



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:56 AM UTC

PDB ID : 4S1F / pdb_00004s1f
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:

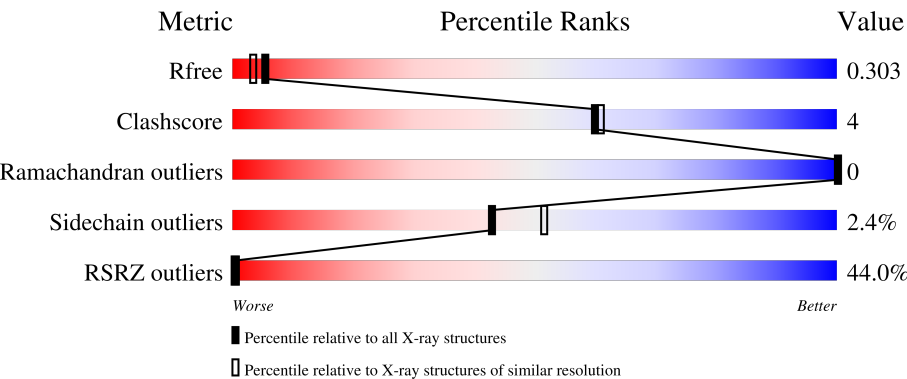
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (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 $\leq 5\%$. 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	27% 87% 9% .
1	B	226	36% 87% 10% .
1	C	226	40% 89% 7% .
1	D	226	25% 90% 6% .
1	E	226	23% 88% 8% ..

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Mol	Chain	Length	Quality of chain
1	F	226	
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	-
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

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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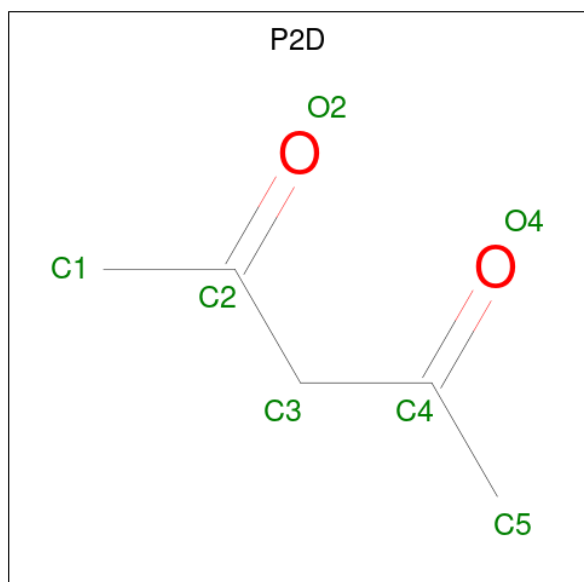
Chain	Residue	Modelled	Actual	Comment	Reference
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K	-1	HIS	-	expression tag	UNP P78055
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K	1	HIS	-	expression tag	UNP P78055
L	-5	MET	-	expression tag	UNP P78055
L	-4	HIS	-	expression tag	UNP P78055
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 (CCD ID: 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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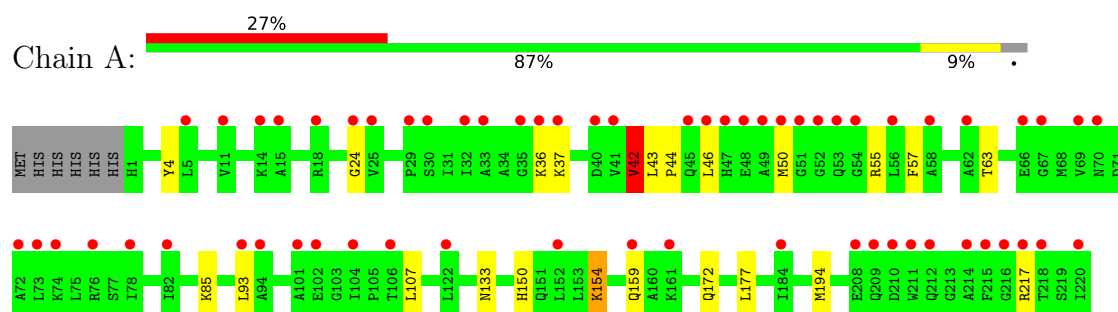
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	33	Total	O	0	0
			33	33		

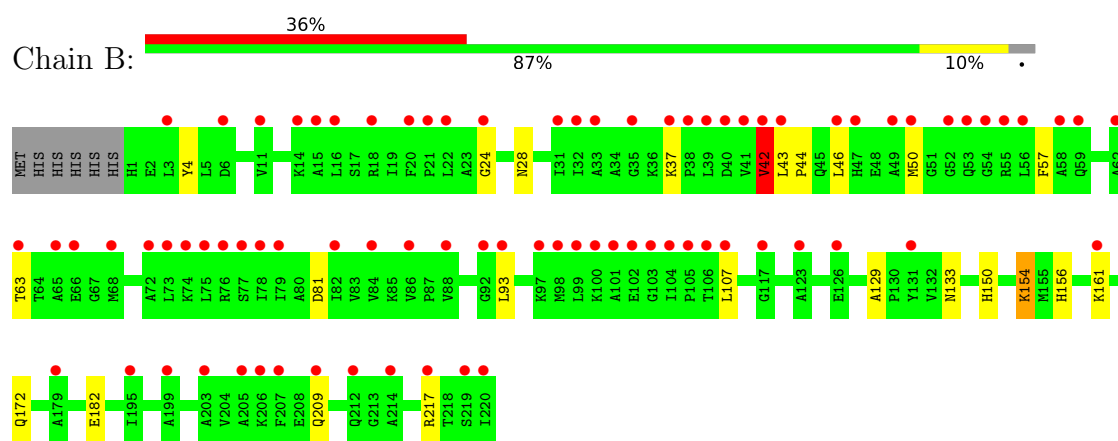
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

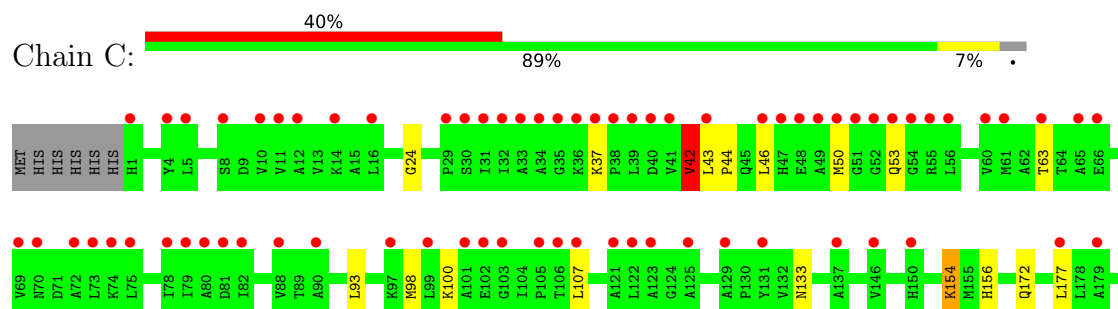
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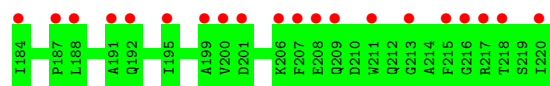


• Molecule 1: Fructose-6-phosphate aldolase 1

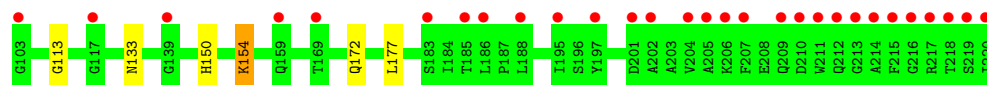
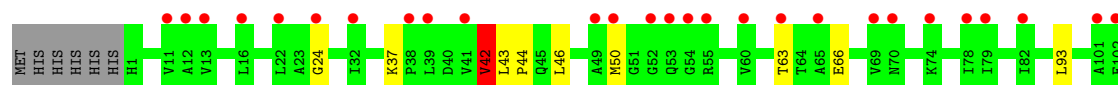
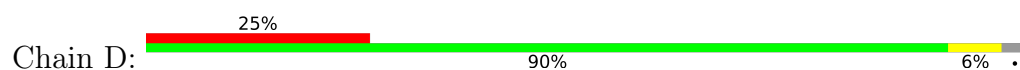


• Molecule 1: Fructose-6-phosphate aldolase 1

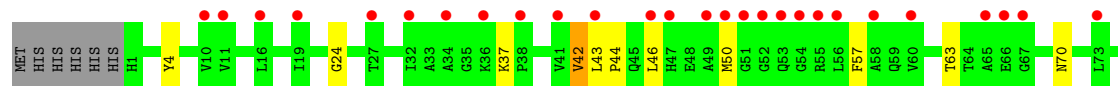
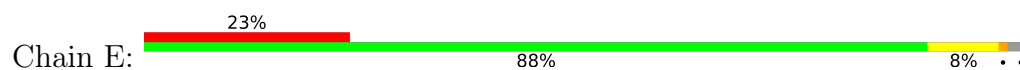




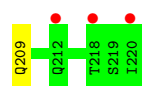
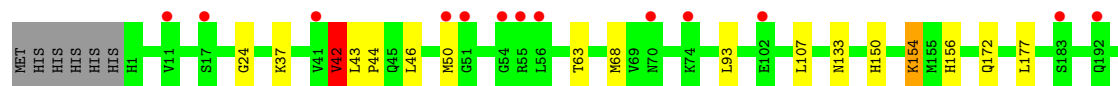
- Molecule 1: Fructose-6-phosphate aldolase 1



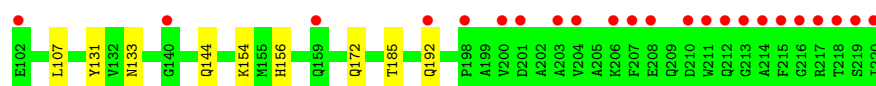
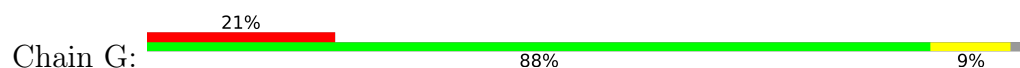
- Molecule 1: Fructose-6-phosphate aldolase 1



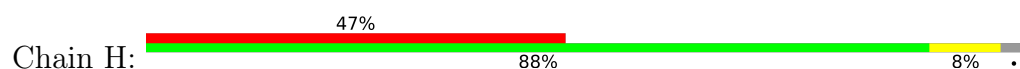
- Molecule 1: Fructose-6-phosphate aldolase 1

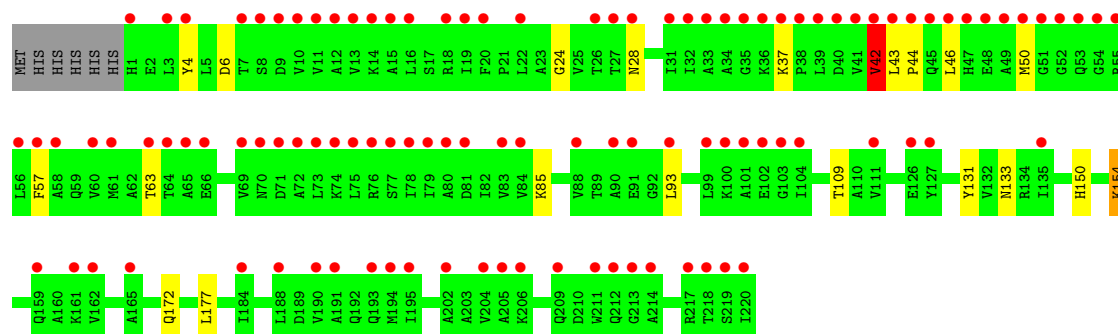


- Molecule 1: Fructose-6-phosphate aldolase 1

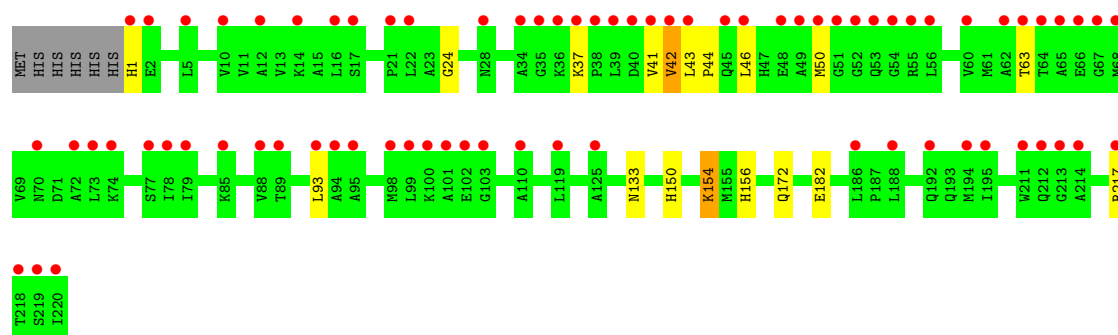
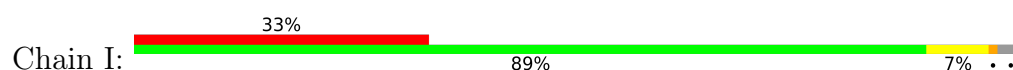


- Molecule 1: Fructose-6-phosphate aldolase 1

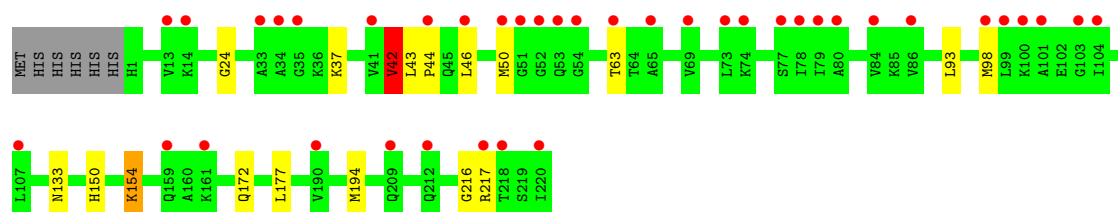
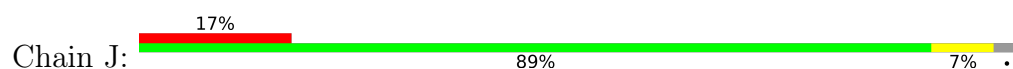




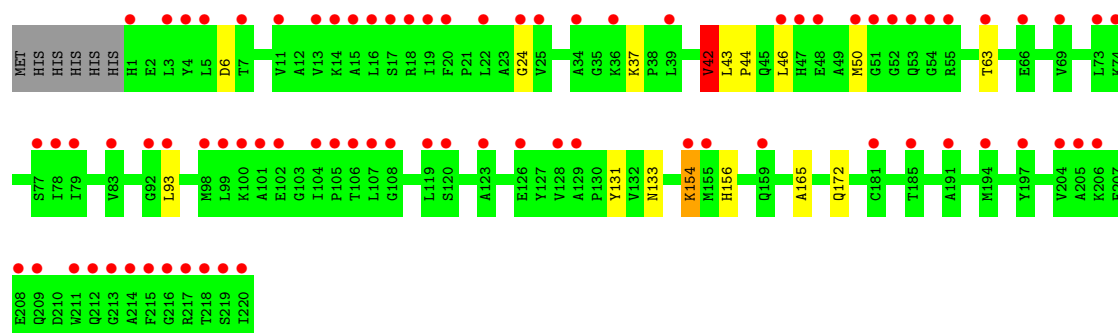
• Molecule 1: Fructose-6-phosphate aldolase 1



• Molecule 1: Fructose-6-phosphate aldolase 1

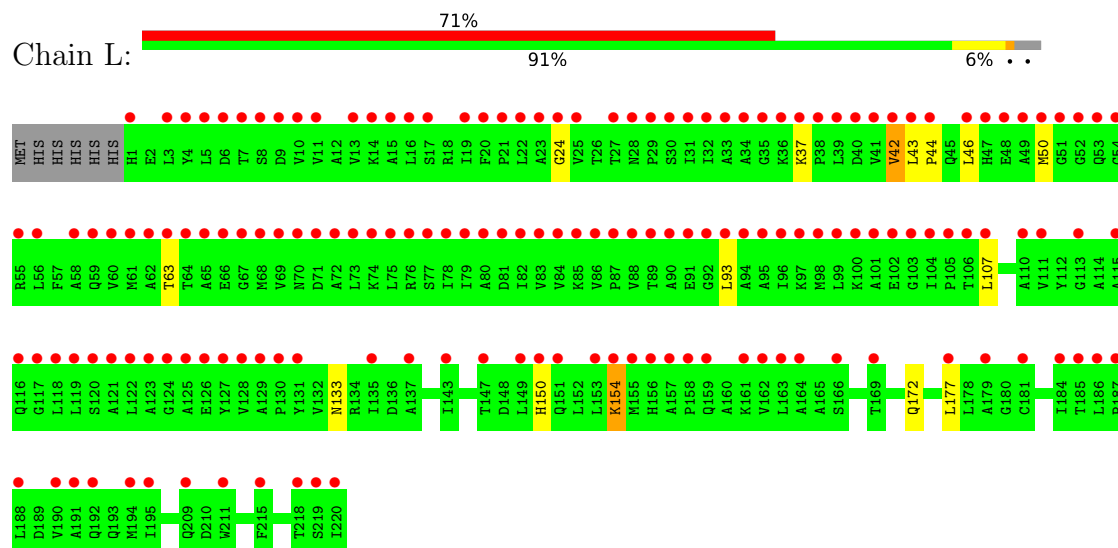


• Molecule 1: Fructose-6-phosphate aldolase 1



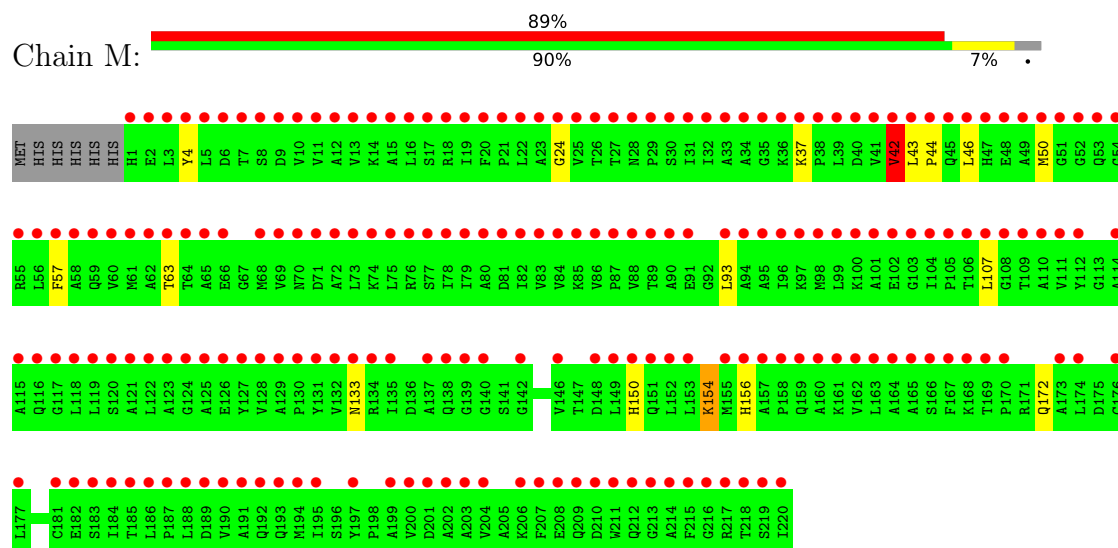
- Molecule 1: Fructose-6-phosphate aldolase 1

Chain L:



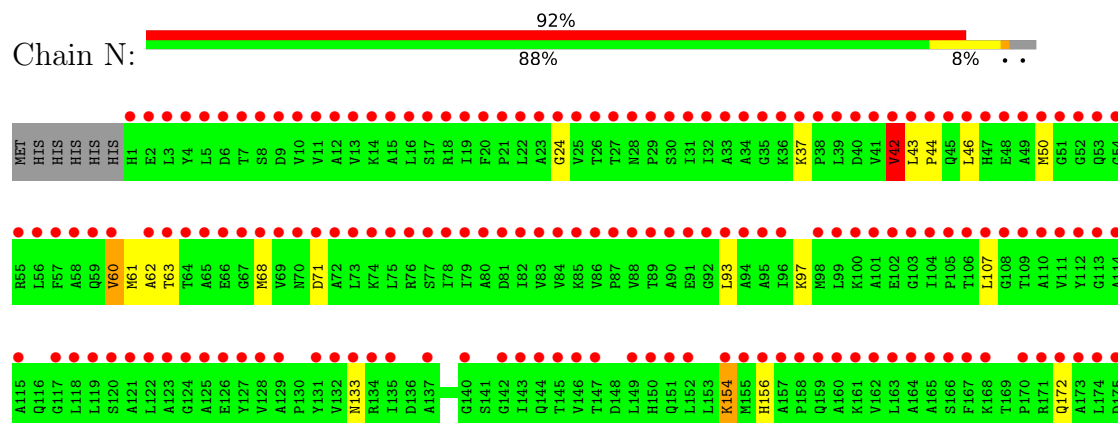
- Molecule 1: Fructose-6-phosphate aldolase 1

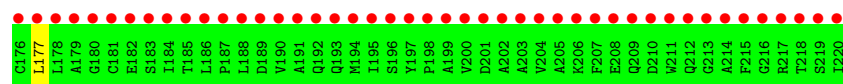
Chain M:



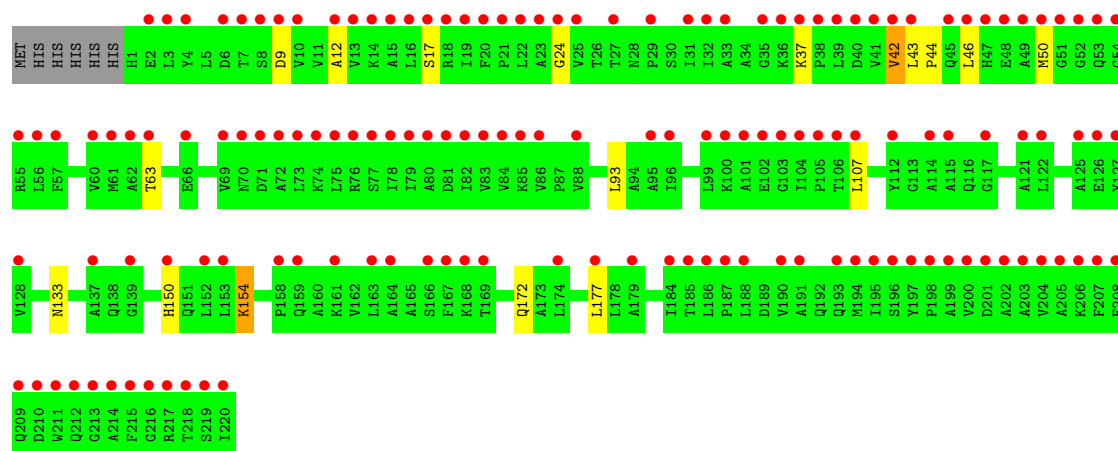
- Molecule 1: Fructose-6-phosphate aldolase 1

Chain N:

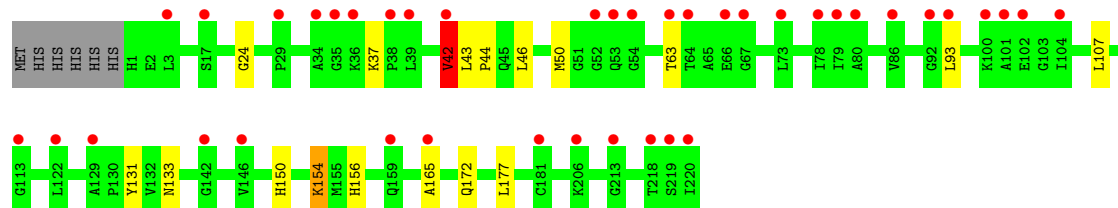
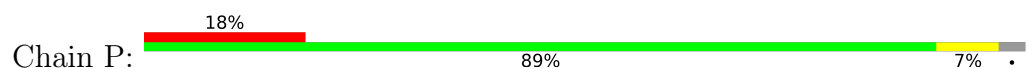




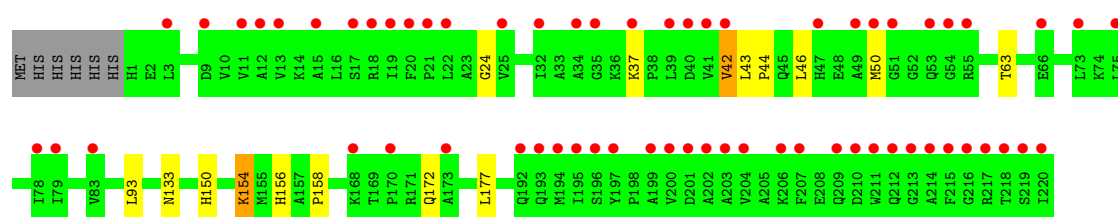
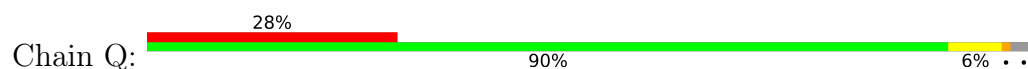
• Molecule 1: Fructose-6-phosphate aldolase 1



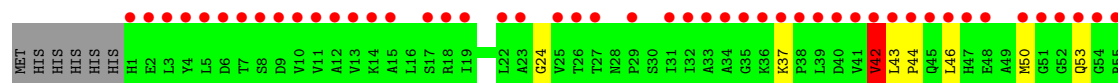
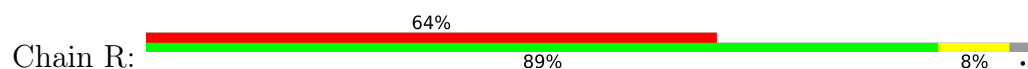
• Molecule 1: Fructose-6-phosphate aldolase 1

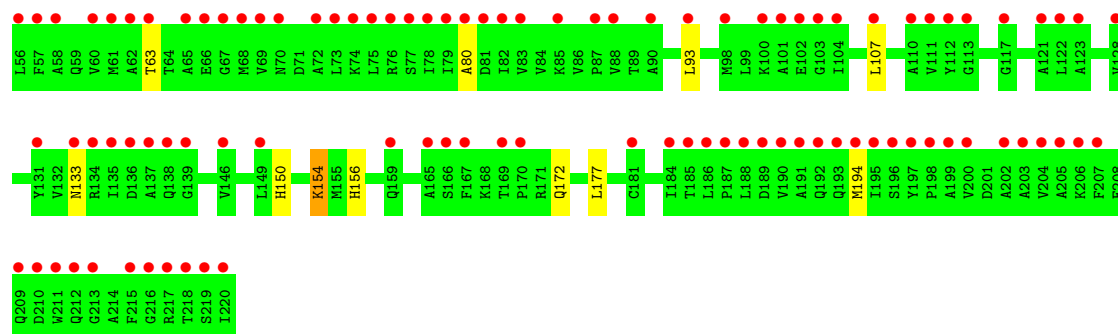


• Molecule 1: Fructose-6-phosphate aldolase 1

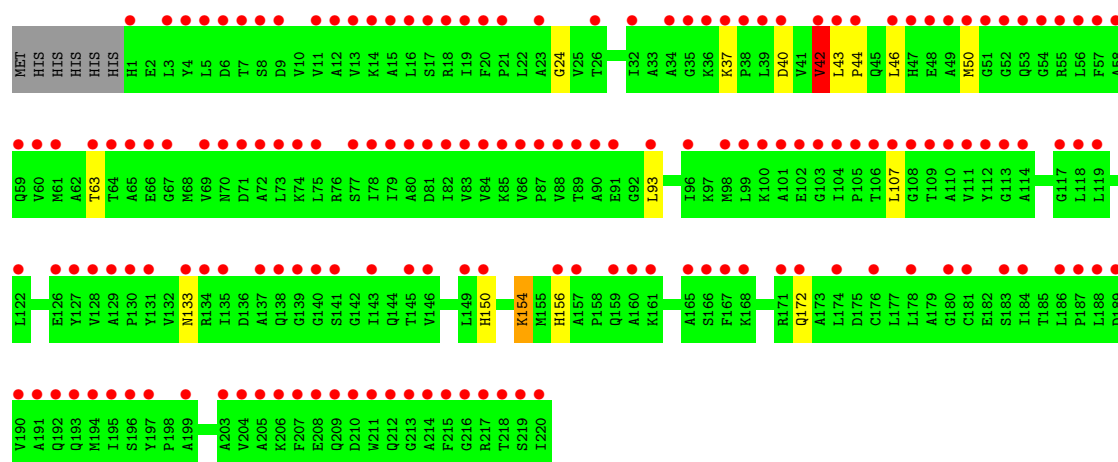
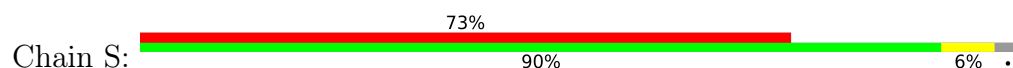


• Molecule 1: Fructose-6-phosphate aldolase 1

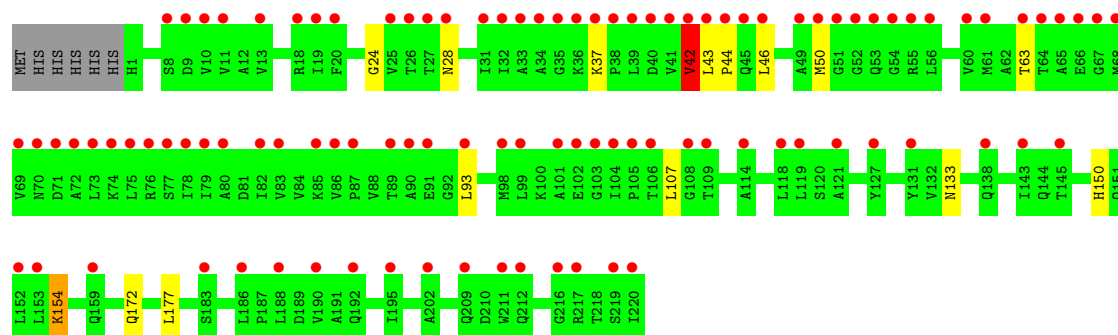
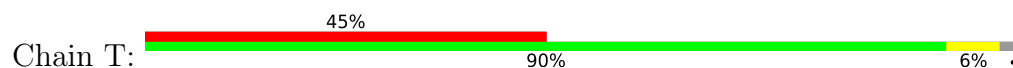




• Molecule 1: Fructose-6-phosphate aldolase 1



• 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 0.277 , 0.303	Depositor DCC
R_{free} test set	11038 reflections (5.03%)	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 , 28.9	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	0.73	0/1641	0.87	1/2232 (0.0%)
1	B	0.77	0/1641	0.88	3/2232 (0.1%)
1	C	0.70	0/1641	0.86	1/2232 (0.0%)
1	D	0.77	0/1641	0.88	2/2232 (0.1%)
1	E	0.75	0/1641	0.90	1/2232 (0.0%)
1	F	0.91	0/1641	0.87	1/2232 (0.0%)
1	G	0.80	0/1641	0.87	1/2232 (0.0%)
1	H	0.67	0/1641	0.86	1/2232 (0.0%)
1	I	0.75	0/1641	0.86	0/2232
1	J	0.84	0/1641	0.88	1/2232 (0.0%)
1	K	0.78	0/1641	0.86	1/2232 (0.0%)
1	L	0.59	0/1641	0.83	0/2232
1	M	0.55	0/1641	0.82	1/2232 (0.0%)
1	N	0.57	0/1641	0.85	2/2232 (0.1%)
1	O	0.65	0/1641	0.82	0/2232
1	P	0.82	0/1641	0.90	1/2232 (0.0%)
1	Q	0.80	0/1641	0.88	0/2232
1	R	0.61	0/1641	0.83	1/2232 (0.0%)
1	S	0.64	1/1641 (0.1%)	0.83	1/2232 (0.0%)
1	T	0.64	0/1641	0.83	1/2232 (0.0%)
All	All	0.72	1/32820 (0.0%)	0.86	20/44640 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	40	ASP	CB-CG	-5.31	1.38	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	GLN	CB-CG-CD	9.56	128.85	112.60
1	N	60	VAL	CB-CA-C	-8.36	102.09	111.45
1	D	66	GLU	CB-CA-C	7.47	123.18	110.79
1	B	161	LYS	CG-CD-CE	6.32	125.84	111.30
1	B	161	LYS	CD-CE-NZ	6.04	131.22	111.90
1	C	42	VAL	CB-CA-C	-5.31	104.97	112.14
1	K	42	VAL	CB-CA-C	-5.30	104.98	112.14
1	T	42	VAL	CB-CA-C	-5.30	104.98	112.14
1	M	42	VAL	CB-CA-C	-5.30	104.98	112.14
1	H	42	VAL	CB-CA-C	-5.28	105.01	112.14
1	P	42	VAL	CB-CA-C	-5.21	105.10	112.14
1	S	42	VAL	CB-CA-C	-5.15	105.19	112.14
1	J	42	VAL	CB-CA-C	-5.14	105.20	112.14
1	B	42	VAL	CB-CA-C	-5.13	105.22	112.14
1	G	42	VAL	CB-CA-C	-5.12	105.23	112.14
1	N	42	VAL	CB-CA-C	-5.11	105.24	112.14
1	F	42	VAL	CB-CA-C	-5.09	105.27	112.14
1	D	42	VAL	CB-CA-C	-5.08	105.29	112.14
1	R	42	VAL	CB-CA-C	-5.05	105.32	112.14
1	A	42	VAL	CB-CA-C	-5.05	105.32	112.14

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	22	0
1	B	1615	0	1671	22	0
1	C	1615	0	1674	13	0
1	D	1615	0	1674	10	0
1	E	1615	0	1674	14	0
1	F	1615	0	1674	14	0
1	G	1615	0	1672	24	0
1	H	1615	0	1672	17	0
1	I	1615	0	1674	14	0
1	J	1615	0	1674	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1615	0	1671	17	0
1	L	1615	0	1674	10	0
1	M	1615	0	1674	12	0
1	N	1615	0	1674	23	0
1	O	1615	0	1674	11	0
1	P	1615	0	1672	20	0
1	Q	1615	0	1674	10	0
1	R	1615	0	1674	20	0
1	S	1615	0	1674	10	0
1	T	1615	0	1674	10	0
2	B	6	0	8	4	0
2	G	6	0	8	10	0
2	H	6	0	8	7	0
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	2	0
3	D	51	0	0	1	0
3	E	63	0	0	2	0
3	F	90	0	0	2	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	1	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	283	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 4.

All (283) 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:F:24:GLY:HA2	1:F:50:MET:HE1	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:131:TYR:CE1	2:P:301:P2D:H8	2.15	0.80
1:A:24:GLY:HA2	1:A:50:MET:HE1	1.64	0.79
1:B:24:GLY:HA2	1:B:50:MET:HE1	1.65	0.79
1:J:24:GLY:HA2	1:J:50:MET:HE1	1.64	0.79
1:I:24:GLY:HA2	1:I:50:MET:HE1	1.65	0.78
1:S:24:GLY:HA2	1:S:50:MET:HE1	1.65	0.78
1:P:50:MET:HE2	3:P:430:HOH:O	1.84	0.78
1:A:217:ARG:CZ	1:R:53:GLN:NE2	2.47	0.78
1:G:24:GLY:HA2	1:G:50:MET:HE1	1.65	0.78
1:P:24:GLY:HA2	1:P:50:MET:HE1	1.65	0.78
1:L:24:GLY:HA2	1:L:50:MET:HE1	1.66	0.77
1:H:24:GLY:HA2	1:H:50:MET:HE1	1.67	0.77
1:R:24:GLY:HA2	1:R:50:MET:HE1	1.67	0.77
1:E:24:GLY:HA2	1:E:50:MET:HE1	1.65	0.77
1:T:24:GLY:HA2	1:T:50:MET:HE1	1.65	0.77
1:C:24:GLY:HA2	1:C:50:MET:HE1	1.67	0.77
1:Q:24:GLY:HA2	1:Q:50:MET:HE1	1.65	0.77
1:N:24:GLY:HA2	1:N:50:MET:HE1	1.66	0.76
1:M:24:GLY:HA2	1:M:50:MET:HE1	1.66	0.76
1:K:24:GLY:HA2	1:K:50:MET:HE1	1.67	0.76
1:D:24:GLY:HA2	1:D:50:MET:HE1	1.67	0.75
1:O:24:GLY:HA2	1:O:50:MET:HE1	1.67	0.73
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: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
1:G:66:GLU:OE1	1:G:66:GLU:C	2.39	0.65
1:F:24:GLY:CA	1:F:50:MET:HE1	2.28	0.64
1:G:28:ASN:ND2	2:G:301:P2D:H7	2.13	0.64
1:J:24:GLY:CA	1:J:50:MET:HE1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:VAL:HG22	1:N:61:MET:N	2.14	0.62
1:C:100:LYS:NZ	3:C:343:HOH:O	2.30	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:P:24:GLY:CA	1:P:50:MET:HE1	2.29	0.61
1:E:24:GLY:CA	1:E:50:MET:HE1	2.30	0.61
1:G:131:TYR:OH	2:G:301:P2D:H6	2.01	0.61
1:A:24:GLY:CA	1:A:50:MET:HE1	2.30	0.60
1:B:24:GLY:CA	1:B:50:MET:HE1	2.30	0.60
1:B:133:ASN:HD22	1:B:172:GLN:HE22	1.50	0.60
1:Q:24:GLY:CA	1:Q:50:MET:HE1	2.32	0.60
1:K:24:GLY:CA	1:K:50:MET:HE1	2.32	0.60
1:M:24:GLY:CA	1:M:50:MET:HE1	2.32	0.60
1:D:150:HIS:CE1	1:D:154:LYS:HD3	2.36	0.59
1:L:24:GLY:CA	1:L:50:MET:HE1	2.32	0.59
1:C:24:GLY:CA	1:C:50:MET:HE1	2.32	0.59
1:S:24:GLY:CA	1:S:50:MET:HE1	2.32	0.59
1:T:24:GLY:CA	1:T:50:MET:HE1	2.32	0.59
1:R:24:GLY:CA	1:R:50:MET:HE1	2.32	0.59
1:G:24:GLY:CA	1:G:50:MET:HE1	2.31	0.59
1:I:24:GLY:CA	1:I:50:MET:HE1	2.32	0.59
1:N:60:VAL:HG22	1:N:62:ALA:H	1.68	0.59
1:H:24:GLY:CA	1:H:50:MET:HE1	2.33	0.58
1:N:24:GLY:CA	1:N:50:MET:HE1	2.32	0.58
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:D:24:GLY:CA	1:D:50:MET:HE1	2.33	0.57
1:O:24:GLY:CA	1:O:50:MET:HE1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:217:ARG:CZ	1:R:53:GLN:CD	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:60:VAL:HG23	1:N:71:ASP:CG	2.42	0.44
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: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:156:HIS:HE1	1:O:177:LEU:O	2.01	0.43
1:F:107:LEU:HD23	1:F:107:LEU:C	2.43	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:A:107:LEU:HD23	1:A:107:LEU:C	2.43	0.42
1:G:66:GLU:OE1	1:G:70:ASN:ND2	2.51	0.42
1:P:150:HIS:NE2	1:P:154:LYS:HD3	2.34	0.42
1:C:107:LEU:C	1:C:107:LEU:HD23	2.44	0.42
1:R:107:LEU:HD23	1:R:107:LEU:C	2.44	0.42
1:N:97:LYS:NZ	1:O:17:SER:O	2.46	0.42
1:S:107:LEU:C	1:S:107:LEU:HD23	2.44	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:L:107:LEU:C	1:L:107:LEU:HD23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:LYS:N	1:A:154:LYS:HD2	2.35	0.41
1:B:107:LEU:C	1:B:107:LEU:HD23	2.45	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:P:107:LEU:C	1:P:107:LEU:HD23	2.45	0.41
1:J:217:ARG:NH2	3:J:311:HOH:O	2.53	0.41
1:K:50:MET:HE2	1:K:50:MET:HB3	1.96	0.41
1:O:150:HIS:NE2	1:O:154:LYS:HD3	2.36	0.41
1:G:107:LEU:HD23	1:G:107:LEU:C	2.45	0.41
1:M:107:LEU:HD23	1:M:107:LEU:C	2.46	0.41
1:N:107:LEU:HD23	1:N:107:LEU:C	2.45	0.41
1:O:107:LEU:C	1:O:107:LEU:HD23	2.46	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
1:B:50:MET:HE2	1:B:50:MET:HB3	1.97	0.40
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:T:107:LEU:C	1:T:107:LEU:HD23	2.46	0.40
1:C:98:MET:HE3	3:D:323:HOH:O	2.21	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:194:MET:HE3	1:R:194:MET:HB2	2.00	0.40
1:A:194:MET:HE3	1:A:194:MET:HB2	1.99	0.40
1:F:68:MET:HE2	3:F:309:HOH:O	2.21	0.40
1:J:194:MET:HE3	1:J:194:MET:HB2	1.98	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
1:E:107:LEU:C	1:E:107:LEU:HD23	2.46	0.40
1:F:50:MET:HE2	1:F:50:MET:HB3	1.96	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
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%)	163 (98%)	4 (2%)	43	51
1	B	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	C	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	D	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	E	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	F	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	G	167/173 (96%)	162 (97%)	5 (3%)	36	43
1	H	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	I	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	J	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	K	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	L	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	M	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	N	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	O	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	P	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	Q	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	R	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	S	167/173 (96%)	163 (98%)	4 (2%)	43	51
1	T	167/173 (96%)	163 (98%)	4 (2%)	43	51
All	All	3340/3460 (96%)	3259 (98%)	81 (2%)	43	51

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	63	THR
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	154	LYS
1	B	42	VAL
1	B	63	THR
1	B	93	LEU
1	B	154	LYS
1	C	42	VAL
1	C	63	THR
1	C	93	LEU
1	C	154	LYS
1	D	42	VAL
1	D	63	THR
1	D	93	LEU
1	D	154	LYS
1	E	42	VAL
1	E	63	THR
1	E	93	LEU
1	E	154	LYS
1	F	42	VAL
1	F	63	THR
1	F	93	LEU
1	F	154	LYS
1	G	42	VAL
1	G	63	THR
1	G	66	GLU
1	G	93	LEU
1	G	154	LYS
1	H	42	VAL
1	H	63	THR
1	H	93	LEU
1	H	154	LYS
1	I	42	VAL
1	I	63	THR
1	I	93	LEU
1	I	154	LYS
1	J	42	VAL
1	J	63	THR
1	J	93	LEU
1	J	154	LYS
1	K	42	VAL
1	K	63	THR
1	K	93	LEU
1	K	154	LYS

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Mol	Chain	Res	Type
1	L	42	VAL
1	L	63	THR
1	L	93	LEU
1	L	154	LYS
1	M	42	VAL
1	M	63	THR
1	M	93	LEU
1	M	154	LYS
1	N	42	VAL
1	N	63	THR
1	N	93	LEU
1	N	154	LYS
1	O	42	VAL
1	O	63	THR
1	O	93	LEU
1	O	154	LYS
1	P	42	VAL
1	P	63	THR
1	P	93	LEU
1	P	154	LYS
1	Q	42	VAL
1	Q	63	THR
1	Q	93	LEU
1	Q	154	LYS
1	R	42	VAL
1	R	63	THR
1	R	93	LEU
1	R	154	LYS
1	S	42	VAL
1	S	63	THR
1	S	93	LEU
1	S	154	LYS
1	T	42	VAL
1	T	63	THR
1	T	93	LEU
1	T	154	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	156	HIS
1	A	192	GLN
1	B	133	ASN
1	B	138	GLN
1	B	150	HIS
1	B	156	HIS
1	B	192	GLN
1	B	212	GLN
1	C	133	ASN
1	C	156	HIS
1	C	192	GLN
1	C	193	GLN
1	D	133	ASN
1	D	138	GLN
1	D	192	GLN
1	E	70	ASN
1	E	133	ASN
1	E	144	GLN
1	E	156	HIS
1	E	193	GLN
1	F	133	ASN
1	F	156	HIS
1	F	192	GLN
1	F	212	GLN
1	G	133	ASN
1	G	144	GLN
1	G	156	HIS
1	G	192	GLN
1	H	133	ASN
1	H	151	GLN
1	H	192	GLN
1	I	133	ASN
1	I	156	HIS
1	I	192	GLN
1	J	133	ASN
1	J	138	GLN
1	J	150	HIS
1	J	156	HIS
1	J	192	GLN
1	J	193	GLN
1	K	133	ASN
1	K	138	GLN

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Mol	Chain	Res	Type
1	K	156	HIS
1	K	192	GLN
1	L	133	ASN
1	L	156	HIS
1	L	192	GLN
1	L	193	GLN
1	M	133	ASN
1	M	138	GLN
1	M	156	HIS
1	M	192	GLN
1	N	133	ASN
1	N	138	GLN
1	N	156	HIS
1	N	192	GLN
1	N	212	GLN
1	O	133	ASN
1	O	138	GLN
1	O	156	HIS
1	O	192	GLN
1	O	212	GLN
1	P	133	ASN
1	P	156	HIS
1	P	192	GLN
1	P	193	GLN
1	Q	133	ASN
1	Q	156	HIS
1	Q	192	GLN
1	Q	193	GLN
1	R	53	GLN
1	R	133	ASN
1	R	156	HIS
1	R	192	GLN
1	S	133	ASN
1	S	156	HIS
1	S	192	GLN
1	T	133	ASN
1	T	138	GLN
1	T	156	HIS
1	T	192	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	P	301	1	5,5,6	1.46	1 (20%)	5,5,7	2.10	2 (40%)
2	P2D	B	301	1	5,5,6	1.81	1 (20%)	5,5,7	1.33	1 (20%)
2	P2D	G	301	1	5,5,6	1.63	1 (20%)	5,5,7	1.82	1 (20%)
2	P2D	H	301	1	5,5,6	1.50	1 (20%)	5,5,7	2.28	3 (60%)
2	P2D	K	301	1	5,5,6	1.83	2 (40%)	5,5,7	1.52	0

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P2D	H	301	1	-	3/3/3/4	-
2	P2D	K	301	1	-	0/3/3/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	P2D	C2-C3	-3.60	1.32	1.51
2	K	301	P2D	C2-C3	-3.53	1.32	1.51
2	G	301	P2D	C2-C3	-3.38	1.33	1.51
2	H	301	P2D	C2-C3	-3.32	1.34	1.51
2	P	301	P2D	C2-C3	-2.85	1.36	1.51
2	K	301	P2D	C3-C4	-2.03	1.44	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	301	P2D	C1-C2-C3	3.78	128.68	112.69
2	H	301	P2D	C5-C4-C3	3.15	126.44	116.85
2	G	301	P2D	C5-C4-C3	-3.01	107.70	116.85
2	H	301	P2D	C1-C2-C3	2.93	125.08	112.69
2	P	301	P2D	O4-C4-C5	-2.32	115.66	121.48
2	H	301	P2D	O4-C4-C5	-2.26	115.82	121.48
2	B	301	P2D	O4-C4-C3	-2.07	115.56	121.47

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	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
2	B	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	P	301	P2D	9	0
2	B	301	P2D	4	0
2	G	301	P2D	10	0
2	H	301	P2D	7	0
2	K	301	P2D	8	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%)	1.52	61 (27%) 1 1	18, 34, 60, 87	0
1	B	220/226 (97%)	1.66	81 (36%) 1 0	17, 36, 57, 79	0
1	C	220/226 (97%)	1.95	91 (41%) 0 0	21, 41, 69, 92	0
1	D	220/226 (97%)	1.47	56 (25%) 1 1	18, 31, 66, 86	0
1	E	220/226 (97%)	1.34	52 (23%) 2 1	16, 32, 52, 82	0
1	F	220/226 (97%)	0.82	16 (7%) 21 19	15, 26, 46, 65	0
1	G	220/226 (97%)	1.32	47 (21%) 2 2	16, 31, 63, 84	0
1	H	220/226 (97%)	2.08	107 (48%) 0 0	21, 42, 68, 96	0
1	I	220/226 (97%)	1.68	75 (34%) 1 0	19, 37, 60, 82	0
1	J	220/226 (97%)	1.09	39 (17%) 4 3	14, 27, 50, 59	0
1	K	220/226 (97%)	1.78	79 (35%) 1 0	19, 39, 64, 89	0
1	L	220/226 (97%)	3.04	160 (72%) 0 0	26, 54, 95, 119	0
1	M	220/226 (97%)	3.96	201 (91%) 0 0	38, 70, 102, 115	0
1	N	220/226 (97%)	4.00	209 (95%) 0 0	37, 68, 100, 119	0
1	O	220/226 (97%)	2.64	146 (66%) 0 0	27, 49, 87, 109	0
1	P	220/226 (97%)	1.20	40 (18%) 3 2	19, 28, 48, 55	0
1	Q	220/226 (97%)	1.51	63 (28%) 1 1	15, 33, 69, 104	0
1	R	220/226 (97%)	2.71	145 (65%) 0 0	26, 52, 73, 91	0
1	S	220/226 (97%)	2.77	166 (75%) 0 0	29, 48, 71, 96	0
1	T	220/226 (97%)	2.09	101 (45%) 0 0	25, 43, 73, 93	0
All	All	4400/4520 (97%)	2.03	1935 (43%) 0 0	14, 40, 80, 119	0

All (1935) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	19	ILE	10.1
1	M	88	VAL	10.0
1	M	83	VAL	9.9
1	I	51	GLY	8.6
1	N	23	ALA	8.2
1	N	195	ILE	8.1
1	S	63	THR	8.1
1	M	72	ALA	8.1
1	K	216	GLY	8.0
1	M	10	VAL	7.9
1	N	79	ILE	7.9
1	N	165	ALA	7.9
1	L	99	LEU	7.9
1	N	82	ILE	7.7
1	R	10	VAL	7.7
1	D	216	GLY	7.6
1	O	101	ALA	7.6
1	L	75	LEU	7.6
1	L	93	LEU	7.6
1	N	46	LEU	7.6
1	N	56	LEU	7.6
1	D	215	PHE	7.5
1	M	215	PHE	7.3
1	N	103	GLY	7.3
1	M	16	LEU	7.2
1	O	202	ALA	7.2
1	N	1	HIS	7.1
1	L	127	TYR	7.1
1	M	32	ILE	7.1
1	N	109	THR	7.1
1	M	20	PHE	7.1
1	G	215	PHE	7.0
1	N	167	PHE	7.0
1	L	119	LEU	7.0
1	Q	220	ILE	7.0
1	O	207	PHE	7.0
1	N	16	LEU	6.9
1	N	41	VAL	6.9
1	L	84	VAL	6.9
1	M	211	TRP	6.8
1	I	101	ALA	6.8
1	L	123	ALA	6.8
1	N	22	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	Q	218	THR	6.7
1	K	215	PHE	6.7
1	M	52	GLY	6.5
1	O	51	GLY	6.5
1	M	101	ALA	6.4
1	O	219	SER	6.4
1	L	78	ILE	6.4
1	O	220	ILE	6.4
1	M	43	LEU	6.4
1	N	194	MET	6.4
1	T	72	ALA	6.4
1	M	131	TYR	6.4
1	N	74	LYS	6.4
1	N	43	LEU	6.4
1	O	205	ALA	6.3
1	M	53	GLN	6.3
1	L	17	SER	6.3
1	N	214	ALA	6.3
1	M	46	LEU	6.2
1	M	73	LEU	6.2
1	N	73	LEU	6.2
1	M	78	ILE	6.2
1	S	74	LYS	6.2
1	N	93	LEU	6.2
1	C	220	ILE	6.1
1	N	4	TYR	6.1
1	M	75	LEU	6.1
1	R	195	ILE	6.1
1	M	107	LEU	6.1
1	T	44	PRO	6.1
1	S	20	PHE	6.1
1	N	60	VAL	6.1
1	L	104	ILE	6.0
1	D	54	GLY	6.0
1	M	186	LEU	6.0
1	N	19	ILE	6.0
1	N	186	LEU	5.9
1	D	52	GLY	5.9
1	L	90	ALA	5.9
1	M	26	THR	5.9
1	N	80	ALA	5.9
1	R	220	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
1	N	39	LEU	5.8
1	M	84	VAL	5.8
1	R	62	ALA	5.8
1	O	55	ARG	5.8
1	M	15	ALA	5.8
1	M	27	THR	5.8
1	N	220	ILE	5.8
1	N	108	GLY	5.8
1	L	107	LEU	5.8
1	M	80	ALA	5.7
1	M	123	ALA	5.7
1	M	54	GLY	5.7
1	H	56	LEU	5.7
1	N	17	SER	5.7
1	L	83	VAL	5.7
1	H	53	GLN	5.7
1	N	75	LEU	5.7
1	O	39	LEU	5.7
1	N	204	VAL	5.7
1	N	207	PHE	5.7
1	S	50	MET	5.7
1	L	73	LEU	5.7
1	L	125	ALA	5.6
1	N	72	ALA	5.6
1	N	50	MET	5.6
1	M	104	ILE	5.6
1	M	28	ASN	5.6
1	N	42	VAL	5.6
1	N	54	GLY	5.6
1	N	123	ALA	5.5
1	M	93	LEU	5.5
1	C	101	ALA	5.5
1	R	139	GLY	5.5
1	M	11	VAL	5.5
1	O	13	VAL	5.5
1	N	3	LEU	5.5
1	M	100	LYS	5.5
1	T	36	LYS	5.5
1	D	213	GLY	5.5
1	M	87	PRO	5.5
1	M	98	MET	5.5
1	O	46	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	T	78	ILE	5.5
1	G	159	GLN	5.5
1	D	214	ALA	5.4
1	M	44	PRO	5.4
1	H	77	SER	5.4
1	K	52	GLY	5.4
1	L	80	ALA	5.4
1	M	129	ALA	5.4
1	N	102	GLU	5.4
1	L	60	VAL	5.4
1	T	39	LEU	5.3
1	L	126	GLU	5.3
1	N	175	ASP	5.3
1	M	82	ILE	5.3
1	R	51	GLY	5.3
1	I	53	GLN	5.3
1	L	39	LEU	5.3
1	H	39	LEU	5.3
1	M	188	LEU	5.3
1	R	74	LYS	5.3
1	M	220	ILE	5.3
1	N	32	ILE	5.3
1	M	64	THR	5.3
1	N	101	ALA	5.3
1	N	183	SER	5.2
1	M	39	LEU	5.2
1	O	42	VAL	5.2
1	S	219	SER	5.2
1	L	35	GLY	5.2
1	N	105	PRO	5.2
1	N	30	SER	5.2
1	C	51	GLY	5.2
1	L	52	GLY	5.2
1	N	203	ALA	5.2
1	C	39	LEU	5.2
1	M	25	VAL	5.2
1	M	42	VAL	5.2
1	L	53	GLN	5.2
1	N	106	THR	5.2
1	L	5	LEU	5.1
1	K	212	GLN	5.1
1	N	159	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	P	213	GLY	5.1
1	H	50	MET	5.1
1	S	16	LEU	5.1
1	N	25	VAL	5.1
1	N	200	VAL	5.1
1	N	166	SER	5.1
1	G	214	ALA	5.1
1	B	102	GLU	5.1
1	R	69	VAL	5.1
1	M	96	ILE	5.1
1	O	35	GLY	5.1
1	L	63	THR	5.0
1	R	5	LEU	5.0
1	E	41	VAL	5.0
1	M	218	THR	5.0
1	M	56	LEU	5.0
1	R	39	LEU	5.0
1	M	13	VAL	5.0
1	L	43	LEU	5.0
1	M	99	LEU	5.0
1	R	46	LEU	5.0
1	H	40	ASP	5.0
1	O	201	ASP	5.0
1	J	217	ARG	5.0
1	N	86	VAL	5.0
1	L	38	PRO	5.0
1	M	89	THR	5.0
1	N	164	ALA	5.0
1	Q	202	ALA	5.0
1	L	69	VAL	4.9
1	M	159	GLN	4.9
1	T	220	ILE	4.9
1	L	22	LEU	4.9
1	N	33	ALA	4.9
1	N	202	ALA	4.9
1	N	205	ALA	4.9
1	H	66	GLU	4.9
1	I	52	GLY	4.9
1	R	215	PHE	4.9
1	S	207	PHE	4.9
1	M	65	ALA	4.9
1	N	13	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	R	7	THR	4.9
1	N	160	ALA	4.9
1	M	17	SER	4.9
1	N	51	GLY	4.9
1	S	88	VAL	4.9
1	L	62	ALA	4.8
1	R	185	THR	4.8
1	S	220	ILE	4.8
1	L	68	MET	4.8
1	M	207	PHE	4.8
1	N	85	LYS	4.8
1	G	51	GLY	4.8
1	I	54	GLY	4.8
1	Q	216	GLY	4.8
1	R	61	MET	4.8
1	L	82	ILE	4.8
1	M	31	ILE	4.8
1	S	93	LEU	4.8
1	M	158	PRO	4.8
1	S	214	ALA	4.8
1	G	220	ILE	4.7
1	M	70	ASN	4.7
1	R	32	ILE	4.7
1	A	56	LEU	4.7
1	R	38	PRO	4.7
1	N	47	HIS	4.7
1	N	58	ALA	4.7
1	M	41	VAL	4.7
1	N	38	PRO	4.7
1	A	49	ALA	4.7
1	M	14	LYS	4.7
1	M	125	ALA	4.7
1	D	53	GLN	4.7
1	M	86	VAL	4.7
1	L	64	THR	4.7
1	N	104	ILE	4.7
1	N	37	LYS	4.7
1	S	17	SER	4.7
1	C	55	ARG	4.7
1	M	109	THR	4.7
1	B	75	LEU	4.6
1	O	22	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	101	ALA	4.6
1	R	77	SER	4.6
1	R	205	ALA	4.6
1	A	159	GLN	4.6
1	R	1	HIS	4.6
1	R	42	VAL	4.6
1	L	50	MET	4.6
1	N	215	PHE	4.6
1	S	217	ARG	4.6
1	C	199	ALA	4.6
1	K	204	VAL	4.6
1	N	10	VAL	4.6
1	O	16	LEU	4.6
1	N	193	GLN	4.6
1	H	101	ALA	4.6
1	N	70	ASN	4.6
1	N	83	VAL	4.6
1	R	79	ILE	4.6
1	O	215	PHE	4.5
1	C	90	ALA	4.5
1	O	203	ALA	4.5
1	N	197	TYR	4.5
1	N	55	ARG	4.5
1	M	135	ILE	4.5
1	N	96	ILE	4.5
1	E	34	ALA	4.5
1	M	156	HIS	4.5
1	O	48	GLU	4.5
1	N	112	TYR	4.5
1	M	122	LEU	4.5
1	O	54	GLY	4.5
1	L	77	SER	4.5
1	L	101	ALA	4.5
1	L	110	ALA	4.5
1	N	18	ARG	4.5
1	C	36	LYS	4.5
1	N	45	GLN	4.5
1	H	75	LEU	4.5
1	O	56	LEU	4.5
1	D	49	ALA	4.5
1	M	95	ALA	4.5
1	M	106	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	195	ILE	4.4
1	N	11	VAL	4.4
1	O	78	ILE	4.4
1	A	35	GLY	4.4
1	D	24	GLY	4.4
1	M	208	GLU	4.4
1	I	77	SER	4.4
1	M	90	ALA	4.4
1	N	206	LYS	4.4
1	O	179	ALA	4.4
1	O	40	ASP	4.4
1	S	107	LEU	4.4
1	S	101	ALA	4.4
1	S	129	ALA	4.4
1	O	10	VAL	4.4
1	R	11	VAL	4.4
1	C	74	LYS	4.4
1	M	36	LYS	4.4
1	R	50	MET	4.4
1	N	20	PHE	4.4
1	I	218	THR	4.4
1	N	7	THR	4.4
1	R	188	LEU	4.4
1	R	198	PRO	4.4
1	T	217	ARG	4.4
1	R	41	VAL	4.4
1	N	189	ASP	4.4
1	R	207	PHE	4.4
1	N	66	GLU	4.3
1	G	218	THR	4.3
1	M	29	PRO	4.3
1	N	149	LEU	4.3
1	H	31	ILE	4.3
1	L	10	VAL	4.3
1	O	50	MET	4.3
1	L	6	ASP	4.3
1	M	160	ALA	4.3
1	M	1	HIS	4.3
1	T	38	PRO	4.3
1	L	96	ILE	4.3
1	L	42	VAL	4.3
1	L	162	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	O	53	GLN	4.3
1	A	48	GLU	4.3
1	L	121	ALA	4.3
1	Q	215	PHE	4.3
1	Q	217	ARG	4.3
1	S	168	LYS	4.3
1	A	106	THR	4.3
1	M	118	LEU	4.3
1	L	86	VAL	4.3
1	T	69	VAL	4.3
1	O	217	ARG	4.3
1	R	70	ASN	4.3
1	S	102	GLU	4.3
1	L	33	ALA	4.3
1	S	15	ALA	4.3
1	M	130	PRO	4.3
1	N	107	LEU	4.3
1	M	194	MET	4.3
1	M	193	GLN	4.3
1	N	209	GLN	4.3
1	N	52	GLY	4.3
1	S	140	GLY	4.3
1	S	195	ILE	4.3
1	N	161	LYS	4.2
1	L	72	ALA	4.2
1	D	212	GLN	4.2
1	N	53	GLN	4.2
1	B	104	ILE	4.2
1	M	128	VAL	4.2
1	A	94	ALA	4.2
1	H	49	ALA	4.2
1	O	15	ALA	4.2
1	N	99	LEU	4.2
1	L	67	GLY	4.2
1	L	102	GLU	4.2
1	T	79	ILE	4.2
1	M	60	VAL	4.2
1	M	40	ASP	4.2
1	L	15	ALA	4.2
1	M	21	PRO	4.2
1	N	49	ALA	4.2
1	N	122	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	O	3	LEU	4.2
1	N	218	THR	4.2
1	C	52	GLY	4.2
1	K	213	GLY	4.2
1	H	219	SER	4.2
1	M	189	ASP	4.2
1	M	190	VAL	4.2
1	N	81	ASP	4.2
1	O	77	SER	4.2
1	R	204	VAL	4.2
1	G	36	LYS	4.2
1	M	94	ALA	4.2
1	N	199	ALA	4.2
1	T	49	ALA	4.2
1	D	22	LEU	4.2
1	M	124	GLY	4.1
1	Q	51	GLY	4.1
1	T	108	GLY	4.1
1	O	79	ILE	4.1
1	M	219	SER	4.1
1	O	204	VAL	4.1
1	Q	209	GLN	4.1
1	I	38	PRO	4.1
1	S	75	LEU	4.1
1	B	106	THR	4.1
1	M	77	SER	4.1
1	O	6	ASP	4.1
1	Q	219	SER	4.1
1	S	210	ASP	4.1
1	D	41	VAL	4.1
1	L	41	VAL	4.1
1	E	54	GLY	4.1
1	M	216	GLY	4.1
1	N	78	ILE	4.1
1	R	31	ILE	4.1
1	M	50	MET	4.1
1	H	84	VAL	4.1
1	H	111	VAL	4.1
1	S	176	CYS	4.1
1	N	87	PRO	4.1
1	H	34	ALA	4.1
1	M	214	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	56	LEU	4.1
1	R	22	LEU	4.1
1	M	7	THR	4.1
1	M	63	THR	4.1
1	M	127	TYR	4.1
1	S	131	TYR	4.1
1	H	52	GLY	4.1
1	N	24	GLY	4.1
1	S	216	GLY	4.1
1	D	74	LYS	4.1
1	M	97	LYS	4.1
1	N	211	TRP	4.1
1	C	79	ILE	4.1
1	E	219	SER	4.1
1	R	196	SER	4.1
1	H	42	VAL	4.1
1	L	129	ALA	4.0
1	M	22	LEU	4.0
1	M	149	LEU	4.0
1	M	24	GLY	4.0
1	S	54	GLY	4.0
1	H	37	LYS	4.0
1	L	74	LYS	4.0
1	O	206	LYS	4.0
1	M	59	GLN	4.0
1	B	220	ILE	4.0
1	M	111	VAL	4.0
1	T	41	VAL	4.0
1	M	137	ALA	4.0
1	G	216	GLY	4.0
1	J	52	GLY	4.0
1	M	35	GLY	4.0
1	M	57	PHE	4.0
1	A	50	MET	4.0
1	E	159	GLN	4.0
1	O	197	TYR	4.0
1	C	69	VAL	4.0
1	O	38	PRO	4.0
1	O	41	VAL	4.0
1	R	34	ALA	4.0
1	R	199	ALA	4.0
1	T	33	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	R	35	GLY	4.0
1	C	207	PHE	4.0
1	R	40	ASP	4.0
1	N	8	SER	4.0
1	N	170	PRO	4.0
1	N	111	VAL	4.0
1	Q	41	VAL	4.0
1	T	34	ALA	4.0
1	T	43	LEU	4.0
1	T	46	LEU	4.0
1	E	53	GLN	4.0
1	M	116	GLN	4.0
1	T	101	ALA	4.0
1	O	7	THR	4.0
1	N	40	ASP	4.0
1	R	197	TYR	4.0
1	O	19	ILE	4.0
1	R	219	SER	4.0
1	H	14	LYS	3.9
1	L	116	GLN	3.9
1	M	153	LEU	3.9
1	G	35	GLY	3.9
1	L	51	GLY	3.9
1	L	124	GLY	3.9
1	M	33	ALA	3.9
1	Q	213	GLY	3.9
1	N	91	GLU	3.9
1	L	71	ASP	3.9
1	N	196	SER	3.9
1	I	79	ILE	3.9
1	M	61	MET	3.9
1	L	91	GLU	3.9
1	L	49	ALA	3.9
1	S	218	THR	3.9
1	I	70	ASN	3.9
1	N	9	ASP	3.9
1	K	220	ILE	3.9
1	A	53	GLN	3.9
1	C	53	GLN	3.9
1	H	61	MET	3.9
1	Q	211	TRP	3.9
1	S	213	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	L	89	THR	3.9
1	Q	214	ALA	3.9
1	R	58	ALA	3.9
1	S	65	ALA	3.9
1	S	14	LYS	3.9
1	O	70	ASN	3.9
1	T	71	ASP	3.9
1	S	135	ILE	3.9
1	R	131	TYR	3.9
1	T	212	GLN	3.9
1	M	69	VAL	3.9
1	L	37	LYS	3.9
1	T	74	LYS	3.9
1	K	218	THR	3.9
1	M	164	ALA	3.9
1	I	40	ASP	3.8
1	D	219	SER	3.8
1	S	104	ILE	3.8
1	T	159	GLN	3.8
1	L	98	MET	3.8
1	M	68	MET	3.8
1	T	50	MET	3.8
1	C	131	TYR	3.8
1	N	162	VAL	3.8
1	S	86	VAL	3.8
1	T	60	VAL	3.8
1	H	54	GLY	3.8
1	L	118	LEU	3.8
1	M	117	GLY	3.8
1	L	94	ALA	3.8
1	R	202	ALA	3.8
1	N	71	ASP	3.8
1	R	211	TRP	3.8
1	K	53	GLN	3.8
1	S	215	PHE	3.8
1	F	11	VAL	3.8
1	H	41	VAL	3.8
1	G	54	GLY	3.8
1	M	119	LEU	3.8
1	R	56	LEU	3.8
1	N	15	ALA	3.8
1	C	209	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	66	GLU	3.8
1	G	17	SER	3.8
1	N	14	LYS	3.8
1	D	220	ILE	3.8
1	C	46	LEU	3.8
1	I	73	LEU	3.8
1	M	3	LEU	3.8
1	N	142	GLY	3.8
1	R	73	LEU	3.8
1	S	188	LEU	3.8
1	A	15	ALA	3.8
1	N	63	THR	3.8
1	R	218	THR	3.8
1	S	72	ALA	3.8
1	L	159	GLN	3.8
1	M	91	GLU	3.8
1	R	53	GLN	3.8
1	R	192	GLN	3.8
1	I	36	LYS	3.8
1	N	158	PRO	3.8
1	L	55	ARG	3.8
1	C	122	LEU	3.8
1	I	56	LEU	3.8
1	P	73	LEU	3.8
1	G	212	GLN	3.7
1	O	191	ALA	3.7
1	Q	212	GLN	3.7
1	S	12	ALA	3.7
1	T	37	LYS	3.7
1	L	44	PRO	3.7
1	J	220	ILE	3.7
1	R	78	ILE	3.7
1	C	56	LEU	3.7
1	N	190	VAL	3.7
1	N	126	GLU	3.7
1	O	209	GLN	3.7
1	S	100	LYS	3.7
1	S	64	THR	3.7
1	P	80	ALA	3.7
1	L	120	SER	3.7
1	B	74	LYS	3.7
1	C	206	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	67	GLY	3.7
1	K	93	LEU	3.7
1	N	188	LEU	3.7
1	O	14	LYS	3.7
1	O	117	GLY	3.7
1	B	88	VAL	3.7
1	M	192	GLN	3.7
1	N	69	VAL	3.7
1	O	25	VAL	3.7
1	S	126	GLU	3.7
1	K	63	THR	3.7
1	S	7	THR	3.7
1	M	165	ALA	3.7
1	O	214	ALA	3.7
1	R	191	ALA	3.7
1	I	55	ARG	3.7
1	M	18	ARG	3.7
1	M	187	PRO	3.7
1	R	187	PRO	3.7
1	S	21	PRO	3.7
1	O	96	ILE	3.7
1	B	53	GLN	3.7
1	R	103	GLY	3.7
1	O	128	VAL	3.7
1	K	219	SER	3.7
1	O	8	SER	3.7
1	O	196	SER	3.7
1	P	78	ILE	3.6
1	N	92	GLY	3.6
1	N	181	CYS	3.6
1	N	216	GLY	3.6
1	H	16	LEU	3.6
1	M	163	LEU	3.6
1	N	98	MET	3.6
1	L	11	VAL	3.6
1	L	40	ASP	3.6
1	M	55	ARG	3.6
1	N	217	ARG	3.6
1	S	106	THR	3.6
1	M	183	SER	3.6
1	C	215	PHE	3.6
1	O	216	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	R	43	LEU	3.6
1	F	41	VAL	3.6
1	M	162	VAL	3.6
1	M	204	VAL	3.6
1	M	45	GLN	3.6
1	Q	192	GLN	3.6
1	S	59	GLN	3.6
1	T	195	ILE	3.6
1	N	76	ARG	3.6
1	M	108	GLY	3.6
1	N	5	LEU	3.6
1	N	174	LEU	3.6
1	S	73	LEU	3.6
1	T	99	LEU	3.6
1	C	106	THR	3.6
1	H	10	VAL	3.6
1	I	10	VAL	3.6
1	M	146	VAL	3.6
1	N	89	THR	3.6
1	M	37	LYS	3.6
1	M	206	LYS	3.6
1	D	205	ALA	3.6
1	S	87	PRO	3.6
1	M	112	TYR	3.6
1	A	215	PHE	3.6
1	K	54	GLY	3.6
1	N	35	GLY	3.6
1	T	51	GLY	3.6
1	D	70	ASN	3.6
1	E	206	LYS	3.6
1	L	7	THR	3.6
1	L	27	THR	3.6
1	N	64	THR	3.6
1	N	185	THR	3.6
1	E	202	ALA	3.6
1	M	115	ALA	3.6
1	M	191	ALA	3.6
1	S	66	GLU	3.6
1	E	77	SER	3.5
1	H	8	SER	3.5
1	J	77	SER	3.5
1	O	212	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	S	53	GLN	3.5
1	N	31	ILE	3.5
1	S	19	ILE	3.5
1	A	54	GLY	3.5
1	N	163	LEU	3.5
1	M	169	THR	3.5
1	H	48	GLU	3.5
1	N	29	PRO	3.5
1	C	33	ALA	3.5
1	I	49	ALA	3.5
1	M	62	ALA	3.5
1	S	212	GLN	3.5
1	A	220	ILE	3.5
1	L	31	ILE	3.5
1	M	103	GLY	3.5
1	R	216	GLY	3.5
1	Q	207	PHE	3.5
1	S	46	LEU	3.5
1	M	71	ASP	3.5
1	M	201	ASP	3.5
1	D	102	GLU	3.5
1	K	48	GLU	3.5
1	T	109	THR	3.5
1	N	44	PRO	3.5
1	E	11	VAL	3.5
1	H	69	VAL	3.5
1	R	13	VAL	3.5
1	R	217	ARG	3.5
1	G	62	ALA	3.5
1	H	214	ALA	3.5
1	R	194	MET	3.5
1	M	74	LYS	3.5
1	O	127	TYR	3.5
1	H	220	ILE	3.5
1	T	54	GLY	3.5
1	A	102	GLU	3.5
1	L	66	GLU	3.5
1	J	63	THR	3.5
1	N	21	PRO	3.5
1	O	218	THR	3.5
1	A	41	VAL	3.5
1	N	84	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	S	60	VAL	3.5
1	M	23	ALA	3.5
1	Q	50	MET	3.5
1	A	36	LYS	3.5
1	B	206	LYS	3.5
1	O	36	LYS	3.5
1	C	54	GLY	3.5
1	C	103	GLY	3.5
1	S	79	ILE	3.5
1	C	5	LEU	3.5
1	K	66	GLU	3.5
1	L	3	LEU	3.5
1	K	20	PHE	3.5
1	L	61	MET	3.4
1	O	84	VAL	3.4
1	O	121	ALA	3.4
1	S	110	ALA	3.4
1	O	211	TRP	3.4
1	K	217	ARG	3.4
1	S	78	ILE	3.4
1	L	122	LEU	3.4
1	Q	22	LEU	3.4
1	R	107	LEU	3.4
1	S	112	TYR	3.4
1	K	209	GLN	3.4
1	B	100	LYS	3.4
1	L	14	LYS	3.4
1	M	161	LYS	3.4
1	Q	206	LYS	3.4
1	R	37	LYS	3.4
1	S	161	LYS	3.4
1	H	88	VAL	3.4
1	O	69	VAL	3.4
1	T	11	VAL	3.4
1	L	58	ALA	3.4
1	H	102	GLU	3.4
1	D	217	ARG	3.4
1	L	103	GLY	3.4
1	F	56	LEU	3.4
1	K	73	LEU	3.4
1	N	177	LEU	3.4
1	S	211	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	85	LYS	3.4
1	R	44	PRO	3.4
1	B	41	VAL	3.4
1	I	41	VAL	3.4
1	N	88	VAL	3.4
1	K	129	ALA	3.4
1	M	49	ALA	3.4
1	O	164	ALA	3.4
1	H	18	ARG	3.4
1	I	217	ARG	3.4
1	S	171	ARG	3.4
1	N	176	CYS	3.4
1	A	51	GLY	3.4
1	N	212	GLN	3.4
1	H	195	ILE	3.4
1	I	220	ILE	3.4
1	L	100	LYS	3.4
1	M	195	ILE	3.4
1	T	63	THR	3.4
1	S	58	ALA	3.4
1	M	51	GLY	3.4
1	A	70	ASN	3.4
1	I	22	LEU	3.3
1	K	79	ILE	3.3
1	O	82	ILE	3.3
1	S	122	LEU	3.3
1	S	98	MET	3.3
1	C	38	PRO	3.3
1	L	158	PRO	3.3
1	O	20	PHE	3.3
1	T	64	THR	3.3
1	O	126	GLU	3.3
1	P	66	GLU	3.3
1	H	11	VAL	3.3
1	Q	200	VAL	3.3
1	Q	53	GLN	3.3
1	H	43	LEU	3.3
1	O	104	ILE	3.3
1	N	187	PRO	3.3
1	S	130	PRO	3.3
1	N	57	PHE	3.3
1	C	14	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	36	LYS	3.3
1	N	100	LYS	3.3
1	R	146	VAL	3.3
1	S	141	SER	3.3
1	L	95	ALA	3.3
1	M	202	ALA	3.3
1	N	95	ALA	3.3
1	R	165	ALA	3.3
1	E	52	GLY	3.3
1	I	50	MET	3.3
1	M	6	ASP	3.3
1	L	195	ILE	3.3
1	L	105	PRO	3.3
1	R	66	GLU	3.3
1	L	1	HIS	3.3
1	N	27	THR	3.3
1	N	36	LYS	3.3
1	O	37	LYS	3.3
1	B	219	SER	3.3
1	R	17	SER	3.3
1	E	58	ALA	3.3
1	H	90	ALA	3.3
1	L	128	VAL	3.3
1	Q	42	VAL	3.3
1	R	200	VAL	3.3
1	S	49	ALA	3.3
1	S	84	VAL	3.3
1	S	137	ALA	3.3
1	R	9	ASP	3.3
1	M	5	LEU	3.3
1	P	122	LEU	3.3
1	E	78	ILE	3.3
1	O	159	GLN	3.3
1	R	209	GLN	3.3
1	B	77	SER	3.3
1	I	88	VAL	3.3
1	M	34	ALA	3.2
1	N	12	ALA	3.2
1	Q	199	ALA	3.2
1	R	60	VAL	3.3
1	R	90	ALA	3.2
1	Q	54	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	73	LEU	3.2
1	M	152	LEU	3.2
1	M	177	LEU	3.2
1	T	93	LEU	3.2
1	N	184	ILE	3.2
1	S	105	PRO	3.2
1	M	47	HIS	3.2
1	D	211	TRP	3.2
1	H	72	ALA	3.2
1	Q	210	ASP	3.2
1	T	70	ASN	3.2
1	T	91	GLU	3.2
1	A	46	LEU	3.2
1	H	99	LEU	3.2
1	O	163	LEU	3.2
1	H	47	HIS	3.2
1	O	21	PRO	3.2
1	T	19	ILE	3.2
1	A	212	GLN	3.2
1	S	138	GLN	3.2
1	T	53	GLN	3.2
1	L	106	THR	3.2
1	M	173	ALA	3.2
1	N	146	VAL	3.2
1	O	62	ALA	3.2
1	G	37	LYS	3.2
1	K	24	GLY	3.2
1	S	42	VAL	3.2
1	K	36	LYS	3.2
1	S	67	GLY	3.2
1	N	133	ASN	3.2
1	T	85	LYS	3.2
1	O	47	HIS	3.2
1	S	5	LEU	3.2
1	H	38	PRO	3.2
1	M	170	PRO	3.2
1	H	104	ILE	3.2
1	O	106	THR	3.2
1	H	57	PHE	3.2
1	A	214	ALA	3.2
1	I	35	GLY	3.2
1	O	80	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	R	80	ALA	3.2
1	L	4	TYR	3.2
1	N	201	ASP	3.2
1	N	119	LEU	3.2
1	R	104	ILE	3.2
1	K	55	ARG	3.1
1	Q	194	MET	3.2
1	L	97	LYS	3.1
1	S	167	PHE	3.1
1	R	102	GLU	3.1
1	A	210	ASP	3.1
1	G	203	ALA	3.1
1	N	157	ALA	3.1
1	R	189	ASP	3.1
1	S	191	ALA	3.1
1	K	11	VAL	3.1
1	T	25	VAL	3.1
1	R	159	GLN	3.1
1	R	193	GLN	3.1
1	S	119	LEU	3.1
1	M	217	ARG	3.1
1	T	55	ARG	3.1
1	I	66	GLU	3.1
1	M	66	GLU	3.1
1	M	181	CYS	3.1
1	M	30	SER	3.1
1	N	219	SER	3.1
1	H	65	ALA	3.1
1	M	9	ASP	3.1
1	R	54	GLY	3.1
1	S	108	GLY	3.1
1	C	60	VAL	3.1
1	D	204	VAL	3.1
1	Q	204	VAL	3.1
1	S	69	VAL	3.1
1	D	209	GLN	3.1
1	E	46	LEU	3.1
1	H	73	LEU	3.1
1	S	99	LEU	3.1
1	S	118	LEU	3.1
1	D	55	ARG	3.1
1	A	78	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	79	ILE	3.1
1	I	211	TRP	3.1
1	H	1	HIS	3.1
1	B	24	GLY	3.1
1	P	142	GLY	3.1
1	Q	9	ASP	3.1
1	S	180	GLY	3.1
1	D	202	ALA	3.1
1	S	11	VAL	3.1
1	G	22	LEU	3.1
1	H	46	LEU	3.1
1	L	130	PRO	3.1
1	L	187	PRO	3.1
1	R	75	LEU	3.1
1	L	143	ILE	3.1
1	S	89	THR	3.1
1	M	167	PHE	3.1
1	Q	35	GLY	3.1
1	T	103	GLY	3.1
1	H	15	ALA	3.1
1	I	62	ALA	3.1
1	Q	12	ALA	3.1
1	L	87	PRO	3.1
1	M	132	VAL	3.1
1	Q	13	VAL	3.1
1	R	190	VAL	3.1
1	S	13	VAL	3.1
1	S	44	PRO	3.1
1	B	93	LEU	3.1
1	M	174	LEU	3.1
1	T	61	MET	3.1
1	M	184	ILE	3.0
1	T	77	SER	3.0
1	H	45	GLN	3.0
1	B	55	ARG	3.0
1	R	55	ARG	3.0
1	E	65	ALA	3.0
1	J	34	ALA	3.0
1	N	129	ALA	3.0
1	S	203	ALA	3.0
1	C	75	LEU	3.0
1	I	194	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	16	LEU	3.0
1	L	163	LEU	3.0
1	C	32	ILE	3.0
1	L	79	ILE	3.0
1	N	143	ILE	3.0
1	D	218	THR	3.0
1	O	18	ARG	3.0
1	A	216	GLY	3.0
1	B	52	GLY	3.0
1	L	54	GLY	3.0
1	S	113	GLY	3.0
1	E	50	MET	3.0
1	I	34	ALA	3.0
1	N	110	ALA	3.0
1	O	158	PRO	3.0
1	O	187	PRO	3.0
1	S	61	MET	3.0
1	C	102	GLU	3.0
1	T	86	VAL	3.0
1	Q	78	ILE	3.0
1	R	135	ILE	3.0
1	H	212	GLN	3.0
1	L	161	LYS	3.0
1	N	168	LYS	3.0
1	A	52	GLY	3.0
1	G	211	TRP	3.0
1	K	211	TRP	3.0
1	L	92	GLY	3.0
1	M	210	ASP	3.0
1	N	213	GLY	3.0
1	O	213	GLY	3.0
1	D	50	MET	3.0
1	B	72	ALA	3.0
1	L	157	ALA	3.0
1	R	33	ALA	3.0
1	N	178	LEU	3.0
1	B	195	ILE	3.0
1	H	74	LYS	3.0
1	H	159	GLN	3.0
1	I	78	ILE	3.0
1	J	159	GLN	3.0
1	L	32	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	217	ARG	3.0
1	N	192	GLN	3.0
1	S	192	GLN	3.0
1	Q	17	SER	3.0
1	P	35	GLY	3.0
1	J	50	MET	3.0
1	R	68	MET	3.0
1	Q	66	GLU	3.0
1	N	198	PRO	3.0
1	B	199	ALA	2.9
1	E	157	ALA	2.9
1	Q	49	ALA	2.9
1	E	73	LEU	2.9
1	R	3	LEU	2.9
1	R	186	LEU	2.9
1	S	39	LEU	2.9
1	I	42	VAL	2.9
1	L	88	VAL	2.9
1	L	111	VAL	2.9
1	R	181	CYS	2.9
1	S	1	HIS	2.9
1	S	111	VAL	2.9
1	T	42	VAL	2.9
1	O	74	LYS	2.9
1	M	120	SER	2.9
1	T	8	SER	2.9
1	A	66	GLU	2.9
1	F	70	ASN	2.9
1	G	213	GLY	2.9
1	N	182	GLU	2.9
1	R	48	GLU	2.9
1	R	117	GLY	2.9
1	B	62	ALA	2.9
1	I	12	ALA	2.9
1	M	114	ALA	2.9
1	P	39	LEU	2.9
1	B	37	LYS	2.9
1	E	97	LYS	2.9
1	H	190	VAL	2.9
1	I	60	VAL	2.9
1	B	31	ILE	2.9
1	C	201	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	183	SER	2.9
1	N	127	TYR	2.9
1	N	131	TYR	2.9
1	N	155	MET	2.9
1	O	4	TYR	2.9
1	S	91	GLU	2.9
1	C	216	GLY	2.9
1	E	117	GLY	2.9
1	H	35	GLY	2.9
1	K	92	GLY	2.9
1	N	6	ASP	2.9
1	M	105	PRO	2.9
1	O	198	PRO	2.9
1	R	87	PRO	2.9
1	E	100	LYS	2.9
1	R	47	HIS	2.9
1	H	211	TRP	2.9
1	I	46	LEU	2.9
1	K	22	LEU	2.9
1	L	188	LEU	2.9
1	N	34	ALA	2.9
1	R	12	ALA	2.9
1	T	152	LEU	2.9
1	A	209	GLN	2.9
1	N	144	GLN	2.9
1	P	159	GLN	2.9
1	D	60	VAL	2.9
1	H	78	ILE	2.9
1	H	184	ILE	2.9
1	O	31	ILE	2.9
1	T	104	ILE	2.9
1	C	63	THR	2.9
1	K	185	THR	2.9
1	G	40	ASP	2.9
1	M	139	GLY	2.9
1	C	37	LYS	2.9
1	C	34	ALA	2.9
1	I	95	ALA	2.9
1	I	125	ALA	2.9
1	J	73	LEU	2.9
1	K	34	ALA	2.9
1	M	110	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	20	PHE	2.9
1	R	72	ALA	2.9
1	C	10	VAL	2.9
1	N	128	VAL	2.9
1	G	48	GLU	2.9
1	M	126	GLU	2.9
1	T	102	GLU	2.9
1	J	104	ILE	2.9
1	R	19	ILE	2.9
1	S	96	ILE	2.9
1	B	6	ASP	2.9
1	G	140	GLY	2.8
1	H	36	LYS	2.8
1	K	51	GLY	2.8
1	O	52	GLY	2.8
1	R	67	GLY	2.8
1	M	4	TYR	2.8
1	I	45	GLN	2.8
1	K	159	GLN	2.8
1	M	212	GLN	2.8
1	H	22	LEU	2.8
1	E	101	ALA	2.8
1	O	72	ALA	2.8
1	Q	15	ALA	2.8
1	R	57	PHE	2.8
1	S	90	ALA	2.8
1	C	11	VAL	2.8
1	R	2	GLU	2.8
1	L	181	CYS	2.8
1	M	176	CYS	2.8
1	O	195	ILE	2.8
1	T	31	ILE	2.8
1	J	74	LYS	2.8
1	B	217	ARG	2.8
1	C	213	GLY	2.8
1	N	113	GLY	2.8
1	R	213	GLY	2.8
1	S	51	GLY	2.8
1	B	105	PRO	2.8
1	P	38	PRO	2.8
1	C	192	GLN	2.8
1	L	34	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	121	ALA	2.8
1	M	157	ALA	2.8
1	C	50	MET	2.8
1	R	98	MET	2.8
1	I	74	LYS	2.8
1	H	135	ILE	2.8
1	L	185	THR	2.8
1	B	47	HIS	2.8
1	H	213	GLY	2.8
1	J	103	GLY	2.8
1	B	46	LEU	2.8
1	T	118	LEU	2.8
1	H	126	GLU	2.8
1	A	58	ALA	2.8
1	D	101	ALA	2.8
1	M	85	LYS	2.8
1	B	18	ARG	2.8
1	E	195	ILE	2.8
1	L	218	THR	2.8
1	I	103	GLY	2.8
1	I	192	GLN	2.8
1	J	54	GLY	2.8
1	L	192	GLN	2.8
1	L	209	GLN	2.8
1	N	180	GLY	2.8
1	P	219	SER	2.8
1	Q	170	PRO	2.8
1	R	170	PRO	2.8
1	C	107	LEU	2.8
1	L	149	LEU	2.8
1	S	3	LEU	2.8
1	S	149	LEU	2.8
1	S	178	LEU	2.8
1	F	74	LYS	2.8
1	N	68	MET	2.8
1	N	154	LYS	2.8
1	L	65	ALA	2.8
1	T	114	ALA	2.8
1	T	121	ALA	2.8
1	J	13	VAL	2.8
1	S	150	HIS	2.7
1	K	106	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	135	ILE	2.7
1	O	184	ILE	2.7
1	P	53	GLN	2.7
1	R	138	GLN	2.7
1	S	71	ASP	2.7
1	I	219	SER	2.7
1	L	117	GLY	2.7
1	T	67	GLY	2.7
1	H	44	PRO	2.7
1	I	21	PRO	2.7
1	J	14	LYS	2.7
1	B	68	MET	2.7
1	L	153	LEU	2.7
1	O	43	LEU	2.7
1	O	177	LEU	2.7
1	T	68	MET	2.7
1	K	214	ALA	2.7
1	B	207	PHE	2.7
1	D	69	VAL	2.7
1	J	69	VAL	2.7
1	L	150	HIS	2.7
1	I	89	THR	2.7
1	Q	40	ASP	2.7
1	R	26	THR	2.7
1	T	106	THR	2.7
1	B	78	ILE	2.7
1	B	82	ILE	2.7
1	K	19	ILE	2.7
1	L	220	ILE	2.7
1	M	79	ILE	2.7
1	O	139	GLY	2.7
1	L	8	SER	2.7
1	R	8	SER	2.7
1	I	100	LYS	2.7
1	S	181	CYS	2.7
1	I	98	MET	2.7
1	B	73	LEU	2.7
1	O	152	LEU	2.7
1	O	188	LEU	2.7
1	T	76	ARG	2.7
1	T	153	LEU	2.7
1	H	12	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	205	ALA	2.7
1	M	12	ALA	2.7
1	O	49	ALA	2.7
1	M	151	GLN	2.7
1	N	172	GLN	2.7
1	O	45	GLN	2.7
1	O	83	VAL	2.7
1	O	200	VAL	2.7
1	S	128	VAL	2.7
1	T	10	VAL	2.7
1	C	70	ASN	2.7
1	N	26	THR	2.7
1	O	63	THR	2.7
1	R	63	THR	2.7
1	T	9	ASP	2.7
1	B	35	GLY	2.7
1	B	54	GLY	2.7
1	I	195	ILE	2.7
1	N	140	GLY	2.7
1	B	66	GLU	2.7
1	G	219	SER	2.7
1	O	100	LYS	2.7
1	Q	18	ARG	2.7
1	L	177	LEU	2.7
1	O	99	LEU	2.7
1	R	93	LEU	2.7
1	B	15	ALA	2.7
1	B	205	ALA	2.7
1	B	97	LYS	2.7
1	G	208	GLU	2.7
1	H	63	THR	2.7
1	M	81	ASP	2.7
1	T	83	VAL	2.7
1	G	19	ILE	2.7
1	H	19	ILE	2.7
1	H	103	GLY	2.7
1	P	67	GLY	2.7
1	J	44	PRO	2.7
1	K	50	MET	2.7
1	B	22	LEU	2.7
1	B	56	LEU	2.7
1	A	47	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	150	HIS	2.6
1	S	156	HIS	2.6
1	B	65	ALA	2.6
1	N	62	ALA	2.6
1	N	90	ALA	2.6
1	N	121	ALA	2.6
1	R	15	ALA	2.6
1	T	45	GLN	2.6
1	B	14	LYS	2.6
1	L	20	PHE	2.6
1	R	14	LYS	2.6
1	A	208	GLU	2.6
1	B	42	VAL	2.6
1	C	146	VAL	2.6
1	H	83	VAL	2.6
1	E	27	THR	2.6
1	P	218	THR	2.6
1	S	145	THR	2.6
1	T	26	THR	2.6
1	I	213	GLY	2.6
1	N	124	GLY	2.6
1	E	38	PRO	2.6
1	K	18	ARG	2.6
1	P	104	ILE	2.6
1	B	98	MET	2.6
1	S	194	MET	2.6
1	C	99	LEU	2.6
1	Q	73	LEU	2.6
1	S	159	GLN	2.6
1	C	12	ALA	2.6
1	L	179	ALA	2.6
1	S	199	ALA	2.6
1	C	66	GLU	2.6
1	I	102	GLU	2.6
1	M	182	GLU	2.6
1	H	20	PHE	2.6
1	S	40	ASP	2.6
1	S	127	TYR	2.6
1	T	40	ASP	2.6
1	C	41	VAL	2.6
1	G	11	VAL	2.6
1	L	190	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	86	VAL	2.6
1	R	25	VAL	2.6
1	G	67	GLY	2.6
1	M	213	GLY	2.6
1	K	78	ILE	2.6
1	T	105	PRO	2.6
1	O	166	SER	2.6
1	B	16	LEU	2.6
1	I	39	LEU	2.6
1	J	212	GLN	2.6
1	K	16	LEU	2.6
1	O	75	LEU	2.6
1	S	186	LEU	2.6
1	S	206	LYS	2.6
1	M	102	GLU	2.6
1	N	114	ALA	2.6
1	R	23	ALA	2.6
1	R	123	ALA	2.6
1	S	114	ALA	2.6
1	M	76	ARG	2.6
1	D	201	ASP	2.6
1	E	81	ASP	2.6
1	G	207	PHE	2.6
1	O	57	PHE	2.6
1	A	69	VAL	2.6
1	B	50	MET	2.6
1	B	84	VAL	2.6
1	B	131	TYR	2.6
1	H	218	THR	2.6
1	J	218	THR	2.6
1	L	131	TYR	2.6
1	S	184	ILE	2.6
1	H	161	LYS	2.6
1	R	36	LYS	2.6
1	C	43	LEU	2.6
1	D	188	LEU	2.6
1	I	119	LEU	2.6
1	N	48	GLU	2.6
1	N	208	GLU	2.6
1	T	18	ARG	2.6
1	A	72	ALA	2.6
1	C	72	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	90	ALA	2.6
1	P	129	ALA	2.6
1	L	81	ASP	2.6
1	N	28	ASN	2.6
1	D	185	THR	2.6
1	E	51	GLY	2.6
1	E	213	GLY	2.6
1	M	142	GLY	2.6
1	N	67	GLY	2.6
1	N	147	THR	2.6
1	S	52	GLY	2.6
1	D	11	VAL	2.6
1	J	84	VAL	2.6
1	R	88	VAL	2.6
1	T	190	VAL	2.6
1	A	184	ILE	2.6
1	C	78	ILE	2.6
1	E	220	ILE	2.6
1	M	8	SER	2.6
1	Q	19	ILE	2.6
1	R	184	ILE	2.6
1	T	127	TYR	2.6
1	C	1	HIS	2.6
1	C	47	HIS	2.6
1	G	206	LYS	2.6
1	B	209	GLN	2.5
1	I	212	GLN	2.5
1	K	119	LEU	2.5
1	P	102	GLU	2.5
1	C	191	ALA	2.5
1	N	94	ALA	2.5
1	H	70	ASN	2.5
1	D	169	THR	2.5
1	F	54	GLY	2.5
1	J	35	GLY	2.5
1	L	29	PRO	2.5
1	M	38	PRO	2.5
1	O	167	PHE	2.5
1	I	14	LYS	2.5
1	J	190	VAL	2.5
1	S	47	HIS	2.5
1	H	193	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	76	ARG	2.5
1	S	43	LEU	2.5
1	K	98	MET	2.5
1	B	123	ALA	2.5
1	E	49	ALA	2.5
1	N	125	ALA	2.5
1	N	179	ALA	2.5
1	O	199	ALA	2.5
1	R	65	ALA	2.5
1	R	121	ALA	2.5
1	L	24	GLY	2.5
1	R	85	LYS	2.5
1	S	117	GLY	2.5
1	T	87	PRO	2.5
1	H	27	THR	2.5
1	K	1	HIS	2.5
1	N	156	HIS	2.5
1	O	27	THR	2.5
1	L	215	PHE	2.5
1	C	200	VAL	2.5
1	K	13	VAL	2.5
1	P	86	VAL	2.5
1	S	83	VAL	2.5
1	T	183	SER	2.5
1	C	184	ILE	2.5
1	D	78	ILE	2.5
1	R	82	ILE	2.5
1	E	55	ARG	2.5
1	H	127	TYR	2.5
1	G	50	MET	2.5
1	O	61	MET	2.5
1	H	28	ASN	2.5
1	K	14	LYS	2.5
1	M	203	ALA	2.5
1	N	65	ALA	2.5
1	N	173	ALA	2.5
1	P	34	ALA	2.5
1	Q	168	LYS	2.5
1	S	85	LYS	2.5
1	C	105	PRO	2.5
1	L	21	PRO	2.5
1	M	150	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	209	GLN	2.5
1	M	209	GLN	2.5
1	O	185	THR	2.5
1	R	45	GLN	2.5
1	B	20	PHE	2.5
1	A	211	TRP	2.5
1	L	25	VAL	2.5
1	N	132	VAL	2.5
1	Q	11	VAL	2.5
1	S	196	SER	2.5
1	S	18	ARG	2.5
1	T	66	GLU	2.5
1	H	4	TYR	2.5
1	T	131	TYR	2.5
1	B	43	LEU	2.5
1	D	186	LEU	2.5
1	I	5	LEU	2.5
1	I	28	ASN	2.5
1	O	9	ASP	2.5
1	S	189	ASP	2.5
1	B	203	ALA	2.5
1	L	164	ALA	2.5
1	O	12	ALA	2.5
1	T	65	ALA	2.5
1	A	24	GLY	2.5
1	A	67	GLY	2.5
1	D	117	GLY	2.5
1	S	103	GLY	2.5
1	C	218	THR	2.4
1	E	102	GLU	2.4
1	S	134	ARG	2.4
1	A	11	VAL	2.4
1	E	10	VAL	2.4
1	E	79	ILE	2.4
1	G	200	VAL	2.4
1	H	32	ILE	2.4
1	H	162	VAL	2.4
1	N	135	ILE	2.4
1	O	190	VAL	2.4
1	T	20	PHE	2.4
1	P	220	ILE	2.4
1	T	82	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	2.4
1	E	16	LEU	2.4
1	R	122	LEU	2.4
1	D	210	ASP	2.4
1	H	81	ASP	2.4
1	L	59	GLN	2.4
1	B	103	GLY	2.4
1	B	117	GLY	2.4
1	K	108	GLY	2.4
1	N	171	ARG	2.4
1	O	66	GLU	2.4
1	O	103	GLY	2.4
1	S	55	ARG	2.4
1	S	208	GLU	2.4
1	T	35	GLY	2.4
1	T	216	GLY	2.4
1	L	147	THR	2.4
1	M	185	THR	2.4
1	T	89	THR	2.4
1	K	181	CYS	2.4
1	N	77	SER	2.4
1	C	82	ILE	2.4
1	D	79	ILE	2.4
1	G	204	VAL	2.4
1	H	60	VAL	2.4
1	T	143	ILE	2.4
1	C	16	LEU	2.4
1	I	93	LEU	2.4
1	K	46	LEU	2.4
1	O	174	LEU	2.4
1	P	3	LEU	2.4
1	K	4	TYR	2.4
1	E	47	HIS	2.4
1	H	76	ARG	2.4
1	S	81	ASP	2.4
1	S	209	GLN	2.4
1	F	102	GLU	2.4
1	B	214	ALA	2.4
1	C	65	ALA	2.4
1	H	33	ALA	2.4
1	H	51	GLY	2.4
1	H	58	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	80	ALA	2.4
1	H	191	ALA	2.4
1	M	58	ALA	2.4
1	O	115	ALA	2.4
1	S	139	GLY	2.4
1	H	64	THR	2.4
1	R	27	THR	2.4
1	K	69	VAL	2.4
1	L	184	ILE	2.4
1	R	206	LYS	2.4
1	S	82	ILE	2.4
1	A	73	LEU	2.4
1	B	99	LEU	2.4
1	L	46	LEU	2.4
1	O	73	LEU	2.4
1	L	211	TRP	2.4
1	G	192	GLN	2.4
1	Q	197	TYR	2.4
1	C	40	ASP	2.4
1	L	70	ASN	2.4
1	O	81	ASP	2.4
1	S	70	ASN	2.4
1	B	92	GLY	2.4
1	C	49	ALA	2.4
1	E	67	GLY	2.4
1	J	51	GLY	2.4
1	L	115	ALA	2.4
1	O	24	GLY	2.4
1	P	92	GLY	2.4
1	Q	203	ALA	2.4
1	I	63	THR	2.4
1	S	36	LYS	2.4
1	B	11	VAL	2.4
1	B	79	ILE	2.4
1	K	128	VAL	2.4
1	P	146	VAL	2.4
1	R	128	VAL	2.4
1	R	167	PHE	2.4
1	E	43	LEU	2.4
1	H	188	LEU	2.4
1	N	118	LEU	2.4
1	S	174	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	217	ARG	2.4
1	R	134	ARG	2.4
1	C	4	TYR	2.3
1	H	9	ASP	2.3
1	N	210	ASP	2.3
1	R	133	ASN	2.3
1	S	197	TYR	2.3
1	A	14	LYS	2.3
1	A	62	ALA	2.3
1	N	115	ALA	2.3
1	P	36	LYS	2.3
1	R	203	ALA	2.3
1	D	63	THR	2.3
1	H	7	THR	2.3
1	S	109	THR	2.3
1	K	120	SER	2.3
1	L	155	MET	2.3
1	Q	79	ILE	2.3
1	L	76	ARG	2.3
1	J	99	LEU	2.3
1	K	5	LEU	2.3
1	O	193	GLN	2.3
1	R	212	GLN	2.3
1	T	138	GLN	2.3
1	K	206	LYS	2.3
1	M	197	TYR	2.3
1	Q	21	PRO	2.3
1	D	139	GLY	2.3
1	N	117	GLY	2.3
1	R	113	GLY	2.3
1	H	165	ALA	2.3
1	I	65	ALA	2.3
1	S	80	ALA	2.3
1	S	160	ALA	2.3
1	T	80	ALA	2.3
1	K	77	SER	2.3
1	K	194	MET	2.3
1	L	166	SER	2.3
1	P	17	SER	2.3
1	R	166	SER	2.3
1	S	8	SER	2.3
1	S	183	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	55	ARG	2.3
1	J	78	ILE	2.3
1	K	104	ILE	2.3
1	M	200	VAL	2.3
1	N	150	HIS	2.3
1	S	32	ILE	2.3
1	D	13	VAL	2.3
1	D	207	PHE	2.3
1	G	2	GLU	2.3
1	J	53	GLN	2.3
1	Q	193	GLN	2.3
1	S	48	GLU	2.3
1	K	99	LEU	2.3
1	R	149	LEU	2.3
1	A	74	LYS	2.3
1	G	210	ASP	2.3
1	H	206	LYS	2.3
1	I	85	LYS	2.3
1	S	187	PRO	2.3
1	S	4	TYR	2.3
1	J	101	ALA	2.3
1	O	95	ALA	2.3
1	T	145	THR	2.3
1	A	217	ARG	2.3
1	Q	196	SER	2.3
1	S	77	SER	2.3
1	K	47	HIS	2.3
1	L	47	HIS	2.3
1	Q	47	HIS	2.3
1	F	192	GLN	2.3
1	O	102	GLU	2.3
1	B	32	ILE	2.3
1	D	32	ILE	2.3
1	P	79	ILE	2.3
1	Q	195	ILE	2.3
1	E	83	VAL	2.3
1	H	13	VAL	2.3
1	J	41	VAL	2.3
1	K	83	VAL	2.3
1	S	204	VAL	2.3
1	B	39	LEU	2.3
1	I	16	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	37	LYS	2.3
1	Q	75	LEU	2.3
1	R	6	ASP	2.3
1	B	21	PRO	2.3
1	T	52	GLY	2.3
1	A	18	ARG	2.3
1	C	125	ALA	2.3
1	G	217	ARG	2.3
1	L	137	ALA	2.3
1	N	137	ALA	2.3
1	R	18	ARG	2.3
1	H	26	THR	2.3
1	A	45	GLN	2.3
1	I	48	GLU	2.3
1	M	48	GLU	2.3
1	O	208	GLU	2.3
1	J	79	ILE	2.3
1	Q	32	ILE	2.3
1	Q	37	LYS	2.3
1	D	39	LEU	2.2
1	H	204	VAL	2.3
1	I	188	LEU	2.2
1	L	186	LEU	2.2
1	O	60	VAL	2.3
1	T	73	LEU	2.2
1	M	133	ASN	2.2
1	L	113	GLY	2.2
1	O	194	MET	2.2
1	P	52	GLY	2.2
1	C	123	ALA	2.2
1	C	208	GLU	2.2
1	D	65	ALA	2.2
1	D	197	TYR	2.2
1	I	214	ALA	2.2
1	K	101	ALA	2.2
1	J	209	GLN	2.2
1	K	7	THR	2.2
1	K	102	GLU	2.2
1	L	48	GLU	2.2
1	R	101	ALA	2.2
1	R	110	ALA	2.2
1	S	205	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	202	ALA	2.2
1	P	64	THR	2.2
1	S	166	SER	2.2
1	H	100	LYS	2.2
1	M	168	LYS	2.2
1	B	86	VAL	2.2
1	C	88	VAL	2.2
1	G	10	VAL	2.2
1	G	41	VAL	2.2
1	P	93	LEU	2.2
1	S	56	LEU	2.2
1	B	40	ASP	2.2
1	L	28	ASN	2.2
1	K	105	PRO	2.2
1	N	134	ARG	2.2
1	S	38	PRO	2.2
1	T	98	MET	2.2
1	F	51	GLY	2.2
1	I	2	GLU	2.2
1	L	156	HIS	2.2
1	B	161	LYS	2.2
1	B	212	GLN	2.2
1	O	168	LYS	2.2
1	S	172	GLN	2.2
1	S	193	GLN	2.2
1	A	101	ALA	2.2
1	B	33	ALA	2.2
1	C	121	ALA	2.2
1	I	64	THR	2.2
1	I	110	ALA	2.2
1	N	145	THR	2.2
1	R	137	ALA	2.2
1	S	165	ALA	2.2
1	C	8	SER	2.2
1	C	30	SER	2.2
1	L	219	SER	2.2
1	M	166	SER	2.2
1	E	32	ILE	2.2
1	O	32	ILE	2.2
1	A	93	LEU	2.2
1	E	56	LEU	2.2
1	E	84	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	25	VAL	2.2
1	S	190	VAL	2.2
1	M	134	ARG	2.2
1	Q	55	ARG	2.2
1	C	61	MET	2.2
1	H	194	MET	2.2
1	M	140	GLY	2.2
1	K	126	GLU	2.2
1	D	159	GLN	2.2
1	E	36	LYS	2.2
1	G	14	LYS	2.2
1	T	209	GLN	2.2
1	H	202	ALA	2.2
1	J	80	ALA	2.2
1	K	123	ALA	2.2
1	D	183	SER	2.2
1	L	169	THR	2.2
1	M	199	ALA	2.2
1	O	125	ALA	2.2
1	O	137	ALA	2.2
1	T	90	ALA	2.2
1	T	211	TRP	2.2
1	A	82	ILE	2.2
1	C	31	ILE	2.2
1	C	188	LEU	2.2
1	F	220	ILE	2.2
1	G	16	LEU	2.2
1	G	73	LEU	2.2
1	I	43	LEU	2.2
1	K	107	LEU	2.2
1	A	40	ASP	2.2
1	Q	83	VAL	2.2
1	B	126	GLU	2.2
1	O	85	LYS	2.2
1	P	181	CYS	2.2
1	I	72	ALA	2.2
1	J	65	ALA	2.2
1	O	114	ALA	2.2
1	R	169	THR	2.2
1	S	34	ALA	2.2
1	A	76	ARG	2.1
1	O	112	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	3	LEU	2.1
1	O	122	LEU	2.1
1	S	143	ILE	2.1
1	G	201	ASP	2.1
1	L	13	VAL	2.1
1	R	210	ASP	2.1
1	T	13	VAL	2.1
1	C	187	PRO	2.1
1	D	38	PRO	2.1
1	C	150	HIS	2.1
1	I	1	HIS	2.1
1	N	151	GLN	2.1
1	T	192	GLN	2.1
1	A	33	ALA	2.1
1	C	80	ALA	2.1
1	I	17	SER	2.1
1	Q	34	ALA	2.1
1	S	157	ALA	2.1
1	F	55	ARG	2.1
1	O	76	ARG	2.1
1	K	197	TYR	2.1
1	A	37	LYS	2.1
1	C	195	ILE	2.1
1	J	46	LEU	2.1
1	L	19	ILE	2.1
1	L	154	LYS	2.1
1	O	153	LEU	2.1
1	O	186	LEU	2.1
1	P	206	LYS	2.1
1	R	100	LYS	2.1
1	T	56	LEU	2.1
1	T	119	LEU	2.1
1	G	66	GLU	2.1
1	G	102	GLU	2.1
1	N	2	GLU	2.1
1	R	136	ASP	2.1
1	S	6	ASP	2.1
1	A	25	VAL	2.1
1	O	88	VAL	2.1
1	P	29	PRO	2.1
1	R	111	VAL	2.1
1	C	35	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	R	52	GLY	2.1
1	B	63	THR	2.1
1	G	63	THR	2.1
1	C	129	ALA	2.1
1	L	23	ALA	2.1
1	O	33	ALA	2.1
1	P	101	ALA	2.1
1	S	23	ALA	2.1
1	O	161	LYS	2.1
1	P	100	LYS	2.1
1	A	32	ILE	2.1
1	B	3	LEU	2.1
1	B	107	LEU	2.1
1	I	99	LEU	2.1
1	K	208	GLU	2.1
1	N	152	LEU	2.1
1	T	32	ILE	2.1
1	T	186	LEU	2.1
1	S	9	ASP	2.1
1	M	138	GLN	2.1
1	N	59	GLN	2.1
1	A	29	PRO	2.1
1	O	29	PRO	2.1
1	Q	25	VAL	2.1
1	S	57	PHE	2.1
1	S	35	GLY	2.1
1	B	76	ARG	2.1
1	E	218	THR	2.1
1	K	17	SER	2.1
1	T	27	THR	2.1
1	D	206	LYS	2.1
1	H	205	ALA	2.1
1	I	94	ALA	2.1
1	K	191	ALA	2.1
1	L	191	ALA	2.1
1	S	37	LYS	2.1
1	K	155	MET	2.1
1	L	194	MET	2.1
1	D	16	LEU	2.1
1	E	107	LEU	2.1
1	I	186	LEU	2.1
1	K	39	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	ILE	2.1
1	L	151	GLN	2.1
1	O	107	LEU	2.1
1	Q	3	LEU	2.1
1	T	188	LEU	2.1
1	R	81	ASP	2.1
1	T	28	ASN	2.1
1	E	127	TYR	2.1
1	R	4	TYR	2.1
1	R	112	TYR	2.1
1	E	60	VAL	2.1
1	J	86	VAL	2.1
1	P	42	VAL	2.1
1	R	83	VAL	2.1
1	S	146	VAL	2.1
1	P	54	GLY	2.1
1	A	161	LYS	2.0
1	J	161	LYS	2.0
1	K	100	LYS	2.0
1	A	30	SER	2.0
1	F	17	SER	2.0
1	L	30	SER	2.0
1	B	49	ALA	2.0
1	B	58	ALA	2.0
1	B	179	ALA	2.0
1	C	48	GLU	2.0
1	C	137	ALA	2.0
1	E	80	ALA	2.0
1	F	50	MET	2.0
1	I	68	MET	2.0
1	J	33	ALA	2.0
1	K	15	ALA	2.0
1	M	2	GLU	2.0
1	O	23	ALA	2.0
1	P	165	ALA	2.0
1	Q	173	ALA	2.0
1	F	212	GLN	2.0
1	H	71	ASP	2.0
1	H	93	LEU	2.0
1	J	107	LEU	2.0
1	K	3	LEU	2.0
1	L	9	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	148	ASP	2.0
1	O	210	ASP	2.0
1	Q	201	ASP	2.0
1	S	133	ASN	2.0
1	E	19	ILE	2.0
1	E	184	ILE	2.0
1	B	38	PRO	2.0
1	R	29	PRO	2.0
1	G	4	TYR	2.0
1	D	103	GLY	2.0
1	P	113	GLY	2.0
1	J	100	LYS	2.0
1	K	154	LYS	2.0
1	C	211	TRP	2.0
1	A	218	THR	2.0
1	F	218	THR	2.0
1	H	91	GLU	2.0
1	J	98	MET	2.0
1	M	155	MET	2.0
1	N	120	SER	2.0
1	O	2	GLU	2.0
1	O	17	SER	2.0
1	O	169	THR	2.0
1	P	63	THR	2.0
1	S	26	THR	2.0
1	T	219	SER	2.0
1	C	179	ALA	2.0
1	D	12	ALA	2.0
1	N	191	ALA	2.0
1	B	59	GLN	2.0
1	G	53	GLN	2.0
1	A	122	LEU	2.0
1	A	152	LEU	2.0
1	C	81	ASP	2.0
1	C	177	LEU	2.0
1	O	71	ASP	2.0
1	Q	39	LEU	2.0
1	T	75	LEU	2.0
1	C	29	PRO	2.0
1	D	82	ILE	2.0
1	G	198	PRO	2.0
1	O	105	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	97	LYS	2.0
1	K	74	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P2D	B	301	6/7	0.68	0.29	43,46,51,55	0
2	P2D	G	301	6/7	0.69	0.29	39,50,54,58	0
2	P2D	H	301	6/7	0.70	0.31	56,60,62,66	0
2	P2D	P	301	6/7	0.75	0.30	41,42,47,50	0
2	P2D	K	301	6/7	0.79	0.21	41,43,53,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.