77	SER	2.7
1	N	188	LEU	2.7
1	O	53	GLN	2.7
1	L	35	GLY	2.7
1	M	20	PHE	2.7
1	I	79	ILE	2.7
1	A	35	GLY	2.7
1	M	33	ALA	2.7
1	N	30	SER	2.7
1	E	41	VAL	2.7
1	M	86	VAL	2.7
1	B	220	ILE	2.7
1	N	175	ASP	2.7
1	R	68	MET	2.7
1	L	41	VAL	2.7
1	R	207	PHE	2.7
1	M	118	LEU	2.7
1	O	163	LEU	2.7
1	S	39	LEU	2.7
1	N	112	TYR	2.7
1	M	194	MET	2.7
1	R	51	GLY	2.7
1	N	32	ILE	2.6
1	O	42	VAL	2.6
1	L	71	ASP	2.6
1	G	220	ILE	2.6
1	H	52	GLY	2.6
1	S	52	GLY	2.6
1	M	25	VAL	2.6
1	N	149	LEU	2.6
1	S	167	PHE	2.6
1	T	39	LEU	2.6
1	R	217	ARG	2.6
1	A	102	GLU	2.6
1	L	91	GLU	2.6
1	S	126	GLU	2.6
1	K	8	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	193	GLN	2.6
1	R	58	ALA	2.6
1	L	81	ASP	2.6
1	A	54	GLY	2.6
1	Q	210	ASP	2.6
1	L	106	THR	2.6
1	R	219	SER	2.6
1	M	99	LEU	2.6
1	N	202	ALA	2.6
1	O	179	ALA	2.6
1	T	108	GLY	2.6
1	N	166	SER	2.5
1	K	204	VAL	2.5
1	T	53	GLN	2.5
1	M	112	TYR	2.5
1	J	52	GLY	2.5
1	D	195	ILE	2.5
1	O	16	LEU	2.5
1	P	73	LEU	2.5
1	M	106	THR	2.5
1	R	32	ILE	2.5
1	T	109	THR	2.5
1	M	3	LEU	2.5
1	S	67	GLY	2.5
1	Q	214	ALA	2.5
1	C	208	GLU	2.5
1	B	100	LYS	2.5
1	M	117	GLY	2.5
1	B	43	LEU	2.5
1	D	53	GLN	2.5
1	I	74	LYS	2.5
1	I	55	ARG	2.5
1	R	198	PRO	2.5
1	M	208	GLU	2.5
1	M	189	ASP	2.5
1	O	6	ASP	2.5
1	R	196	SER	2.5
1	M	121	ALA	2.5
1	N	199	ALA	2.5
1	H	18	ARG	2.5
1	B	47	HIS	2.5
1	L	52	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	159	GLN	2.5
1	C	69	VAL	2.4
1	C	199	ALA	2.4
1	N	205	ALA	2.4
1	E	66	GLU	2.4
1	I	56	LEU	2.4
1	R	188	LEU	2.4
1	N	157	ALA	2.4
1	Q	215	PHE	2.4
1	R	7	THR	2.4
1	L	66	GLU	2.4
1	O	19	ILE	2.4
1	R	56	LEU	2.4
1	S	118	LEU	2.4
1	T	159	GLN	2.4
1	D	24	GLY	2.4
1	S	130	PRO	2.4
1	M	218	THR	2.4
1	I	66	GLU	2.4
1	H	211	TRP	2.4
1	H	159	GLN	2.4
1	M	149	LEU	2.4
1	K	52	GLY	2.4
1	O	213	GLY	2.4
1	R	1	HIS	2.4
1	M	109	THR	2.4
1	N	71	ASP	2.4
1	Q	41	VAL	2.4
1	H	219	SER	2.4
1	N	129	ALA	2.4
1	C	42	VAL	2.4
1	O	106	THR	2.4
1	E	219	SER	2.4
1	S	220	ILE	2.4
1	O	217	ARG	2.4
1	C	103	GLY	2.4
1	H	75	LEU	2.4
1	S	16	LEU	2.4
1	N	68	MET	2.4
1	R	191	ALA	2.4
1	B	20	PHE	2.4
1	M	212	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	177	LEU	2.3
1	S	80	ALA	2.3
1	M	132	VAL	2.3
1	M	156	HIS	2.3
1	O	48	GLU	2.3
1	N	44	PRO	2.3
1	O	197	TYR	2.3
1	K	73	LEU	2.3
1	M	125	ALA	2.3
1	N	58	ALA	2.3
1	N	90	ALA	2.3
1	B	106	THR	2.3
1	R	146	VAL	2.3
1	T	60	VAL	2.3
1	P	66	GLU	2.3
1	H	31	ILE	2.3
1	J	220	ILE	2.3
1	B	56	LEU	2.3
1	E	157	ALA	2.3
1	H	46	LEU	2.3
1	M	122	LEU	2.3
1	N	160	ALA	2.3
1	S	129	ALA	2.3
1	T	50	MET	2.3
1	H	41	VAL	2.3
1	E	51	GLY	2.3
1	O	35	GLY	2.3
1	S	216	GLY	2.3
1	O	32	ILE	2.3
1	L	40	ASP	2.3
1	S	58	ALA	2.3
1	L	64	THR	2.3
1	N	183	SER	2.3
1	P	213	GLY	2.3
1	H	10	VAL	2.3
1	K	13	VAL	2.3
1	M	207	PHE	2.3
1	N	86	VAL	2.3
1	N	204	VAL	2.3
1	N	76	ARG	2.3
1	L	120	SER	2.3
1	T	33	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	59	GLN	2.3
1	C	41	VAL	2.3
1	M	204	VAL	2.3
1	M	36	LYS	2.3
1	O	14	LYS	2.3
1	O	100	LYS	2.3
1	M	104	ILE	2.3
1	R	104	ILE	2.3
1	N	13	VAL	2.2
1	R	193	GLN	2.2
1	B	219	SER	2.2
1	L	16	LEU	2.2
1	A	70	ASN	2.2
1	H	61	MET	2.2
1	M	192	GLN	2.2
1	C	215	PHE	2.2
1	D	218	THR	2.2
1	E	27	THR	2.2
1	B	74	LYS	2.2
1	N	85	LYS	2.2
1	G	214	ALA	2.2
1	M	23	ALA	2.2
1	M	90	ALA	2.2
1	C	206	LYS	2.2
1	M	37	LYS	2.2
1	N	132	VAL	2.2
1	R	42	VAL	2.2
1	E	53	GLN	2.2
1	M	115	ALA	2.2
1	M	30	SER	2.2
1	E	159	GLN	2.2
1	R	205	ALA	2.2
1	R	78	ILE	2.2
1	K	209	GLN	2.2
1	O	20	PHE	2.1
1	T	195	ILE	2.1
1	F	56	LEU	2.1
1	K	93	LEU	2.1
1	M	97	LYS	2.1
1	T	74	LYS	2.1
1	D	51	GLY	2.1
1	R	67	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	182	GLU	2.1
1	R	131	TYR	2.1
1	N	78	ILE	2.1
1	T	212	GLN	2.1
1	B	21	PRO	2.1
1	F	70	ASN	2.1
1	I	70	ASN	2.1
1	P	38	PRO	2.1
1	R	8	SER	2.1
1	M	55	ARG	2.1
1	T	55	ARG	2.1
1	H	88	VAL	2.1
1	N	10	VAL	2.1
1	O	218	THR	2.1
1	L	213	GLY	2.1
1	M	124	GLY	2.1
1	R	79	ILE	2.1
1	S	77	SER	2.1
1	K	36	LYS	2.1
1	A	49	ALA	2.1
1	M	89	THR	2.1
1	H	69	VAL	2.1
1	S	91	GLU	2.1
1	C	8	SER	2.1
1	I	103	GLY	2.1
1	N	52	GLY	2.1
1	O	104	ILE	2.1
1	C	65	ALA	2.1
1	K	69	VAL	2.1
1	O	54	GLY	2.1
1	O	77	SER	2.1
1	O	196	SER	2.1
1	S	112	TYR	2.1
1	B	73	LEU	2.1
1	K	159	GLN	2.1
1	L	39	LEU	2.1
1	M	59	GLN	2.1
1	N	133	ASN	2.1
1	C	49	ALA	2.1
1	O	211	TRP	2.1
1	Q	42	VAL	2.1
1	N	21	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	197	TYR	2.1
1	M	48	GLU	2.0
1	M	56	LEU	2.0
1	E	54	GLY	2.0
1	N	69	VAL	2.0
1	B	93	LEU	2.0
1	C	82	ILE	2.0
1	M	177	LEU	2.0
1	B	66	GLU	2.0
1	E	202	ALA	2.0
1	P	80	ALA	2.0
1	B	44	PRO	2.0
1	K	55	ARG	2.0
1	B	88	VAL	2.0
1	M	60	VAL	2.0
1	N	162	VAL	2.0
1	A	215	PHE	2.0
1	M	66	GLU	2.0
1	D	209	GLN	2.0
1	N	193	GLN	2.0
1	R	212	GLN	2.0
1	S	35	GLY	2.0
1	M	8	SER	2.0
1	R	71	ASP	2.0
1	R	23	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	P2D	B	301	6/7	0.73	0.34	43,46,51,55	0
2	P2D	P	301	6/7	0.80	0.37	41,42,47,50	0
2	P2D	H	301	6/7	0.82	0.30	56,60,62,66	0
2	P2D	G	301	6/7	0.86	0.32	39,50,54,58	0
2	P2D	K	301	6/7	0.89	0.21	41,43,53,57	0

6.5 Other polymers (i)

There are no such residues in this entry.