



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 09:42 PM EDT

PDB ID : 2O1T
Title : Structure of Middle plus C-terminal domains (M+C) of GRP94
Authors : Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.
Deposited on : unknown
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

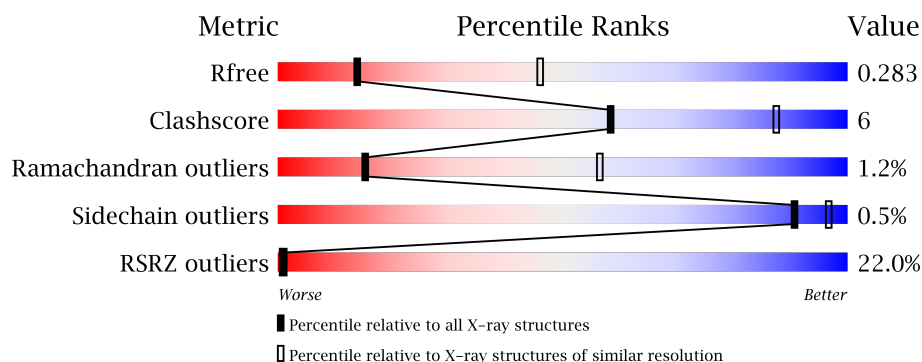
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




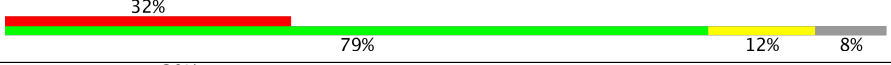
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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

Mol	Chain	Length	Quality of chain
1	A	450	
1	B	450	
1	C	450	
1	D	450	
1	E	450	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	450	
1	G	450	
1	H	450	
1	I	450	
1	J	450	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33009 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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	B	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	C	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	D	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	E	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	F	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	G	413	Total	C	N	O	S	0	0	0
			3300	2101	548	638	13			
1	H	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	I	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	J	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	MET	-	EXPRESSION TAG	UNP P41148
A	317	GLY	-	EXPRESSION TAG	UNP P41148
A	318	SER	-	EXPRESSION TAG	UNP P41148
A	319	SER	-	EXPRESSION TAG	UNP P41148
A	320	HIS	-	EXPRESSION TAG	UNP P41148
A	321	HIS	-	EXPRESSION TAG	UNP P41148
A	322	HIS	-	EXPRESSION TAG	UNP P41148
A	323	HIS	-	EXPRESSION TAG	UNP P41148
A	324	HIS	-	EXPRESSION TAG	UNP P41148

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	HIS	-	EXPRESSION TAG	UNP P41148
A	326	SER	-	EXPRESSION TAG	UNP P41148
A	327	SER	-	EXPRESSION TAG	UNP P41148
A	328	GLY	-	EXPRESSION TAG	UNP P41148
A	329	LEU	-	EXPRESSION TAG	UNP P41148
A	330	VAL	-	EXPRESSION TAG	UNP P41148
A	331	PRO	-	EXPRESSION TAG	UNP P41148
A	332	ARG	-	EXPRESSION TAG	UNP P41148
A	333	GLY	-	EXPRESSION TAG	UNP P41148
A	334	SER	-	EXPRESSION TAG	UNP P41148
A	335	HIS	-	EXPRESSION TAG	UNP P41148
B	316	MET	-	EXPRESSION TAG	UNP P41148
B	317	GLY	-	EXPRESSION TAG	UNP P41148
B	318	SER	-	EXPRESSION TAG	UNP P41148
B	319	SER	-	EXPRESSION TAG	UNP P41148
B	320	HIS	-	EXPRESSION TAG	UNP P41148
B	321	HIS	-	EXPRESSION TAG	UNP P41148
B	322	HIS	-	EXPRESSION TAG	UNP P41148
B	323	HIS	-	EXPRESSION TAG	UNP P41148
B	324	HIS	-	EXPRESSION TAG	UNP P41148
B	325	HIS	-	EXPRESSION TAG	UNP P41148
B	326	SER	-	EXPRESSION TAG	UNP P41148
B	327	SER	-	EXPRESSION TAG	UNP P41148
B	328	GLY	-	EXPRESSION TAG	UNP P41148
B	329	LEU	-	EXPRESSION TAG	UNP P41148
B	330	VAL	-	EXPRESSION TAG	UNP P41148
B	331	PRO	-	EXPRESSION TAG	UNP P41148
B	332	ARG	-	EXPRESSION TAG	UNP P41148
B	333	GLY	-	EXPRESSION TAG	UNP P41148
B	334	SER	-	EXPRESSION TAG	UNP P41148
B	335	HIS	-	EXPRESSION TAG	UNP P41148
C	316	MET	-	EXPRESSION TAG	UNP P41148
C	317	GLY	-	EXPRESSION TAG	UNP P41148
C	318	SER	-	EXPRESSION TAG	UNP P41148
C	319	SER	-	EXPRESSION TAG	UNP P41148
C	320	HIS	-	EXPRESSION TAG	UNP P41148
C	321	HIS	-	EXPRESSION TAG	UNP P41148
C	322	HIS	-	EXPRESSION TAG	UNP P41148
C	323	HIS	-	EXPRESSION TAG	UNP P41148
C	324	HIS	-	EXPRESSION TAG	UNP P41148
C	325	HIS	-	EXPRESSION TAG	UNP P41148
C	326	SER	-	EXPRESSION TAG	UNP P41148

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	327	SER	-	EXPRESSION TAG	UNP P41148
C	328	GLY	-	EXPRESSION TAG	UNP P41148
C	329	LEU	-	EXPRESSION TAG	UNP P41148
C	330	VAL	-	EXPRESSION TAG	UNP P41148
C	331	PRO	-	EXPRESSION TAG	UNP P41148
C	332	ARG	-	EXPRESSION TAG	UNP P41148
C	333	GLY	-	EXPRESSION TAG	UNP P41148
C	334	SER	-	EXPRESSION TAG	UNP P41148
C	335	HIS	-	EXPRESSION TAG	UNP P41148
D	316	MET	-	EXPRESSION TAG	UNP P41148
D	317	GLY	-	EXPRESSION TAG	UNP P41148
D	318	SER	-	EXPRESSION TAG	UNP P41148
D	319	SER	-	EXPRESSION TAG	UNP P41148
D	320	HIS	-	EXPRESSION TAG	UNP P41148
D	321	HIS	-	EXPRESSION TAG	UNP P41148
D	322	HIS	-	EXPRESSION TAG	UNP P41148
D	323	HIS	-	EXPRESSION TAG	UNP P41148
D	324	HIS	-	EXPRESSION TAG	UNP P41148
D	325	HIS	-	EXPRESSION TAG	UNP P41148
D	326	SER	-	EXPRESSION TAG	UNP P41148
D	327	SER	-	EXPRESSION TAG	UNP P41148
D	328	GLY	-	EXPRESSION TAG	UNP P41148
D	329	LEU	-	EXPRESSION TAG	UNP P41148
D	330	VAL	-	EXPRESSION TAG	UNP P41148
D	331	PRO	-	EXPRESSION TAG	UNP P41148
D	332	ARG	-	EXPRESSION TAG	UNP P41148
D	333	GLY	-	EXPRESSION TAG	UNP P41148
D	334	SER	-	EXPRESSION TAG	UNP P41148
D	335	HIS	-	EXPRESSION TAG	UNP P41148
E	316	MET	-	EXPRESSION TAG	UNP P41148
E	317	GLY	-	EXPRESSION TAG	UNP P41148
E	318	SER	-	EXPRESSION TAG	UNP P41148
E	319	SER	-	EXPRESSION TAG	UNP P41148
E	320	HIS	-	EXPRESSION TAG	UNP P41148
E	321	HIS	-	EXPRESSION TAG	UNP P41148
E	322	HIS	-	EXPRESSION TAG	UNP P41148
E	323	HIS	-	EXPRESSION TAG	UNP P41148
E	324	HIS	-	EXPRESSION TAG	UNP P41148
E	325	HIS	-	EXPRESSION TAG	UNP P41148
E	326	SER	-	EXPRESSION TAG	UNP P41148
E	327	SER	-	EXPRESSION TAG	UNP P41148
E	328	GLY	-	EXPRESSION TAG	UNP P41148

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	329	LEU	-	EXPRESSION TAG	UNP P41148
E	330	VAL	-	EXPRESSION TAG	UNP P41148
E	331	PRO	-	EXPRESSION TAG	UNP P41148
E	332	ARG	-	EXPRESSION TAG	UNP P41148
E	333	GLY	-	EXPRESSION TAG	UNP P41148
E	334	SER	-	EXPRESSION TAG	UNP P41148
E	335	HIS	-	EXPRESSION TAG	UNP P41148
F	316	MET	-	EXPRESSION TAG	UNP P41148
F	317	GLY	-	EXPRESSION TAG	UNP P41148
F	318	SER	-	EXPRESSION TAG	UNP P41148
F	319	SER	-	EXPRESSION TAG	UNP P41148
F	320	HIS	-	EXPRESSION TAG	UNP P41148
F	321	HIS	-	EXPRESSION TAG	UNP P41148
F	322	HIS	-	EXPRESSION TAG	UNP P41148
F	323	HIS	-	EXPRESSION TAG	UNP P41148
F	324	HIS	-	EXPRESSION TAG	UNP P41148
F	325	HIS	-	EXPRESSION TAG	UNP P41148
F	326	SER	-	EXPRESSION TAG	UNP P41148
F	327	SER	-	EXPRESSION TAG	UNP P41148
F	328	GLY	-	EXPRESSION TAG	UNP P41148
F	329	LEU	-	EXPRESSION TAG	UNP P41148
F	330	VAL	-	EXPRESSION TAG	UNP P41148
F	331	PRO	-	EXPRESSION TAG	UNP P41148
F	332	ARG	-	EXPRESSION TAG	UNP P41148
F	333	GLY	-	EXPRESSION TAG	UNP P41148
F	334	SER	-	EXPRESSION TAG	UNP P41148
F	335	HIS	-	EXPRESSION TAG	UNP P41148
G	316	MET	-	EXPRESSION TAG	UNP P41148
G	317	GLY	-	EXPRESSION TAG	UNP P41148
G	318	SER	-	EXPRESSION TAG	UNP P41148
G	319	SER	-	EXPRESSION TAG	UNP P41148
G	320	HIS	-	EXPRESSION TAG	UNP P41148
G	321	HIS	-	EXPRESSION TAG	UNP P41148
G	322	HIS	-	EXPRESSION TAG	UNP P41148
G	323	HIS	-	EXPRESSION TAG	UNP P41148
G	324	HIS	-	EXPRESSION TAG	UNP P41148
G	325	HIS	-	EXPRESSION TAG	UNP P41148
G	326	SER	-	EXPRESSION TAG	UNP P41148
G	327	SER	-	EXPRESSION TAG	UNP P41148
G	328	GLY	-	EXPRESSION TAG	UNP P41148
G	329	LEU	-	EXPRESSION TAG	UNP P41148
G	330	VAL	-	EXPRESSION TAG	UNP P41148

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	331	PRO	-	EXPRESSION TAG	UNP P41148
G	332	ARG	-	EXPRESSION TAG	UNP P41148
G	333	GLY	-	EXPRESSION TAG	UNP P41148
G	334	SER	-	EXPRESSION TAG	UNP P41148
G	335	HIS	-	EXPRESSION TAG	UNP P41148
H	316	MET	-	EXPRESSION TAG	UNP P41148
H	317	GLY	-	EXPRESSION TAG	UNP P41148
H	318	SER	-	EXPRESSION TAG	UNP P41148
H	319	SER	-	EXPRESSION TAG	UNP P41148
H	320	HIS	-	EXPRESSION TAG	UNP P41148
H	321	HIS	-	EXPRESSION TAG	UNP P41148
H	322	HIS	-	EXPRESSION TAG	UNP P41148
H	323	HIS	-	EXPRESSION TAG	UNP P41148
H	324	HIS	-	EXPRESSION TAG	UNP P41148
H	325	HIS	-	EXPRESSION TAG	UNP P41148
H	326	SER	-	EXPRESSION TAG	UNP P41148
H	327	SER	-	EXPRESSION TAG	UNP P41148
H	328	GLY	-	EXPRESSION TAG	UNP P41148
H	329	LEU	-	EXPRESSION TAG	UNP P41148
H	330	VAL	-	EXPRESSION TAG	UNP P41148
H	331	PRO	-	EXPRESSION TAG	UNP P41148
H	332	ARG	-	EXPRESSION TAG	UNP P41148
H	333	GLY	-	EXPRESSION TAG	UNP P41148
H	334	SER	-	EXPRESSION TAG	UNP P41148
H	335	HIS	-	EXPRESSION TAG	UNP P41148
I	316	MET	-	EXPRESSION TAG	UNP P41148
I	317	GLY	-	EXPRESSION TAG	UNP P41148
I	318	SER	-	EXPRESSION TAG	UNP P41148
I	319	SER	-	EXPRESSION TAG	UNP P41148
I	320	HIS	-	EXPRESSION TAG	UNP P41148
I	321	HIS	-	EXPRESSION TAG	UNP P41148
I	322	HIS	-	EXPRESSION TAG	UNP P41148
I	323	HIS	-	EXPRESSION TAG	UNP P41148
I	324	HIS	-	EXPRESSION TAG	UNP P41148
I	325	HIS	-	EXPRESSION TAG	UNP P41148
I	326	SER	-	EXPRESSION TAG	UNP P41148
I	327	SER	-	EXPRESSION TAG	UNP P41148
I	328	GLY	-	EXPRESSION TAG	UNP P41148
I	329	LEU	-	EXPRESSION TAG	UNP P41148
I	330	VAL	-	EXPRESSION TAG	UNP P41148
I	331	PRO	-	EXPRESSION TAG	UNP P41148
I	332	ARG	-	EXPRESSION TAG	UNP P41148

Continued on next page...

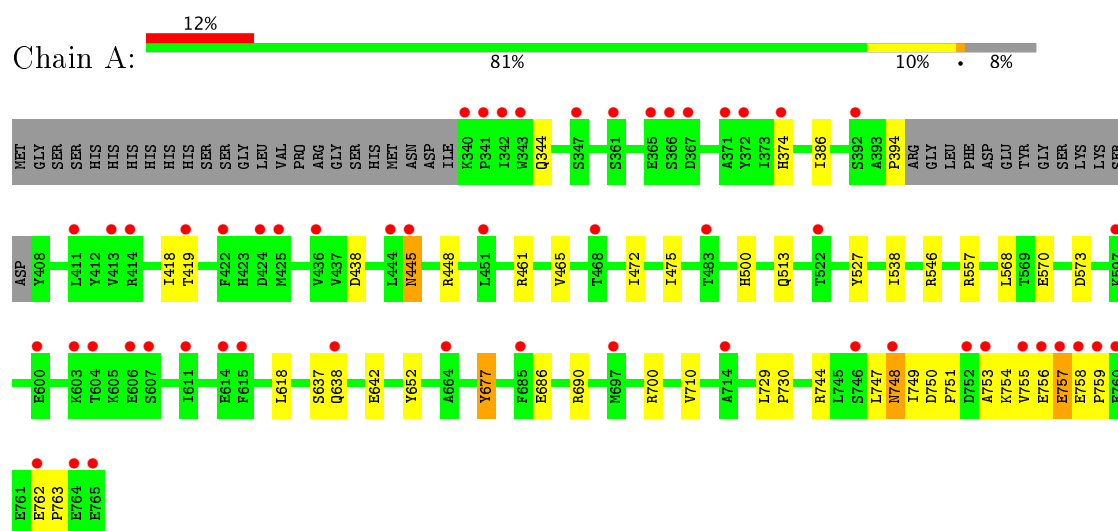
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	333	GLY	-	EXPRESSION TAG	UNP P41148
I	334	SER	-	EXPRESSION TAG	UNP P41148
I	335	HIS	-	EXPRESSION TAG	UNP P41148
J	316	MET	-	EXPRESSION TAG	UNP P41148
J	317	GLY	-	EXPRESSION TAG	UNP P41148
J	318	SER	-	EXPRESSION TAG	UNP P41148
J	319	SER	-	EXPRESSION TAG	UNP P41148
J	320	HIS	-	EXPRESSION TAG	UNP P41148
J	321	HIS	-	EXPRESSION TAG	UNP P41148
J	322	HIS	-	EXPRESSION TAG	UNP P41148
J	323	HIS	-	EXPRESSION TAG	UNP P41148
J	324	HIS	-	EXPRESSION TAG	UNP P41148
J	325	HIS	-	EXPRESSION TAG	UNP P41148
J	326	SER	-	EXPRESSION TAG	UNP P41148
J	327	SER	-	EXPRESSION TAG	UNP P41148
J	328	GLY	-	EXPRESSION TAG	UNP P41148
J	329	LEU	-	EXPRESSION TAG	UNP P41148
J	330	VAL	-	EXPRESSION TAG	UNP P41148
J	331	PRO	-	EXPRESSION TAG	UNP P41148
J	332	ARG	-	EXPRESSION TAG	UNP P41148
J	333	GLY	-	EXPRESSION TAG	UNP P41148
J	334	SER	-	EXPRESSION TAG	UNP P41148
J	335	HIS	-	EXPRESSION TAG	UNP P41148

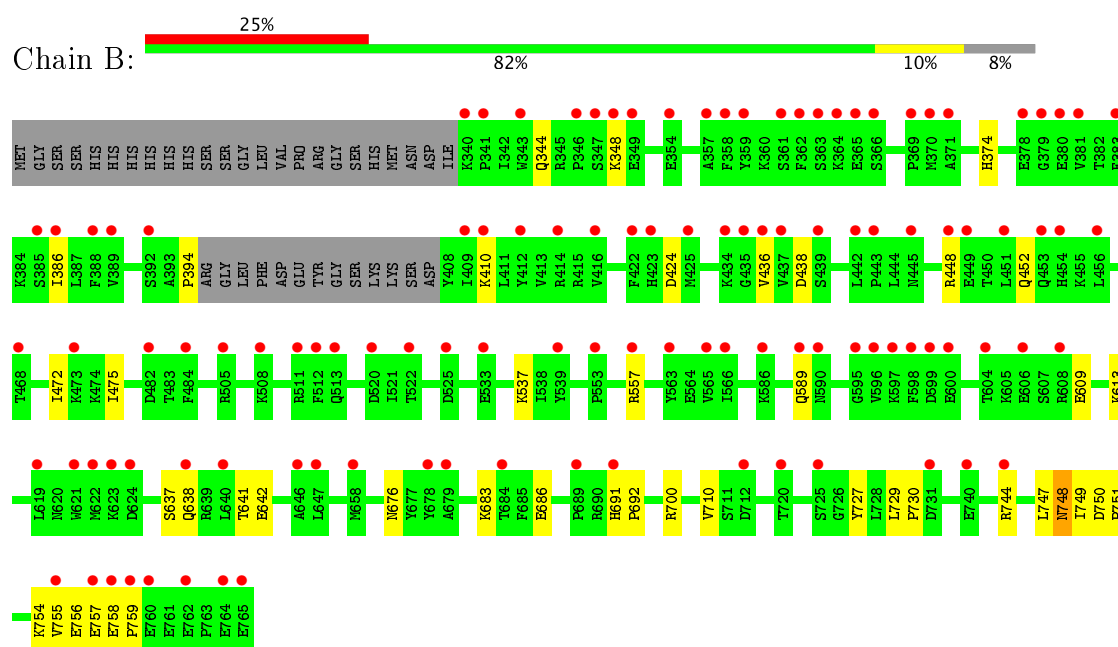
3 Residue-property plots [i](#)

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

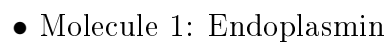
• Molecule 1: Endoplasmic



• Molecule 1: Endoplasmic



• Molecule 1: Endoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.30Å 129.54Å 184.78Å 90.00° 99.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 45.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.20) 99.6 (45.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.284 , 0.294 0.270 , 0.283	Depositor DCC
R_{free} test set	5004 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	109.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 163.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33009	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.54	1/3368 (0.0%)	0.68	2/4543 (0.0%)
1	B	0.37	0/3368	0.61	1/4543 (0.0%)
1	C	0.42	0/3368	0.64	1/4543 (0.0%)
1	D	0.43	0/3368	0.64	1/4543 (0.0%)
1	E	0.53	0/3368	0.68	1/4543 (0.0%)
1	F	0.51	0/3368	0.66	1/4543 (0.0%)
1	G	0.43	0/3366	0.65	2/4540 (0.0%)
1	H	0.36	0/3368	0.61	1/4543 (0.0%)
1	I	0.35	0/3368	0.62	1/4543 (0.0%)
1	J	0.48	0/3368	0.65	1/4543 (0.0%)
All	All	0.45	1/33678 (0.0%)	0.64	12/45427 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	TYR	CA-CB	-6.37	1.40	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	394	PRO	N-CA-CB	7.79	112.64	103.30
1	B	394	PRO	N-CA-CB	7.39	112.16	103.30
1	E	394	PRO	N-CA-CB	7.35	112.12	103.30
1	A	394	PRO	N-CA-CB	7.34	112.11	103.30
1	J	394	PRO	N-CA-CB	7.33	112.10	103.30
1	G	394	PRO	N-CA-CB	7.29	112.05	103.30
1	C	394	PRO	N-CA-CB	7.24	111.99	103.30
1	H	394	PRO	N-CA-CB	7.23	111.98	103.30
1	D	394	PRO	N-CA-CB	7.11	111.83	103.30
1	I	394	PRO	N-CA-CB	7.01	111.72	103.30
1	G	618	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	618	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3301	0	3196	44	4
1	B	3301	0	3196	25	0
1	C	3301	0	3196	40	0
1	D	3301	0	3196	51	1
1	E	3301	0	3196	69	1
1	F	3301	0	3196	59	5
1	G	3300	0	3194	47	1
1	H	3301	0	3196	36	0
1	I	3301	0	3196	29	2
1	J	3301	0	3196	62	0
All	All	33009	0	31958	360	7

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 6.

All (360) 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:757:GLU:OE2	1:J:677:TYR:HA	1.21	1.31
1:E:500:HIS:CE1	1:J:704:ASP:HB2	1.80	1.16
1:D:759:PRO:HD3	1:E:692:PRO:HD3	1.38	1.05
1:A:754:LYS:HD3	1:E:678:TYR:OH	1.61	1.00
1:C:757:GLU:OE2	1:J:677:TYR:CA	2.11	0.98
1:A:750:ASP:CG	1:E:652:TYR:HB2	1.84	0.97
1:F:652:TYR:CE2	1:J:756:GLU:CD	2.40	0.95
1:E:500:HIS:NE2	1:J:703:GLU:HB3	1.83	0.93
1:D:743:LEU:HD22	1:E:713:LEU:HG	1.52	0.91
1:C:757:GLU:CD	1:J:677:TYR:HA	1.91	0.90
1:E:500:HIS:HE1	1:J:704:ASP:HB2	1.39	0.87
1:C:754:LYS:HD3	1:J:678:TYR:CD2	2.10	0.85
1:H:692:PRO:HB3	1:I:754:LYS:HE3	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:743:LEU:HD22	1:G:713:LEU:HG	1.66	0.78
1:D:637:SER:HB2	1:D:686:GLU:HB3	1.66	0.78
1:F:637:SER:HB2	1:F:686:GLU:HB3	1.64	0.77
1:C:754:LYS:HD3	1:J:678:TYR:HD2	1.49	0.76
1:A:637:SER:HB2	1:A:686:GLU:HB3	1.68	0.75
1:I:637:SER:HB2	1:I:686:GLU:HB3	1.68	0.75
1:E:637:SER:HB2	1:E:686:GLU:HB3	1.68	0.75
1:H:637:SER:HB2	1:H:686:GLU:HB3	1.69	0.75
1:J:637:SER:HB2	1:J:686:GLU:HB3	1.69	0.74
1:B:637:SER:HB2	1:B:686:GLU:HB3	1.69	0.74
1:A:753:ALA:O	1:E:678:TYR:CE2	2.40	0.74
1:C:637:SER:HB2	1:C:686:GLU:HB3	1.69	0.73
1:D:758:GLU:HG3	1:E:695:LYS:HD3	1.73	0.71
1:A:642:GLU:HA	1:J:759:PRO:HB3	1.73	0.70
1:A:750:ASP:O	1:A:754:LYS:HB2	1.92	0.70
1:G:637:SER:HB2	1:G:686:GLU:HB3	1.74	0.69
1:C:750:ASP:O	1:C:754:LYS:HB2	1.92	0.69
1:D:750:ASP:HB3	1:D:754:LYS:HG2	1.75	0.68
1:E:750:ASP:O	1:E:754:LYS:HB2	1.93	0.68
1:A:750:ASP:CB	1:E:652:TYR:HB2	2.24	0.68
1:A:750:ASP:OD1	1:E:652:TYR:HB2	1.93	0.68
1:E:500:HIS:CD2	1:J:703:GLU:HB3	2.29	0.67
1:D:744:ARG:HG2	1:E:693:LEU:HD13	1.77	0.66
1:D:759:PRO:HD3	1:E:692:PRO:CD	2.22	0.65
1:D:742:MET:CE	1:E:742:MET:HE3	2.26	0.65
1:F:740:GLU:OE2	1:G:691:HIS:NE2	2.28	0.65
1:D:729:LEU:HD12	1:D:730:PRO:HD2	1.79	0.65
1:I:750:ASP:O	1:I:754:LYS:HB2	1.95	0.65
1:F:744:ARG:HD3	1:G:693:LEU:HB2	1.80	0.64
1:D:744:ARG:HD3	1:E:693:LEU:HB2	1.79	0.64
1:F:729:LEU:HD12	1:F:730:PRO:HD2	1.79	0.64
1:D:713:LEU:HG	1:E:743:LEU:HD22	1.81	0.63
1:F:652:TYR:CE2	1:J:756:GLU:OE2	2.50	0.63
1:F:717:LEU:HD13	1:G:743:LEU:HD13	1.81	0.63
1:A:753:ALA:O	1:E:678:TYR:CD2	2.52	0.62
1:C:748:ASN:O	1:J:652:TYR:CE1	2.52	0.62
1:J:729:LEU:HD12	1:J:730:PRO:HD2	1.79	0.62
1:B:729:LEU:HD12	1:B:730:PRO:HD2	1.83	0.61
1:A:690:ARG:O	1:J:758:GLU:HB3	2.00	0.61
1:C:757:GLU:CG	1:J:677:TYR:HA	2.30	0.61
1:H:750:ASP:HB3	1:H:754:LYS:HG2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:750:ASP:O	1:G:754:LYS:HB2	2.00	0.61
1:A:750:ASP:HB3	1:A:754:LYS:HG2	1.82	0.61
1:F:374:HIS:HD2	1:F:386:ILE:HG12	1.65	0.61
1:H:729:LEU:HD12	1:H:730:PRO:HD2	1.83	0.61
1:C:750:ASP:HB3	1:C:754:LYS:HG2	1.83	0.60
1:A:700:ARG:HD2	1:A:710:VAL:HG22	1.84	0.60
1:D:744:ARG:NH2	1:D:755:VAL:HB	2.16	0.60
1:C:754:LYS:HD3	1:J:678:TYR:CE2	2.37	0.59
1:H:569:THR:O	1:I:667:TYR:OH	2.18	0.59
1:A:729:LEU:HD12	1:A:730:PRO:HD2	1.85	0.59
1:F:652:TYR:HE2	1:J:756:GLU:OE2	1.84	0.59
1:F:743:LEU:CD2	1:G:713:LEU:HG	2.32	0.59
1:B:374:HIS:HD2	1:B:386:ILE:HG12	1.67	0.58
1:H:374:HIS:HD2	1:H:386:ILE:HG12	1.68	0.58
1:A:642:GLU:HG2	1:J:759:PRO:HB2	1.85	0.58
1:C:700:ARG:HD2	1:C:710:VAL:HG22	1.84	0.58
1:E:500:HIS:CD2	1:E:500:HIS:H	2.20	0.58
1:F:691:HIS:HE1	1:G:744:ARG:HD3	1.67	0.58
1:D:692:PRO:HD3	1:E:758:GLU:HB2	1.86	0.58
1:F:742:MET:CE	1:G:742:MET:HE3	2.34	0.58
1:I:700:ARG:HD2	1:I:710:VAL:HG22	1.86	0.58
1:G:683:LYS:HE3	1:G:727:TYR:CE1	2.38	0.57
1:A:642:GLU:HG2	1:J:759:PRO:CB	2.33	0.57
1:A:418:ILE:HG22	1:A:419:THR:HG22	1.86	0.57
1:H:557:ARG:HD3	1:H:638:GLN:O	2.04	0.57
1:B:744:ARG:NH2	1:B:755:VAL:HB	2.20	0.57
1:D:374:HIS:HD2	1:D:386:ILE:HG12	1.70	0.57
1:I:729:LEU:HD12	1:I:730:PRO:HD2	1.85	0.57
1:F:557:ARG:HD3	1:F:638:GLN:O	2.05	0.56
1:G:700:ARG:HD2	1:G:710:VAL:HG22	1.88	0.56
1:G:729:LEU:HD12	1:G:730:PRO:HD2	1.88	0.56
1:C:344:GLN:NE2	1:C:438:ASP:OD2	2.37	0.56
1:I:750:ASP:HB3	1:I:754:LYS:HG2	1.87	0.56
1:J:744:ARG:NH2	1:J:755:VAL:HB	2.21	0.56
1:D:557:ARG:HD3	1:D:638:GLN:O	2.05	0.56
1:D:750:ASP:HB3	1:D:754:LYS:CG	2.36	0.56
1:E:750:ASP:HB3	1:E:754:LYS:HG2	1.88	0.56
1:J:374:HIS:HD2	1:J:386:ILE:HG12	1.69	0.55
1:C:757:GLU:OE2	1:J:676:ASN:O	2.25	0.55
1:B:557:ARG:HD3	1:B:638:GLN:O	2.06	0.55
1:F:743:LEU:HD13	1:G:717:LEU:HD13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:344:GLN:NE2	1:I:438:ASP:OD2	2.38	0.55
1:G:750:ASP:HB3	1:G:754:LYS:HG2	1.89	0.55
1:E:729:LEU:HD12	1:E:730:PRO:HD2	1.88	0.55
1:F:742:MET:HE3	1:G:742:MET:CE	2.37	0.55
1:E:700:ARG:HD2	1:E:710:VAL:HG22	1.89	0.55
1:F:652:TYR:CD2	1:J:756:GLU:OE1	2.60	0.54
1:A:754:LYS:HD3	1:E:678:TYR:HH	1.68	0.54
1:H:744:ARG:NH2	1:H:755:VAL:HB	2.23	0.54
1:F:652:TYR:CZ	1:J:756:GLU:HG2	2.43	0.54
1:B:750:ASP:HB3	1:B:754:LYS:HG2	1.90	0.54
1:J:557:ARG:HD3	1:J:638:GLN:O	2.08	0.53
1:F:750:ASP:HB3	1:F:754:LYS:HG2	1.88	0.53
1:F:744:ARG:HG2	1:G:693:LEU:HD13	1.91	0.53
1:H:693:LEU:HD13	1:I:744:ARG:HG2	1.91	0.53
1:A:344:GLN:NE2	1:A:438:ASP:OD2	2.38	0.53
1:D:759:PRO:HA	1:E:690:ARG:O	2.08	0.53
1:F:742:MET:HE3	1:G:742:MET:HE1	1.91	0.53
1:D:742:MET:HE2	1:E:742:MET:CE	2.39	0.53
1:A:754:LYS:HD3	1:E:678:TYR:CZ	2.43	0.53
1:C:729:LEU:HD12	1:C:730:PRO:HD2	1.92	0.52
1:D:750:ASP:O	1:D:754:LYS:HB2	2.10	0.52
1:G:344:GLN:NE2	1:G:438:ASP:OD2	2.41	0.52
1:J:344:GLN:NE2	1:J:438:ASP:OD2	2.39	0.52
1:G:744:ARG:NH2	1:G:755:VAL:HB	2.24	0.52
1:A:570:GLU:HB2	1:A:573:ASP:CG	2.30	0.52
1:H:467:LYS:HD3	1:J:529:GLU:OE2	2.10	0.52
1:C:761:GLU:OE2	1:J:676:ASN:O	2.28	0.52
1:A:374:HIS:HD2	1:A:386:ILE:HG12	1.73	0.52
1:E:570:GLU:HB2	1:E:573:ASP:CG	2.30	0.52
1:E:744:ARG:NH2	1:E:755:VAL:HB	2.25	0.52
1:E:344:GLN:NE2	1:E:438:ASP:OD2	2.40	0.52
1:E:683:LYS:HE3	1:E:727:TYR:CE1	2.45	0.52
1:D:742:MET:HE3	1:E:742:MET:HE3	1.92	0.52
1:I:374:HIS:HD2	1:I:386:ILE:HG12	1.75	0.51
1:J:750:ASP:HB3	1:J:754:LYS:HG2	1.93	0.51
1:D:528:VAL:HA	1:D:531:MET:SD	2.50	0.51
1:C:500:HIS:CD2	1:C:500:HIS:H	2.29	0.51
1:A:750:ASP:HB2	1:E:652:TYR:HB2	1.92	0.51
1:D:759:PRO:HG3	1:E:692:PRO:HD2	1.92	0.51
1:F:374:HIS:CD2	1:F:386:ILE:HG12	2.46	0.50
1:F:744:ARG:NH2	1:F:755:VAL:HB	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:742:MET:HE1	1:G:742:MET:HE3	1.92	0.50
1:I:570:GLU:HB2	1:I:573:ASP:CG	2.31	0.50
1:F:424:ASP:CG	1:F:452:GLN:HE21	2.15	0.50
1:A:500:HIS:H	1:A:500:HIS:CD2	2.28	0.50
1:I:744:ARG:NH2	1:I:755:VAL:HB	2.27	0.50
1:G:374:HIS:HD2	1:G:386:ILE:HG12	1.77	0.50
1:D:742:MET:HE2	1:E:742:MET:HE3	1.92	0.50
1:H:374:HIS:CD2	1:H:386:ILE:HG12	2.47	0.50
1:F:414:ARG:O	1:F:415:ARG:HB2	2.12	0.50
1:I:557:ARG:HD3	1:I:638:GLN:O	2.11	0.50
1:C:557:ARG:HD3	1:C:638:GLN:O	2.11	0.49
1:E:374:HIS:HD2	1:E:386:ILE:HG12	1.77	0.49
1:F:700:ARG:HD2	1:F:710:VAL:HG22	1.94	0.49
1:H:380:GLU:CD	1:J:533:GLU:HB2	2.33	0.49
1:C:744:ARG:NH2	1:C:755:VAL:HB	2.26	0.49
1:G:570:GLU:HB2	1:G:573:ASP:CG	2.32	0.49
1:H:692:PRO:HB3	1:I:754:LYS:CE	2.40	0.49
1:H:750:ASP:O	1:H:754:LYS:HB2	2.12	0.49
1:F:472:ILE:O	1:F:475:ILE:HG12	2.13	0.49
1:C:418:ILE:HG22	1:C:419:THR:HG22	1.95	0.49
1:F:742:MET:CE	1:G:742:MET:CE	2.90	0.49
1:H:344:GLN:NE2	1:H:438:ASP:OD2	2.43	0.49
1:F:652:TYR:CD2	1:J:756:GLU:CD	2.86	0.49
1:F:683:LYS:HE3	1:F:727:TYR:CE1	2.48	0.48
1:C:374:HIS:HD2	1:C:386:ILE:HG12	1.78	0.48
1:A:750:ASP:HB2	1:E:652:TYR:CB	2.44	0.48
1:B:344:GLN:NE2	1:B:438:ASP:OD2	2.41	0.48
1:E:418:ILE:HG22	1:E:419:THR:HG22	1.94	0.48
1:F:691:HIS:CE1	1:G:744:ARG:HD3	2.47	0.48
1:H:743:LEU:HD22	1:I:713:LEU:HG	1.94	0.48
1:C:757:GLU:HG2	1:J:677:TYR:CA	2.44	0.48
1:G:557:ARG:HD3	1:G:638:GLN:O	2.13	0.48
1:J:754:LYS:C	1:J:756:GLU:H	2.16	0.48
1:F:652:TYR:CE2	1:J:756:GLU:CG	2.97	0.48
1:D:472:ILE:O	1:D:475:ILE:HG12	2.14	0.48
1:D:742:MET:CE	1:E:742:MET:CE	2.91	0.48
1:F:537:LYS:HE2	1:F:589:GLN:HB2	1.96	0.48
1:F:700:ARG:HD2	1:F:710:VAL:CG2	2.44	0.48
1:I:418:ILE:HG22	1:I:419:THR:HG22	1.95	0.48
1:D:739:ILE:HD12	1:E:739:ILE:HD12	1.96	0.48
1:F:750:ASP:O	1:F:754:LYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:SER:OG	1:E:554:PHE:HD1	1.97	0.47
1:G:418:ILE:HG22	1:G:419:THR:HG22	1.96	0.47
1:H:750:ASP:HB3	1:H:754:LYS:CG	2.44	0.47
1:C:700:ARG:HD2	1:C:710:VAL:CG2	2.43	0.47
1:D:759:PRO:CD	1:E:692:PRO:HD3	2.27	0.47
1:I:700:ARG:HD2	1:I:710:VAL:CG2	2.44	0.47
1:A:700:ARG:HD2	1:A:710:VAL:CG2	2.44	0.47
1:A:744:ARG:NH2	1:A:755:VAL:HB	2.30	0.47
1:C:747:LEU:O	1:C:748:ASN:CB	2.62	0.47
1:E:461:ARG:O	1:E:465:VAL:HG23	2.15	0.47
1:I:500:HIS:H	1:I:500:HIS:CD2	2.32	0.47
1:B:750:ASP:O	1:B:754:LYS:HB2	2.15	0.47
1:D:344:GLN:NE2	1:D:438:ASP:OD2	2.41	0.47
1:E:700:ARG:HD2	1:E:710:VAL:CG2	2.45	0.47
1:F:644:PRO:HD3	1:G:740:GLU:OE2	2.14	0.47
1:E:557:ARG:HD3	1:E:638:GLN:O	2.15	0.47
1:J:472:ILE:O	1:J:475:ILE:HG12	2.15	0.47
1:A:461:ARG:O	1:A:465:VAL:HG23	2.15	0.47
1:I:461:ARG:O	1:I:465:VAL:HG23	2.15	0.47
1:B:759:PRO:HB3	1:C:642:GLU:HA	1.97	0.46
1:B:374:HIS:CD2	1:B:386:ILE:HG12	2.48	0.46
1:F:693:LEU:HD13	1:G:744:ARG:HG2	1.97	0.46
1:H:424:ASP:CG	1:H:452:GLN:HE21	2.19	0.46
1:C:570:GLU:HB2	1:C:573:ASP:CG	2.35	0.46
1:B:683:LYS:HE3	1:B:727:TYR:CE1	2.51	0.46
1:G:700:ARG:HD2	1:G:710:VAL:CG2	2.46	0.46
1:J:641:THR:HG22	1:J:642:GLU:HG3	1.97	0.46
1:E:500:HIS:CD2	1:J:703:GLU:OE1	2.68	0.46
1:B:700:ARG:HD2	1:B:710:VAL:HG22	1.97	0.46
1:B:609:GLU:O	1:B:613:LYS:HD3	2.15	0.46
1:G:461:ARG:O	1:G:465:VAL:HG23	2.16	0.46
1:H:692:PRO:HD3	1:I:758:GLU:HB2	1.97	0.46
1:F:754:LYS:C	1:F:756:GLU:H	2.18	0.46
1:C:757:GLU:HG2	1:J:677:TYR:CB	2.46	0.46
1:H:472:ILE:O	1:H:475:ILE:HG12	2.16	0.45
1:H:700:ARG:HD2	1:H:710:VAL:HG22	1.98	0.45
1:J:348:LYS:HB2	1:J:348:LYS:HE3	1.73	0.45
1:C:568:LEU:HB3	1:C:573:ASP:HB3	1.98	0.45
1:F:344:GLN:NE2	1:F:438:ASP:OD2	2.43	0.45
1:A:557:ARG:HD3	1:A:638:GLN:O	2.17	0.45
1:C:748:ASN:O	1:J:652:TYR:CD1	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:GLU:N	1:C:759:PRO:CD	2.80	0.45
1:H:609:GLU:O	1:H:613:LYS:HD3	2.17	0.45
1:I:683:LYS:HE3	1:I:727:TYR:CE1	2.51	0.45
1:C:683:LYS:HE3	1:C:727:TYR:CE1	2.51	0.45
1:F:410:LYS:HB2	1:F:436:VAL:HG12	1.99	0.45
1:F:609:GLU:O	1:F:613:LYS:HD3	2.17	0.45
1:J:424:ASP:CG	1:J:452:GLN:HE21	2.20	0.45
1:E:747:LEU:O	1:E:748:ASN:CB	2.64	0.45
1:B:700:ARG:HD2	1:B:710:VAL:CG2	2.47	0.45
1:D:754:LYS:C	1:D:756:GLU:H	2.19	0.45
1:C:754:LYS:CE	1:J:678:TYR:HE2	2.30	0.45
1:D:759:PRO:HG3	1:E:691:HIS:HA	1.98	0.45
1:I:568:LEU:HB3	1:I:573:ASP:HB3	1.98	0.45
1:A:374:HIS:CD2	1:A:386:ILE:HG12	2.51	0.45
1:A:758:GLU:N	1:A:759:PRO:CD	2.80	0.45
1:E:695:LYS:HE2	1:E:695:LYS:HB3	1.79	0.44
1:F:528:VAL:HA	1:F:531:MET:SD	2.57	0.44
1:H:537:LYS:HE2	1:H:589:GLN:HB2	1.99	0.44
1:A:750:ASP:OD1	1:A:753:ALA:HB3	2.17	0.44
1:G:568:LEU:HB3	1:G:573:ASP:HB3	2.00	0.44
1:H:641:THR:HG22	1:H:642:GLU:HG3	1.99	0.44
1:D:568:LEU:HB3	1:D:573:ASP:HB3	1.99	0.44
1:D:374:HIS:CD2	1:D:386:ILE:HG12	2.50	0.44
1:F:568:LEU:HB3	1:F:573:ASP:HB3	2.00	0.44
1:G:758:GLU:N	1:G:759:PRO:CD	2.81	0.44
1:F:754:LYS:HB3	1:G:692:PRO:HB3	1.99	0.44
1:H:528:VAL:HA	1:H:531:MET:SD	2.57	0.44
1:H:700:ARG:HD2	1:H:710:VAL:CG2	2.48	0.44
1:B:754:LYS:C	1:B:756:GLU:H	2.21	0.44
1:F:641:THR:HG22	1:F:642:GLU:HG3	2.00	0.44
1:D:348:LYS:HE3	1:D:348:LYS:HB2	1.71	0.44
1:F:691:HIS:HA	1:F:692:PRO:HD2	1.78	0.44
1:J:374:HIS:CD2	1:J:386:ILE:HG12	2.50	0.44
1:F:750:ASP:HB3	1:F:754:LYS:CG	2.48	0.43
1:H:348:LYS:HE3	1:H:348:LYS:HB2	1.74	0.43
1:F:418:ILE:HG22	1:F:419:THR:HG22	2.00	0.43
1:D:759:PRO:CG	1:E:692:PRO:HD2	2.48	0.43
1:J:410:LYS:HB2	1:J:436:VAL:HG12	2.00	0.43
1:J:537:LYS:HE2	1:J:589:GLN:HB2	2.00	0.43
1:I:747:LEU:O	1:I:748:ASN:CB	2.66	0.43
1:B:641:THR:HG22	1:B:642:GLU:HG3	1.98	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:513:GLN:HB3	1:C:546:ARG:NH1	2.33	0.43
1:B:472:ILE:O	1:B:475:ILE:HG12	2.18	0.43
1:E:374:HIS:CD2	1:E:386:ILE:HG12	2.53	0.43
1:A:757:GLU:HB2	1:E:677:TYR:CB	2.49	0.43
1:B:691:HIS:HA	1:B:692:PRO:HD2	1.80	0.43
1:B:537:LYS:HE2	1:B:589:GLN:HB2	2.01	0.43
1:D:424:ASP:CG	1:D:452:GLN:HE21	2.22	0.43
1:D:691:HIS:HA	1:D:692:PRO:HD2	1.79	0.43
1:H:380:GLU:OE1	1:J:533:GLU:HB2	2.19	0.43
1:B:348:LYS:HB2	1:B:348:LYS:HE3	1.76	0.43
1:C:517:HIS:HA	1:C:518:PRO:HD2	1.78	0.43
1:H:754:LYS:C	1:H:756:GLU:H	2.21	0.43
1:I:374:HIS:CD2	1:I:386:ILE:HG12	2.53	0.43
1:J:609:GLU:O	1:J:613:LYS:HD3	2.19	0.43
1:B:410:LYS:HB2	1:B:436:VAL:HG12	1.99	0.43
1:D:729:LEU:HA	1:D:730:PRO:HD2	1.85	0.43
1:H:602:GLU:O	1:H:606:GLU:HG3	2.19	0.43
1:J:500:HIS:CD2	1:J:500:HIS:H	2.37	0.42
1:C:472:ILE:O	1:C:475:ILE:HG12	2.20	0.42
1:D:758:GLU:N	1:D:759:PRO:CD	2.82	0.42
1:F:492:ILE:O	1:F:496:VAL:HG23	2.19	0.42
1:D:418:ILE:HG22	1:D:419:THR:HG22	2.01	0.42
1:D:410:LYS:HB2	1:D:436:VAL:HG12	2.01	0.42
1:D:755:VAL:HA	1:E:692:PRO:HG3	2.00	0.42
1:F:693:LEU:HB2	1:G:744:ARG:HD3	1.99	0.42
1:G:500:HIS:H	1:G:500:HIS:CD2	2.36	0.42
1:H:463:LYS:NZ	1:J:529:GLU:O	2.53	0.42
1:A:568:LEU:HB3	1:A:573:ASP:HB3	2.00	0.42
1:A:729:LEU:HA	1:A:730:PRO:HD2	1.81	0.42
1:E:568:LEU:HB3	1:E:573:ASP:HB3	2.01	0.42
1:G:374:HIS:CD2	1:G:386:ILE:HG12	2.55	0.42
1:C:729:LEU:HA	1:C:730:PRO:HD2	1.80	0.42
1:J:683:LYS:HE3	1:J:727:TYR:CE1	2.54	0.42
1:B:750:ASP:HB3	1:B:754:LYS:CG	2.50	0.42
1:C:552:SER:HA	1:C:553:PRO:HD3	1.94	0.42
1:G:633:LYS:HG3	1:G:684:THR:HG23	2.01	0.42
1:H:410:LYS:HB2	1:H:436:VAL:HG12	2.02	0.42
1:A:527:TYR:CE2	1:A:538:ILE:HG23	2.54	0.42
1:A:750:ASP:HB3	1:A:754:LYS:CG	2.49	0.42
1:J:747:LEU:O	1:J:748:ASN:CB	2.68	0.42
1:A:642:GLU:HG2	1:J:759:PRO:HB3	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:HIS:CD2	1:C:386:ILE:HG12	2.55	0.42
1:D:742:MET:SD	1:E:743:LEU:HD23	2.60	0.42
1:E:758:GLU:N	1:E:759:PRO:CD	2.83	0.42
1:F:517:HIS:HA	1:F:518:PRO:HD2	1.87	0.42
1:I:348:LYS:HB2	1:I:348:LYS:HE3	1.90	0.42
1:J:418:ILE:HG22	1:J:419:THR:HG22	2.01	0.42
1:A:747:LEU:O	1:A:748:ASN:CB	2.68	0.42
1:F:747:LEU:O	1:F:748:ASN:CB	2.67	0.42
1:C:754:LYS:HZ3	1:J:678:TYR:HE2	1.62	0.41
1:E:633:LYS:HG3	1:E:684:THR:HG23	2.02	0.41
1:F:692:PRO:HG3	1:G:754:LYS:HB3	2.02	0.41
1:B:424:ASP:CG	1:B:452:GLN:HE21	2.23	0.41
1:F:590:ASN:HD22	1:F:593:LYS:HE3	1.85	0.41
1:C:757:GLU:CG	1:J:677:TYR:CA	2.98	0.41
1:G:747:LEU:O	1:G:748:ASN:CB	2.67	0.41
1:A:513:GLN:HB3	1:A:546:ARG:NH1	2.35	0.41
1:D:641:THR:HG22	1:D:642:GLU:HG3	2.02	0.41
1:G:695:LYS:HE2	1:G:695:LYS:HB3	1.88	0.41
1:I:758:GLU:N	1:I:759:PRO:CD	2.83	0.41
1:A:754:LYS:C	1:A:756:GLU:N	2.74	0.41
1:G:527:TYR:CE2	1:G:538:ILE:HG23	2.55	0.41
1:J:700:ARG:HD2	1:J:710:VAL:HG22	2.02	0.41
1:J:750:ASP:O	1:J:754:LYS:HB2	2.20	0.41
1:J:758:GLU:N	1:J:759:PRO:CD	2.82	0.41
1:A:472:ILE:O	1:A:475:ILE:HG12	2.20	0.41
1:A:762:GLU:N	1:A:763:PRO:CD	2.84	0.41
1:B:758:GLU:N	1:B:759:PRO:CD	2.84	0.41
1:D:759:PRO:CA	1:E:690:ARG:O	2.68	0.41
1:A:570:GLU:HB2	1:A:573:ASP:OD2	2.21	0.41
1:D:700:ARG:HD2	1:D:710:VAL:CG2	2.50	0.41
1:D:765:GLU:O	1:E:604:THR:HG23	2.21	0.41
1:F:642:GLU:HA	1:G:759:PRO:HB3	2.03	0.41
1:D:537:LYS:HE2	1:D:589:GLN:HB2	2.01	0.41
1:G:552:SER:OG	1:G:554:PHE:HD1	2.04	0.41
1:F:744:ARG:CD	1:G:693:LEU:HB2	2.50	0.41
1:H:747:LEU:O	1:H:748:ASN:CB	2.68	0.41
1:B:747:LEU:O	1:B:748:ASN:CB	2.68	0.41
1:E:511:ARG:HA	1:E:511:ARG:HD3	1.97	0.41
1:E:524:LEU:HD23	1:E:524:LEU:HA	1.87	0.41
1:G:597:LYS:HE3	1:G:597:LYS:HB2	1.94	0.41
1:I:762:GLU:N	1:I:763:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:568:LEU:HB3	1:J:573:ASP:HB3	2.03	0.41
1:E:348:LYS:HB2	1:E:348:LYS:HE3	1.91	0.41
1:G:762:GLU:N	1:G:763:PRO:CD	2.84	0.41
1:H:683:LYS:HE3	1:H:727:TYR:CE1	2.55	0.41
1:A:750:ASP:CB	1:E:652:TYR:CB	2.95	0.41
1:I:695:LYS:HE2	1:I:695:LYS:HB3	1.87	0.40
1:E:609:GLU:O	1:E:613:LYS:HD3	2.22	0.40
1:E:729:LEU:HA	1:E:730:PRO:HD2	1.79	0.40
1:F:602:GLU:O	1:F:606:GLU:HG3	2.21	0.40
1:F:691:HIS:NE2	1:G:740:GLU:OE2	2.54	0.40
1:H:570:GLU:HB2	1:H:573:ASP:CG	2.41	0.40
1:H:627:LEU:HB3	1:H:630:LYS:HB2	2.03	0.40
1:D:552:SER:HA	1:D:553:PRO:HD3	1.96	0.40
1:D:609:GLU:O	1:D:613:LYS:HD3	2.21	0.40
1:D:700:ARG:HD2	1:D:710:VAL:HG22	2.02	0.40
1:D:747:LEU:O	1:D:748:ASN:CB	2.70	0.40
1:E:500:HIS:CD2	1:E:500:HIS:N	2.85	0.40
1:I:513:GLN:HB3	1:I:546:ARG:NH1	2.36	0.40
1:E:500:HIS:ND1	1:J:704:ASP:HB2	2.28	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:753:ALA:O	1:G:652:TYR:OH[1_455]	1.62	0.58
1:A:677:TYR:CB	1:D:757:GLU:OE1[2_655]	1.73	0.47
1:F:699:ARG:NH2	1:I:445:ASN:O[1_655]	1.74	0.46
1:A:445:ASN:ND2	1:F:412:TYR:CD1[1_565]	1.91	0.29
1:F:696:ASP:OD2	1:I:445:ASN:ND2[1_655]	2.03	0.17
1:A:445:ASN:O	1:F:415:ARG:O[1_565]	2.07	0.13
1:A:445:ASN:OD1	1:F:343:TRP:CZ2[1_565]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/450 (91%)	361 (88%)	44 (11%)	4 (1%)	18	61
1	B	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	15	56
1	C	409/450 (91%)	365 (89%)	40 (10%)	4 (1%)	18	61
1	D	409/450 (91%)	368 (90%)	35 (9%)	6 (2%)	12	51
1	E	409/450 (91%)	357 (87%)	47 (12%)	5 (1%)	15	56
1	F	409/450 (91%)	365 (89%)	36 (9%)	8 (2%)	9	44
1	G	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	18	61
1	H	409/450 (91%)	367 (90%)	36 (9%)	6 (2%)	12	51
1	I	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	18	61
1	J	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	15	56
All	All	4090/4500 (91%)	3637 (89%)	402 (10%)	51 (1%)	15	56

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	ILE
1	C	749	ILE
1	D	757	GLU
1	E	749	ILE
1	I	749	ILE
1	A	748	ASN
1	B	748	ASN
1	B	749	ILE
1	B	757	GLU
1	C	748	ASN
1	D	748	ASN
1	D	749	ILE
1	E	748	ASN
1	E	757	GLU
1	F	748	ASN
1	F	749	ILE
1	F	757	GLU
1	G	748	ASN
1	G	749	ILE
1	G	757	GLU
1	H	748	ASN
1	H	749	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	757	GLU
1	I	748	ASN
1	I	757	GLU
1	J	748	ASN
1	J	749	ILE
1	J	757	GLU
1	A	751	PRO
1	A	757	GLU
1	C	751	PRO
1	C	757	GLU
1	E	751	PRO
1	G	751	PRO
1	I	751	PRO
1	F	420	ASP
1	J	420	ASP
1	B	676	ASN
1	D	420	ASP
1	D	751	PRO
1	E	746	SER
1	F	419	THR
1	F	676	ASN
1	F	751	PRO
1	H	420	ASP
1	H	676	ASN
1	B	751	PRO
1	D	676	ASN
1	H	751	PRO
1	J	751	PRO
1	F	581	PRO

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	352/410 (86%)	349 (99%)	3 (1%)	82	94
1	B	352/410 (86%)	351 (100%)	1 (0%)	94	98

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	352/410 (86%)	350 (99%)	2 (1%)	89	96
1	D	352/410 (86%)	351 (100%)	1 (0%)	94	98
1	E	352/410 (86%)	349 (99%)	3 (1%)	82	94
1	F	352/410 (86%)	350 (99%)	2 (1%)	89	96
1	G	352/410 (86%)	350 (99%)	2 (1%)	89	96
1	H	352/410 (86%)	351 (100%)	1 (0%)	94	98
1	I	352/410 (86%)	351 (100%)	1 (0%)	94	98
1	J	352/410 (86%)	350 (99%)	2 (1%)	89	96
All	All	3520/4100 (86%)	3502 (100%)	18 (0%)	91	97

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	448	ARG
1	A	652	TYR
1	B	448	ARG
1	C	448	ARG
1	C	652	TYR
1	D	448	ARG
1	E	448	ARG
1	E	652	TYR
1	E	760	GLU
1	F	448	ARG
1	F	491	ASN
1	G	448	ARG
1	G	652	TYR
1	H	448	ARG
1	I	448	ARG
1	J	448	ARG
1	J	678	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	452	GLN
1	D	452	GLN
1	E	500	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	452	GLN
1	H	452	GLN
1	J	452	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	413/450 (91%)	0.88	54 (13%) 4 2	129, 151, 152, 165	0
1	B	413/450 (91%)	1.53	112 (27%) 1 1	129, 151, 152, 165	0
1	C	413/450 (91%)	0.94	62 (15%) 3 1	129, 151, 152, 165	0
1	D	413/450 (91%)	1.21	87 (21%) 1 1	129, 151, 152, 165	0
1	E	413/450 (91%)	1.02	57 (13%) 3 2	129, 151, 152, 165	0
1	F	413/450 (91%)	0.87	55 (13%) 4 2	129, 151, 152, 165	0
1	G	413/450 (91%)	1.52	102 (24%) 1 1	129, 151, 152, 165	0
1	H	413/450 (91%)	1.79	142 (34%) 0 0	129, 151, 152, 165	0
1	I	413/450 (91%)	2.65	176 (42%) 0 0	129, 151, 152, 165	0
1	J	413/450 (91%)	0.88	63 (15%) 2 1	129, 151, 152, 165	0
All	All	4130/4500 (91%)	1.33	910 (22%) 1 1	129, 151, 153, 165	0

All (910) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	443	PRO	22.7
1	I	443	PRO	21.6
1	I	437	VAL	18.8
1	I	392	SER	17.7
1	D	765	GLU	17.2
1	I	363	SER	15.9
1	I	364	LYS	15.7
1	E	753	ALA	14.9
1	I	386	ILE	14.4
1	I	444	LEU	14.4
1	G	347	SER	14.1
1	I	651	GLN	14.0
1	I	387	LEU	13.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	755	VAL	13.2
1	A	758	GLU	13.2
1	D	366	SER	12.7
1	I	447	SER	12.6
1	I	436	VAL	12.4
1	I	449	GLU	12.2
1	C	755	VAL	12.1
1	G	600	GLU	12.0
1	I	349	GLU	11.9
1	I	457	LEU	11.8
1	H	697	MET	11.7
1	I	765	GLU	11.5
1	B	759	PRO	11.4
1	E	342	ILE	11.3
1	I	634	ALA	11.3
1	I	442	LEU	11.3
1	I	446	VAL	10.9
1	I	764	GLU	10.9
1	G	448	ARG	10.8
1	G	381	VAL	10.8
1	D	755	VAL	10.7
1	B	599	ASP	10.6
1	D	762	GLU	10.5
1	G	375	PHE	10.4
1	A	765	GLU	10.0
1	H	757	GLU	10.0
1	H	760	GLU	9.7
1	H	761	GLU	9.7
1	H	753	ALA	9.7
1	G	388	PHE	9.6
1	D	411	LEU	9.6
1	E	452	GLN	9.5
1	B	388	PHE	9.5
1	D	443	PRO	9.5
1	H	598	PHE	9.5
1	H	638	GLN	9.4
1	I	450	THR	9.2
1	H	436	VAL	9.2
1	I	677	TYR	9.2
1	B	436	VAL	8.8
1	I	635	VAL	8.8
1	I	468	THR	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	763	PRO	8.7
1	B	435	GLY	8.6
1	A	759	PRO	8.6
1	B	755	VAL	8.6
1	B	600	GLU	8.5
1	G	433	VAL	8.3
1	E	757	GLU	8.3
1	H	619	LEU	8.3
1	E	763	PRO	8.2
1	I	445	ASN	8.2
1	B	762	GLU	8.2
1	A	341	PRO	8.1
1	C	435	GLY	8.1
1	D	437	VAL	8.0
1	I	746	SER	8.0
1	D	388	PHE	7.9
1	D	753	ALA	7.9
1	G	451	LEU	7.9
1	J	765	GLU	7.9
1	E	366	SER	7.9
1	H	597	LYS	7.8
1	I	600	GLU	7.6
1	I	366	SER	7.6
1	E	380	GLU	7.6
1	B	765	GLU	7.6
1	G	446	VAL	7.6
1	F	754	LYS	7.5
1	B	760	GLU	7.4
1	J	390	PRO	7.4
1	G	370	MET	7.4
1	H	622	MET	7.4
1	F	753	ALA	7.4
1	H	758	GLU	7.3
1	J	451	LEU	7.2
1	G	368	ASP	7.2
1	G	444	LEU	7.2
1	I	373	ILE	7.1
1	I	385	SER	7.1
1	H	358	PHE	7.1
1	H	617	PRO	7.0
1	D	367	ASP	7.0
1	B	437	VAL	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	678	TYR	6.9
1	G	454	HIS	6.9
1	I	646	ALA	6.8
1	A	340	LYS	6.8
1	G	604	THR	6.8
1	G	442	LEU	6.8
1	D	754	LYS	6.8
1	B	608	ARG	6.8
1	H	678	TYR	6.8
1	H	704	ASP	6.7
1	H	765	GLU	6.7
1	B	646	ALA	6.7
1	C	765	GLU	6.6
1	C	388	PHE	6.6
1	B	363	SER	6.6
1	I	510	LEU	6.6
1	G	765	GLU	6.5
1	B	359	TYR	6.3
1	I	411	LEU	6.3
1	B	386	ILE	6.3
1	C	714	ALA	6.3
1	G	411	LEU	6.3
1	H	675	THR	6.3
1	E	754	LYS	6.3
1	I	456	LEU	6.3
1	I	341	PRO	6.2
1	B	423	HIS	6.2
1	I	464	LEU	6.2
1	F	760	GLU	6.2
1	I	754	LYS	6.2
1	J	760	GLU	6.2
1	E	451	LEU	6.2
1	E	341	PRO	6.2
1	I	362	PHE	6.1
1	C	760	GLU	6.1
1	I	759	PRO	6.1
1	I	356	LYS	6.1
1	I	342	ILE	6.0
1	I	448	ARG	6.0
1	F	761	GLU	6.0
1	H	613	LYS	6.0
1	G	421	ASP	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	764	GLU	6.0
1	I	391	THR	6.0
1	B	679	ALA	6.0
1	I	451	LEU	6.0
1	F	599	ASP	6.0
1	A	764	GLU	6.0
1	F	435	GLY	5.9
1	G	374	HIS	5.9
1	I	414	ARG	5.9
1	H	730	PRO	5.8
1	H	606	GLU	5.8
1	I	624	ASP	5.8
1	G	380	GLU	5.8
1	B	442	LEU	5.8
1	F	451	LEU	5.8
1	G	458	LYS	5.8
1	A	444	LEU	5.7
1	H	615	PHE	5.7
1	D	451	LEU	5.7
1	I	433	VAL	5.7
1	D	342	ILE	5.7
1	I	684	THR	5.7
1	I	393	ALA	5.7
1	F	764	GLU	5.6
1	G	356	LYS	5.6
1	I	619	LEU	5.6
1	E	762	GLU	5.6
1	I	454	HIS	5.6
1	D	758	GLU	5.6
1	H	645	CYS	5.6
1	I	352	ASP	5.5
1	D	447	SER	5.5
1	B	725	SER	5.5
1	D	436	VAL	5.5
1	G	596	VAL	5.5
1	B	451	LEU	5.4
1	I	422	PHE	5.4
1	I	340	LYS	5.4
1	I	355	TYR	5.4
1	B	364	LYS	5.4
1	F	757	GLU	5.4
1	H	592	ALA	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	658	MET	5.3
1	E	764	GLU	5.3
1	H	553	PRO	5.3
1	H	612	GLU	5.3
1	G	366	SER	5.2
1	C	434	LYS	5.2
1	J	358	PHE	5.2
1	H	589	GLN	5.2
1	A	342	ILE	5.2
1	A	760	GLU	5.2
1	C	762	GLU	5.2
1	C	697	MET	5.2
1	D	600	GLU	5.2
1	C	599	ASP	5.1
1	I	745	LEU	5.1
1	I	435	GLY	5.1
1	I	687	ILE	5.1
1	H	648	VAL	5.1
1	F	765	GLU	5.1
1	J	380	GLU	5.1
1	I	514	SER	5.1
1	A	600	GLU	5.0
1	H	752	ASP	5.0
1	I	761	GLU	5.0
1	H	688	ASN	5.0
1	C	694	ILE	5.0
1	G	606	GLU	5.0
1	G	389	VAL	4.9
1	H	654	TRP	4.9
1	I	360	LYS	4.9
1	H	604	THR	4.9
1	B	369	PRO	4.9
1	J	437	VAL	4.9
1	G	419	THR	4.9
1	I	612	GLU	4.9
1	B	389	VAL	4.9
1	F	755	VAL	4.9
1	I	354	GLU	4.9
1	D	422	PHE	4.9
1	J	606	GLU	4.9
1	I	408	TYR	4.8
1	G	755	VAL	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	367	ASP	4.8
1	A	422	PHE	4.8
1	G	492	ILE	4.8
1	I	686	GLU	4.8
1	H	516	HIS	4.8
1	I	460	ILE	4.8
1	I	419	THR	4.8
1	H	413	VAL	4.8
1	H	759	PRO	4.8
1	B	358	PHE	4.7
1	B	340	LYS	4.7
1	F	340	LYS	4.7
1	I	347	SER	4.7
1	F	678	TYR	4.7
1	J	418	ILE	4.7
1	I	560	LYS	4.7
1	B	422	PHE	4.7
1	J	762	GLU	4.7
1	G	450	THR	4.7
1	H	691	HIS	4.7
1	E	746	SER	4.7
1	H	632	GLU	4.7
1	B	757	GLU	4.6
1	D	361	SER	4.6
1	A	445	ASN	4.6
1	I	659	GLU	4.6
1	E	350	VAL	4.6
1	F	361	SER	4.6
1	I	648	VAL	4.6
1	G	376	THR	4.6
1	F	342	ILE	4.6
1	G	598	PHE	4.6
1	I	434	LYS	4.6
1	G	599	ASP	4.6
1	A	753	ALA	4.5
1	F	422	PHE	4.5
1	I	458	LYS	4.5
1	G	447	SER	4.5
1	F	394	PRO	4.5
1	J	349	GLU	4.5
1	E	444	LEU	4.5
1	E	340	LYS	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	730	PRO	4.5
1	A	604	THR	4.4
1	H	762	GLU	4.4
1	G	360	LYS	4.4
1	J	408	TYR	4.4
1	F	600	GLU	4.4
1	H	422	PHE	4.4
1	I	498	GLU	4.4
1	I	384	LYS	4.4
1	G	533	GLU	4.4
1	F	752	ASP	4.4
1	I	374	HIS	4.4
1	I	617	PRO	4.4
1	I	461	ARG	4.4
1	I	541	MET	4.4
1	B	758	GLU	4.4
1	G	559	LEU	4.3
1	G	386	ILE	4.3
1	H	764	GLU	4.3
1	B	589	GLN	4.3
1	H	554	PHE	4.3
1	D	764	GLU	4.3
1	H	540	PHE	4.3
1	I	762	GLU	4.3
1	G	385	SER	4.3
1	I	538	ILE	4.3
1	I	372	TYR	4.3
1	I	415	ARG	4.3
1	B	380	GLU	4.3
1	D	634	ALA	4.3
1	H	591	VAL	4.3
1	I	598	PHE	4.3
1	H	683	LYS	4.3
1	I	705	GLU	4.3
1	H	374	HIS	4.3
1	J	357	ALA	4.3
1	A	392	SER	4.3
1	I	756	GLU	4.3
1	H	672	ASP	4.3
1	I	511	ARG	4.3
1	E	388	PHE	4.2
1	I	750	ASP	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	607	SER	4.2
1	B	365	GLU	4.2
1	E	674	SER	4.2
1	D	446	VAL	4.2
1	A	697	MET	4.2
1	I	348	LYS	4.2
1	B	604	THR	4.2
1	B	712	ASP	4.2
1	F	762	GLU	4.2
1	A	366	SER	4.2
1	C	629	ASP	4.1
1	G	445	ASN	4.1
1	H	689	PRO	4.1
1	C	437	VAL	4.1
1	H	623	LYS	4.1
1	I	607	SER	4.1
1	D	757	GLU	4.1
1	E	765	GLU	4.1
1	A	607	SER	4.1
1	J	374	HIS	4.1
1	I	678	TYR	4.1
1	H	410	LYS	4.1
1	J	764	GLU	4.1
1	F	654	TRP	4.1
1	H	740	GLU	4.1
1	B	647	LEU	4.1
1	B	448	ARG	4.0
1	I	367	ASP	4.0
1	H	698	LEU	4.0
1	B	366	SER	4.0
1	B	764	GLU	4.0
1	B	453	GLN	4.0
1	B	381	VAL	4.0
1	E	379	GLY	4.0
1	F	601	SER	4.0
1	B	563	TYR	4.0
1	C	453	GLN	3.9
1	D	419	THR	3.9
1	I	425	MET	3.9
1	E	362	PHE	3.9
1	B	606	GLU	3.9
1	G	344	GLN	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	380	GLU	3.8
1	B	744	ARG	3.8
1	H	418	ILE	3.8
1	I	515	SER	3.8
1	H	647	LEU	3.8
1	H	659	GLU	3.8
1	I	662	MET	3.8
1	C	746	SER	3.8
1	I	361	SER	3.8
1	J	439	SER	3.8
1	E	391	THR	3.8
1	H	630	LYS	3.7
1	I	685	PHE	3.8
1	C	543	GLY	3.7
1	H	483	THR	3.7
1	F	366	SER	3.7
1	H	484	PHE	3.7
1	B	370	MET	3.7
1	C	747	LEU	3.7
1	D	387	LEU	3.7
1	G	349	GLU	3.7
1	H	380	GLU	3.7
1	I	412	TYR	3.7
1	B	598	PHE	3.7
1	D	575	TYR	3.7
1	C	366	SER	3.7
1	H	451	LEU	3.7
1	H	627	LEU	3.7
1	I	432	PHE	3.7
1	I	633	LYS	3.7
1	D	444	LEU	3.7
1	F	442	LEU	3.7
1	C	757	GLU	3.7
1	I	638	GLN	3.7
1	H	729	LEU	3.7
1	H	701	VAL	3.6
1	I	540	PHE	3.6
1	B	678	TYR	3.6
1	H	370	MET	3.6
1	I	423	HIS	3.6
1	D	365	GLU	3.6
1	H	599	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	449	GLU	3.6
1	H	737	ASP	3.6
1	B	443	PRO	3.6
1	F	597	LYS	3.5
1	J	452	GLN	3.5
1	E	422	PHE	3.5
1	G	418	ILE	3.5
1	I	383	PHE	3.5
1	G	449	GLU	3.5
1	J	421	ASP	3.5
1	D	591	VAL	3.5
1	H	644	PRO	3.5
1	I	542	ALA	3.5
1	C	701	VAL	3.5
1	H	537	LYS	3.5
1	I	567	TYR	3.5
1	I	703	GLU	3.5
1	J	350	VAL	3.5
1	G	342	ILE	3.5
1	I	599	ASP	3.5
1	J	385	SER	3.5
1	G	585	GLY	3.5
1	B	624	ASP	3.4
1	C	600	GLU	3.4
1	J	703	GLU	3.4
1	H	569	THR	3.4
1	H	643	SER	3.4
1	H	728	LEU	3.4
1	J	388	PHE	3.4
1	H	575	TYR	3.4
1	B	341	PRO	3.4
1	H	746	SER	3.4
1	I	753	ALA	3.4
1	A	451	LEU	3.4
1	G	461	ARG	3.4
1	J	419	THR	3.4
1	D	472	ILE	3.4
1	E	761	GLU	3.4
1	B	511	ARG	3.4
1	A	614	GLU	3.4
1	I	606	GLU	3.4
1	D	568	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	525	ASP	3.4
1	J	342	ILE	3.4
1	B	371	ALA	3.4
1	H	388	PHE	3.3
1	D	706	ASP	3.3
1	I	558	LEU	3.3
1	G	557	ARG	3.3
1	H	744	ARG	3.3
1	H	600	GLU	3.3
1	H	705	GLU	3.3
1	G	343	TRP	3.3
1	E	464	LEU	3.3
1	J	379	GLY	3.3
1	A	424	ASP	3.3
1	B	638	GLN	3.3
1	F	367	ASP	3.3
1	E	418	ILE	3.3
1	I	522	THR	3.3
1	F	701	VAL	3.3
1	H	695	LYS	3.3
1	A	367	ASP	3.2
1	I	513	GLN	3.2
1	J	697	MET	3.2
1	D	714	ALA	3.2
1	J	411	LEU	3.2
1	I	381	VAL	3.2
1	A	419	THR	3.2
1	G	348	LYS	3.2
1	G	613	LYS	3.2
1	F	684	THR	3.2
1	B	622	MET	3.2
1	I	681	GLN	3.2
1	F	341	PRO	3.2
1	D	410	LYS	3.2
1	H	596	VAL	3.2
1	H	755	VAL	3.2
1	F	705	GLU	3.2
1	G	457	LEU	3.2
1	C	340	LYS	3.2
1	J	638	GLN	3.2
1	H	408	TYR	3.2
1	E	411	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	386	ILE	3.2
1	J	362	PHE	3.2
1	D	705	GLU	3.2
1	H	550	GLU	3.2
1	A	361	SER	3.2
1	H	607	SER	3.2
1	D	750	ASP	3.2
1	B	434	LYS	3.1
1	I	539	TYR	3.1
1	H	368	ASP	3.1
1	H	634	ALA	3.1
1	I	760	GLU	3.1
1	J	340	LYS	3.1
1	B	619	LEU	3.1
1	B	482	ASP	3.1
1	G	369	PRO	3.1
1	J	642	GLU	3.1
1	G	357	ALA	3.1
1	A	468	THR	3.1
1	I	465	VAL	3.1
1	G	413	VAL	3.1
1	I	609	GLU	3.1
1	A	374	HIS	3.1
1	C	436	VAL	3.1
1	G	436	VAL	3.1
1	C	422	PHE	3.1
1	I	546	ARG	3.1
1	H	754	LYS	3.1
1	E	419	THR	3.1
1	B	566	ILE	3.1
1	J	389	VAL	3.1
1	E	619	LEU	3.1
1	H	717	LEU	3.0
1	D	383	PHE	3.0
1	C	648	VAL	3.0
1	I	641	THR	3.0
1	B	357	ALA	3.0
1	B	354	GLU	3.0
1	F	441	ASP	3.0
1	H	732	THR	3.0
1	G	423	HIS	3.0
1	B	553	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	744	ARG	3.0
1	C	613	LYS	3.0
1	B	565	VAL	3.0
1	B	383	PHE	3.0
1	A	606	GLU	3.0
1	B	416	VAL	3.0
1	I	438	ASP	3.0
1	I	587	ARG	3.0
1	G	560	LYS	3.0
1	I	579	ALA	3.0
1	J	755	VAL	3.0
1	E	748	ASN	3.0
1	H	685	PHE	3.0
1	F	704	ASP	2.9
1	G	387	LEU	2.9
1	I	597	LYS	2.9
1	C	561	LYS	2.9
1	C	357	ALA	2.9
1	G	753	ALA	2.9
1	H	350	VAL	2.9
1	H	633	LYS	2.9
1	A	483	THR	2.9
1	E	755	VAL	2.9
1	I	346	PRO	2.9
1	G	468	THR	2.9
1	H	708	LYS	2.9
1	H	452	GLN	2.9
1	I	623	LYS	2.9
1	I	732	THR	2.9
1	E	410	LYS	2.9
1	C	620	ASN	2.9
1	A	343	TRP	2.9
1	B	658	MET	2.9
1	C	743	LEU	2.9
1	J	416	VAL	2.9
1	B	392	SER	2.9
1	E	381	VAL	2.9
1	E	752	ASP	2.9
1	D	759	PRO	2.9
1	H	655	SER	2.9
1	B	410	LYS	2.9
1	G	394	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	652	TYR	2.9
1	D	616	GLU	2.8
1	J	678	TYR	2.8
1	I	636	VAL	2.8
1	C	358	PHE	2.8
1	A	755	VAL	2.8
1	F	746	SER	2.8
1	B	590	ASN	2.8
1	I	652	TYR	2.8
1	G	432	PHE	2.8
1	G	437	VAL	2.8
1	J	354	GLU	2.8
1	E	561	LYS	2.8
1	E	437	VAL	2.8
1	G	541	MET	2.8
1	D	592	ALA	2.8
1	D	747	LEU	2.8
1	J	344	GLN	2.8
1	D	746	SER	2.8
1	D	343	TRP	2.8
1	G	417	PHE	2.8
1	D	648	VAL	2.8
1	J	515	SER	2.8
1	C	759	PRO	2.8
1	E	443	PRO	2.8
1	I	343	TRP	2.7
1	D	658	MET	2.7
1	I	390	PRO	2.7
1	I	487	GLU	2.7
1	C	597	LYS	2.7
1	F	744	ARG	2.7
1	E	500	HIS	2.7
1	I	556	GLU	2.7
1	C	615	PHE	2.7
1	B	347	SER	2.7
1	F	618	LEU	2.7
1	F	698	LEU	2.7
1	B	343	TRP	2.7
1	J	598	PHE	2.7
1	G	626	ALA	2.7
1	I	359	TYR	2.7
1	D	341	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	390	PRO	2.7
1	E	527	TYR	2.7
1	H	437	VAL	2.7
1	B	586	LYS	2.7
1	I	484	PHE	2.7
1	E	737	ASP	2.7
1	J	343	TRP	2.7
1	G	558	LEU	2.7
1	B	361	SER	2.7
1	B	484	PHE	2.7
1	D	748	ASN	2.7
1	D	604	THR	2.7
1	H	441	ASP	2.7
1	H	682	LYS	2.7
1	A	748	ASN	2.7
1	D	386	ILE	2.7
1	H	590	ASN	2.7
1	B	512	PHE	2.7
1	F	362	PHE	2.7
1	G	660	ARG	2.7
1	I	738	ARG	2.7
1	H	435	GLY	2.7
1	D	484	PHE	2.6
1	D	394	PRO	2.6
1	I	647	LEU	2.6
1	I	748	ASN	2.6
1	C	449	GLU	2.6
1	G	534	LYS	2.6
1	H	706	ASP	2.6
1	I	482	ASP	2.6
1	I	536	ASP	2.6
1	A	522	THR	2.6
1	I	697	MET	2.6
1	A	615	PHE	2.6
1	F	374	HIS	2.6
1	B	740	GLU	2.6
1	I	376	THR	2.6
1	J	457	LEU	2.6
1	H	610	ALA	2.6
1	F	585	GLY	2.6
1	H	653	GLY	2.6
1	A	752	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	513	GLN	2.6
1	D	364	LYS	2.6
1	B	596	VAL	2.6
1	I	563	TYR	2.6
1	B	522	THR	2.6
1	G	654	TRP	2.6
1	G	687	ILE	2.6
1	A	371	ALA	2.6
1	G	392	SER	2.6
1	C	748	ASN	2.6
1	H	636	VAL	2.6
1	C	472	ILE	2.6
1	J	371	ALA	2.6
1	B	623	LYS	2.6
1	G	759	PRO	2.6
1	D	424	ASP	2.6
1	D	459	VAL	2.6
1	A	347	SER	2.5
1	C	644	PRO	2.5
1	E	442	LEU	2.5
1	B	346	PRO	2.5
1	F	598	PHE	2.5
1	I	533	GLU	2.5
1	D	418	ILE	2.5
1	J	361	SER	2.5
1	B	412	TYR	2.5
1	H	389	VAL	2.5
1	H	608	ARG	2.5
1	E	363	SER	2.5
1	H	671	LYS	2.5
1	I	537	LYS	2.5
1	A	756	GLU	2.5
1	A	757	GLU	2.5
1	D	761	GLU	2.5
1	J	486	LYS	2.5
1	A	685	PHE	2.5
1	D	362	PHE	2.5
1	D	375	PHE	2.5
1	A	638	GLN	2.5
1	I	568	LEU	2.5
1	C	544	SER	2.5
1	G	346	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	748	ASN	2.5
1	C	370	MET	2.5
1	E	732	THR	2.5
1	G	647	LEU	2.5
1	I	615	PHE	2.5
1	B	425	MET	2.5
1	H	440	ASP	2.5
1	I	365	GLU	2.5
1	B	597	LYS	2.4
1	H	442	LEU	2.4
1	J	434	LYS	2.4
1	D	417	PHE	2.4
1	D	608	ARG	2.4
1	G	350	VAL	2.4
1	I	596	VAL	2.4
1	J	619	LEU	2.4
1	F	638	GLN	2.4
1	G	556	GLU	2.4
1	H	438	ASP	2.4
1	E	357	ALA	2.4
1	C	732	THR	2.4
1	D	360	LYS	2.4
1	E	349	GLU	2.4
1	F	444	LEU	2.4
1	G	516	HIS	2.4
1	B	445	ASN	2.4
1	I	740	GLU	2.4
1	J	394	PRO	2.4
1	J	540	PHE	2.4
1	E	747	LEU	2.4
1	B	362	PHE	2.4
1	A	664	ALA	2.4
1	A	762	GLU	2.4
1	D	659	GLU	2.4
1	B	439	SER	2.4
1	C	744	ARG	2.4
1	I	534	LYS	2.4
1	C	408	TYR	2.4
1	H	574	GLU	2.4
1	E	421	ASP	2.4
1	H	416	VAL	2.4
1	B	349	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	689	PRO	2.4
1	C	689	PRO	2.4
1	D	624	ASP	2.4
1	F	421	ASP	2.4
1	F	740	GLU	2.4
1	G	574	GLU	2.4
1	A	413	VAL	2.3
1	F	436	VAL	2.3
1	H	665	GLN	2.3
1	I	588	PHE	2.3
1	H	605	LYS	2.3
1	D	372	TYR	2.3
1	D	442	LEU	2.3
1	I	353	ASP	2.3
1	J	422	PHE	2.3
1	B	505	ARG	2.3
1	F	411	LEU	2.3
1	G	393	ALA	2.3
1	I	429	TYR	2.3
1	B	378	GLU	2.3
1	H	584	ASP	2.3
1	J	448	ARG	2.3
1	H	578	GLN	2.3
1	I	731	ASP	2.3
1	H	342	ILE	2.3
1	H	580	LEU	2.3
1	C	347	SER	2.3
1	H	356	LYS	2.3
1	H	686	GLU	2.3
1	D	744	ARG	2.3
1	C	421	ASP	2.3
1	B	473	LYS	2.3
1	I	463	LYS	2.3
1	A	411	LEU	2.3
1	E	648	VAL	2.3
1	H	710	VAL	2.3
1	I	426	MET	2.3
1	H	640	LEU	2.3
1	I	430	LEU	2.3
1	J	430	LEU	2.3
1	E	568	LEU	2.3
1	H	444	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	691	HIS	2.3
1	H	411	LEU	2.3
1	A	611	ILE	2.3
1	A	597	LYS	2.3
1	G	429	TYR	2.3
1	D	559	LEU	2.3
1	H	611	ILE	2.3
1	E	347	SER	2.3
1	H	674	SER	2.3
1	B	456	LEU	2.2
1	G	620	ASN	2.2
1	I	706	ASP	2.2
1	B	379	GLY	2.2
1	I	380	GLU	2.2
1	B	640	LEU	2.2
1	G	510	LEU	2.2
1	J	687	ILE	2.2
1	E	758	GLU	2.2
1	A	746	SER	2.2
1	G	590	ASN	2.2
1	G	704	ASP	2.2
1	B	414	ARG	2.2
1	C	740	GLU	2.2
1	G	513	GLN	2.2
1	J	602	GLU	2.2
1	B	525	ASP	2.2
1	H	448	ARG	2.2
1	D	555	VAL	2.2
1	J	386	ILE	2.2
1	B	539	TYR	2.2
1	B	731	ASP	2.2
1	E	584	ASP	2.2
1	G	499	ASP	2.2
1	B	409	ILE	2.2
1	F	360	LYS	2.2
1	A	365	GLU	2.2
1	B	557	ARG	2.2
1	E	360	LYS	2.2
1	D	389	VAL	2.2
1	G	496	VAL	2.2
1	H	539	TYR	2.2
1	D	553	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	631	ILE	2.2
1	B	621	TRP	2.2
1	C	652	TYR	2.2
1	C	756	GLU	2.2
1	D	425	MET	2.2
1	E	450	THR	2.2
1	C	619	LEU	2.2
1	G	695	LYS	2.2
1	J	513	GLN	2.2
1	I	565	VAL	2.2
1	J	365	GLU	2.2
1	B	454	HIS	2.2
1	D	569	THR	2.2
1	I	410	LYS	2.2
1	F	364	LYS	2.1
1	H	541	MET	2.1
1	I	481	ASN	2.1
1	J	677	TYR	2.1
1	D	704	ASP	2.1
1	C	411	LEU	2.1
1	D	456	LEU	2.1
1	G	359	TYR	2.1
1	H	355	TYR	2.1
1	J	557	ARG	2.1
1	J	436	VAL	2.1
1	C	585	GLY	2.1
1	B	348	LYS	2.1
1	D	597	LYS	2.1
1	G	588	PHE	2.1
1	B	385	SER	2.1
1	C	596	VAL	2.1
1	E	445	ASN	2.1
1	I	529	GLU	2.1
1	A	603	LYS	2.1
1	C	763	PRO	2.1
1	H	439	SER	2.1
1	G	422	PHE	2.1
1	H	460	ILE	2.1
1	H	676	ASN	2.1
1	A	414	ARG	2.1
1	D	737	ASP	2.1
1	I	649	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	596	VAL	2.1
1	B	684	THR	2.1
1	D	510	LEU	2.1
1	A	372	TYR	2.1
1	B	533	GLU	2.1
1	D	544	SER	2.1
1	F	392	SER	2.1
1	A	436	VAL	2.1
1	H	525	ASP	2.1
1	F	660	ARG	2.1
1	H	694	ILE	2.1
1	G	619	LEU	2.1
1	J	387	LEU	2.1
1	F	439	SER	2.1
1	G	439	SER	2.1
1	G	565	VAL	2.1
1	H	555	VAL	2.1
1	B	595	GLY	2.1
1	D	452	GLN	2.1
1	H	343	TRP	2.1
1	G	688	ASN	2.1
1	A	714	ALA	2.1
1	G	572	VAL	2.1
1	H	414	ARG	2.1
1	C	499	ASP	2.1
1	I	512	PHE	2.1
1	G	582	GLU	2.1
1	J	561	LYS	2.1
1	G	648	VAL	2.1
1	C	451	LEU	2.1
1	B	520	ASP	2.1
1	D	513	GLN	2.0
1	E	353	ASP	2.1
1	C	371	ALA	2.0
1	F	748	ASN	2.0
1	D	656	GLY	2.0
1	G	762	GLU	2.0
1	D	627	LEU	2.0
1	I	472	ILE	2.0
1	D	655	SER	2.0
1	H	624	ASP	2.0
1	B	508	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	614	GLU	2.0
1	J	426	MET	2.0
1	C	693	LEU	2.0
1	D	441	ASP	2.0
1	D	708	LYS	2.0
1	I	561	LYS	2.0
1	I	572	VAL	2.0
1	J	420	ASP	2.0
1	H	409	ILE	2.0
1	A	425	MET	2.0
1	B	468	THR	2.0
1	B	720	THR	2.0
1	D	481	ASN	2.0
1	C	638	GLN	2.0
1	C	651	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.