



Preliminary Full wwPDB X-ray Structure Validation Report ⓘ

May 6, 2020 – 02:01 PM EDT

Deposition ID : D_1000241405

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

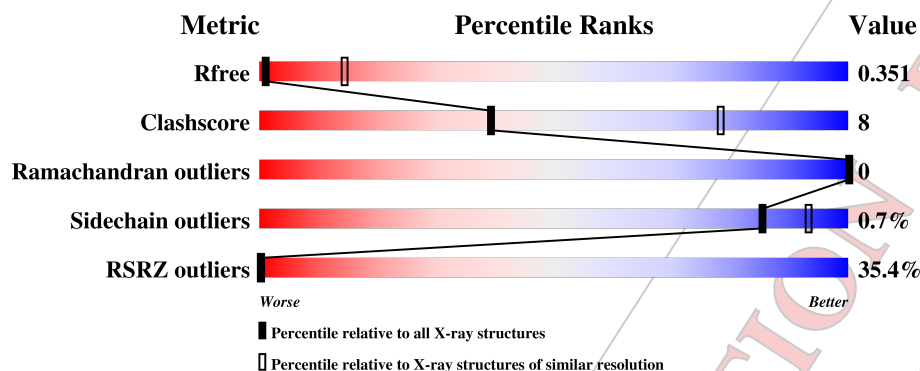
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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}	111664	1018 (4.08-3.60)
Clashscore	122126	1087 (4.08-3.60)
Ramachandran outliers	120053	1050 (4.08-3.60)
Sidechain outliers	120020	1044 (4.08-3.60)
RSRZ outliers	108989	1002 (4.10-3.58)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	387	<div> <div>36%</div> <div>65%</div> <div>19%</div> <div>15%</div> </div>
1	B	387	<div> <div>26%</div> <div>68%</div> <div>17%</div> <div>15%</div> </div>
1	C	387	<div> <div>28%</div> <div>67%</div> <div>17%</div> <div>15%</div> </div>
1	D	387	<div> <div>32%</div> <div>71%</div> <div>14%</div> <div>15%</div> </div>
1	E	387	<div> <div>30%</div> <div>66%</div> <div>19%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain			
1	F	387	27%	70%	15%	15%
1	G	387	25%	68%	17%	15%
1	H	387	36%	64%	21%	15%

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
3	SO4	I	1	-	-	-	X
3	SO4	I	5	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21808 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 Calsequestrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	B	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	C	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	D	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	E	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	F	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	G	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	H	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O14958
A	14	HIS	-	expression tag	UNP O14958
A	15	MET	-	expression tag	UNP O14958
A	16	ALA	-	expression tag	UNP O14958
A	17	SER	-	expression tag	UNP O14958
B	13	GLY	-	expression tag	UNP O14958
B	14	HIS	-	expression tag	UNP O14958
B	15	MET	-	expression tag	UNP O14958
B	16	ALA	-	expression tag	UNP O14958
B	17	SER	-	expression tag	UNP O14958
C	13	GLY	-	expression tag	UNP O14958
C	14	HIS	-	expression tag	UNP O14958
C	15	MET	-	expression tag	UNP O14958

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	ALA	-	expression tag	UNP O14958
C	17	SER	-	expression tag	UNP O14958
D	13	GLY	-	expression tag	UNP O14958
D	14	HIS	-	expression tag	UNP O14958
D	15	MET	-	expression tag	UNP O14958
D	16	ALA	-	expression tag	UNP O14958
D	17	SER	-	expression tag	UNP O14958
E	13	GLY	-	expression tag	UNP O14958
E	14	HIS	-	expression tag	UNP O14958
E	15	MET	-	expression tag	UNP O14958
E	16	ALA	-	expression tag	UNP O14958
E	17	SER	-	expression tag	UNP O14958
F	13	GLY	-	expression tag	UNP O14958
F	14	HIS	-	expression tag	UNP O14958
F	15	MET	-	expression tag	UNP O14958
F	16	ALA	-	expression tag	UNP O14958
F	17	SER	-	expression tag	UNP O14958
G	13	GLY	-	expression tag	UNP O14958
G	14	HIS	-	expression tag	UNP O14958
G	15	MET	-	expression tag	UNP O14958
G	16	ALA	-	expression tag	UNP O14958
G	17	SER	-	expression tag	UNP O14958
H	13	GLY	-	expression tag	UNP O14958
H	14	HIS	-	expression tag	UNP O14958
H	15	MET	-	expression tag	UNP O14958
H	16	ALA	-	expression tag	UNP O14958
H	17	SER	-	expression tag	UNP O14958

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: Yb) (formula: Yb).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0
2	Y	1	Total Yb 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		

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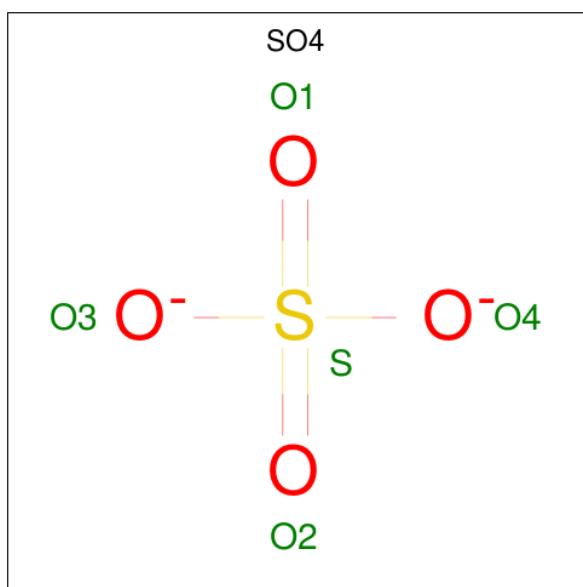
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		
2	Y	1	Total	Yb	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



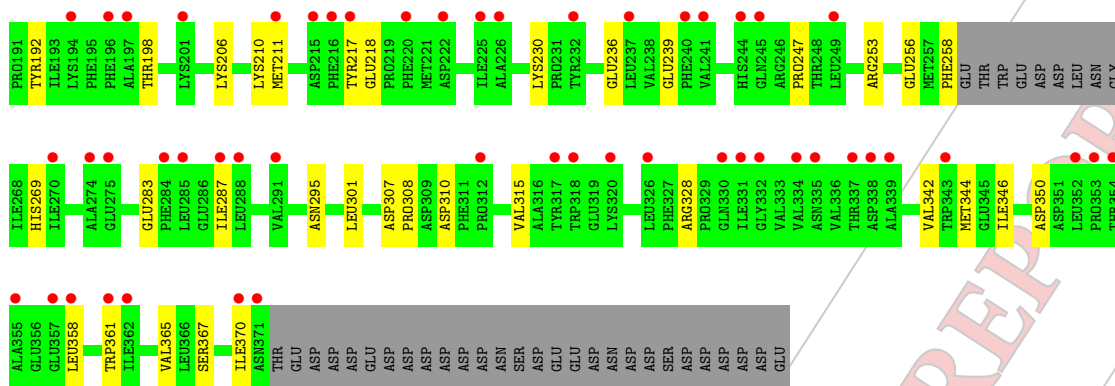
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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

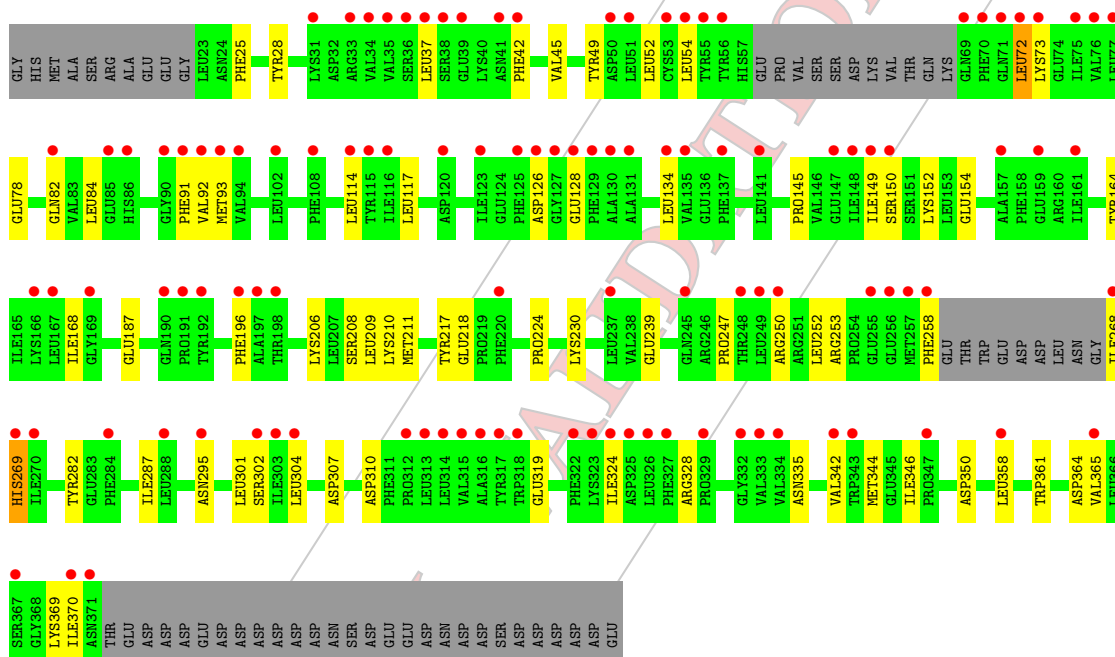
[illegible]

Chain B:

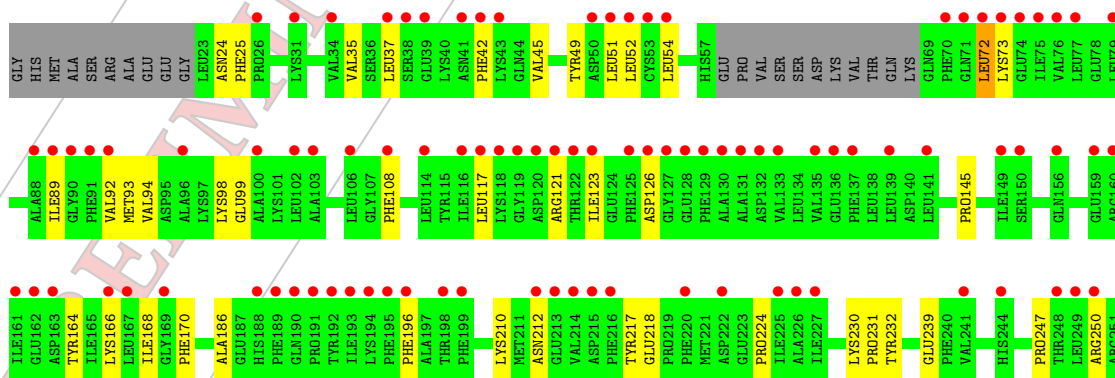
Position	Most Conserved AA	Information Content (bits)
1	GLY	0.22
2	GLY90	0.22
3	HIS	0.22
4	MET	0.22
5	ALA	0.22
6	SER	0.22
7	ARG	0.22
8	ALA	0.22
9	GLU	0.22
10	GLU	0.22
11	GLY	0.22
12	LEU23	0.22
13	ASP24	0.22
14	PHE25	0.22
15	TYR28	0.22
16	ARG33	0.22
17	VAL34	0.22
18	LEU37	0.22
19	SER38	0.22
20	GLU39	0.22
21	PHE42	0.22
22	VAL45	0.22
23	TYR49	0.22
24	ASP50	0.22
25	LEU51	0.22
26	LEU52	0.22
27	CYS53	0.22
28	LEU54	0.22
29	TYR55	0.22
30	TYR56	0.22
31	HIS57	0.22
32	GLU	0.22
33	PRO	0.22
34	SER	0.22
35	SER	0.22
36	ASP	0.22
37	LYS	0.22
38	VAL	0.22
39	THR	0.22
40	GLN	0.22
41	LYS	0.22
42	GLN69	0.22
43	PHE70	0.22
44	GLN71	0.22
45	LEU72	0.22
46	LYS73	0.22
47	GLU74	0.22
48	ILE75	0.22
49	VAL76	0.22
50	LEU77	0.22
51	GLU78	0.22
52	VAL83	0.22
53	PHE84	0.22
54	TYR89	0.22



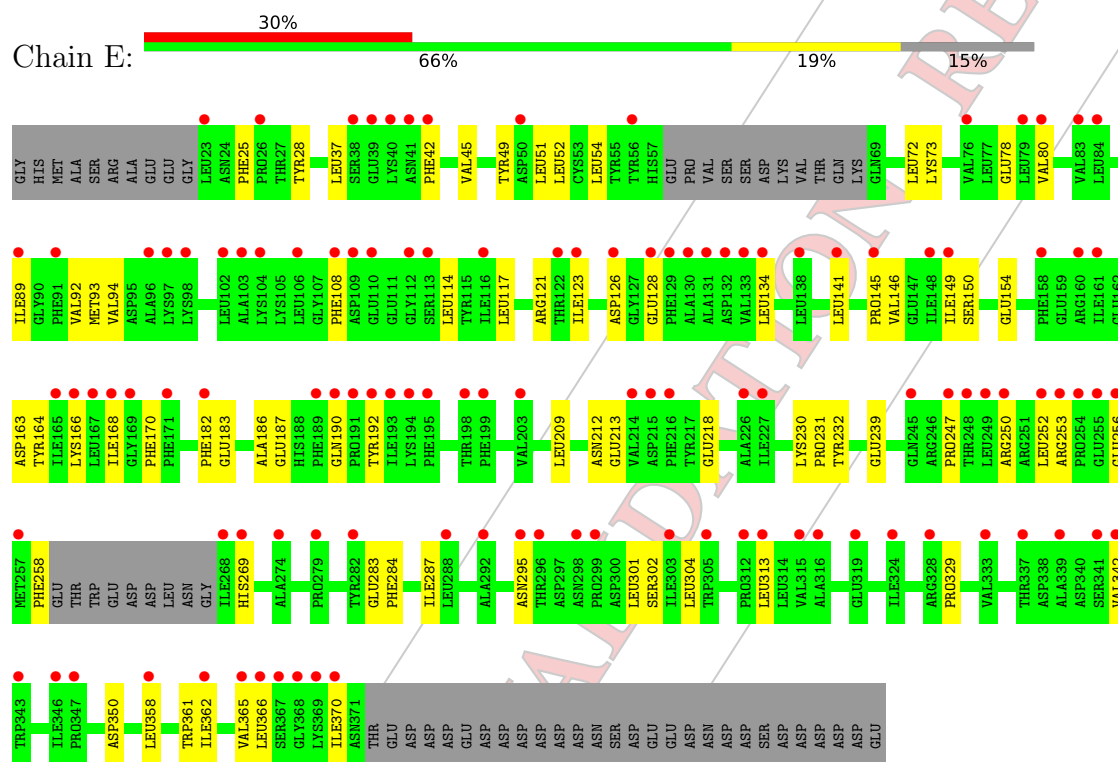
• Molecule 1: Calsequestrin-2



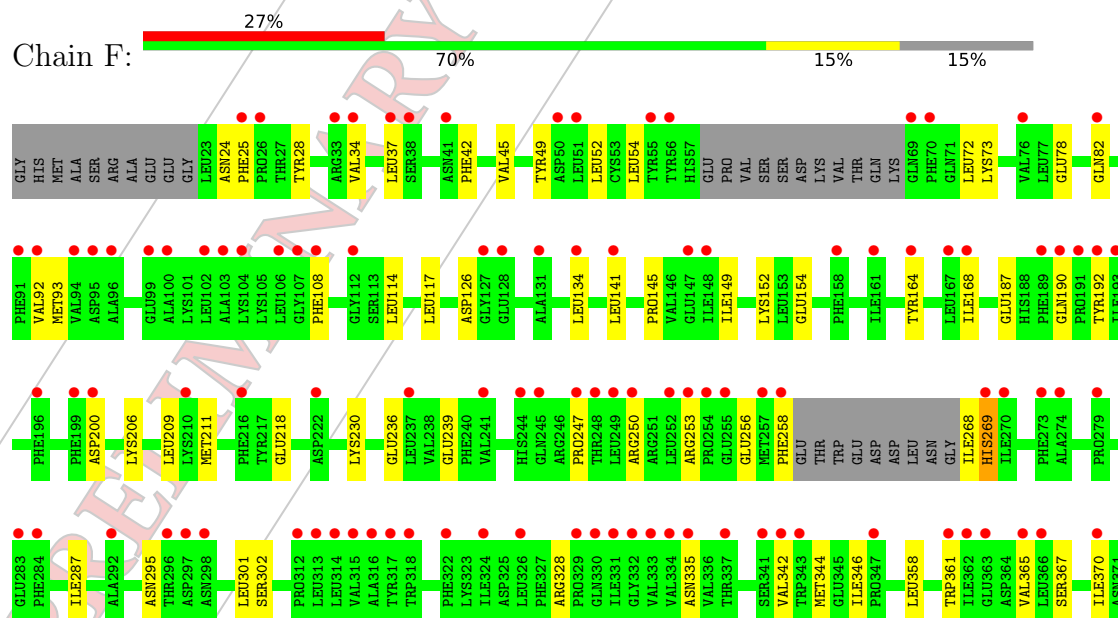
• Molecule 1: Calsequestrin-2



- Molecule 1: Calsequestrin-2



- Molecule 1: Calsequestrin-2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.83Å 86.02Å 214.34Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	214.34 – 3.84 214.34 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.4 (214.34-3.84) 98.0 (214.34-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.290 , 0.340 0.296 , 0.351	Depositor DCC
R_{free} test set	1440 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.266 for k,h,-l 0.266 for -k,-h,-l 0.266 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	21808	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YB, SO4

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	0.38	0/2779	0.56	1/3758 (0.0%)
1	B	0.40	0/2779	0.57	0/3758
1	C	0.40	0/2779	0.58	1/3758 (0.0%)
1	D	0.39	0/2779	0.57	1/3758 (0.0%)
1	E	0.40	0/2779	0.56	0/3758
1	F	0.40	0/2779	0.58	0/3758
1	G	0.40	0/2779	0.56	0/3758
1	H	0.39	0/2779	0.57	0/3758
All	All	0.40	0/22232	0.57	3/30064 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	LEU	CA-CB-CG	5.98	129.05	115.30
1	D	72	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	72	LEU	CA-CB-CG	5.13	127.11	115.30

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	2715	0	2653	49	0
1	B	2715	0	2653	45	0
1	C	2715	0	2653	49	0
1	D	2715	0	2653	37	0
1	E	2715	0	2653	48	0
1	F	2715	0	2653	42	0
1	G	2715	0	2653	41	0
1	H	2715	0	2653	53	0
2	Y	63	0	0	0	0
3	I	25	0	0	0	0
All	All	21808	0	21224	346	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 8.

All (346) 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:C:211:MET:O	1:C:230:LYS:NZ	2.19	0.76
1:F:211:MET:O	1:F:230:LYS:NZ	2.19	0.73
1:H:342:VAL:HG11	1:H:370:ILE:HG23	1.70	0.71
1:C:164:TYR:HD2	1:C:253:ARG:HH22	1.38	0.71
1:A:152:LYS:HB3	1:A:206:LYS:HE3	1.73	0.69
1:B:211:MET:O	1:B:230:LYS:NZ	2.25	0.69
1:G:211:MET:O	1:G:230:LYS:NZ	2.22	0.68
1:D:250:ARG:NH1	1:D:302:SER:OG	2.26	0.68
1:G:342:VAL:HG11	1:G:370:ILE:HG23	1.76	0.67
1:E:342:VAL:HG11	1:E:370:ILE:HG23	1.77	0.66
1:F:164:TYR:HD2	1:F:253:ARG:HH22	1.42	0.66
1:D:342:VAL:HG11	1:D:370:ILE:HG23	1.77	0.66
1:E:250:ARG:NH1	1:E:302:SER:OG	2.29	0.66
1:A:164:TYR:HD2	1:A:253:ARG:HH22	1.45	0.65
1:A:342:VAL:HG11	1:A:370:ILE:HG23	1.79	0.64
1:B:164:TYR:HD2	1:B:253:ARG:HH22	1.45	0.64
1:G:161:ILE:O	1:G:166:LYS:NZ	2.23	0.64
1:B:52:LEU:HB2	1:B:117:LEU:HB2	1.79	0.63
1:F:287:ILE:HG22	1:F:358:LEU:HD12	1.79	0.63
1:B:287:ILE:HG22	1:B:358:LEU:HD12	1.81	0.62
1:F:342:VAL:HG11	1:F:370:ILE:HG23	1.81	0.62
1:H:212:ASN:HB3	1:H:231:PRO:HB3	1.80	0.62
1:C:52:LEU:HB2	1:C:117:LEU:HB2	1.81	0.62
1:C:287:ILE:HG22	1:C:358:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ARG:NH2	1:A:310:ASP:OD2	2.28	0.60
1:A:218:GLU:OE1	1:A:247:PRO:HB3	2.02	0.60
1:B:37:LEU:HD11	1:B:42:PHE:HA	1.84	0.60
1:B:342:VAL:HG11	1:B:370:ILE:HG23	1.84	0.59
1:A:54:LEU:HG	1:A:92:VAL:HG23	1.84	0.59
1:F:168:ILE:HG23	1:F:209:LEU:HD11	1.84	0.59
1:H:250:ARG:NH1	1:H:302:SER:OG	2.36	0.59
1:A:72:LEU:HD12	1:A:73:LYS:HG3	1.85	0.59
1:C:218:GLU:OE1	1:C:247:PRO:HB3	2.03	0.59
1:E:72:LEU:HD12	1:E:73:LYS:HG3	1.85	0.58
1:E:126:ASP:HB3	1:E:258:PHE:HB3	1.85	0.58
1:H:121:ARG:NH1	1:H:123:ILE:HD11	2.18	0.58
1:A:80:VAL:HG21	1:A:134:LEU:HD23	1.86	0.58
1:E:247:PRO:HD2	1:E:250:ARG:HD3	1.86	0.58
1:B:149:ILE:HG23	1:B:154:GLU:HB3	1.85	0.58
1:D:247:PRO:HD2	1:D:250:ARG:HD3	1.85	0.58
1:G:152:LYS:HB3	1:G:206:LYS:HE3	1.86	0.58
1:C:149:ILE:HG23	1:C:154:GLU:HB3	1.86	0.57
1:E:218:GLU:OE1	1:E:247:PRO:HB3	2.03	0.57
1:F:218:GLU:OE1	1:F:247:PRO:HB3	2.05	0.57
1:B:72:LEU:HD12	1:B:73:LYS:HG3	1.86	0.57
1:H:72:LEU:HD12	1:H:73:LYS:HG3	1.86	0.57
1:G:168:ILE:HG23	1:G:209:LEU:HD11	1.85	0.57
1:C:342:VAL:HG11	1:C:370:ILE:HG23	1.85	0.57
1:G:287:ILE:HG22	1:G:358:LEU:HD12	1.85	0.57
1:B:152:LYS:HB3	1:B:206:LYS:HE3	1.87	0.56
1:A:84:LEU:HD22	1:A:87:LYS:HG3	1.85	0.56
1:F:52:LEU:HB2	1:F:117:LEU:HB2	1.86	0.56
1:B:367:SER:O	1:F:236:GLU:HA	2.04	0.56
1:D:72:LEU:HD12	1:D:73:LYS:HG3	1.87	0.56
1:G:28:TYR:CE1	1:G:78:GLU:HB3	2.40	0.56
1:H:149:ILE:HG23	1:H:154:GLU:HB3	1.88	0.56
1:A:283:GLU:O	1:A:287:ILE:HG12	2.06	0.56
1:A:126:ASP:HB3	1:A:258:PHE:HB3	1.88	0.55
1:D:54:LEU:HG	1:D:92:VAL:HG23	1.88	0.55
1:G:164:TYR:HD2	1:G:253:ARG:HH22	1.53	0.55
1:C:168:ILE:HG23	1:C:209:LEU:HD11	1.88	0.55
1:D:218:GLU:OE1	1:D:247:PRO:HB3	2.06	0.55
1:B:28:TYR:CE1	1:B:78:GLU:HB3	2.41	0.55
1:F:149:ILE:HG23	1:F:154:GLU:HB3	1.89	0.55
1:C:152:LYS:HB3	1:C:206:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:LYS:HB3	1:F:206:LYS:HE3	1.88	0.55
1:H:126:ASP:HB3	1:H:258:PHE:HB3	1.89	0.55
1:C:72:LEU:HD12	1:C:73:LYS:HG3	1.88	0.54
1:H:218:GLU:OE1	1:H:247:PRO:HB3	2.07	0.54
1:G:37:LEU:HD11	1:G:42:PHE:HA	1.89	0.54
1:G:149:ILE:HG23	1:G:154:GLU:HB3	1.88	0.54
1:G:52:LEU:HB2	1:G:117:LEU:HB2	1.88	0.54
1:B:141:LEU:HD23	1:B:190:GLN:HG2	1.90	0.54
1:C:45:VAL:HG13	1:C:49:TYR:CE2	2.43	0.53
1:H:80:VAL:HG21	1:H:134:LEU:HD23	1.89	0.53
1:A:149:ILE:HG23	1:A:154:GLU:HB3	1.91	0.53
1:E:287:ILE:HG22	1:E:358:LEU:HD12	1.91	0.53
1:H:54:LEU:HG	1:H:92:VAL:HG23	1.91	0.53
1:A:287:ILE:HG22	1:A:358:LEU:HD12	1.90	0.53
1:E:168:ILE:HG23	1:E:209:LEU:HD11	1.91	0.53
1:G:308:PRO:HA	1:G:315:VAL:HG21	1.90	0.53
1:G:328:ARG:NH1	1:G:346:ILE:O	2.41	0.53
1:H:37:LEU:HD11	1:H:42:PHE:HA	1.91	0.53
1:E:54:LEU:HG	1:E:92:VAL:HG23	1.91	0.52
1:C:344:MET:HG3	1:C:361:TRP:CD1	2.44	0.52
1:E:37:LEU:HD11	1:E:42:PHE:HA	1.91	0.52
1:F:37:LEU:HD11	1:F:42:PHE:HA	1.91	0.52
1:B:236:GLU:HA	1:F:367:SER:O	2.10	0.52
1:H:247:PRO:HD2	1:H:250:ARG:HD3	1.91	0.52
1:F:268:ILE:HD12	1:F:335:ASN:HA	1.91	0.52
1:D:126:ASP:HB3	1:D:258:PHE:HB3	1.92	0.52
1:H:287:ILE:HG22	1:H:358:LEU:HD12	1.92	0.52
1:G:218:GLU:OE1	1:G:247:PRO:HB3	2.09	0.52
1:E:212:ASN:HB3	1:E:231:PRO:HB3	1.92	0.52
1:G:72:LEU:HD12	1:G:73:LYS:HG3	1.92	0.52
1:B:344:MET:HG3	1:B:361:TRP:CD1	2.45	0.52
1:F:72:LEU:HD12	1:F:73:LYS:HG3	1.92	0.51
1:F:114:LEU:HD23	1:F:134:LEU:HD11	1.92	0.51
1:C:37:LEU:HD11	1:C:42:PHE:HA	1.92	0.51
1:G:57:HIS:ND1	1:G:111:GLU:OE2	2.43	0.51
1:H:251:ARG:NH2	1:H:310:ASP:OD2	2.38	0.51
1:E:252:LEU:HD13	1:E:304:LEU:HD21	1.91	0.51
1:F:344:MET:HG3	1:F:361:TRP:CD1	2.46	0.51
1:C:328:ARG:NH1	1:C:346:ILE:O	2.37	0.50
1:E:45:VAL:HG13	1:E:49:TYR:CE2	2.45	0.50
1:A:37:LEU:HD11	1:A:42:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:VAL:HG13	1:C:49:TYR:HE2	1.74	0.50
1:C:28:TYR:CE1	1:C:78:GLU:HB3	2.46	0.50
1:D:252:LEU:HD13	1:D:304:LEU:HD21	1.92	0.50
1:F:328:ARG:NH1	1:F:346:ILE:O	2.35	0.50
1:B:308:PRO:HA	1:B:315:VAL:HG21	1.94	0.50
1:E:149:ILE:HG23	1:E:154:GLU:HB3	1.94	0.50
1:D:25:PHE:CZ	1:G:128:GLU:HB2	2.48	0.49
1:C:128:GLU:HB2	1:H:25:PHE:CZ	2.47	0.49
1:G:307:ASP:HB3	1:G:310:ASP:OD2	2.12	0.49
1:H:28:TYR:CE1	1:H:78:GLU:HB3	2.47	0.49
1:A:164:TYR:CE1	1:A:166:LYS:HG2	2.48	0.49
1:B:350:ASP:CG	1:E:150:SER:HB2	2.33	0.49
1:D:247:PRO:HG2	1:D:250:ARG:HB3	1.94	0.48
1:A:247:PRO:HD2	1:A:250:ARG:HD3	1.94	0.48
1:B:295:ASN:HB2	1:B:301:LEU:HD23	1.93	0.48
1:F:45:VAL:HG13	1:F:49:TYR:CE2	2.49	0.48
1:G:114:LEU:HD23	1:G:134:LEU:HD11	1.95	0.48
1:G:54:LEU:HD13	1:G:117:LEU:HG	1.94	0.48
1:F:28:TYR:HA	1:F:82:GLN:OE1	2.13	0.48
1:H:163:ASP:HB3	1:H:253:ARG:HH21	1.78	0.48
1:C:210:LYS:HB3	1:C:230:LYS:HZ1	1.79	0.48
1:C:307:ASP:HB3	1:C:310:ASP:OD2	2.12	0.48
1:E:80:VAL:HG21	1:E:134:LEU:HD23	1.95	0.48
1:F:200:ASP:OD1	1:G:347:PRO:HB3	2.13	0.48
1:D:37:LEU:HD11	1:D:42:PHE:HA	1.96	0.48
1:G:45:VAL:HG13	1:G:49:TYR:CE2	2.49	0.48
1:C:250:ARG:NH1	1:C:302:SER:OG	2.47	0.48
1:H:192:TYR:CE1	1:H:256:GLU:HA	2.49	0.48
1:A:289:LYS:HB3	1:A:293:ARG:HH12	1.79	0.47
1:E:45:VAL:HG13	1:E:49:TYR:HE2	1.78	0.47
1:G:295:ASN:HB2	1:G:301:LEU:HD23	1.96	0.47
1:B:45:VAL:HG13	1:B:49:TYR:CE2	2.50	0.47
1:E:145:PRO:HB2	1:E:186:ALA:HB1	1.95	0.47
1:B:210:LYS:HB3	1:B:230:LYS:NZ	2.30	0.47
1:A:212:ASN:HB3	1:A:231:PRO:HB3	1.96	0.47
1:A:275:GLU:HG2	1:A:308:PRO:HD2	1.95	0.47
1:H:54:LEU:HD23	1:H:94:VAL:HG21	1.97	0.47
1:A:328:ARG:O	1:A:330:GLN:HG2	2.15	0.47
1:D:210:LYS:HB3	1:D:230:LYS:HZ3	1.80	0.47
1:D:287:ILE:HG22	1:D:358:LEU:HD12	1.95	0.47
1:E:54:LEU:HD13	1:E:117:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:NH1	1:A:346:ILE:O	2.47	0.47
1:D:93:MET:HB3	1:D:93:MET:HE2	1.73	0.47
1:C:145:PRO:HG2	1:C:187:GLU:HG2	1.96	0.47
1:A:54:LEU:HD13	1:A:117:LEU:HG	1.97	0.47
1:D:145:PRO:HB2	1:D:186:ALA:HB1	1.96	0.47
1:B:57:HIS:ND1	1:B:111:GLU:OE2	2.48	0.47
1:D:54:LEU:HD22	1:D:108:PHE:HZ	1.80	0.47
1:F:141:LEU:HD23	1:F:190:GLN:HG2	1.97	0.47
1:H:164:TYR:CE1	1:H:166:LYS:HG2	2.50	0.47
1:H:247:PRO:HG2	1:H:250:ARG:HB3	1.97	0.47
1:A:54:LEU:HD22	1:A:108:PHE:HZ	1.80	0.46
1:F:54:LEU:HD22	1:F:108:PHE:HZ	1.79	0.46
1:G:268:ILE:HD12	1:G:335:ASN:HA	1.96	0.46
1:G:344:MET:HG3	1:G:361:TRP:CD1	2.49	0.46
1:E:54:LEU:HD23	1:E:94:VAL:HG21	1.97	0.46
1:G:54:LEU:HD22	1:G:108:PHE:HZ	1.80	0.46
1:C:114:LEU:HD23	1:C:134:LEU:HD11	1.97	0.46
1:C:54:LEU:HG	1:C:92:VAL:HG23	1.97	0.46
1:G:291:VAL:HG13	1:G:359:GLU:HG3	1.98	0.46
1:A:168:ILE:HA	1:A:196:PHE:O	2.16	0.46
1:G:72:LEU:HD12	1:G:73:LYS:N	2.31	0.46
1:H:152:LYS:HB3	1:H:206:LYS:HE3	1.97	0.46
1:D:212:ASN:HB3	1:D:231:PRO:HB3	1.98	0.46
1:G:54:LEU:HD22	1:G:108:PHE:CZ	2.51	0.46
1:G:141:LEU:HD23	1:G:190:GLN:HG2	1.98	0.46
1:H:40:LYS:NZ	1:H:44:GLN:OE1	2.49	0.46
1:C:54:LEU:HD13	1:C:117:LEU:HG	1.98	0.45
1:G:361:TRP:O	1:G:365:VAL:HG23	2.15	0.45
1:B:34:VAL:HG12	1:B:93:MET:HG2	1.97	0.45
1:B:93:MET:HE2	1:B:93:MET:HB3	1.85	0.45
1:E:163:ASP:HB3	1:E:253:ARG:HH21	1.81	0.45
1:E:230:LYS:HB3	1:E:232:TYR:OH	2.16	0.45
1:F:54:LEU:HG	1:F:92:VAL:HG23	1.98	0.45
1:A:93:MET:HE2	1:A:93:MET:HB3	1.76	0.45
1:E:283:GLU:O	1:E:287:ILE:HG12	2.16	0.45
1:F:54:LEU:HD22	1:F:108:PHE:CZ	2.51	0.45
1:D:121:ARG:NH1	1:D:123:ILE:HD11	2.32	0.45
1:A:81:ALA:HA	1:A:91:PHE:CE1	2.51	0.45
1:A:94:VAL:HG13	1:A:99:GLU:HB2	1.98	0.45
1:B:218:GLU:OE1	1:B:247:PRO:HB3	2.17	0.45
1:D:361:TRP:O	1:D:365:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:ALA:HA	1:H:91:PHE:CE1	2.52	0.45
1:A:295:ASN:HB2	1:A:301:LEU:HD23	1.99	0.45
1:A:284:PHE:HB2	1:A:352:LEU:HD13	1.99	0.45
1:D:54:LEU:HD23	1:D:94:VAL:HG21	1.99	0.45
1:H:181:ALA:HB1	1:H:234:GLU:N	2.32	0.45
1:B:192:TYR:CE1	1:B:256:GLU:HA	2.51	0.45
1:E:361:TRP:O	1:E:365:VAL:HG23	2.17	0.45
1:E:51:LEU:HB2	1:E:89:ILE:HG12	1.99	0.45
1:F:54:LEU:HD13	1:F:117:LEU:HG	1.98	0.45
1:G:273:PHE:O	1:G:329:PRO:HA	2.17	0.45
1:D:230:LYS:HB3	1:D:232:TYR:OH	2.16	0.45
1:E:295:ASN:HB2	1:E:301:LEU:HD23	1.97	0.45
1:F:145:PRO:HG2	1:F:187:GLU:HG2	1.99	0.45
1:H:283:GLU:O	1:H:287:ILE:HG12	2.17	0.45
1:H:93:MET:HE2	1:H:93:MET:HB3	1.72	0.45
1:B:166:LYS:HB2	1:B:217:TYR:HB2	1.98	0.45
1:F:28:TYR:CE1	1:F:78:GLU:HB3	2.52	0.45
1:G:81:ALA:HA	1:G:91:PHE:CE1	2.52	0.45
1:H:95:ASP:HB3	1:H:98:LYS:HB3	1.98	0.45
1:D:52:LEU:HB2	1:D:117:LEU:HB2	1.98	0.44
1:E:52:LEU:HB2	1:E:117:LEU:HB2	1.98	0.44
1:F:45:VAL:HG13	1:F:49:TYR:HE2	1.81	0.44
1:B:126:ASP:HB3	1:B:258:PHE:HD2	1.83	0.44
1:B:361:TRP:O	1:B:365:VAL:HG23	2.17	0.44
1:C:168:ILE:HA	1:C:196:PHE:O	2.18	0.44
1:C:84:LEU:HD12	1:C:91:PHE:HZ	1.82	0.44
1:E:54:LEU:HD22	1:E:108:PHE:HZ	1.82	0.44
1:E:284:PHE:CG	1:E:329:PRO:HB3	2.53	0.44
1:F:295:ASN:HB2	1:F:301:LEU:HD23	2.00	0.44
1:D:283:GLU:OE1	1:G:154:GLU:HG3	2.17	0.44
1:C:350:ASP:CG	1:H:150:SER:HB2	2.38	0.44
1:F:126:ASP:HB3	1:F:258:PHE:CD2	2.52	0.44
1:C:350:ASP:O	1:H:151:SER:HB2	2.18	0.44
1:H:230:LYS:HB3	1:H:232:TYR:OH	2.17	0.44
1:B:308:PRO:HB3	1:B:315:VAL:HG11	2.00	0.44
1:H:52:LEU:HB2	1:H:117:LEU:HB2	1.99	0.44
1:C:268:ILE:HG22	1:C:269:HIS:ND1	2.33	0.44
1:E:121:ARG:NH1	1:E:123:ILE:HD11	2.33	0.44
1:G:166:LYS:HB2	1:G:217:TYR:HB2	1.98	0.44
1:G:54:LEU:HG	1:G:92:VAL:HG23	2.00	0.44
1:G:54:LEU:HD23	1:G:94:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:PHE:CZ	1:E:128:GLU:HB2	2.53	0.44
1:F:126:ASP:HB3	1:F:258:PHE:HD2	1.83	0.44
1:F:192:TYR:CE1	1:F:256:GLU:HA	2.53	0.44
1:H:183:GLU:O	1:H:187:GLU:HG3	2.18	0.44
1:A:247:PRO:HG2	1:A:250:ARG:HB3	2.00	0.43
1:A:163:ASP:HB3	1:A:253:ARG:HH21	1.83	0.43
1:H:168:ILE:HA	1:H:196:PHE:O	2.18	0.43
1:A:28:TYR:CE1	1:A:78:GLU:HB3	2.53	0.43
1:A:54:LEU:HG	1:A:92:VAL:CG2	2.49	0.43
1:B:72:LEU:HD12	1:B:73:LYS:N	2.33	0.43
1:C:361:TRP:O	1:C:365:VAL:HG23	2.19	0.43
1:D:51:LEU:HB2	1:D:89:ILE:HG12	2.01	0.43
1:E:28:TYR:CE1	1:E:78:GLU:HB3	2.53	0.43
1:H:52:LEU:HD23	1:H:52:LEU:HA	1.79	0.43
1:D:24:ASN:HB3	1:D:25:PHE:H	1.69	0.43
1:E:93:MET:HE2	1:E:93:MET:HB3	1.73	0.43
1:H:54:LEU:HD22	1:H:108:PHE:HZ	1.83	0.43
1:A:361:TRP:O	1:A:365:VAL:HG23	2.19	0.43
1:E:141:LEU:HD23	1:E:190:GLN:HG2	2.00	0.43
1:A:95:ASP:HB3	1:A:98:LYS:HB3	2.00	0.43
1:H:211:MET:O	1:H:230:LYS:NZ	2.47	0.43
1:D:170:PHE:O	1:D:212:ASN:N	2.43	0.43
1:F:268:ILE:HG22	1:F:269:HIS:ND1	2.33	0.43
1:F:361:TRP:O	1:F:365:VAL:HG23	2.19	0.43
1:A:45:VAL:HG13	1:A:49:TYR:CE2	2.54	0.43
1:D:54:LEU:HD13	1:D:117:LEU:HG	2.00	0.43
1:E:183:GLU:O	1:E:187:GLU:HG3	2.19	0.43
1:C:25:PHE:CZ	1:H:128:GLU:HB2	2.54	0.43
1:B:150:SER:HB2	1:E:350:ASP:CG	2.38	0.42
1:B:145:PRO:HG2	1:B:187:GLU:HG2	2.02	0.42
1:C:217:TYR:CZ	1:C:224:PRO:HB3	2.54	0.42
1:B:328:ARG:NH1	1:B:346:ILE:O	2.38	0.42
1:B:54:LEU:HD22	1:B:108:PHE:CZ	2.54	0.42
1:D:168:ILE:HA	1:D:196:PHE:O	2.18	0.42
1:F:72:LEU:HD12	1:F:73:LYS:N	2.33	0.42
1:B:45:VAL:HG13	1:B:49:TYR:HE2	1.84	0.42
1:C:252:LEU:HB2	1:C:304:LEU:HD11	2.01	0.42
1:E:284:PHE:CD2	1:E:329:PRO:HB3	2.54	0.42
1:E:72:LEU:HD12	1:E:73:LYS:N	2.34	0.42
1:H:45:VAL:HG13	1:H:49:TYR:CE2	2.54	0.42
1:D:54:LEU:HD22	1:D:108:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:HB2	1:E:25:PHE:CZ	2.53	0.42
1:A:114:LEU:HD23	1:A:134:LEU:HD11	2.02	0.42
1:B:170:PHE:HA	1:B:198:THR:O	2.19	0.42
1:B:283:GLU:O	1:B:287:ILE:HG12	2.19	0.42
1:E:247:PRO:HG2	1:E:250:ARG:HB3	2.01	0.42
1:D:164:TYR:CE1	1:D:166:LYS:HG2	2.55	0.42
1:E:213:GLU:HB2	1:E:230:LYS:HD3	2.02	0.42
1:H:284:PHE:CG	1:H:329:PRO:HB3	2.55	0.42
1:H:94:VAL:HG13	1:H:99:GLU:HB2	2.02	0.42
1:C:319:GLU:HG2	1:C:324:ILE:O	2.18	0.42
1:E:164:TYR:CE1	1:E:166:LYS:HG2	2.55	0.42
1:G:45:VAL:HG13	1:G:49:TYR:HE2	1.85	0.42
1:H:164:TYR:HD2	1:H:253:ARG:HH22	1.66	0.42
1:C:150:SER:HB2	1:H:350:ASP:CG	2.40	0.42
1:C:126:ASP:HB3	1:C:258:PHE:HD2	1.85	0.42
1:D:94:VAL:HG13	1:D:99:GLU:HB2	2.01	0.42
1:H:252:LEU:HD13	1:H:304:LEU:HD21	2.01	0.42
1:A:24:ASN:HB3	1:A:25:PHE:H	1.68	0.42
1:D:284:PHE:CG	1:D:329:PRO:HB3	2.55	0.42
1:F:24:ASN:HB3	1:F:25:PHE:H	1.69	0.42
1:B:126:ASP:HB3	1:B:258:PHE:CD2	2.54	0.42
1:C:268:ILE:HD12	1:C:335:ASN:HA	2.02	0.42
1:D:35:VAL:O	1:D:92:VAL:HA	2.20	0.42
1:B:83:VAL:HG21	1:E:313:LEU:HD11	2.01	0.42
1:H:51:LEU:HB2	1:H:89:ILE:HG12	2.01	0.42
1:C:126:ASP:HB3	1:C:258:PHE:CD2	2.55	0.41
1:C:364:ASP:O	1:C:369:LYS:HB2	2.19	0.41
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.79	0.41
1:E:114:LEU:HD23	1:E:134:LEU:HD11	2.01	0.41
1:F:93:MET:HB3	1:F:93:MET:HE2	1.95	0.41
1:G:45:VAL:HG12	1:G:52:LEU:HD21	2.02	0.41
1:A:281:GLY:HA2	1:A:329:PRO:HG3	2.01	0.41
1:B:210:LYS:HB3	1:B:230:LYS:HZ1	1.86	0.41
1:A:289:LYS:HB3	1:A:293:ARG:NH1	2.36	0.41
1:C:72:LEU:HD12	1:C:73:LYS:N	2.35	0.41
1:E:362:ILE:O	1:E:366:LEU:HG	2.21	0.41
1:F:54:LEU:O	1:F:114:LEU:HD12	2.20	0.41
1:A:158:PHE:HE1	1:A:196:PHE:CD1	2.39	0.41
1:A:284:PHE:CD2	1:A:329:PRO:HB3	2.55	0.41
1:F:250:ARG:NH1	1:F:302:SER:OG	2.53	0.41
1:D:164:TYR:HD2	1:D:253:ARG:HH22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:NH1	1:A:123:ILE:HD11	2.36	0.41
1:C:295:ASN:HB2	1:C:301:LEU:HD23	2.02	0.41
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.86	0.41
1:F:200:ASP:CG	1:G:347:PRO:HB3	2.41	0.41
1:C:282:TYR:OH	1:H:160:ARG:HD3	2.21	0.41
1:A:274:ALA:HB1	1:A:281:GLY:O	2.20	0.41
1:A:291:VAL:HG13	1:A:359:GLU:HG3	2.03	0.41
1:B:54:LEU:HD23	1:B:94:VAL:HG21	2.02	0.41
1:H:295:ASN:HB2	1:H:301:LEU:HD23	2.02	0.41
1:H:328:ARG:O	1:H:330:GLN:HG2	2.20	0.41
1:A:126:ASP:HB3	1:A:258:PHE:CD2	2.56	0.41
1:C:37:LEU:HD21	1:C:42:PHE:HD1	1.86	0.41
1:D:217:TYR:CZ	1:D:224:PRO:HB3	2.56	0.41
1:E:146:VAL:HG13	1:E:182:PHE:HE2	1.86	0.41
1:G:192:TYR:CE1	1:G:256:GLU:HA	2.55	0.41
1:H:72:LEU:HD12	1:H:73:LYS:N	2.36	0.41
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.86	0.40
1:B:54:LEU:HD13	1:B:117:LEU:HG	2.02	0.40
1:D:45:VAL:HG13	1:D:49:TYR:CE2	2.55	0.40
1:B:307:ASP:HB3	1:B:310:ASP:OD2	2.20	0.40
1:B:57:HIS:CE1	1:B:97:LYS:HE2	2.56	0.40
1:F:247:PRO:HD2	1:F:250:ARG:HD3	2.02	0.40
1:A:31:LYS:HB3	1:A:33:ARG:NH1	2.36	0.40
1:C:28:TYR:HA	1:C:82:GLN:OE1	2.21	0.40
1:E:170:PHE:O	1:E:212:ASN:N	2.46	0.40
1:H:210:LYS:HB3	1:H:230:LYS:HZ3	1.87	0.40
1:H:185:ALA:N	1:H:234:GLU:HG3	2.36	0.40
1:C:208:SER:OG	1:D:98:LYS:HE3	2.21	0.40
1:C:247:PRO:HG2	1:C:250:ARG:HB3	2.03	0.40
1:C:93:MET:HE2	1:C:93:MET:HB3	1.94	0.40
1:F:34:VAL:HG12	1:F:93:MET:HG2	2.04	0.40
1:H:289:LYS:HB3	1:H:293:ARG:HH12	1.86	0.40
1:A:54:LEU:HD23	1:A:94:VAL:HG21	2.02	0.40
1:E:192:TYR:CE1	1:E:256:GLU:HA	2.57	0.40
1:H:54:LEU:HD13	1:H:117:LEU:HG	2.04	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	323/387 (84%)	309 (96%)	14 (4%)	0	100	100
1	B	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	C	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	D	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	E	323/387 (84%)	309 (96%)	14 (4%)	0	100	100
1	F	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	G	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	H	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
All	All	2584/3096 (84%)	2478 (96%)	106 (4%)	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	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	B	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	C	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	D	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	E	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	F	297/351 (85%)	295 (99%)	2 (1%)	85	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	H	297/351 (85%)	295 (99%)	2 (1%)	85	93
All	All	2376/2808 (85%)	2360 (99%)	16 (1%)	85	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	269	HIS
1	B	239	GLU
1	B	269	HIS
1	C	239	GLU
1	C	269	HIS
1	D	239	GLU
1	D	269	HIS
1	E	239	GLU
1	E	269	HIS
1	F	239	GLU
1	F	269	HIS
1	G	239	GLU
1	G	269	HIS
1	H	239	GLU
1	H	269	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	HIS
1	F	188	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 63 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	I	5	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	I	2	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	I	1	2	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	I	4	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	I	3	-	4,4,4	0.16	0	6,6,6	0.19	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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(Å²)	Q<0.9
1	A	329/387 (85%)	2.15	139 (42%)	0	0	69, 99, 134, 141	0
1	B	329/387 (85%)	1.46	101 (30%)	0	0	54, 89, 137, 152	0
1	C	329/387 (85%)	1.53	110 (33%)	0	0	51, 87, 132, 154	0
1	D	329/387 (85%)	1.79	125 (37%)	0	0	57, 99, 133, 146	0
1	E	329/387 (85%)	1.64	116 (35%)	0	0	56, 97, 137, 148	0
1	F	329/387 (85%)	1.42	105 (31%)	0	0	48, 91, 133, 160	0
1	G	329/387 (85%)	1.40	98 (29%)	0	0	50, 92, 132, 156	0
1	H	329/387 (85%)	2.01	139 (42%)	0	0	61, 96, 133, 143	0
All	All	2632/3096 (85%)	1.68	933 (35%)	0	0	48, 94, 135, 160	0

All (933) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ALA	13.0
1	H	115	TYR	11.6
1	H	150	SER	10.5
1	D	257	MET	10.4
1	A	96	ALA	10.3
1	E	248	THR	9.6
1	H	113	SER	9.3
1	E	257	MET	9.3
1	C	127	GLY	8.9
1	H	114	LEU	8.9
1	C	92	VAL	8.7
1	A	114	LEU	8.7
1	D	190	GLN	8.6
1	C	128	GLU	8.6
1	A	169	GLY	8.6
1	C	93	MET	8.4

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Mol	Chain	Res	Type	RSRZ
1	A	215	ASP	8.3
1	G	54	LEU	8.2
1	A	95	ASP	8.0
1	G	73	LYS	7.9
1	A	116	ILE	7.9
1	H	53	CYS	7.9
1	A	23	LEU	7.9
1	C	257	MET	7.8
1	E	128	GLU	7.8
1	A	115	TYR	7.8
1	H	102	LEU	7.7
1	H	112	GLY	7.7
1	H	54	LEU	7.6
1	G	92	VAL	7.6
1	B	71	GLN	7.6
1	D	128	GLU	7.6
1	H	212	ASN	7.5
1	D	248	THR	7.4
1	A	102	LEU	7.4
1	A	113	SER	7.3
1	H	88	ALA	7.3
1	D	53	CYS	7.2
1	A	97	LYS	7.2
1	G	116	ILE	7.2
1	A	55	TYR	7.2
1	E	249	LEU	7.1
1	B	55	TYR	7.1
1	H	129	PHE	7.0
1	A	227	ILE	7.0
1	A	150	SER	6.9
1	H	169	GLY	6.9
1	H	96	ALA	6.9
1	D	302	SER	6.9
1	D	191	PRO	6.7
1	E	190	GLN	6.6
1	A	283	GLU	6.6
1	A	198	THR	6.6
1	G	55	TYR	6.5
1	F	191	PRO	6.5
1	H	149	ILE	6.5
1	G	94	VAL	6.4
1	H	92	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	LEU	6.4
1	F	108	PHE	6.4
1	F	315	VAL	6.4
1	G	53	CYS	6.3
1	C	71	GLN	6.3
1	H	302	SER	6.2
1	D	71	GLN	6.2
1	E	192	TYR	6.2
1	G	93	MET	6.2
1	A	149	ILE	6.2
1	H	44	GLN	6.2
1	D	192	TYR	6.1
1	D	90	GLY	6.1
1	D	256	GLU	6.0
1	F	128	GLU	6.0
1	H	226	ALA	6.0
1	B	94	VAL	6.0
1	F	318	TRP	6.0
1	C	269	HIS	6.0
1	H	215	ASP	6.0
1	D	102	LEU	5.9
1	G	70	PHE	5.9
1	A	216	PHE	5.9
1	A	117	LEU	5.9
1	H	248	THR	5.8
1	D	91	PHE	5.8
1	E	108	PHE	5.8
1	H	168	ILE	5.8
1	A	355	ALA	5.7
1	A	225	ILE	5.7
1	G	56	TYR	5.7
1	E	226	ALA	5.7
1	F	94	VAL	5.7
1	C	37	LEU	5.7
1	H	283	GLU	5.7
1	D	324	ILE	5.7
1	H	55	TYR	5.7
1	D	74	GLU	5.7
1	E	193	ILE	5.7
1	B	92	VAL	5.6
1	E	367	SER	5.6
1	A	301	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	214	VAL	5.6
1	H	296	THR	5.5
1	C	94	VAL	5.5
1	C	334	VAL	5.5
1	G	114	LEU	5.5
1	C	258	PHE	5.5
1	F	192	TYR	5.5
1	C	54	LEU	5.4
1	E	191	PRO	5.4
1	B	23	LEU	5.4
1	B	96	ALA	5.4
1	B	149	ILE	5.4
1	D	268	ILE	5.4
1	C	192	TYR	5.4
1	H	198	THR	5.4
1	B	95	ASP	5.4
1	B	91	PHE	5.3
1	A	359	GLU	5.3
1	C	75	ILE	5.3
1	C	191	PRO	5.3
1	D	301	LEU	5.3
1	H	116	ILE	5.3
1	E	130	ALA	5.2
1	D	129	PHE	5.2
1	A	129	PHE	5.2
1	E	102	LEU	5.2
1	H	119	GLY	5.2
1	D	70	PHE	5.2
1	G	76	VAL	5.1
1	G	212	ASN	5.1
1	A	286	GLU	5.1
1	F	314	LEU	5.1
1	B	102	LEU	5.1
1	C	91	PHE	5.1
1	G	102	LEU	5.1
1	H	237	LEU	5.1
1	E	141	LEU	5.1
1	C	333	VAL	5.1
1	E	131	ALA	5.1
1	D	42	PHE	5.1
1	F	257	MET	5.0
1	D	125	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	129	PHE	5.0
1	C	318	TRP	5.0
1	D	39	GLU	5.0
1	F	95	ASP	5.0
1	B	114	LEU	5.0
1	B	54	LEU	4.9
1	A	132	ASP	4.9
1	E	109	ASP	4.9
1	E	41	ASN	4.9
1	D	249	LEU	4.9
1	A	125	PHE	4.9
1	H	301	LEU	4.9
1	H	117	LEU	4.9
1	B	38	SER	4.9
1	B	196	PHE	4.9
1	G	52	LEU	4.9
1	H	56	TYR	4.9
1	A	100	ALA	4.9
1	A	358	LEU	4.9
1	A	303	ILE	4.9
1	F	190	GLN	4.9
1	B	116	ILE	4.9
1	F	50	ASP	4.8
1	A	112	GLY	4.8
1	E	40	LYS	4.8
1	F	107	GLY	4.8
1	E	366	LEU	4.8
1	A	248	THR	4.8
1	D	73	LYS	4.8
1	D	226	ALA	4.8
1	D	130	ALA	4.8
1	A	123	ILE	4.8
1	A	91	PHE	4.8
1	A	357	GLU	4.7
1	B	106	LEU	4.7
1	E	292	ALA	4.7
1	A	295	ASN	4.7
1	B	72	LEU	4.7
1	A	39	GLU	4.7
1	A	339	ALA	4.7
1	G	115	TYR	4.7
1	D	88	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	313	LEU	4.7
1	B	354	THR	4.7
1	H	99	GLU	4.7
1	D	250	ARG	4.7
1	H	216	PHE	4.6
1	H	303	ILE	4.6
1	D	54	LEU	4.6
1	B	361	TRP	4.6
1	C	53	CYS	4.6
1	B	99	GLU	4.6
1	A	136	GLU	4.5
1	G	77	LEU	4.5
1	H	52	LEU	4.5
1	E	149	ILE	4.5
1	A	53	CYS	4.5
1	C	324	ILE	4.5
1	H	23	LEU	4.5
1	D	215	ASP	4.5
1	H	245	GLN	4.5
1	A	302	SER	4.5
1	E	296	THR	4.5
1	G	74	GLU	4.4
1	D	141	LEU	4.4
1	D	194	LYS	4.4
1	H	238	VAL	4.4
1	C	38	SER	4.4
1	H	151	SER	4.4
1	H	163	ASP	4.4
1	G	117	LEU	4.4
1	B	318	TRP	4.4
1	D	106	LEU	4.4
1	D	227	ILE	4.3
1	C	125	PHE	4.3
1	E	103	ALA	4.3
1	A	84	LEU	4.3
1	F	26	PRO	4.3
1	B	197	ALA	4.3
1	D	89	ILE	4.3
1	H	43	LYS	4.2
1	F	333	VAL	4.2
1	B	370	ILE	4.2
1	F	92	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	194	LYS	4.2
1	H	337	THR	4.2
1	D	298	ASN	4.2
1	E	295	ASN	4.2
1	H	217	TYR	4.2
1	A	298	ASN	4.2
1	E	50	ASP	4.1
1	C	55	TYR	4.1
1	D	50	ASP	4.1
1	F	245	GLN	4.1
1	E	250	ARG	4.1
1	A	94	VAL	4.1
1	E	370	ILE	4.1
1	F	37	LEU	4.1
1	D	96	ALA	4.1
1	D	72	LEU	4.1
1	H	160	ARG	4.1
1	E	23	LEU	4.0
1	D	316	ALA	4.0
1	H	249	LEU	4.0
1	G	176	SER	4.0
1	D	114	LEU	4.0
1	B	70	PHE	4.0
1	A	217	TYR	4.0
1	A	249	LEU	4.0
1	B	93	MET	4.0
1	G	217	TYR	4.0
1	C	82	GLN	4.0
1	E	123	ILE	4.0
1	E	161	ILE	4.0
1	A	354	THR	4.0
1	A	168	ILE	3.9
1	A	284	PHE	3.9
1	B	332	GLY	3.9
1	C	126	ASP	3.9
1	G	95	ASP	3.9
1	H	111	GLU	3.9
1	A	87	LYS	3.9
1	F	337	THR	3.9
1	D	161	ILE	3.9
1	H	355	ALA	3.9
1	A	88	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	145	PRO	3.9
1	A	141	LEU	3.9
1	A	257	MET	3.9
1	G	241	VAL	3.9
1	F	91	PHE	3.9
1	B	84	LEU	3.9
1	C	313	LEU	3.9
1	E	368	GLY	3.8
1	E	160	ARG	3.8
1	B	284	PHE	3.8
1	A	154	GLU	3.8
1	G	169	GLY	3.8
1	A	352	LEU	3.8
1	B	117	LEU	3.8
1	D	52	LEU	3.8
1	D	269	HIS	3.8
1	C	72	LEU	3.8
1	A	197	ALA	3.8
1	F	193	ILE	3.8
1	H	89	ILE	3.8
1	A	332	GLY	3.8
1	A	368	GLY	3.8
1	F	112	GLY	3.8
1	E	198	THR	3.8
1	E	227	ILE	3.8
1	G	257	MET	3.8
1	C	190	GLN	3.8
1	C	325	ASP	3.8
1	A	44	GLN	3.8
1	D	137	PHE	3.8
1	F	322	PHE	3.7
1	A	289	LYS	3.7
1	G	72	LEU	3.7
1	F	103	ALA	3.7
1	D	131	ALA	3.7
1	F	366	LEU	3.7
1	D	244	HIS	3.7
1	B	241	VAL	3.7
1	C	76	VAL	3.7
1	D	121	ARG	3.7
1	E	365	VAL	3.7
1	D	150	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	315	VAL	3.7
1	D	369	LYS	3.7
1	C	102	LEU	3.7
1	G	168	ILE	3.7
1	B	52	LEU	3.7
1	A	24	ASN	3.7
1	F	342	VAL	3.7
1	G	167	LEU	3.7
1	H	91	PHE	3.6
1	H	232	TYR	3.6
1	H	165	ILE	3.6
1	G	222	ASP	3.6
1	E	333	VAL	3.6
1	H	73	LYS	3.6
1	B	74	GLU	3.6
1	C	147	GLU	3.6
1	A	241	VAL	3.6
1	C	33	ARG	3.6
1	A	99	GLU	3.6
1	C	149	ILE	3.6
1	C	317	TYR	3.6
1	H	213	GLU	3.6
1	H	76	VAL	3.6
1	D	368	GLY	3.6
1	E	324	ILE	3.6
1	H	39	GLU	3.6
1	D	76	VAL	3.6
1	D	123	ILE	3.6
1	G	245	GLN	3.6
1	C	36	SER	3.6
1	E	182	PHE	3.6
1	A	52	LEU	3.6
1	B	245	GLN	3.6
1	C	120	ASP	3.6
1	H	167	LEU	3.6
1	E	113	SER	3.5
1	D	313	LEU	3.5
1	H	220	PHE	3.5
1	B	244	HIS	3.5
1	A	240	PHE	3.5
1	C	197	ALA	3.5
1	A	119	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	93	MET	3.5
1	C	312	PRO	3.5
1	H	80	VAL	3.5
1	D	303	ILE	3.5
1	H	171	PHE	3.5
1	H	49	TYR	3.5
1	E	97	LYS	3.5
1	H	132	ASP	3.5
1	B	353	PRO	3.5
1	E	313	LEU	3.5
1	H	257	MET	3.5
1	H	97	LYS	3.5
1	E	254	PRO	3.5
1	H	288	LEU	3.5
1	E	96	ALA	3.5
1	D	120	ASP	3.4
1	C	130	ALA	3.4
1	D	299	PRO	3.4
1	B	115	TYR	3.4
1	F	248	THR	3.4
1	G	237	LEU	3.4
1	B	317	TYR	3.4
1	H	94	VAL	3.4
1	B	331	ILE	3.4
1	C	196	PHE	3.4
1	D	136	GLU	3.4
1	B	312	PRO	3.4
1	H	154	GLU	3.4
1	E	305	TRP	3.4
1	D	169	GLY	3.4
1	E	203	VAL	3.4
1	C	347	PRO	3.4
1	C	134	LEU	3.4
1	E	252	LEU	3.4
1	G	343	TRP	3.4
1	B	215	ASP	3.4
1	E	369	LYS	3.4
1	A	285	LEU	3.4
1	E	83	VAL	3.4
1	E	195	PHE	3.4
1	G	149	ILE	3.4
1	H	123	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	298	ASN	3.4
1	A	362	ILE	3.4
1	D	198	THR	3.3
1	F	131	ALA	3.3
1	G	355	ALA	3.3
1	A	160	ARG	3.3
1	B	150	SER	3.3
1	H	90	GLY	3.3
1	A	268	ILE	3.3
1	C	343	TRP	3.3
1	G	332	GLY	3.3
1	F	269	HIS	3.3
1	E	167	LEU	3.3
1	D	122	THR	3.3
1	H	106	LEU	3.3
1	E	268	ILE	3.3
1	B	125	PHE	3.3
1	C	323	LYS	3.3
1	H	225	ILE	3.3
1	B	222	ASP	3.3
1	C	268	ILE	3.3
1	B	168	ILE	3.3
1	H	48	LYS	3.3
1	G	313	LEU	3.3
1	A	213	GLU	3.3
1	C	250	ARG	3.3
1	D	222	ASP	3.3
1	A	101	LYS	3.3
1	A	42	PHE	3.3
1	D	193	ILE	3.3
1	E	312	PRO	3.2
1	F	341	SER	3.2
1	F	335	ASN	3.2
1	E	362	ILE	3.2
1	B	56	TYR	3.2
1	E	215	ASP	3.2
1	D	367	SER	3.2
1	A	287	ILE	3.2
1	H	162	GLU	3.2
1	B	216	PHE	3.2
1	E	339	ALA	3.2
1	F	249	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	115	TYR	3.2
1	A	288	LEU	3.2
1	F	250	ARG	3.2
1	A	89	ILE	3.2
1	G	129	PHE	3.2
1	A	361	TRP	3.2
1	E	122	THR	3.2
1	B	128	GLU	3.2
1	D	214	VAL	3.2
1	H	196	PHE	3.2
1	G	287	ILE	3.2
1	G	215	ASP	3.2
1	A	106	LEU	3.2
1	C	314	LEU	3.2
1	B	69	GLN	3.1
1	D	41	ASN	3.1
1	A	279	PRO	3.1
1	F	33	ARG	3.1
1	H	95	ASP	3.1
1	H	282	TYR	3.1
1	F	141	LEU	3.1
1	E	189	PHE	3.1
1	B	77	LEU	3.1
1	C	249	LEU	3.1
1	C	326	LEU	3.1
1	D	220	PHE	3.1
1	G	274	ALA	3.1
1	B	34	VAL	3.1
1	G	196	PHE	3.1
1	E	110	GLU	3.1
1	A	118	LYS	3.1
1	D	126	ASP	3.1
1	D	162	GLU	3.1
1	F	99	GLU	3.1
1	A	254	PRO	3.1
1	C	70	PHE	3.1
1	D	216	PHE	3.1
1	H	30	GLY	3.1
1	A	271	VAL	3.1
1	C	316	ALA	3.1
1	D	334	VAL	3.1
1	G	69	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	229	ASN	3.0
1	D	279	PRO	3.0
1	D	333	VAL	3.0
1	B	330	GLN	3.0
1	C	108	PHE	3.0
1	E	158	PHE	3.0
1	E	91	PHE	3.0
1	H	224	PRO	3.0
1	B	53	CYS	3.0
1	A	296	THR	3.0
1	A	369	LYS	3.0
1	D	116	ILE	3.0
1	H	103	ALA	3.0
1	B	357	GLU	3.0
1	H	42	PHE	3.0
1	A	223	GLU	3.0
1	F	34	VAL	3.0
1	F	102	LEU	3.0
1	C	322	PHE	3.0
1	F	147	GLU	3.0
1	F	331	ILE	3.0
1	D	77	LEU	3.0
1	A	92	VAL	3.0
1	F	317	TYR	3.0
1	G	108	PHE	3.0
1	H	197	ALA	3.0
1	C	161	ILE	3.0
1	H	273	PHE	3.0
1	C	90	GLY	2.9
1	B	141	LEU	2.9
1	F	199	PHE	2.9
1	B	287	ILE	2.9
1	C	256	GLU	2.9
1	E	26	PRO	2.9
1	E	299	PRO	2.9
1	G	99	GLU	2.9
1	H	177	GLU	2.9
1	H	125	PHE	2.9
1	H	284	PHE	2.9
1	C	86	HIS	2.9
1	B	123	ILE	2.9
1	E	256	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	92	VAL	2.9
1	B	355	ALA	2.9
1	C	131	ALA	2.9
1	G	175	ASP	2.9
1	H	289	LYS	2.9
1	F	96	ALA	2.9
1	H	31	LYS	2.9
1	A	270	ILE	2.9
1	E	106	LEU	2.9
1	D	315	VAL	2.9
1	G	232	TYR	2.9
1	B	37	LEU	2.9
1	H	158	PHE	2.9
1	D	135	VAL	2.9
1	H	214	VAL	2.9
1	F	312	PRO	2.9
1	G	223	GLU	2.9
1	A	105	LYS	2.9
1	E	269	HIS	2.9
1	A	90	GLY	2.9
1	B	288	LEU	2.9
1	G	361	TRP	2.9
1	H	352	LEU	2.9
1	F	279	PRO	2.9
1	H	313	LEU	2.8
1	F	127	GLY	2.8
1	G	331	ILE	2.8
1	C	304	LEU	2.8
1	E	38	SER	2.8
1	A	337	THR	2.8
1	B	352	LEU	2.8
1	C	69	GLN	2.8
1	C	270	ILE	2.8
1	C	329	PRO	2.8
1	E	199	PHE	2.8
1	G	284	PHE	2.8
1	H	370	ILE	2.8
1	A	73	LYS	2.8
1	E	214	VAL	2.8
1	B	73	LYS	2.8
1	D	79	LEU	2.8
1	D	139	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	74	GLU	2.8
1	B	169	GLY	2.8
1	C	39	GLU	2.8
1	F	56	TYR	2.8
1	F	334	VAL	2.8
1	H	241	VAL	2.8
1	A	122	THR	2.8
1	F	189	PHE	2.8
1	G	353	PRO	2.8
1	E	255	GLU	2.8
1	E	274	ALA	2.8
1	F	332	GLY	2.8
1	F	316	ALA	2.8
1	C	137	PHE	2.8
1	D	103	ALA	2.8
1	F	252	LEU	2.8
1	C	35	VAL	2.7
1	H	227	ILE	2.7
1	A	220	PHE	2.7
1	B	343	TRP	2.7
1	F	106	LEU	2.7
1	B	249	LEU	2.7
1	E	42	PHE	2.7
1	B	103	ALA	2.7
1	F	326	LEU	2.7
1	C	85	GLU	2.7
1	H	28	TYR	2.7
1	H	108	PHE	2.7
1	E	245	GLN	2.7
1	A	367	SER	2.7
1	C	114	LEU	2.7
1	F	158	PHE	2.7
1	G	91	PHE	2.7
1	H	148	ILE	2.7
1	E	288	LEU	2.7
1	H	87	LYS	2.7
1	F	270	ILE	2.7
1	G	288	LEU	2.7
1	G	270	ILE	2.7
1	D	159	GLU	2.7
1	E	79	LEU	2.7
1	C	135	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	135	VAL	2.7
1	B	24	ASN	2.7
1	B	217	TYR	2.7
1	F	365	VAL	2.7
1	H	131	ALA	2.7
1	H	223	GLU	2.7
1	H	203	VAL	2.7
1	B	98	LYS	2.7
1	D	326	LEU	2.7
1	H	128	GLU	2.7
1	B	335	ASN	2.7
1	A	251	ARG	2.7
1	D	189	PHE	2.7
1	F	244	HIS	2.7
1	E	337	THR	2.7
1	B	371	ASN	2.7
1	B	194	LYS	2.7
1	D	132	ASP	2.7
1	F	38	SER	2.7
1	D	212	ASN	2.7
1	H	166	LYS	2.7
1	H	322	PHE	2.7
1	A	370	ILE	2.6
1	C	148	ILE	2.6
1	F	330	GLN	2.6
1	C	284	PHE	2.6
1	G	37	LEU	2.6
1	C	370	ILE	2.6
1	C	73	LYS	2.6
1	C	167	LEU	2.6
1	F	254	PRO	2.6
1	A	163	ASP	2.6
1	D	255	GLU	2.6
1	E	39	GLU	2.6
1	G	29	ASP	2.6
1	G	283	GLU	2.6
1	F	324	ILE	2.6
1	H	362	ILE	2.6
1	A	77	LEU	2.6
1	D	312	PRO	2.6
1	F	298	ASN	2.6
1	A	74	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	237	LEU	2.6
1	A	45	VAL	2.6
1	B	131	ALA	2.6
1	E	216	PHE	2.6
1	E	346	ILE	2.6
1	A	108	PHE	2.6
1	A	293	ARG	2.6
1	B	39	GLU	2.6
1	E	253	ARG	2.6
1	A	331	ILE	2.6
1	E	116	ILE	2.6
1	F	168	ILE	2.6
1	B	50	ASP	2.6
1	D	241	VAL	2.6
1	D	325	ASP	2.6
1	A	43	LYS	2.6
1	H	141	LEU	2.6
1	C	42	PHE	2.6
1	F	200	ASP	2.6
1	C	157	ALA	2.6
1	E	282	TYR	2.5
1	B	132	ASP	2.5
1	D	156	GLN	2.5
1	G	103	ALA	2.5
1	E	279	PRO	2.5
1	C	141	LEU	2.5
1	G	38	SER	2.5
1	E	129	PHE	2.5
1	G	349	ASP	2.5
1	D	108	PHE	2.5
1	E	84	LEU	2.5
1	G	358	LEU	2.5
1	D	26	PRO	2.5
1	F	343	TRP	2.5
1	H	156	GLN	2.5
1	A	137	PHE	2.5
1	E	166	LYS	2.5
1	B	225	ILE	2.5
1	G	148	ILE	2.5
1	B	33	ARG	2.5
1	B	337	THR	2.5
1	C	342	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	245	GLN	2.5
1	E	171	PHE	2.5
1	D	163	ASP	2.5
1	G	164	TYR	2.5
1	H	358	LEU	2.5
1	H	155	VAL	2.5
1	G	200	ASP	2.4
1	A	237	LEU	2.4
1	G	134	LEU	2.4
1	B	270	ILE	2.4
1	A	239	GLU	2.4
1	G	39	GLU	2.4
1	G	197	ALA	2.4
1	F	255	GLU	2.4
1	H	164	TYR	2.4
1	G	166	LYS	2.4
1	E	303	ILE	2.4
1	G	220	PHE	2.4
1	A	165	ILE	2.4
1	A	299	PRO	2.4
1	F	161	ILE	2.4
1	F	222	ASP	2.4
1	A	305	TRP	2.4
1	E	343	TRP	2.4
1	A	80	VAL	2.4
1	A	147	GLU	2.4
1	F	241	VAL	2.4
1	G	105	LYS	2.4
1	H	287	ILE	2.4
1	B	226	ALA	2.4
1	F	284	PHE	2.4
1	B	237	LEU	2.4
1	H	211	MET	2.4
1	H	312	PRO	2.4
1	C	31	LYS	2.4
1	H	51	LEU	2.4
1	C	371	ASN	2.4
1	D	119	GLY	2.4
1	E	316	ALA	2.4
1	G	233	THR	2.4
1	H	157	ALA	2.4
1	G	249	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	154	GLU	2.4
1	D	188	HIS	2.4
1	G	71	GLN	2.4
1	C	303	ILE	2.4
1	D	118	LYS	2.4
1	C	51	LEU	2.4
1	F	69	GLN	2.4
1	A	182	PHE	2.4
1	E	76	VAL	2.4
1	C	123	ILE	2.4
1	F	283	GLU	2.4
1	F	329	PRO	2.4
1	G	195	PHE	2.4
1	D	300	ASP	2.4
1	F	363	GLU	2.4
1	C	169	GLY	2.4
1	C	332	GLY	2.4
1	D	160	ARG	2.4
1	H	46	LEU	2.4
1	C	327	PHE	2.4
1	F	55	TYR	2.4
1	G	163	ASP	2.4
1	F	347	PRO	2.3
1	G	312	PRO	2.3
1	D	51	LEU	2.3
1	C	116	ILE	2.3
1	E	132	ASP	2.3
1	F	370	ILE	2.3
1	B	211	MET	2.3
1	B	127	GLY	2.3
1	C	198	THR	2.3
1	D	358	LEU	2.3
1	A	244	HIS	2.3
1	B	285	LEU	2.3
1	D	43	LYS	2.3
1	G	338	ASP	2.3
1	H	331	ILE	2.3
1	H	24	ASN	2.3
1	F	274	ALA	2.3
1	F	296	THR	2.3
1	B	291	VAL	2.3
1	C	302	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	169	GLY	2.3
1	D	322	PHE	2.3
1	C	34	VAL	2.3
1	D	37	LEU	2.3
1	A	304	LEU	2.3
1	H	365	VAL	2.3
1	F	362	ILE	2.3
1	F	210	LYS	2.3
1	B	240	PHE	2.3
1	H	293	ARG	2.3
1	B	76	VAL	2.3
1	D	314	LEU	2.3
1	E	358	LEU	2.3
1	G	34	VAL	2.3
1	D	196	PHE	2.3
1	D	75	ILE	2.3
1	H	347	PRO	2.3
1	A	103	ALA	2.3
1	A	272	ALA	2.3
1	H	118	LYS	2.3
1	B	90	GLY	2.3
1	C	56	TYR	2.3
1	C	220	PHE	2.3
1	A	335	ASN	2.2
1	D	343	TRP	2.2
1	A	356	GLU	2.2
1	B	275	GLU	2.2
1	D	34	VAL	2.2
1	G	25	PHE	2.2
1	E	315	VAL	2.2
1	F	148	ILE	2.2
1	F	237	LEU	2.2
1	B	232	TYR	2.2
1	F	216	PHE	2.2
1	C	166	LYS	2.2
1	G	23	LEU	2.2
1	H	84	LEU	2.2
1	H	130	ALA	2.2
1	G	24	ASN	2.2
1	A	224	PRO	2.2
1	G	339	ALA	2.2
1	E	104	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	164	TYR	2.2
1	A	238	VAL	2.2
1	E	112	GLY	2.2
1	B	339	ALA	2.2
1	D	199	PHE	2.2
1	D	167	LEU	2.2
1	B	201	LYS	2.2
1	G	244	HIS	2.2
1	G	254	PRO	2.2
1	H	50	ASP	2.2
1	H	72	LEU	2.2
1	A	49	TYR	2.2
1	B	220	PHE	2.2
1	E	328	ARG	2.2
1	C	295	ASN	2.2
1	F	82	GLN	2.2
1	B	338	ASP	2.2
1	D	133	VAL	2.2
1	E	80	VAL	2.2
1	H	353	PRO	2.2
1	D	166	LYS	2.2
1	C	50	ASP	2.2
1	D	100	ALA	2.2
1	B	358	LEU	2.2
1	F	167	LEU	2.2
1	G	250	ARG	2.2
1	G	158	PHE	2.2
1	C	367	SER	2.2
1	G	131	ALA	2.2
1	E	133	VAL	2.2
1	B	362	ILE	2.2
1	F	258	PHE	2.2
1	F	134	LEU	2.2
1	G	214	VAL	2.2
1	C	255	GLU	2.2
1	E	148	ILE	2.2
1	F	25	PHE	2.2
1	F	361	TRP	2.2
1	H	25	PHE	2.2
1	F	100	ALA	2.1
1	D	304	LEU	2.1
1	H	101	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	305	TRP	2.1
1	E	165	ILE	2.1
1	F	273	PHE	2.1
1	H	292	ALA	2.1
1	G	51	LEU	2.1
1	G	27	THR	2.1
1	H	38	SER	2.1
1	D	213	GLU	2.1
1	C	365	VAL	2.1
1	G	150	SER	2.1
1	H	161	ILE	2.1
1	A	72	LEU	2.1
1	E	347	PRO	2.1
1	E	56	TYR	2.1
1	G	285	LEU	2.1
1	E	168	ILE	2.1
1	H	107	GLY	2.1
1	A	131	ALA	2.1
1	A	70	PHE	2.1
1	F	70	PHE	2.1
1	E	319	GLU	2.1
1	G	146	VAL	2.1
1	D	195	PHE	2.1
1	F	247	PRO	2.1
1	E	126	ASP	2.1
1	F	76	VAL	2.1
1	A	40	LYS	2.1
1	A	232	TYR	2.1
1	F	196	PHE	2.1
1	A	50	ASP	2.1
1	A	37	LEU	2.1
1	E	134	LEU	2.1
1	D	31	LYS	2.1
1	E	98	LYS	2.1
1	A	109	ASP	2.1
1	B	334	VAL	2.1
1	B	320	LYS	2.1
1	D	225	ILE	2.1
1	D	38	SER	2.1
1	C	77	LEU	2.1
1	E	89	ILE	2.1
1	C	159	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	138	LEU	2.1
1	E	342	VAL	2.1
1	A	292	ALA	2.1
1	A	317	TYR	2.1
1	C	288	LEU	2.1
1	E	341	SER	2.1
1	H	233	THR	2.1
1	F	253	ARG	2.1
1	B	134	LEU	2.0
1	F	41	ASN	2.0
1	F	297	ASP	2.0
1	C	41	ASN	2.0
1	A	228	PRO	2.0
1	A	76	VAL	2.0
1	B	326	LEU	2.0
1	C	248	THR	2.0
1	F	51	LEU	2.0
1	D	149	ILE	2.0
1	E	247	PRO	2.0
1	H	142	ILE	2.0
1	C	150	SER	2.0
1	G	35	VAL	2.0
1	G	106	LEU	2.0
1	G	198	THR	2.0
1	B	274	ALA	2.0
1	F	292	ALA	2.0
1	C	358	LEU	2.0
1	H	206	LYS	2.0
1	D	127	GLY	2.0
1	D	319	GLU	2.0
1	H	336	VAL	2.0
1	A	189	PHE	2.0
1	H	346	ILE	2.0
1	D	117	LEU	2.0
1	F	104	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	YB	Y	15	1/?	0.48	0.14	133,133,133,133	1
2	YB	Y	42	1/?	0.52	0.16	115,115,115,115	1
2	YB	Y	47	1/?	0.58	0.10	202,202,202,202	0
2	YB	Y	24	1/?	0.59	0.10	124,124,124,124	1
3	SO4	I	1	5/?	0.68	0.61	119,129,144,148	0
2	YB	Y	83	1/?	0.69	0.14	94,94,94,94	1
2	YB	Y	34	1/?	0.71	0.17	129,129,129,129	1
2	YB	Y	51	1/?	0.72	0.14	88,88,88,88	1
2	YB	Y	10	1/?	0.73	0.08	165,165,165,165	1
2	YB	Y	38	1/?	0.74	0.17	159,159,159,159	0
3	SO4	I	3	5/?	0.75	0.23	105,113,123,123	0
2	YB	Y	41	1/?	0.75	0.17	100,100,100,100	1
2	YB	Y	20	1/?	0.76	0.16	129,129,129,129	1
2	YB	Y	14	1/?	0.76	0.11	135,135,135,135	1
2	YB	Y	76	1/?	0.76	0.15	105,105,105,105	1
2	YB	Y	85	1/?	0.77	0.12	307,307,307,307	0
2	YB	Y	27	1/?	0.77	0.19	111,111,111,111	1
2	YB	Y	40	1/?	0.78	0.07	149,149,149,149	1
2	YB	Y	37	1/?	0.78	0.27	116,116,116,116	1
3	SO4	I	5	5/?	0.78	0.53	112,121,124,127	0
2	YB	Y	35	1/?	0.78	0.12	182,182,182,182	1
2	YB	Y	57	1/?	0.78	0.17	120,120,120,120	1
2	YB	Y	23	1/?	0.79	0.05	184,184,184,184	0
2	YB	Y	87	1/?	0.79	0.17	347,347,347,347	1
2	YB	Y	77	1/?	0.79	0.10	97,97,97,97	1
2	YB	Y	13	1/?	0.81	0.07	149,149,149,149	1
2	YB	Y	33	1/?	0.81	0.09	170,170,170,170	0
2	YB	Y	11	1/?	0.81	0.13	130,130,130,130	1
2	YB	Y	80	1/?	0.81	0.18	184,184,184,184	1
2	YB	Y	16	1/?	0.82	0.16	123,123,123,123	1
2	YB	Y	82	1/?	0.82	0.31	169,169,169,169	1
2	YB	Y	18	1/?	0.83	0.16	120,120,120,120	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	YB	Y	12	1/?	0.84	0.11	134,134,134,134	1
2	YB	Y	84	1/?	0.84	0.17	325,325,325,325	1
2	YB	Y	7	1/?	0.85	0.19	149,149,149,149	1
2	YB	Y	6	1/?	0.85	0.14	127,127,127,127	0
2	YB	Y	78	1/?	0.85	0.26	116,116,116,116	1
2	YB	Y	75	1/?	0.85	0.17	130,130,130,130	1
3	SO4	I	2	5/?	0.85	0.20	99,100,111,111	0
2	YB	Y	49	1/?	0.85	0.14	115,115,115,115	1
2	YB	Y	73	1/?	0.85	0.19	109,109,109,109	1
2	YB	Y	9	1/?	0.86	0.08	148,148,148,148	1
2	YB	Y	55	1/?	0.87	0.12	123,123,123,123	1
2	YB	Y	86	1/?	0.87	0.14	315,315,315,315	0
2	YB	Y	30	1/?	0.87	0.11	161,161,161,161	0
3	SO4	I	4	5/?	0.87	0.17	100,107,113,117	0
2	YB	Y	2	1/?	0.87	0.13	165,165,165,165	0
2	YB	Y	32	1/?	0.88	0.11	166,166,166,166	1
2	YB	Y	53	1/?	0.88	0.16	100,100,100,100	1
2	YB	Y	54	1/?	0.88	0.16	85,85,85,85	1
2	YB	Y	26	1/?	0.90	0.07	150,150,150,150	1
2	YB	Y	4	1/?	0.90	0.11	153,153,153,153	1
2	YB	Y	45	1/?	0.91	0.09	160,160,160,160	0
2	YB	Y	1	1/?	0.91	0.13	142,142,142,142	0
2	YB	Y	28	1/?	0.91	0.27	122,122,122,122	1
2	YB	Y	48	1/?	0.91	0.22	92,92,92,92	1
2	YB	Y	3	1/?	0.92	0.13	134,134,134,134	0
2	YB	Y	36	1/?	0.92	0.09	94,94,94,94	1
2	YB	Y	5	1/?	0.93	0.17	158,158,158,158	1
2	YB	Y	70	1/?	0.93	0.21	137,137,137,137	1
2	YB	Y	21	1/?	0.93	0.09	162,162,162,162	0
2	YB	Y	22	1/?	0.93	0.07	130,130,130,130	1
2	YB	Y	31	1/?	0.93	0.17	129,129,129,129	1
2	YB	Y	8	1/?	0.94	0.19	157,157,157,157	1
2	YB	Y	29	1/?	0.94	0.06	92,92,92,92	1
2	YB	Y	19	1/?	0.95	0.11	161,161,161,161	1
2	YB	Y	17	1/?	0.96	0.19	115,115,115,115	1
2	YB	Y	81	1/?	0.96	0.14	130,130,130,130	1

6.5 Other polymers

There are no such residues in this entry.