



# Full wwPDB X-ray Structure Validation Report i

Aug 16, 2022 – 01:28 pm BST

PDB ID : 7QX8  
Title : Crystal structure of serine hydroxymethyltransferase, isoform 7 from Arabidopsis thaliana (SHM7)  
Authors : Ruszkowski, M.; Grzechowiak, M.; Sekula, B.  
Deposited on : 2022-01-26  
Resolution : 2.74 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](mailto: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 i symbol.

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

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The following versions of software and data (see references ①) were used in the production of this report:

MolProbitiy : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.29  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

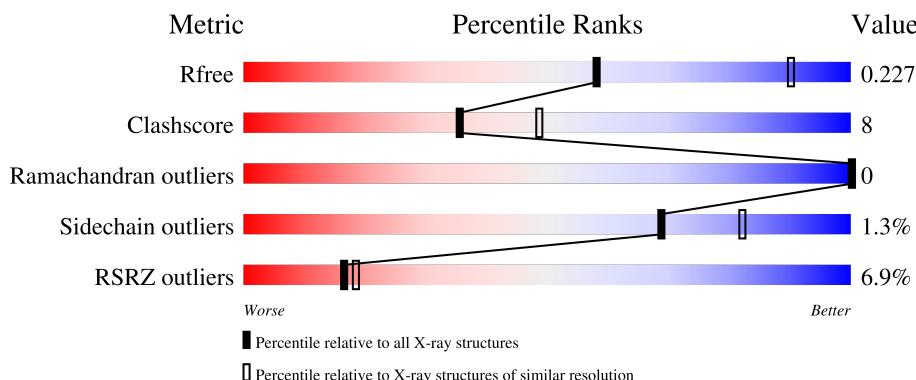
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 Å.

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



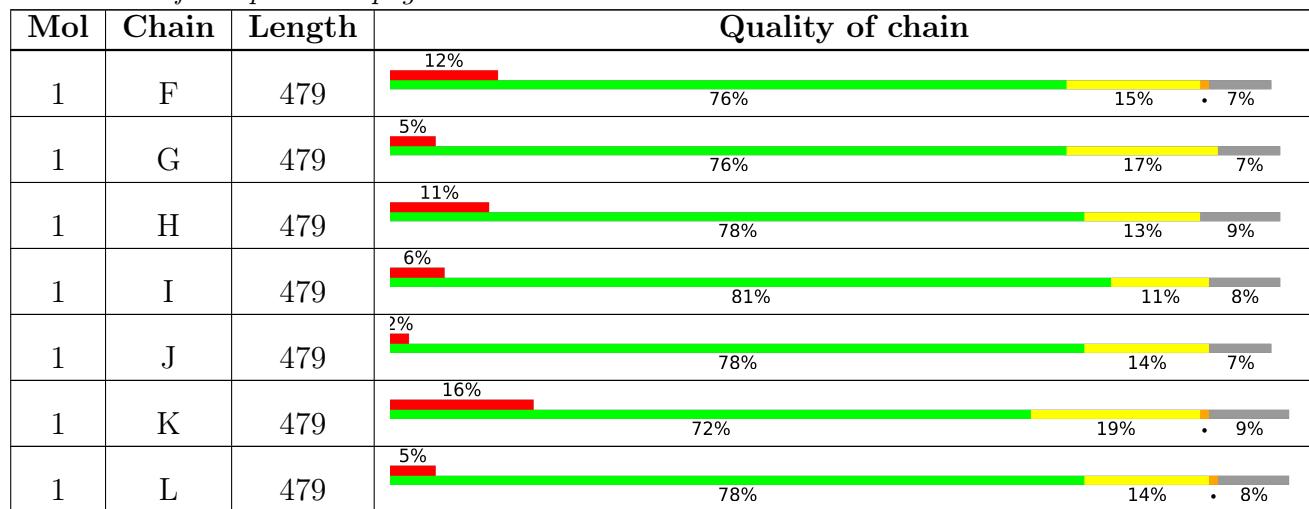
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



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## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 41696 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 Serine hydroxymethyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3454	2183	608	638	25			
1	B	443	Total	C	N	O	S	0	0	0
			3454	2181	608	640	25			
1	C	447	Total	C	N	O	S	0	0	0
			3486	2199	613	649	25			
1	D	438	Total	C	N	O	S	0	1	0
			3429	2167	603	634	25			
1	E	442	Total	C	N	O	S	0	1	0
			3460	2186	609	640	25			
1	F	444	Total	C	N	O	S	0	1	0
			3467	2186	612	644	25			
1	G	444	Total	C	N	O	S	0	0	0
			3460	2183	609	643	25			
1	H	438	Total	C	N	O	S	0	1	0
			3431	2169	604	633	25			
1	I	442	Total	C	N	O	S	0	1	0
			3456	2182	610	639	25			
1	J	444	Total	C	N	O	S	0	0	0
			3461	2185	609	642	25			
1	K	437	Total	C	N	O	S	0	1	0
			3419	2158	604	632	25			
1	L	443	Total	C	N	O	S	0	1	0
			3463	2187	610	641	25			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	SER	-	expression tag	UNP Q84WV0
A	121	ASN	-	expression tag	UNP Q84WV0
A	122	ALA	-	expression tag	UNP Q84WV0
B	120	SER	-	expression tag	UNP Q84WV0
B	121	ASN	-	expression tag	UNP Q84WV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	122	ALA	-	expression tag	UNP Q84WV0
C	120	SER	-	expression tag	UNP Q84WV0
C	121	ASN	-	expression tag	UNP Q84WV0
C	122	ALA	-	expression tag	UNP Q84WV0
D	120	SER	-	expression tag	UNP Q84WV0
D	121	ASN	-	expression tag	UNP Q84WV0
D	122	ALA	-	expression tag	UNP Q84WV0
E	120	SER	-	expression tag	UNP Q84WV0
E	121	ASN	-	expression tag	UNP Q84WV0
E	122	ALA	-	expression tag	UNP Q84WV0
F	120	SER	-	expression tag	UNP Q84WV0
F	121	ASN	-	expression tag	UNP Q84WV0
F	122	ALA	-	expression tag	UNP Q84WV0
G	120	SER	-	expression tag	UNP Q84WV0
G	121	ASN	-	expression tag	UNP Q84WV0
G	122	ALA	-	expression tag	UNP Q84WV0
H	120	SER	-	expression tag	UNP Q84WV0
H	121	ASN	-	expression tag	UNP Q84WV0
H	122	ALA	-	expression tag	UNP Q84WV0
I	120	SER	-	expression tag	UNP Q84WV0
I	121	ASN	-	expression tag	UNP Q84WV0
I	122	ALA	-	expression tag	UNP Q84WV0
J	120	SER	-	expression tag	UNP Q84WV0
J	121	ASN	-	expression tag	UNP Q84WV0
J	122	ALA	-	expression tag	UNP Q84WV0
K	120	SER	-	expression tag	UNP Q84WV0
K	121	ASN	-	expression tag	UNP Q84WV0
K	122	ALA	-	expression tag	UNP Q84WV0
L	120	SER	-	expression tag	UNP Q84WV0
L	121	ASN	-	expression tag	UNP Q84WV0
L	122	ALA	-	expression tag	UNP Q84WV0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	32	Total O 32 32	0	0
2	B	24	Total O 24 24	0	0
2	C	35	Total O 35 35	0	0
2	D	12	Total O 12 12	0	0

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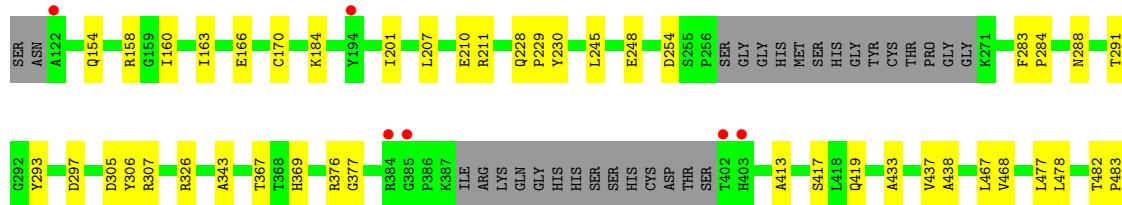
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	30	Total O 30 30	0	0
2	F	18	Total O 18 18	0	0
2	G	15	Total O 15 15	0	0
2	H	6	Total O 6 6	0	0
2	I	24	Total O 24 24	0	0
2	J	26	Total O 26 26	0	0
2	K	14	Total O 14 14	0	0
2	L	20	Total O 20 20	0	0

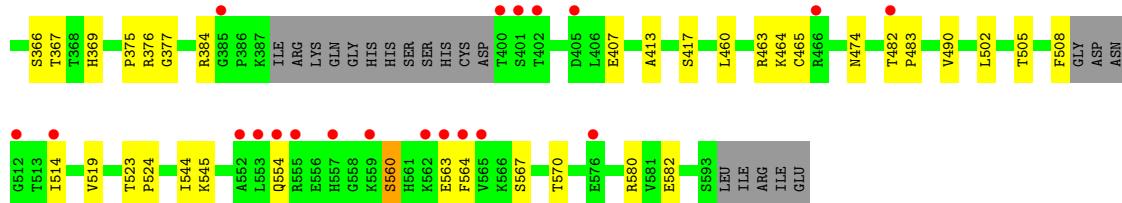
### 3 Residue-property plots [\(i\)](#)

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

- Molecule 1: Serine hydroxymethyltransferase 7

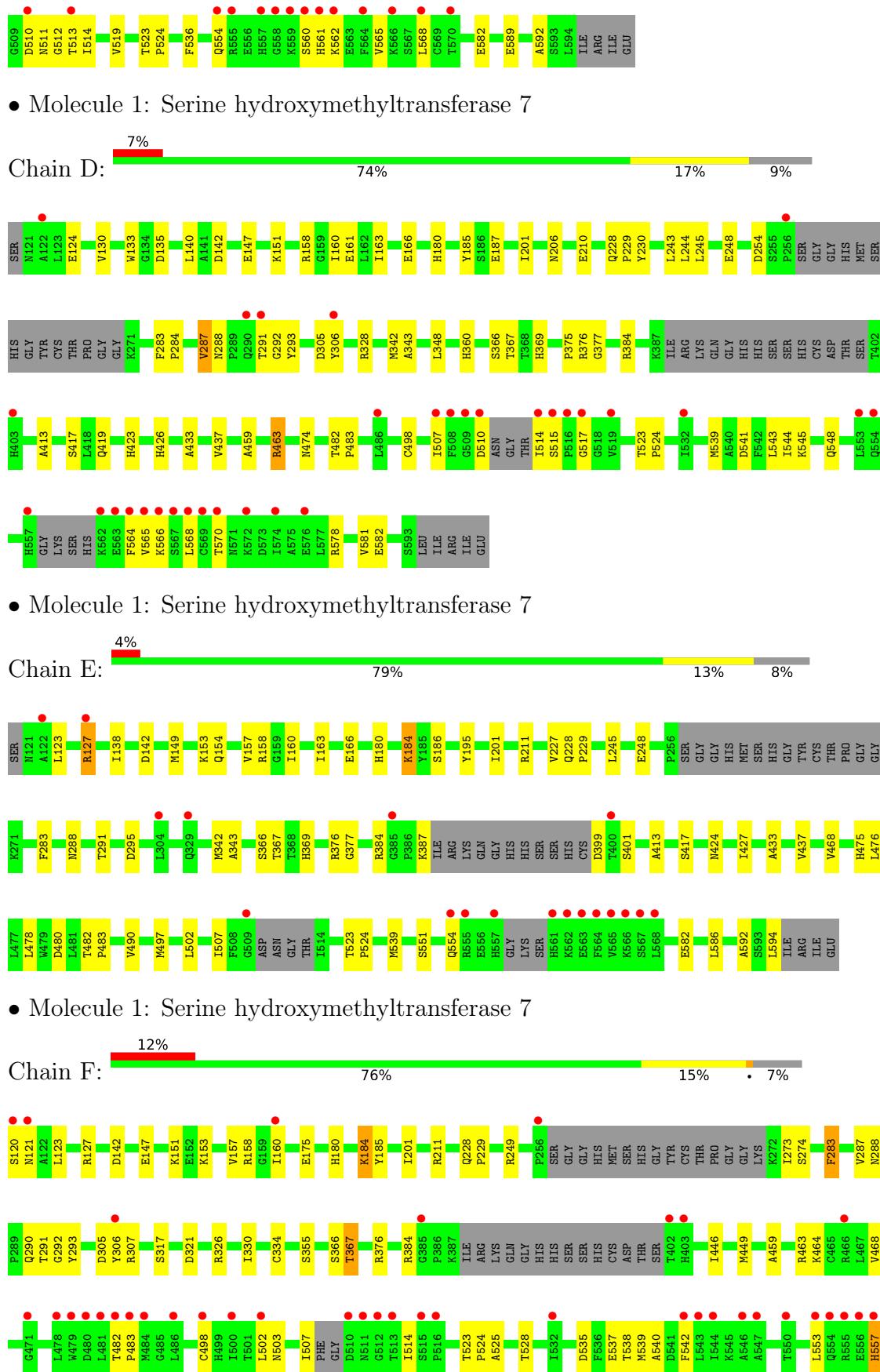


- Molecule 1: Serine hydroxymethyltransferase 7



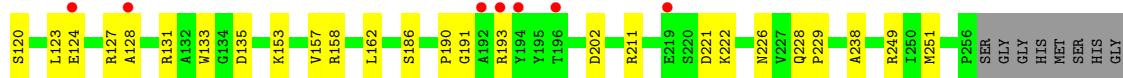
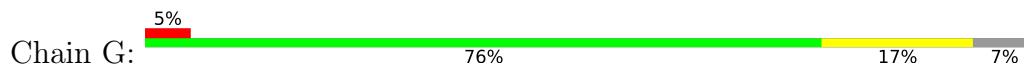
- Molecule 1: Serine hydroxymethyltransferase 7



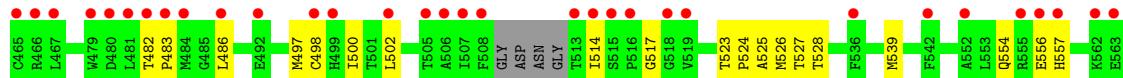
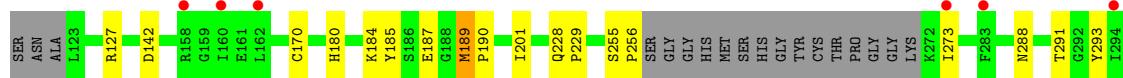
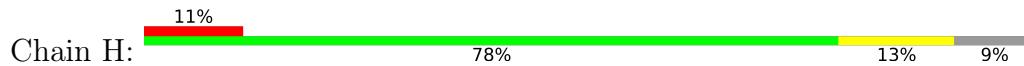




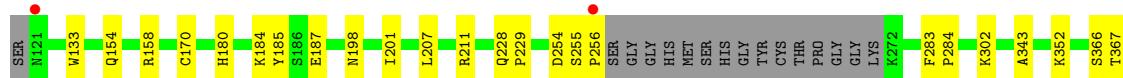
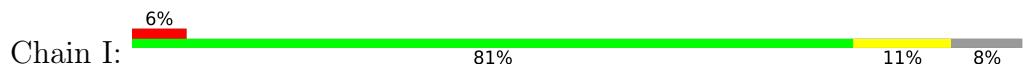
- Molecule 1: Serine hydroxymethyltransferase 7



- Molecule 1: Serine hydroxymethyltransferase 7

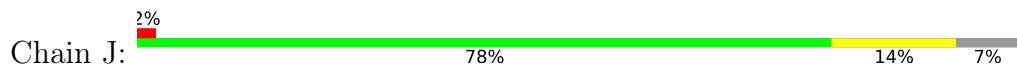


- Molecule 1: Serine hydroxymethyltransferase 7

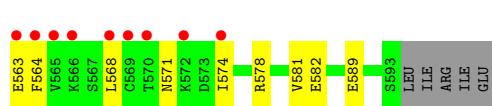
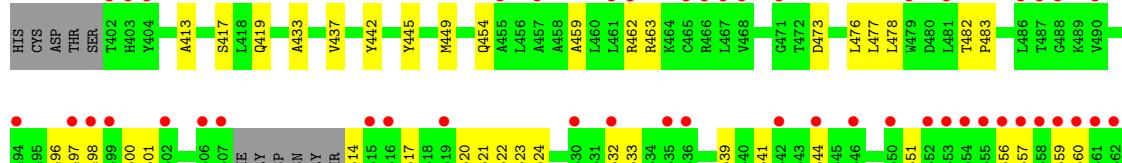




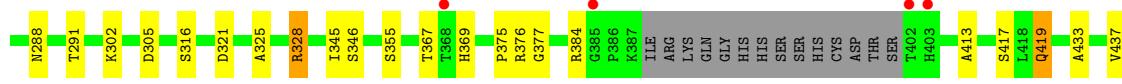
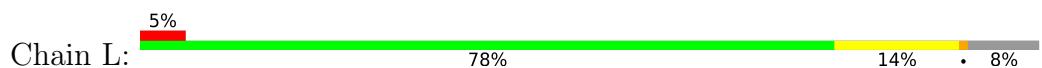
- Molecule 1: Serine hydroxymethyltransferase 7

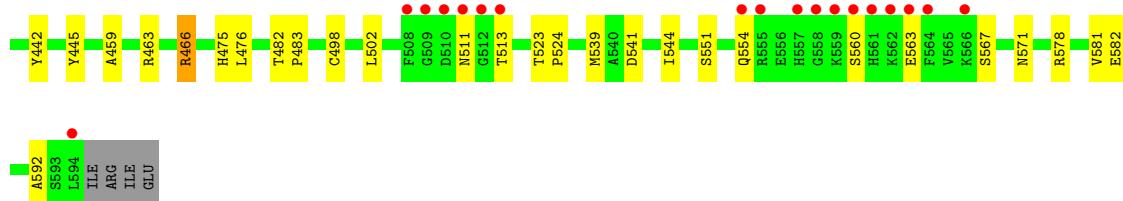


- Molecule 1: Serine hydroxymethyltransferase 7



- Molecule 1: Serine hydroxymethyltransferase 7





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.83Å    123.95Å    290.54Å 90.00°    93.17°    90.00°	Depositor
Resolution (Å)	58.00 – 2.74 58.02 – 2.74	Depositor EDS
% Data completeness (in resolution range)	65.2 (58.00-2.74) 65.2 (58.02-2.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.76 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
$R$ , $R_{free}$	0.187 , 0.227 0.188 , 0.227	Depositor DCC
$R_{free}$ test set	1220 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.51$ , $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	41696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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	0.74	0/3524	0.88	0/4757
1	B	0.71	0/3524	0.86	0/4757
1	C	0.74	0/3557	0.88	0/4804
1	D	0.71	0/3501	0.86	0/4726
1	E	0.73	0/3533	0.88	0/4770
1	F	0.69	0/3540	0.86	0/4781
1	G	0.68	0/3530	0.88	0/4767
1	H	0.67	0/3505	0.85	0/4733
1	I	0.73	0/3530	0.88	0/4767
1	J	0.74	0/3531	0.90	0/4768
1	K	0.67	0/3491	0.83	0/4713
1	L	0.69	0/3538	0.87	0/4779
All	All	0.71	0/42304	0.87	0/57122

There are no bond length outliers.

There are no bond angle outliers.

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	3454	0	3446	50	0
1	B	3454	0	3442	44	0
1	C	3486	0	3468	55	0
1	D	3429	0	3413	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3460	0	3443	52	0
1	F	3467	0	3449	66	0
1	G	3460	0	3442	72	0
1	H	3431	0	3418	62	0
1	I	3456	0	3438	48	0
1	J	3461	0	3446	56	0
1	K	3419	0	3406	94	0
1	L	3463	0	3446	58	0
2	A	32	0	0	2	0
2	B	24	0	0	0	0
2	C	35	0	0	2	0
2	D	12	0	0	0	0
2	E	30	0	0	0	0
2	F	18	0	0	5	0
2	G	15	0	0	1	0
2	H	6	0	0	0	0
2	I	24	0	0	1	0
2	J	26	0	0	1	0
2	K	14	0	0	1	0
2	L	20	0	0	0	0
All	All	41696	0	41257	668	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 (668) 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:A:526:MET:HG3	1:A:539:MET:HE1	1.27	1.12
1:I:497:MET:HG3	1:I:568:LEU:HD21	1.11	1.10
1:H:452:ASN:HD22	1:H:527:THR:HG22	1.10	1.08
1:G:249:ARG:HB3	1:G:306:TYR:HE1	1.16	1.05
1:B:560:SER:OG	1:B:563:GLU:HB2	1.60	1.01
1:I:497:MET:CG	1:I:568:LEU:HD21	1.92	0.98
1:A:526:MET:HG3	1:A:539:MET:CE	1.95	0.97
1:G:186:SER:HB3	1:G:193:ARG:HH11	1.28	0.96
1:F:449:MET:HE2	1:F:524:PRO:HG3	1.48	0.94
1:G:186:SER:HB3	1:G:193:ARG:NH1	1.83	0.93
1:K:253:LEU:HD23	1:K:254:ASP:N	1.85	0.92
1:G:249:ARG:HB3	1:G:306:TYR:CE1	2.06	0.91
1:G:589:GLU:HG2	1:H:127:ARG:HG3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:ARG:O	1:D:581:VAL:HG12	1.71	0.90
1:D:230:TYR:CE2	1:D:419:GLN:HB3	2.07	0.89
1:K:578:ARG:O	1:K:581:VAL:HG12	1.73	0.89
1:D:369:HIS:CD2	1:D:376:ARG:HA	2.10	0.86
1:G:251:MET:HG3	1:G:283:PHE:O	1.76	0.85
1:D:463:ARG:HG3	1:D:463:ARG:HH11	1.38	0.85
1:F:449:MET:CE	1:F:524:PRO:HG3	2.07	0.85
1:I:497:MET:HG3	1:I:568:LEU:CD2	2.04	0.84
1:D:539:MET:O	1:D:543:LEU:HD13	1.79	0.83
1:I:498:CYS:O	1:I:581:VAL:HG21	1.78	0.82
1:H:436:GLN:O	1:H:439:THR:HG22	1.82	0.80
1:G:369:HIS:CD2	1:G:376:ARG:HA	2.17	0.80
1:H:452:ASN:ND2	1:H:527:THR:HG22	1.93	0.80
1:L:232:CYS:HB2	1:L:367:THR:HG22	1.64	0.79
1:H:497:MET:HG3	1:H:568:LEU:HG	1.63	0.79
1:C:387:LYS:NZ	1:C:401:SER:HB3	1.98	0.77
1:D:498:CYS:O	1:D:581:VAL:HG11	1.84	0.76
1:G:128:ALA:HA	1:G:131:ARG:HG2	1.67	0.76
1:G:251:MET:CE	1:G:308:PRO:HG3	2.16	0.76
1:L:498:CYS:O	1:L:581:VAL:HG11	1.85	0.76
1:A:438:ALA:O	1:I:352:LYS:HE3	1.86	0.75
1:H:557:HIS:HB3	1:H:564:PHE:HD1	1.51	0.75
1:G:251:MET:HE3	1:G:308:PRO:HG3	1.68	0.74
1:K:180[B]:HIS:NE2	1:L:592:ALA:O	2.21	0.73
1:H:557:HIS:HB3	1:H:564:PHE:CD1	2.22	0.73
1:F:305:ASP:HB3	1:G:283:PHE:HZ	1.53	0.73
1:F:459:ALA:O	1:F:463:ARG:HG2	1.89	0.73
1:F:464:LYS:HG3	1:F:464:LYS:O	1.89	0.73
1:C:592:ALA:O	1:D:180[B]:HIS:NE2	2.22	0.72
1:E:369:HIS:CD2	1:E:376:ARG:HA	2.23	0.72
1:F:572:LYS:O	1:F:576:GLU:HG3	1.89	0.72
1:A:160:ILE:HG23	1:A:539:MET:CE	2.19	0.72
1:K:317:SER:HB2	1:K:476:LEU:HD21	1.72	0.72
1:G:249:ARG:HD3	1:G:306:TYR:CE1	2.25	0.71
1:L:578:ARG:O	1:L:581:VAL:HG12	1.90	0.71
1:G:251:MET:HE1	1:G:303:ALA:HA	1.72	0.71
1:K:166:GLU:HA	1:L:185:TYR:CE2	2.27	0.70
1:K:501:THR:HG22	1:L:196:THR:HG22	1.72	0.70
1:D:463:ARG:HG3	1:D:463:ARG:NH1	2.07	0.70
1:G:283:PHE:HB2	1:G:306:TYR:CE2	2.25	0.70
1:E:184:LYS:HG2	1:E:201:ILE:CD1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HG23	1:A:539:MET:HE3	1.72	0.69
1:F:498:CYS:O	1:F:581:VAL:HG11	1.93	0.69
1:H:369:HIS:CD2	1:H:376:ARG:HA	2.27	0.69
1:F:578:ARG:O	1:F:581:VAL:HG12	1.94	0.68
1:F:184:LYS:HG2	1:F:201:ILE:HD13	1.75	0.67
1:H:498:CYS:HA	1:H:578:ARG:HG3	1.76	0.67
1:H:288:ASN:HB3	1:H:291:THR:HG22	1.77	0.67
1:B:369:HIS:CD2	1:B:376:ARG:HA	2.30	0.66
1:G:369:HIS:HD2	1:G:377:GLY:H	1.44	0.66
1:H:439:THR:HG23	1:H:442:TYR:H	1.59	0.66
1:F:184:LYS:HG2	1:F:201:ILE:CD1	2.25	0.66
1:L:560:SER:HB3	1:L:563:GLU:HG2	1.77	0.66
1:F:291:THR:HG22	1:F:293:TYR:HD2	1.61	0.66
1:E:149:MET:O	1:F:180[A]:HIS:NE2	2.28	0.66
1:E:387:LYS:HZ2	1:E:401:SER:HB3	1.61	0.66
1:A:523:THR:N	1:A:524:PRO:HD3	2.11	0.66
1:C:387:LYS:HZ3	1:C:401:SER:HB3	1.61	0.66
1:I:463:ARG:HD2	1:I:544:ILE:HD11	1.78	0.66
1:B:560:SER:HG	1:B:563:GLU:HB2	1.62	0.65
1:G:574:ILE:HD12	1:G:578:ARG:HH12	1.62	0.65
1:F:123:LEU:HD11	2:F:608:HOH:O	1.96	0.65
1:D:283:PHE:HB2	1:D:306:TYR:CZ	2.32	0.65
1:K:317:SER:HB2	1:K:476:LEU:CD2	2.28	0.64
1:K:164:ALA:CB	1:K:476:LEU:HD13	2.26	0.64
1:J:228:GLN:N	1:J:229:PRO:CD	2.60	0.64
1:J:307:ARG:NH1	1:J:334:CYS:HA	2.13	0.64
1:E:387:LYS:NZ	1:E:401:SER:HB3	2.12	0.64
1:D:291:THR:HG23	1:D:293:TYR:H	1.62	0.64
1:B:185:TYR:CE1	1:B:187:GLU:HG3	2.32	0.64
1:E:586:LEU:HD12	1:J:586:LEU:HD12	1.79	0.64
1:D:342:MET:O	1:D:342:MET:HG2	1.99	0.63
1:I:464:LYS:HG2	1:I:464:LYS:O	1.97	0.63
1:K:496:GLU:CG	1:L:196:THR:HG23	2.29	0.62
1:L:511:ASN:OD1	1:L:513:THR:HG22	2.00	0.62
1:D:288:ASN:HB3	1:D:291:THR:HG22	1.82	0.62
1:E:283:PHE:CE1	1:H:305:ASP:OD1	2.52	0.62
1:J:232:CYS:HB2	1:J:367:THR:HG22	1.81	0.62
1:C:291:THR:HG23	1:C:293:TYR:H	1.63	0.62
1:H:497:MET:HG3	1:H:568:LEU:CG	2.29	0.62
1:C:514:ILE:N	1:C:514:ILE:HD12	2.15	0.62
1:D:369:HIS:HD2	1:D:377:GLY:H	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ASN:HB3	1:C:291:THR:HG22	1.82	0.61
1:F:538:THR:HG22	1:F:542:PHE:CE1	2.35	0.61
1:C:288:ASN:CG	1:C:291:THR:HG22	2.20	0.61
1:D:228:GLN:N	1:D:229:PRO:CD	2.64	0.61
1:I:578:ARG:O	1:I:581:VAL:HG22	2.01	0.61
1:C:228:GLN:N	1:C:229:PRO:CD	2.64	0.61
1:L:466:ARG:HH11	1:L:466:ARG:HG3	1.66	0.61
1:A:523:THR:N	1:A:524:PRO:CD	2.64	0.60
1:J:124:GLU:OE2	1:J:127:ARG:HD3	2.01	0.60
1:I:589:GLU:HG2	1:J:127:ARG:HG3	1.82	0.60
1:C:433:ALA:O	1:C:437:VAL:HG23	2.02	0.60
1:F:127:ARG:HD3	2:F:608:HOH:O	2.00	0.60
1:B:228:GLN:N	1:B:229:PRO:CD	2.65	0.60
1:K:288:ASN:HB3	1:K:291:THR:HG22	1.82	0.60
1:K:476:LEU:HD12	1:K:521:ILE:O	2.01	0.60
1:K:164:ALA:HB2	1:K:476:LEU:HD13	1.83	0.59
1:D:523:THR:N	1:D:524:PRO:HD3	2.17	0.59
1:G:523:THR:N	1:G:524:PRO:HD3	2.17	0.59
1:K:463:ARG:NH1	1:K:541:ASP:OD1	2.35	0.59
1:K:291:THR:HG23	1:K:293:TYR:H	1.68	0.59
1:K:454:GLN:HA	1:K:454:GLN:OE1	2.03	0.59
1:G:191:GLY:N	1:G:202:ASP:OD2	2.36	0.59
1:K:589:GLU:OE2	1:L:127:ARG:HG2	2.03	0.59
1:B:490:VAL:HG11	1:B:554:GLN:NE2	2.18	0.59
1:K:169:VAL:HB	1:K:173:VAL:HG21	1.85	0.58
1:K:523:THR:N	1:K:524:PRO:HD2	2.17	0.58
1:K:476:LEU:HD11	1:K:520:ARG:CG	2.33	0.58
1:B:570:THR:O	1:B:570:THR:HG22	2.04	0.58
1:A:502:LEU:HD21	1:A:521:ILE:HG12	1.84	0.58
1:C:288:ASN:CB	1:C:291:THR:HG22	2.33	0.58
1:G:283:PHE:CB	1:G:306:TYR:CE2	2.86	0.58
1:H:452:ASN:HD22	1:H:527:THR:CG2	2.01	0.58
1:G:499:HIS:NE2	1:G:578:ARG:HD2	2.18	0.58
1:I:523:THR:N	1:I:524:PRO:HD3	2.18	0.58
1:J:502:LEU:CD2	1:J:521:ILE:HG12	2.33	0.58
1:K:319:PRO:HG3	1:K:478:LEU:HD13	1.85	0.58
1:L:162:LEU:HB2	1:L:502:LEU:CD2	2.33	0.58
1:L:228:GLN:N	1:L:229:PRO:CD	2.66	0.58
1:F:305:ASP:HB3	1:G:283:PHE:CZ	2.35	0.58
1:G:589:GLU:HG2	1:H:127:ARG:CG	2.29	0.58
1:G:523:THR:N	1:G:524:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:449:MET:HA	1:H:527:THR:HG21	1.85	0.58
1:G:228:GLN:N	1:G:229:PRO:CD	2.67	0.58
1:J:218:LEU:HD11	1:J:358:PHE:CE2	2.39	0.58
1:D:124:GLU:OE1	1:D:124:GLU:HA	2.04	0.57
1:B:185:TYR:HE1	1:B:187:GLU:CG	2.17	0.57
1:L:245:LEU:O	1:L:248:GLU:HG3	2.03	0.57
1:L:523:THR:N	1:L:524:PRO:CD	2.68	0.57
1:H:288:ASN:CB	1:H:291:THR:HG22	2.34	0.57
1:H:288:ASN:HB3	1:H:291:THR:CG2	2.34	0.57
1:E:227:VAL:HG23	1:E:427:ILE:CD1	2.35	0.57
1:C:497:MET:HG3	1:C:568:LEU:HD11	1.87	0.57
1:F:562:LYS:HA	1:F:565:VAL:HG22	1.87	0.57
1:L:523:THR:N	1:L:524:PRO:HD3	2.20	0.57
1:C:376:ARG:NH1	1:D:185:TYR:CD1	2.72	0.57
1:G:211:ARG:NH1	1:H:142:ASP:OD2	2.34	0.57
1:K:253:LEU:HD23	1:K:254:ASP:H	1.66	0.57
1:D:523:THR:N	1:D:524:PRO:CD	2.68	0.56
1:E:180[B]:HIS:NE2	1:F:592:ALA:O	2.26	0.56
1:J:306:TYR:HD1	1:K:306:TYR:HE1	1.50	0.56
1:L:463:ARG:HD2	1:L:544:ILE:HG13	1.87	0.56
1:L:466:ARG:HH11	1:L:466:ARG:CG	2.17	0.56
1:E:228:GLN:N	1:E:229:PRO:CD	2.68	0.56
1:F:228:GLN:N	1:F:229:PRO:CD	2.68	0.56
1:I:366:SER:OG	1:I:367:THR:N	2.38	0.56
1:A:369:HIS:CD2	1:A:376:ARG:HA	2.40	0.56
1:B:523:THR:N	1:B:524:PRO:HD3	2.21	0.56
1:A:523:THR:H	1:A:524:PRO:HD3	1.70	0.56
1:E:490:VAL:HG11	1:E:554:GLN:NE2	2.21	0.56
1:K:369:HIS:O	1:L:185:TYR:OH	2.24	0.56
1:L:560:SER:HB3	1:L:563:GLU:CG	2.34	0.56
1:C:523:THR:N	1:C:524:PRO:HD3	2.21	0.56
1:C:562:LYS:HB2	2:C:628:HOH:O	2.06	0.56
1:K:228:GLN:N	1:K:229:PRO:CD	2.69	0.56
1:A:487:THR:OG1	1:A:490:VAL:HG12	2.06	0.56
1:B:502:LEU:HD13	1:B:519:VAL:HG13	1.88	0.56
1:G:402:THR:HG23	1:G:403:HIS:ND1	2.21	0.56
1:D:283:PHE:CD2	1:D:306:TYR:CD1	2.94	0.56
1:H:288:ASN:CG	1:H:291:THR:HG22	2.26	0.56
1:C:149:MET:O	1:D:180[A]:HIS:NE2	2.38	0.56
1:H:557:HIS:CB	1:H:564:PHE:CD1	2.87	0.56
1:I:228:GLN:N	1:I:229:PRO:CD	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:VAL:HA	1:D:568:LEU:HD12	1.88	0.55
1:F:307:ARG:NH2	1:F:334:CYS:HA	2.21	0.55
1:H:523:THR:N	1:H:524:PRO:HD3	2.21	0.55
1:J:342:MET:CE	1:J:366:SER:HB2	2.36	0.55
1:E:475:HIS:CE1	1:E:476:LEU:HD23	2.41	0.55
1:J:307:ARG:HH12	1:J:334:CYS:HA	1.72	0.55
1:L:463:ARG:NH1	1:L:541:ASP:OD1	2.38	0.55
1:D:328:ARG:HD2	1:D:360:HIS:O	2.06	0.55
1:C:511:ASN:OD1	1:C:513:THR:HG23	2.07	0.55
1:C:387:LYS:HZ1	1:C:401:SER:HB3	1.70	0.55
1:I:180[B]:HIS:NE2	1:J:149:MET:O	2.37	0.55
1:J:228:GLN:N	1:J:229:PRO:HD3	2.22	0.55
1:C:497:MET:HG3	1:C:568:LEU:CD1	2.36	0.55
1:I:463:ARG:CD	1:I:544:ILE:CD1	2.85	0.55
1:G:361:CYS:O	1:G:383:ARG:NH2	2.39	0.55
1:F:249:ARG:CD	1:F:283:PHE:HZ	2.19	0.55
1:L:369:HIS:CD2	1:L:376:ARG:HA	2.41	0.55
1:H:500:ILE:HG22	1:H:502:LEU:HD13	1.88	0.55
1:K:342:MET:HE3	1:K:364:VAL:HG12	1.88	0.55
1:B:343:ALA:HA	1:B:367:THR:HG22	1.88	0.54
1:L:369:HIS:HD2	1:L:377:GLY:H	1.54	0.54
1:A:160:ILE:CG2	1:A:539:MET:HE3	2.37	0.54
1:B:523:THR:N	1:B:524:PRO:CD	2.70	0.54
1:I:523:THR:N	1:I:524:PRO:CD	2.70	0.54
1:L:466:ARG:HG3	1:L:466:ARG:NH1	2.22	0.54
1:H:442:TYR:O	1:H:445:TYR:HB3	2.08	0.54
1:E:592:ALA:O	1:F:180[B]:HIS:NE2	2.40	0.54
1:K:228:GLN:N	1:K:229:PRO:HD3	2.23	0.54
1:E:184:LYS:HG2	1:E:201:ILE:HD13	1.88	0.54
1:G:153:LYS:HE2	1:G:593:SER:HB3	1.89	0.54
1:J:523:THR:N	1:J:524:PRO:HD3	2.22	0.54
1:K:522:GLY:C	1:K:524:PRO:HD2	2.28	0.54
1:F:523:THR:N	1:F:524:PRO:CD	2.71	0.54
1:H:557:HIS:HB2	1:H:564:PHE:CE1	2.43	0.54
1:I:502:LEU:HD12	1:I:503:ASN:N	2.23	0.54
1:A:291:THR:HG22	1:A:293:TYR:HD1	1.72	0.54
1:F:127:ARG:CD	2:F:608:HOH:O	2.55	0.54
1:C:502:LEU:HD13	1:C:519:VAL:HG21	1.88	0.54
1:E:195:TYR:HE1	1:F:503:ASN:ND2	2.06	0.54
1:A:228:GLN:N	1:A:229:PRO:CD	2.71	0.54
1:D:463:ARG:HD2	1:D:544:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180[B]:HIS:CE1	1:L:592:ALA:O	2.61	0.54
1:D:366:SER:OG	1:D:367:THR:N	2.40	0.54
1:C:288:ASN:HB3	1:C:291:THR:CG2	2.38	0.53
1:B:502:LEU:HD13	1:B:519:VAL:CG1	2.38	0.53
1:E:369:HIS:HD2	1:E:377:GLY:H	1.55	0.53
1:J:523:THR:N	1:J:524:PRO:CD	2.71	0.53
1:K:185:TYR:CE2	1:K:187:GLU:HG3	2.43	0.53
1:D:369:HIS:HD2	1:D:376:ARG:HA	1.66	0.53
1:L:158:ARG:HD3	1:L:582:GLU:OE2	2.07	0.53
1:D:287:VAL:HG21	1:D:292:GLY:O	2.08	0.53
1:B:154:GLN:O	1:B:158:ARG:HG3	2.09	0.53
1:H:228:GLN:N	1:H:229:PRO:CD	2.72	0.53
1:K:322:TRP:HB2	1:K:324:PHE:CZ	2.43	0.53
1:K:523:THR:N	1:K:524:PRO:CD	2.72	0.53
1:I:568:LEU:C	1:I:568:LEU:HD23	2.29	0.53
1:I:343:ALA:HA	1:I:367:THR:HG22	1.90	0.53
1:G:190:PRO:HB2	1:G:202:ASP:OD1	2.09	0.53
1:G:131:ARG:NH1	1:H:589:GLU:OE1	2.41	0.53
1:K:342:MET:HE3	1:K:364:VAL:CG1	2.39	0.53
1:D:566:LYS:O	1:D:570:THR:HG22	2.08	0.53
1:K:498:CYS:O	1:K:581:VAL:HG11	2.09	0.53
1:K:288:ASN:CB	1:K:291:THR:HG22	2.39	0.52
1:D:287:VAL:HG22	1:D:293:TYR:O	2.09	0.52
1:D:369:HIS:HB3	1:D:375:PRO:O	2.08	0.52
1:I:560:SER:O	1:I:564:PHE:HB2	2.10	0.52
1:K:288:ASN:HB3	1:K:291:THR:CG2	2.40	0.52
1:L:162:LEU:HB2	1:L:502:LEU:HD23	1.89	0.52
1:E:523:THR:N	1:E:524:PRO:HD3	2.25	0.52
1:A:154:GLN:O	1:A:158:ARG:HG3	2.09	0.52
1:J:158:ARG:HB3	1:J:582:GLU:HG3	1.92	0.52
1:E:138:ILE:HG22	1:F:175:GLU:OE2	2.09	0.52
1:K:287:VAL:HG21	1:K:292:GLY:O	2.09	0.52
1:D:459:ALA:O	1:D:463:ARG:NH1	2.43	0.52
1:K:496:GLU:HG3	1:L:196:THR:HG23	1.91	0.52
1:F:523:THR:N	1:F:524:PRO:HD3	2.25	0.52
1:B:184:LYS:HG2	1:B:201:ILE:CD1	2.40	0.52
1:B:185:TYR:CE1	1:B:187:GLU:CG	2.92	0.52
1:D:287:VAL:HG22	1:D:293:TYR:C	2.31	0.52
1:D:433:ALA:O	1:D:437:VAL:HG23	2.10	0.52
1:C:369:HIS:CD2	1:C:376:ARG:HA	2.45	0.52
1:D:288:ASN:HB3	1:D:291:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ASN:CB	1:D:291:THR:HG22	2.40	0.52
1:K:367:THR:OG1	1:K:369:HIS:CD2	2.63	0.52
1:L:283:PHE:CE2	1:L:302:LYS:HE3	2.45	0.52
1:L:459:ALA:HB1	1:L:463:ARG:HH21	1.75	0.52
1:D:230:TYR:CZ	1:D:419:GLN:HB3	2.44	0.51
1:G:433:ALA:O	1:G:437:VAL:HG23	2.10	0.51
1:H:369:HIS:HD2	1:H:377:GLY:H	1.58	0.51
1:E:154:GLN:O	1:E:158:ARG:HG3	2.10	0.51
1:G:162:LEU:HB2	1:G:502:LEU:HD23	1.92	0.51
1:H:514:ILE:O	1:H:514:ILE:HG13	2.11	0.51
1:J:342:MET:HE3	1:J:366:SER:HB2	1.91	0.51
1:K:288:ASN:CG	1:K:291:THR:HG22	2.30	0.51
1:G:592:ALA:O	1:H:180[A]:HIS:NE2	2.43	0.51
1:H:523:THR:N	1:H:524:PRO:CD	2.73	0.51
1:J:482:THR:HG23	1:J:517:GLY:HA3	1.92	0.51
1:K:342:MET:CE	1:K:364:VAL:HG11	2.40	0.51
1:K:497:MET:SD	1:K:568:LEU:HD21	2.50	0.51
1:E:211:ARG:NH1	1:F:142:ASP:OD2	2.37	0.51
1:F:514:ILE:HG13	1:F:514:ILE:O	2.10	0.51
1:C:482:THR:N	1:C:483:PRO:CD	2.74	0.51
1:K:294:ILE:CG2	1:K:296:TYR:CE2	2.93	0.51
1:F:249:ARG:HB3	1:F:283:PHE:CE1	2.45	0.51
1:F:283:PHE:CG	1:F:306:TYR:CD2	2.99	0.51
1:H:343:ALA:HA	1:H:367:THR:HG22	1.93	0.51
1:J:433:ALA:O	1:J:437:VAL:HG23	2.11	0.51
1:K:449:MET:CE	1:K:524:PRO:HB3	2.41	0.51
1:C:446:ILE:O	1:C:449:MET:HB3	2.11	0.50
1:G:482:THR:HG23	1:G:517:GLY:HA3	1.93	0.50
1:I:283:PHE:CE1	1:L:305:ASP:HB3	2.46	0.50
1:B:366:SER:OG	1:B:367:THR:N	2.40	0.50
1:F:449:MET:HE2	1:F:524:PRO:CG	2.31	0.50
1:H:184:LYS:HG2	1:H:201:ILE:CD1	2.41	0.50
1:J:283:PHE:HZ	1:K:305:ASP:HB3	1.75	0.50
1:A:291:THR:HG22	1:A:293:TYR:CD1	2.47	0.50
1:F:468:VAL:CG2	1:F:507:ILE:HD11	2.41	0.50
1:F:525:ALA:O	1:F:528:THR:HB	2.11	0.50
1:I:154:GLN:O	1:I:158:ARG:HG3	2.11	0.50
1:J:459:ALA:HB1	1:J:463:ARG:HH12	1.77	0.50
1:K:442:TYR:O	1:K:445:TYR:HB3	2.11	0.50
1:A:343:ALA:HA	1:A:367:THR:HG22	1.92	0.50
1:K:449:MET:HE3	1:K:524:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:CD1	1:D:244:LEU:N	2.74	0.50
1:E:127:ARG:HE	1:F:589:GLU:HG2	1.76	0.50
1:E:186:SER:HB2	1:E:424:ASN:HD21	1.77	0.50
1:C:523:THR:N	1:C:524:PRO:CD	2.75	0.49
1:G:190:PRO:HA	1:G:193:ARG:HE	1.77	0.49
1:B:283:PHE:CZ	1:C:305:ASP:OD2	2.65	0.49
1:G:158:ARG:HB3	1:G:582:GLU:HG3	1.94	0.49
1:K:557:HIS:O	1:K:564:PHE:HD1	1.95	0.49
1:F:557:HIS:HB2	1:F:564:PHE:CE1	2.48	0.49
1:K:476:LEU:HD11	1:K:520:ARG:HG3	1.95	0.49
1:J:160:ILE:HG23	1:J:539:MET:HE3	1.95	0.49
1:L:230:TYR:CE2	1:L:419:GLN:HB3	2.48	0.49
1:A:305:ASP:OD2	1:D:283:PHE:CZ	2.66	0.49
1:D:288:ASN:CG	1:D:291:THR:HG22	2.32	0.49
1:E:480:ASP:HB2	1:E:507:ILE:HD11	1.94	0.49
1:F:120:SER:HA	1:F:123:LEU:HB3	1.93	0.49
1:F:158:ARG:HB3	1:F:582:GLU:HG3	1.95	0.49
1:H:367:THR:OG1	1:H:369:HIS:NE2	2.46	0.49
1:J:482:THR:N	1:J:483:PRO:CD	2.75	0.49
1:D:206:ASN:O	1:D:210:GLU:HG3	2.11	0.49
1:E:127:ARG:HG3	1:F:589:GLU:HG2	1.95	0.49
1:F:273:ILE:HG13	1:F:274:SER:H	1.76	0.49
1:I:574:ILE:HG13	1:I:575:ALA:N	2.26	0.49
1:B:228:GLN:N	1:B:229:PRO:HD3	2.28	0.49
1:D:158:ARG:HB3	1:D:582:GLU:HG3	1.94	0.49
1:D:185:TYR:CE2	1:D:187:GLU:HG3	2.48	0.49
1:I:207:LEU:O	1:I:211:ARG:HG3	2.13	0.49
1:E:228:GLN:N	1:E:229:PRO:HD3	2.28	0.49
1:A:291:THR:CG2	1:A:293:TYR:HB2	2.43	0.48
1:B:514:ILE:HG13	1:B:514:ILE:O	2.13	0.48
1:D:160:ILE:HG23	1:D:539:MET:HE3	1.95	0.48
1:D:342:MET:HE2	1:D:366:SER:HB2	1.95	0.48
1:F:446:ILE:O	1:F:449:MET:HB3	2.13	0.48
1:B:413:ALA:O	1:B:417:SER:HB2	2.13	0.48
1:H:366:SER:OG	1:H:367:THR:N	2.46	0.48
1:J:288:ASN:ND2	1:J:291:THR:HG23	2.28	0.48
1:C:245:LEU:O	1:C:248:GLU:HG3	2.13	0.48
1:I:463:ARG:HD3	1:I:544:ILE:HD12	1.94	0.48
1:K:343:ALA:HA	1:K:367:THR:HG22	1.96	0.48
1:A:291:THR:HG22	1:A:293:TYR:H	1.79	0.48
1:I:254:ASP:HB2	1:I:284:PRO:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:342:MET:O	1:J:342:MET:HG2	2.13	0.48
1:D:463:ARG:NH2	1:D:541:ASP:OD1	2.42	0.48
1:F:538:THR:HG22	1:F:542:PHE:HE1	1.77	0.48
1:G:190:PRO:CB	1:G:202:ASP:OD1	2.62	0.48
1:L:253:LEU:HD23	1:L:316:SER:HB2	1.94	0.48
1:A:560:SER:OG	1:A:563:GLU:CB	2.61	0.48
1:C:228:GLN:N	1:C:229:PRO:HD3	2.29	0.48
1:H:189:MET:HG3	1:H:190:PRO:HD2	1.96	0.48
1:H:288:ASN:ND2	1:H:291:THR:HG22	2.29	0.48
1:I:463:ARG:HD2	1:I:544:ILE:CD1	2.41	0.48
1:E:180[B]:HIS:CE1	1:F:153:LYS:HE3	2.49	0.48
1:J:342:MET:HB3	1:J:342:MET:HE2	1.77	0.48
1:J:369:HIS:HD2	1:J:377:GLY:H	1.61	0.48
1:K:369:HIS:CG	1:K:376:ARG:HG2	2.49	0.48
1:F:290:GLN:OE1	1:F:290:GLN:N	2.47	0.47
1:G:476:LEU:O	1:G:477:LEU:HD12	2.14	0.47
1:G:482:THR:N	1:G:483:PRO:CD	2.77	0.47
1:C:211:ARG:NH1	1:D:142:ASP:OD2	2.38	0.47
1:C:291:THR:HG23	1:C:293:TYR:N	2.29	0.47
1:C:490:VAL:HG11	1:C:554:GLN:HE21	1.78	0.47
1:G:162:LEU:HB2	1:G:502:LEU:CD2	2.44	0.47
1:J:369:HIS:CD2	1:J:376:ARG:HA	2.48	0.47
1:L:433:ALA:O	1:L:437:VAL:HG23	2.14	0.47
1:C:387:LYS:HZ1	1:C:401:SER:CB	2.28	0.47
1:F:283:PHE:CG	1:F:306:TYR:HD2	2.32	0.47
1:J:171:ARG:HH11	1:J:594:LEU:HD23	1.79	0.47
1:J:207:LEU:O	1:J:211:ARG:HG3	2.15	0.47
1:K:571:ASN:O	1:K:574:ILE:HG13	2.15	0.47
1:C:561:HIS:O	1:C:565:VAL:HG23	2.15	0.47
1:G:342:MET:CE	1:G:366:SER:HB2	2.45	0.47
1:J:312:ILE:HA	1:J:339:MET:O	2.14	0.47
1:K:559:LYS:HD2	1:K:559:LYS:O	2.14	0.47
1:L:328:ARG:HA	1:L:328:ARG:HD3	1.58	0.47
1:D:228:GLN:N	1:D:229:PRO:HD3	2.29	0.47
1:F:160:ILE:HG23	1:F:539:MET:HE3	1.95	0.47
1:G:283:PHE:HB2	1:G:306:TYR:HE2	1.75	0.47
1:I:185:TYR:CE2	1:I:187:GLU:HG3	2.50	0.47
1:K:254:ASP:HB2	1:K:284:PRO:HB2	1.97	0.47
1:B:463:ARG:O	1:B:464:LYS:CG	2.62	0.47
1:G:490:VAL:HG11	1:G:554:GLN:NE2	2.30	0.47
1:H:446:ILE:O	1:H:449:MET:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:551:SER:O	1:L:554:GLN:HG3	2.15	0.47
1:A:288:ASN:OD1	1:A:288:ASN:C	2.53	0.47
1:E:482:THR:N	1:E:483:PRO:CD	2.78	0.47
1:G:312:ILE:HD13	1:G:339:MET:HB3	1.97	0.47
1:G:342:MET:HG2	1:G:342:MET:O	2.15	0.47
1:A:482:THR:N	1:A:483:PRO:CD	2.77	0.47
1:J:249:ARG:HB3	1:J:306:TYR:CE2	2.50	0.47
1:H:571:ASN:O	1:H:574:ILE:HG13	2.15	0.47
1:I:497:MET:SD	1:I:568:LEU:HD21	2.55	0.47
1:L:482:THR:N	1:L:483:PRO:CD	2.78	0.47
1:A:245:LEU:O	1:A:248:GLU:HG3	2.15	0.47
1:D:245:LEU:O	1:D:248:GLU:HG3	2.15	0.47
1:G:562:LYS:O	1:G:565:VAL:HG12	2.15	0.47
1:L:153:LYS:O	1:L:157:VAL:HG13	2.15	0.47
1:D:243:LEU:HB2	1:D:244:LEU:HD13	1.96	0.46
1:H:557:HIS:CB	1:H:564:PHE:CE1	2.99	0.46
1:J:306:TYR:CD1	1:K:306:TYR:HE1	2.30	0.46
1:L:325:ALA:O	1:L:328:ARG:HB3	2.15	0.46
1:G:153:LYS:O	1:G:157:VAL:HG12	2.16	0.46
1:K:342:MET:HE2	1:K:364:VAL:HG11	1.95	0.46
1:B:564:PHE:O	1:B:567:SER:OG	2.27	0.46
1:C:158:ARG:HB3	1:C:582:GLU:HG3	1.98	0.46
1:E:245:LEU:O	1:E:248:GLU:HG3	2.15	0.46
1:E:288:ASN:ND2	1:E:291:THR:HG23	2.30	0.46
1:G:288:ASN:ND2	1:G:291:THR:HG23	2.30	0.46
1:L:228:GLN:N	1:L:229:PRO:HD3	2.29	0.46
1:D:523:THR:H	1:D:524:PRO:HD3	1.81	0.46
1:B:502:LEU:C	1:B:502:LEU:HD12	2.36	0.46
1:E:195:TYR:CE1	1:F:503:ASN:ND2	2.84	0.46
1:E:343:ALA:HA	1:E:367:THR:HG22	1.96	0.46
1:I:532:ILE:HD11	1:I:534:SER:OG	2.16	0.46
1:L:163:ILE:HB	1:L:166:GLU:HG3	1.97	0.46
1:I:198:ASN:HB2	2:I:616:HOH:O	2.15	0.46
1:K:163:ILE:HB	1:K:166:GLU:HG3	1.97	0.46
1:A:291:THR:HG22	1:A:293:TYR:HB2	1.97	0.46
1:B:288:ASN:ND2	1:B:291:THR:HG23	2.31	0.46
1:G:251:MET:CG	1:G:283:PHE:O	2.55	0.46
1:G:523:THR:H	1:G:524:PRO:HD3	1.81	0.46
1:A:184:LYS:HG2	1:A:201:ILE:HD13	1.98	0.46
1:A:210:GLU:HB3	2:A:609:HOH:O	2.17	0.46
1:B:185:TYR:CD1	1:B:187:GLU:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482:THR:N	1:H:483:PRO:CD	2.79	0.46
1:K:317:SER:CB	1:K:476:LEU:HD21	2.42	0.46
1:L:369:HIS:CD2	1:L:377:GLY:H	2.34	0.46
1:K:369:HIS:CD2	1:K:376:ARG:HA	2.51	0.45
1:A:369:HIS:HD2	1:A:377:GLY:H	1.64	0.45
1:C:207:LEU:O	1:C:211:ARG:HG3	2.15	0.45
1:E:342:MET:CE	1:E:366:SER:HB2	2.47	0.45
1:E:523:THR:N	1:E:524:PRO:CD	2.78	0.45
1:H:500:ILE:HG22	1:H:502:LEU:CD1	2.45	0.45
1:G:127:ARG:HG3	1:H:589:GLU:HG2	1.97	0.45
1:I:133:TRP:CZ2	1:J:170:CYS:HB3	2.51	0.45
1:J:157:VAL:HG22	1:J:590:MET:HG2	1.99	0.45
1:J:468:VAL:HB	1:J:478:LEU:HB2	1.98	0.45
1:L:442:TYR:O	1:L:445:TYR:HB3	2.16	0.45
1:B:369:HIS:HD2	1:B:377:GLY:H	1.63	0.45
1:F:123:LEU:CD1	2:F:608:HOH:O	2.59	0.45
1:F:535:ASP:O	1:F:539:MET:HG3	2.16	0.45
1:H:185:TYR:CE2	1:H:187:GLU:HG3	2.51	0.45
1:K:160:ILE:HG23	1:K:539:MET:CE	2.47	0.45
1:K:290:GLN:NE2	1:K:290:GLN:HA	2.30	0.45
1:K:560:SER:OG	1:K:563:GLU:CB	2.65	0.45
1:L:413:ALA:O	1:L:417:SER:HB2	2.17	0.45
1:E:594:LEU:O	1:E:594:LEU:HD12	2.17	0.45
1:K:291:THR:HG23	1:K:293:TYR:N	2.30	0.45
1:E:283:PHE:CZ	1:H:305:ASP:OD1	2.70	0.45
1:F:287:VAL:CG1	1:F:292:GLY:C	2.85	0.45
1:F:567:SER:HB2	2:F:611:HOH:O	2.16	0.45
1:K:514:ILE:O	1:K:514:ILE:HG13	2.17	0.45
1:G:123:LEU:C	1:G:123:LEU:HD23	2.37	0.45
1:L:369:HIS:HB3	1:L:375:PRO:O	2.17	0.45
1:L:232:CYS:HB2	1:L:367:THR:CG2	2.40	0.45
1:A:297:ASP:OD1	1:A:326:ARG:NH2	2.50	0.45
1:A:560:SER:OG	1:A:563:GLU:HB3	2.17	0.45
1:B:545:LYS:HD2	1:B:580:ARG:HH12	1.82	0.45
1:D:545:LYS:HA	1:D:548:GLN:HG2	1.99	0.45
1:E:160:ILE:HG23	1:E:539:MET:CE	2.47	0.45
1:E:497:MET:HA	1:E:497:MET:CE	2.46	0.45
1:I:482:THR:N	1:I:483:PRO:CD	2.80	0.45
1:J:463:ARG:O	1:J:464:LYS:HG2	2.17	0.45
1:J:502:LEU:HD21	1:J:521:ILE:HG12	1.99	0.45
1:A:467:LEU:HD13	1:A:477:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:VAL:HB	1:C:478:LEU:HB2	1.99	0.44
1:D:291:THR:HG23	1:D:293:TYR:N	2.29	0.44
1:K:476:LEU:HD11	1:K:520:ARG:HG2	1.98	0.44
1:K:501:THR:HG22	1:L:196:THR:CG2	2.45	0.44
1:A:283:PHE:CZ	1:D:305:ASP:HB3	2.53	0.44
1:C:514:ILE:HD12	1:C:514:ILE:H	1.80	0.44
1:L:160:ILE:HG23	1:L:539:MET:CE	2.48	0.44
1:A:413:ALA:O	1:A:417:SER:HB2	2.18	0.44
1:B:482:THR:N	1:B:483:PRO:CD	2.80	0.44
1:K:185:TYR:CD1	1:L:376:ARG:NH1	2.85	0.44
1:L:160:ILE:HG23	1:L:539:MET:HE3	1.99	0.44
1:B:256:PRO:HG3	1:B:508:PHE:CE2	2.52	0.44
1:C:123:LEU:C	1:C:123:LEU:HD23	2.37	0.44
1:I:158:ARG:HB3	1:I:582:GLU:HG3	2.00	0.44
1:K:294:ILE:CG2	1:K:296:TYR:CZ	3.01	0.44
1:K:560:SER:OG	1:K:563:GLU:HB2	2.18	0.44
1:D:482:THR:HG23	1:D:517:GLY:HA3	2.00	0.44
1:F:249:ARG:HB3	1:F:283:PHE:HE1	1.82	0.44
1:K:532:ILE:HG12	1:K:533:GLU:OE1	2.18	0.44
1:B:367:THR:OG1	1:B:369:HIS:NE2	2.50	0.44
1:C:343:ALA:HA	1:C:367:THR:HG22	1.99	0.44
1:D:147:GLU:OE2	1:D:151:LYS:HE3	2.18	0.44
1:F:287:VAL:HG11	1:F:292:GLY:O	2.17	0.44
1:H:413:ALA:O	1:H:417:SER:HB2	2.16	0.44
1:J:254:ASP:HB2	1:J:284:PRO:HB2	1.98	0.44
1:K:287:VAL:HG22	1:K:293:TYR:C	2.38	0.44
1:B:463:ARG:O	1:B:464:LYS:HG2	2.17	0.44
1:E:413:ALA:O	1:E:417:SER:HB2	2.17	0.44
1:G:120:SER:O	1:G:124:GLU:HB3	2.18	0.44
1:I:184:LYS:HG2	1:I:201:ILE:CD1	2.48	0.44
1:C:497:MET:HG3	1:C:568:LEU:HG	1.99	0.44
1:F:553:LEU:HG	1:F:564:PHE:CE2	2.53	0.44
1:H:255:SER:O	1:H:256:PRO:C	2.57	0.44
1:K:124:GLU:OE1	1:K:124:GLU:HA	2.18	0.44
1:K:324:PHE:CE2	1:K:355:SER:HB2	2.52	0.44
1:E:123:LEU:C	1:E:123:LEU:HD23	2.39	0.43
1:E:295:ASP:OD1	1:E:295:ASP:C	2.56	0.43
1:F:537:GLU:O	1:F:540:ALA:HB3	2.18	0.43
1:G:371:GLY:O	1:G:442:TYR:OH	2.33	0.43
1:G:446:ILE:O	1:G:449:MET:HB3	2.18	0.43
1:K:127:ARG:NH2	2:K:603:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:HB	1:A:166:GLU:HG3	1.99	0.43
1:C:366:SER:OG	1:C:367:THR:N	2.52	0.43
1:E:433:ALA:O	1:E:437:VAL:HG23	2.18	0.43
1:H:291:THR:HG23	1:H:293:TYR:N	2.33	0.43
1:H:525:ALA:O	1:H:528:THR:HB	2.18	0.43
1:J:463:ARG:O	1:J:464:LYS:CG	2.66	0.43
1:A:562:LYS:O	1:A:566:LYS:HG3	2.18	0.43
1:B:369:HIS:HB3	1:B:375:PRO:O	2.19	0.43
1:D:243:LEU:C	1:D:244:LEU:HD12	2.38	0.43
1:G:228:GLN:N	1:G:229:PRO:HD3	2.32	0.43
1:F:147:GLU:HG2	1:F:151:LYS:HE3	2.00	0.43
1:G:226:ASN:HA	2:G:603:HOH:O	2.18	0.43
1:J:160:ILE:HG23	1:J:539:MET:CE	2.48	0.43
1:J:476:LEU:O	1:J:477:LEU:HD12	2.19	0.43
1:K:342:MET:O	1:K:342:MET:HG2	2.17	0.43
1:K:482:THR:N	1:K:483:PRO:CD	2.81	0.43
1:L:321:ASP:CG	1:L:355:SER:HG	2.22	0.43
1:D:413:ALA:O	1:D:417:SER:HB2	2.18	0.43
1:D:564:PHE:O	1:D:568:LEU:HG	2.17	0.43
1:E:163:ILE:HB	1:E:166:GLU:HG3	1.99	0.43
1:G:133:TRP:CZ2	1:H:170:CYS:HB3	2.54	0.43
1:I:228:GLN:N	1:I:229:PRO:HD3	2.34	0.43
1:J:306:TYR:HD1	1:K:306:TYR:CE1	2.35	0.43
1:K:476:LEU:HD12	1:K:477:LEU:H	1.82	0.43
1:A:307:ARG:NE	2:A:601:HOH:O	2.42	0.43
1:D:514:ILE:HD12	1:D:514:ILE:N	2.33	0.43
1:G:251:MET:HE2	1:G:308:PRO:HG3	1.96	0.43
1:I:367:THR:OG1	1:I:369:HIS:CD2	2.72	0.43
1:K:556:GLU:HG3	1:K:557:HIS:CD2	2.54	0.43
1:A:553:LEU:HD23	1:A:568:LEU:HD23	2.00	0.43
1:D:482:THR:N	1:D:483:PRO:CD	2.82	0.43
1:E:366:SER:OG	1:E:367:THR:N	2.52	0.43
1:I:413:ALA:O	1:I:417:SER:HB2	2.18	0.43
1:D:507:ILE:HG23	1:D:515:SER:OG	2.19	0.43
1:E:142:ASP:OD2	1:F:211:ARG:NH1	2.43	0.43
1:F:326:ARG:O	1:F:330:ILE:HG13	2.18	0.43
1:G:572:LYS:HG3	1:G:573:ASP:N	2.33	0.43
1:J:466:ARG:HG3	2:J:621:HOH:O	2.17	0.43
1:D:283:PHE:HB2	1:D:306:TYR:CE1	2.54	0.43
1:E:184:LYS:O	1:F:376:ARG:NH1	2.52	0.43
1:F:228:GLN:N	1:F:229:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:O	1:A:211:ARG:HG3	2.18	0.43
1:A:228:GLN:N	1:A:229:PRO:HD3	2.33	0.43
1:B:348:LEU:HD11	1:B:474:ASN:HB2	2.00	0.43
1:C:367:THR:OG1	1:C:369:HIS:NE2	2.52	0.43
1:F:153:LYS:O	1:F:157:VAL:HG12	2.19	0.43
1:A:306:TYR:HA	1:D:283:PHE:CE1	2.54	0.42
1:B:369:HIS:CD2	1:B:377:GLY:H	2.37	0.42
1:F:482:THR:N	1:F:483:PRO:CD	2.82	0.42
1:H:228:GLN:N	1:H:229:PRO:HD3	2.34	0.42
1:K:185:TYR:CE2	1:K:187:GLU:CG	3.02	0.42
1:C:367:THR:OG1	1:C:369:HIS:CD2	2.72	0.42
1:D:160:ILE:HG23	1:D:539:MET:CE	2.49	0.42
1:J:526:MET:HG3	1:J:539:MET:HE1	2.01	0.42
1:K:317:SER:CB	1:K:476:LEU:CD2	2.97	0.42
1:C:369:HIS:HD2	1:C:377:GLY:H	1.67	0.42
1:D:423:HIS:HB3	1:D:426:HIS:CD2	2.54	0.42
1:G:251:MET:HE2	1:G:251:MET:HB2	1.78	0.42
1:C:560:SER:HB3	2:C:628:HOH:O	2.19	0.42
1:G:576:GLU:O	1:G:580:ARG:HG3	2.20	0.42
1:H:442:TYR:OH	1:H:446:ILE:HD11	2.20	0.42
1:I:170:CYS:HB3	1:J:133:TRP:CZ2	2.54	0.42
1:J:184:LYS:O	1:J:424:ASN:ND2	2.52	0.42
1:L:131:ARG:NH2	1:L:135:ASP:OD2	2.53	0.42
1:E:367:THR:OG1	1:E:369:HIS:NE2	2.53	0.42
1:G:415:PHE:CG	1:G:416:PRO:HA	2.54	0.42
1:I:369:HIS:CE1	1:I:376:ARG:NH2	2.88	0.42
1:I:482:THR:HG23	1:I:517:GLY:HA3	2.00	0.42
1:L:475:HIS:CE1	1:L:476:LEU:HD23	2.54	0.42
1:G:238:ALA:HA	1:G:418:LEU:CD1	2.50	0.42
1:G:490:VAL:HG11	1:G:554:GLN:HE22	1.85	0.42
1:I:562:LYS:HD3	1:I:562:LYS:HA	1.70	0.42
1:J:294:ILE:CD1	1:J:322:TRP:CH2	3.02	0.42
1:E:153:LYS:O	1:E:157:VAL:HG12	2.20	0.42
1:B:254:ASP:HB2	1:B:284:PRO:HB2	2.02	0.42
1:D:140:LEU:HD11	1:G:555:ARG:CD	2.50	0.42
1:G:343:ALA:HA	1:G:367:THR:HG22	2.01	0.42
1:K:482:THR:HG23	1:K:517:GLY:HA3	2.01	0.42
1:C:376:ARG:NH1	1:C:376:ARG:HG2	2.35	0.42
1:D:140:LEU:HD11	1:G:555:ARG:HD3	2.02	0.42
1:D:343:ALA:HA	1:D:367:THR:HG22	2.02	0.42
1:F:288:ASN:OD1	1:F:288:ASN:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:497:MET:O	1:H:578:ARG:HD3	2.19	0.42
1:H:556:GLU:HG2	1:H:557:HIS:ND1	2.35	0.42
1:A:367:THR:OG1	1:A:369:HIS:NE2	2.52	0.42
1:C:170:CYS:HB3	1:D:133:TRP:CZ2	2.55	0.41
1:C:206:ASN:O	1:C:210:GLU:HG3	2.20	0.41
1:H:342:MET:CE	1:H:366:SER:HB2	2.50	0.41
1:J:209:ILE:HG23	1:J:225:VAL:CG1	2.49	0.41
1:A:160:ILE:CG2	1:A:539:MET:CE	2.94	0.41
1:A:433:ALA:O	1:A:437:VAL:HG23	2.20	0.41
1:A:468:VAL:HB	1:A:478:LEU:HB2	2.02	0.41
1:C:209:ILE:HG23	1:C:225:VAL:CG1	2.50	0.41
1:G:221:ASP:OD1	1:G:222:LYS:HG3	2.19	0.41
1:I:255:SER:HA	1:I:256:PRO:HD2	1.96	0.41
1:K:170:CYS:O	1:K:173:VAL:HG22	2.20	0.41
1:L:345:ILE:O	1:L:346:SER:C	2.56	0.41
1:A:526:MET:CG	1:A:539:MET:HE1	2.21	0.41
1:K:433:ALA:O	1:K:437:VAL:HG23	2.21	0.41
1:B:158:ARG:HB3	1:B:582:GLU:HG3	2.01	0.41
1:C:452:ASN:HB3	1:C:536:PHE:CE2	2.55	0.41
1:D:163:ILE:HB	1:D:166:GLU:HG3	2.03	0.41
1:E:468:VAL:HB	1:E:478:LEU:HB2	2.02	0.41
1:F:366:SER:OG	1:F:367:THR:N	2.53	0.41
1:K:160:ILE:HG23	1:K:539:MET:HE3	2.03	0.41
1:K:230:TYR:CZ	1:K:419:GLN:HB3	2.55	0.41
1:C:387:LYS:NZ	1:C:401:SER:CB	2.76	0.41
1:H:291:THR:HG23	1:H:293:TYR:H	1.84	0.41
1:H:526:MET:HG3	1:H:539:MET:HE1	2.02	0.41
1:A:170:CYS:HB3	1:B:133:TRP:CZ2	2.56	0.41
1:D:185:TYR:CE2	1:D:187:GLU:CG	3.03	0.41
1:I:463:ARG:CD	1:I:544:ILE:HD12	2.50	0.41
1:A:230:TYR:CE2	1:A:419:GLN:HB3	2.55	0.41
1:A:554:GLN:O	1:A:558:GLY:HA3	2.21	0.41
1:C:511:ASN:OD1	1:C:512:GLY:N	2.54	0.41
1:C:592:ALA:O	1:D:180[B]:HIS:CE1	2.73	0.41
1:E:288:ASN:C	1:E:288:ASN:OD1	2.58	0.41
1:G:413:ALA:O	1:G:417:SER:HB2	2.21	0.41
1:I:369:HIS:CD2	1:I:376:ARG:HA	2.56	0.41
1:I:502:LEU:HD12	1:I:502:LEU:C	2.40	0.41
1:F:123:LEU:C	1:F:123:LEU:HD13	2.41	0.41
1:J:283:PHE:CZ	1:K:305:ASP:HB3	2.55	0.41
1:K:581:VAL:HG13	1:K:582:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:567:SER:O	1:L:571:ASN:HB2	2.20	0.41
1:B:460:LEU:O	1:B:465:CYS:HB2	2.21	0.41
1:D:348:LEU:HD11	1:D:474:ASN:HB2	2.02	0.41
1:E:342:MET:O	1:E:342:MET:HG2	2.21	0.41
1:F:249:ARG:CG	1:F:283:PHE:HZ	2.34	0.41
1:G:416:PRO:HG2	1:H:273:ILE:HG23	2.03	0.41
1:J:184:LYS:HG2	1:J:201:ILE:HD13	2.03	0.41
1:K:294:ILE:HG21	1:K:296:TYR:CZ	2.56	0.41
1:K:342:MET:CE	1:K:364:VAL:CG1	2.98	0.41
1:K:459:ALA:O	1:K:462:ARG:HG2	2.21	0.41
1:K:463:ARG:HD2	1:K:544:ILE:HD11	2.03	0.41
1:B:384:ARG:HD3	1:B:407:GLU:OE2	2.21	0.41
1:C:589:GLU:HB3	1:D:130:VAL:HG11	2.02	0.41
1:G:589:GLU:HG3	1:H:127:ARG:O	2.21	0.41
1:H:482:THR:HG23	1:H:517:GLY:HA3	2.03	0.41
1:I:589:GLU:HG2	1:J:127:ARG:CG	2.51	0.41
1:C:185:TYR:CE2	1:C:187:GLU:HG3	2.56	0.40
1:D:570:THR:HG23	1:D:570:THR:O	2.20	0.40
1:I:502:LEU:HD13	1:I:519:VAL:HB	2.02	0.40
1:J:230:TYR:CE2	1:J:419:GLN:HB3	2.56	0.40
1:L:288:ASN:ND2	1:L:291:THR:HG23	2.36	0.40
1:B:463:ARG:HD3	1:B:544:ILE:HG13	2.03	0.40
1:E:158:ARG:HB3	1:E:582:GLU:HG3	2.03	0.40
1:E:342:MET:HE2	1:E:366:SER:HB2	2.03	0.40
1:A:537:GLU:O	1:A:540:ALA:HB3	2.21	0.40
1:B:294:ILE:HG13	1:B:318:TYR:CZ	2.56	0.40
1:B:490:VAL:HG11	1:B:554:GLN:HE22	1.86	0.40
1:H:433:ALA:O	1:H:437:VAL:HG23	2.21	0.40
1:H:486:LEU:HD23	1:H:554:GLN:OE1	2.20	0.40
1:B:245:LEU:O	1:B:248:GLU:HG3	2.22	0.40
1:D:254:ASP:HB2	1:D:284:PRO:HB2	2.03	0.40
1:I:302:LYS:NZ	1:L:305:ASP:OD2	2.51	0.40
1:J:154:GLN:O	1:J:158:ARG:HG3	2.22	0.40
1:J:574:ILE:HG13	1:J:575:ALA:N	2.37	0.40
1:K:123:LEU:O	1:K:126:ARG:HG2	2.22	0.40
1:K:376:ARG:HH21	1:L:185:TYR:HE1	1.69	0.40
1:K:413:ALA:O	1:K:417:SER:HB2	2.21	0.40
1:A:254:ASP:HB2	1:A:284:PRO:HB2	2.03	0.40
1:C:413:ALA:O	1:C:417:SER:HB2	2.21	0.40
1:J:342:MET:HE2	1:J:366:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	435/479 (91%)	417 (96%)	18 (4%)	0	100 100
1	B	435/479 (91%)	418 (96%)	17 (4%)	0	100 100
1	C	441/479 (92%)	419 (95%)	22 (5%)	0	100 100
1	D	429/479 (90%)	411 (96%)	18 (4%)	0	100 100
1	E	433/479 (90%)	415 (96%)	18 (4%)	0	100 100
1	F	437/479 (91%)	417 (95%)	20 (5%)	0	100 100
1	G	436/479 (91%)	418 (96%)	18 (4%)	0	100 100
1	H	431/479 (90%)	410 (95%)	21 (5%)	0	100 100
1	I	435/479 (91%)	418 (96%)	17 (4%)	0	100 100
1	J	436/479 (91%)	419 (96%)	17 (4%)	0	100 100
1	K	430/479 (90%)	410 (95%)	20 (5%)	0	100 100
1	L	438/479 (91%)	409 (93%)	29 (7%)	0	100 100
All	All	5216/5748 (91%)	4981 (96%)	235 (4%)	0	100 100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	366/396 (92%)	365 (100%)	1 (0%)	92 95
1	B	367/396 (93%)	363 (99%)	4 (1%)	73 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	371/396 (94%)	365 (98%)	6 (2%)	62	78
1	D	364/396 (92%)	357 (98%)	7 (2%)	57	74
1	E	368/396 (93%)	362 (98%)	6 (2%)	62	78
1	F	369/396 (93%)	357 (97%)	12 (3%)	38	59
1	G	368/396 (93%)	366 (100%)	2 (0%)	88	92
1	H	365/396 (92%)	361 (99%)	4 (1%)	73	84
1	I	367/396 (93%)	366 (100%)	1 (0%)	92	95
1	J	368/396 (93%)	367 (100%)	1 (0%)	92	95
1	K	363/396 (92%)	354 (98%)	9 (2%)	47	67
1	L	368/396 (93%)	364 (99%)	4 (1%)	73	84
All	All	4404/4752 (93%)	4347 (99%)	57 (1%)	69	82

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	THR
1	B	317	SER
1	B	321	ASP
1	B	505	THR
1	B	560	SER
1	C	135	ASP
1	C	321	ASP
1	C	355	SER
1	C	502	LEU
1	C	505	THR
1	C	510	ASP
1	D	135	ASP
1	D	161	GLU
1	D	201	ILE
1	D	287	VAL
1	D	384	ARG
1	D	463	ARG
1	D	510	ASP
1	E	127	ARG
1	E	184	LYS
1	E	384	ARG
1	E	399	ASP
1	E	502	LEU

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Mol	Chain	Res	Type
1	E	551	SER
1	F	121	ASN
1	F	184	LYS
1	F	185	TYR
1	F	283	PHE
1	F	317	SER
1	F	321	ASP
1	F	355	SER
1	F	367	THR
1	F	384	ARG
1	F	502	LEU
1	F	557	HIS
1	F	564	PHE
1	G	135	ASP
1	G	560	SER
1	H	189	MET
1	H	384	ARG
1	H	567	SER
1	H	578	ARG
1	I	384	ARG
1	J	534	SER
1	K	135	ASP
1	K	287	VAL
1	K	290	GLN
1	K	321	ASP
1	K	355	SER
1	K	384	ARG
1	K	473	ASP
1	K	500	ILE
1	K	551	SER
1	L	328	ARG
1	L	384	ARG
1	L	419	GLN
1	L	466	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	424	ASN
1	E	554	GLN
1	F	503	ASN
1	G	360	HIS

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Mol	Chain	Res	Type
1	G	369	HIS
1	H	448	GLN
1	H	452	ASN
1	H	579	ASN
1	I	199	GLN
1	J	554	GLN
1	K	136	GLN
1	K	290	GLN
1	K	557	HIS
1	L	369	HIS

### 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 monosaccharides 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	443/479 (92%)	0.11	8 (1%) 68 74	43, 56, 97, 147	0
1	B	443/479 (92%)	0.23	21 (4%) 31 34	39, 70, 125, 174	0
1	C	447/479 (93%)	0.05	16 (3%) 42 47	42, 56, 124, 183	0
1	D	438/479 (91%)	0.37	32 (7%) 15 17	41, 79, 135, 179	0
1	E	442/479 (92%)	0.31	18 (4%) 37 41	41, 64, 122, 195	0
1	F	444/479 (92%)	0.70	58 (13%) 3 3	41, 89, 151, 209	0
1	G	444/479 (92%)	0.44	25 (5%) 24 27	53, 97, 142, 178	0
1	H	438/479 (91%)	0.58	51 (11%) 4 4	53, 94, 180, 219	0
1	I	442/479 (92%)	0.31	28 (6%) 20 22	41, 64, 143, 193	0
1	J	444/479 (92%)	0.15	10 (2%) 60 67	41, 66, 107, 134	0
1	K	437/479 (91%)	0.85	75 (17%) 1 1	46, 106, 156, 199	0
1	L	443/479 (92%)	0.32	25 (5%) 24 27	51, 75, 139, 182	0
All	All	5305/5748 (92%)	0.37	367 (6%) 16 18	39, 74, 146, 219	0

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	568	LEU	8.0
1	E	564	PHE	7.1
1	F	563	GLU	6.5
1	H	557	HIS	6.4
1	B	565	VAL	6.4
1	E	563	GLU	6.3
1	K	486	LEU	6.3
1	H	568	LEU	6.0
1	E	557	HIS	5.9
1	E	561	HIS	5.9
1	I	513	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	F	486	LEU	5.7
1	K	560	SER	5.6
1	B	564	PHE	5.5
1	B	554	GLN	5.4
1	K	557	HIS	5.4
1	B	555	ARG	5.3
1	F	565	VAL	5.3
1	L	563	GLU	5.3
1	H	569	CYS	5.2
1	K	552	ALA	5.1
1	H	515	SER	5.1
1	F	569	CYS	5.0
1	H	479	TRP	5.0
1	C	557	HIS	4.9
1	K	461	LEU	4.9
1	I	564	PHE	4.9
1	F	546	ALA	4.8
1	G	385	GLY	4.8
1	K	569	CYS	4.8
1	K	223	TRP	4.8
1	D	507	ILE	4.8
1	F	479	TRP	4.7
1	F	556	GLU	4.7
1	K	467	LEU	4.7
1	F	564	PHE	4.7
1	F	511	ASN	4.6
1	K	564	PHE	4.6
1	K	563	GLU	4.6
1	C	555	ARG	4.6
1	K	553	LEU	4.6
1	I	568	LEU	4.5
1	K	487	THR	4.5
1	H	481	LEU	4.5
1	K	385	GLY	4.4
1	K	561	HIS	4.4
1	L	403	HIS	4.4
1	F	481	LEU	4.4
1	K	479	TRP	4.4
1	I	553	LEU	4.4
1	H	508	PHE	4.4
1	H	565	VAL	4.3
1	B	553	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	577	LEU	4.3
1	K	568	LEU	4.3
1	D	567	SER	4.3
1	I	557	HIS	4.3
1	F	562	LYS	4.2
1	I	567	SER	4.2
1	F	570	THR	4.2
1	K	462	ARG	4.2
1	F	559	LYS	4.2
1	I	566	LYS	4.2
1	K	565	VAL	4.1
1	G	512	GLY	4.1
1	H	516	PRO	4.1
1	F	484	MET	4.1
1	G	403	HIS	4.1
1	F	560	SER	4.1
1	F	557	HIS	4.1
1	F	561	HIS	4.1
1	D	568	LEU	4.1
1	D	564	PHE	4.0
1	D	570	THR	4.0
1	D	515	SER	4.0
1	D	566	LYS	4.0
1	K	555	ARG	3.9
1	L	402	THR	3.9
1	F	567	SER	3.8
1	I	563	GLU	3.8
1	B	466	ARG	3.8
1	K	465	CYS	3.8
1	K	224	GLY	3.8
1	F	555	ARG	3.8
1	I	121	ASN	3.8
1	K	536	PHE	3.8
1	L	560	SER	3.8
1	K	383	ARG	3.7
1	E	565	VAL	3.7
1	L	564	PHE	3.7
1	K	558	GLY	3.6
1	I	560	SER	3.6
1	C	564	PHE	3.6
1	C	558	GLY	3.6
1	H	518	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	574	ILE	3.6
1	E	562	LYS	3.6
1	F	547	ALA	3.6
1	F	554	GLN	3.6
1	B	563	GLU	3.6
1	H	467	LEU	3.6
1	L	511	ASN	3.6
1	G	194	TYR	3.6
1	K	384	ARG	3.6
1	F	480	ASP	3.5
1	F	544	ILE	3.5
1	H	584	PHE	3.5
1	E	555	ARG	3.5
1	L	557	HIS	3.5
1	D	569	CYS	3.5
1	D	554	GLN	3.5
1	K	386	PRO	3.5
1	H	403	HIS	3.4
1	C	510	ASP	3.4
1	F	581	VAL	3.4
1	B	400	THR	3.4
1	D	510	ASP	3.4
1	D	572	LYS	3.4
1	D	508	PHE	3.4
1	H	459	ALA	3.4
1	D	563	GLU	3.4
1	D	532	ILE	3.3
1	K	507	ILE	3.3
1	F	512	GLY	3.3
1	I	572	LYS	3.3
1	K	559	LYS	3.3
1	A	403	HIS	3.3
1	F	515	SER	3.3
1	F	542	PHE	3.3
1	K	515	SER	3.3
1	L	561	HIS	3.3
1	H	507	ILE	3.3
1	F	498	CYS	3.3
1	E	509	GLY	3.3
1	G	568	LEU	3.3
1	K	554	GLN	3.3
1	D	509	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	486	LEU	3.2
1	K	532	ILE	3.2
1	L	508	PHE	3.2
1	F	256	PRO	3.2
1	K	574	ILE	3.2
1	I	464	LYS	3.2
1	F	403	HIS	3.2
1	F	483	PRO	3.2
1	H	466	ARG	3.2
1	J	385	GLY	3.2
1	E	554	GLN	3.2
1	G	402	THR	3.1
1	A	594	LEU	3.1
1	F	510	ASP	3.1
1	J	403	HIS	3.1
1	L	509	GLY	3.1
1	B	552	ALA	3.1
1	G	128	ALA	3.1
1	F	516	PRO	3.1
1	D	557	HIS	3.1
1	K	488	GLY	3.1
1	K	361	CYS	3.1
1	K	546	ALA	3.0
1	E	385	GLY	3.0
1	K	457	ALA	3.0
1	H	498	CYS	3.0
1	F	482	THR	3.0
1	L	554	GLN	3.0
1	K	516	PRO	3.0
1	I	489	LYS	3.0
1	B	270	GLY	2.9
1	F	478	LEU	2.9
1	I	562	LYS	2.9
1	L	566	LYS	2.9
1	C	568	LEU	2.9
1	D	516	PRO	2.9
1	K	544	ILE	2.9
1	E	567	SER	2.9
1	G	124	GLU	2.9
1	K	455	ALA	2.9
1	F	385	GLY	2.9
1	F	532	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	512	GLY	2.8
1	F	566	LYS	2.8
1	G	401	SER	2.8
1	K	499	HIS	2.8
1	K	562	LYS	2.8
1	L	196	THR	2.8
1	K	494	VAL	2.8
1	G	404	TYR	2.8
1	I	514	ILE	2.8
1	I	574	ILE	2.8
1	K	542	PHE	2.8
1	F	306	TYR	2.8
1	H	294	ILE	2.8
1	H	505	THR	2.8
1	K	402	THR	2.7
1	K	550	THR	2.7
1	H	581	VAL	2.7
1	K	519	VAL	2.7
1	G	515	SER	2.7
1	H	583	ALA	2.7
1	H	563	GLU	2.7
1	F	500	ILE	2.7
1	E	400	THR	2.7
1	G	193	ARG	2.7
1	F	120	SER	2.7
1	C	559	LYS	2.7
1	D	306	TYR	2.7
1	I	555	ARG	2.7
1	H	579	ASN	2.7
1	G	304	LEU	2.7
1	B	401	SER	2.6
1	G	465	CYS	2.6
1	C	508	PHE	2.6
1	A	402	THR	2.6
1	F	558	GLY	2.6
1	I	570	THR	2.6
1	K	121	ASN	2.6
1	K	556	GLU	2.6
1	J	121	ASN	2.6
1	D	256	PRO	2.6
1	F	160	ILE	2.6
1	L	513	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	461	LEU	2.6
1	B	385	GLY	2.6
1	D	517	GLY	2.6
1	K	466	ARG	2.6
1	L	555	ARG	2.6
1	K	570	THR	2.5
1	H	506	ALA	2.5
1	F	582	GLU	2.5
1	K	490	VAL	2.5
1	K	290	GLN	2.5
1	J	122	ALA	2.5
1	H	273	ILE	2.5
1	J	402	THR	2.5
1	K	222	LYS	2.5
1	K	530	GLY	2.5
1	B	576	GLU	2.5
1	L	559	LYS	2.5
1	B	557	HIS	2.5
1	I	561	HIS	2.5
1	K	158	ARG	2.5
1	K	498	CYS	2.5
1	I	554	GLN	2.5
1	C	554	GLN	2.5
1	C	560	SER	2.5
1	H	283	PHE	2.5
1	H	536	PHE	2.5
1	I	559	LYS	2.5
1	J	405	ASP	2.5
1	H	556	GLU	2.5
1	K	255	SER	2.5
1	K	497	MET	2.5
1	D	576	GLU	2.4
1	D	562	LYS	2.4
1	F	402	THR	2.4
1	H	482	THR	2.4
1	J	594	LEU	2.4
1	L	558	GLY	2.4
1	K	360	HIS	2.4
1	L	126	ARG	2.4
1	L	512	GLY	2.4
1	I	256	PRO	2.4
1	I	552	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	594	LEU	2.4
1	J	404	TYR	2.4
1	K	404	TYR	2.4
1	F	513	THR	2.4
1	A	385	GLY	2.4
1	D	565	VAL	2.4
1	F	471	GLY	2.4
1	E	127	ARG	2.4
1	C	487	THR	2.4
1	D	122	ALA	2.4
1	D	403	HIS	2.4
1	H	306	TYR	2.3
1	A	512	GLY	2.3
1	K	251	MET	2.3
1	K	471	GLY	2.3
1	L	128	ALA	2.3
1	C	562	LYS	2.3
1	H	562	LYS	2.3
1	F	574	ILE	2.3
1	G	219	GLU	2.3
1	G	314	GLY	2.3
1	A	194	TYR	2.3
1	E	329	GLN	2.3
1	H	513	THR	2.3
1	L	368	THR	2.3
1	G	327	VAL	2.3
1	K	322	TRP	2.3
1	G	593	SER	2.3
1	H	162	LEU	2.3
1	K	403	HIS	2.3
1	K	502	LEU	2.3
1	A	122	ALA	2.2
1	B	562	LYS	2.2
1	D	553	LEU	2.2
1	K	535	ASP	2.2
1	D	290	GLN	2.2
1	I	569	CYS	2.2
1	K	481	LEU	2.2
1	L	562	LYS	2.2
1	E	122	ALA	2.2
1	E	566	LYS	2.2
1	F	121	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	457	ALA	2.2
1	K	221	ASP	2.2
1	F	584	PHE	2.2
1	G	508	PHE	2.2
1	K	468	VAL	2.2
1	F	466	ARG	2.2
1	F	553	LEU	2.2
1	H	486	LEU	2.2
1	H	499	HIS	2.2
1	B	405	ASP	2.2
1	G	192	ALA	2.2
1	G	513	THR	2.2
1	H	492	GLU	2.2
1	H	542	PHE	2.2
1	K	376	ARG	2.2
1	H	502	LEU	2.2
1	H	552	ALA	2.2
1	K	506	ALA	2.2
1	E	568	LEU	2.2
1	G	557	HIS	2.2
1	I	508	PHE	2.2
1	F	587	GLN	2.1
1	H	483	PRO	2.1
1	H	484	MET	2.1
1	I	571	ASN	2.1
1	D	514	ILE	2.1
1	H	160	ILE	2.1
1	H	480	ASP	2.1
1	B	402	THR	2.1
1	A	384	ARG	2.1
1	L	385	GLY	2.1
1	C	570	THR	2.1
1	C	566	LYS	2.1
1	F	543	LEU	2.1
1	G	196	THR	2.1
1	C	561	HIS	2.1
1	K	566	LYS	2.1
1	B	482	THR	2.1
1	H	158	ARG	2.1
1	H	555	ARG	2.1
1	H	593	SER	2.1
1	J	401	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	558	GLY	2.1
1	E	304	LEU	2.1
1	B	514	ILE	2.1
1	H	514	ILE	2.1
1	K	286	LYS	2.1
1	K	572	LYS	2.1
1	H	465	CYS	2.1
1	B	559	LYS	2.0
1	F	502	LEU	2.0
1	D	519	VAL	2.0
1	H	519	VAL	2.0
1	D	291	THR	2.0
1	H	460	LEU	2.0
1	J	386	PRO	2.0
1	G	405	ASP	2.0
1	I	515	SER	2.0
1	K	220	SER	2.0
1	L	510	ASP	2.0
1	C	513	THR	2.0
1	F	550	THR	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.