Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 03:40 PM EDT

PDB ID	:	5W79
Title	:	Crystal Structure of the Group II Chaperonin from Methanococcus Maripaludis, Cysteine-less mutant in the Apo State
Authors	:	Dalton, K.M.; Lopez, T.; Liu, C.; Ralston, C.Y.; Pereira, J.H.; Chartron, J.W.; McAndrew, R.P.; Douglas, N.R.; Adams, P.D.; Pande, V.S.; Frydman, J.
Deposited on	:	2017-06-19
Resolution	:	3.12 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

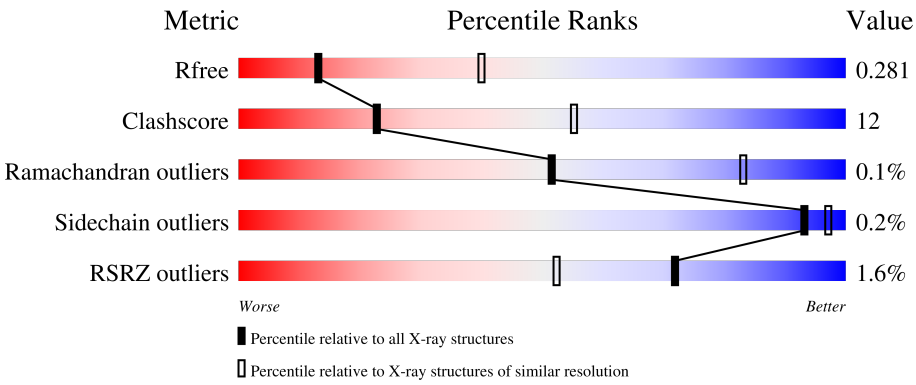
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.12 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	543	2% 69% 26% 5%
1	B	543	2% 73% 21% 5%
1	C	543	. % 69% 26% 5%
1	D	543	. % 70% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	543	3% 71% 23% 5%
1	F	543	.% 70% 25% 5%
1	G	543	.% 71% 24% 5%
1	H	543	2% 70% 25% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31143 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	515	3887	2419	670	778	20	0	0	0
1	B	515	3887	2419	670	778	20	0	0	0
1	C	515	3887	2419	670	778	20	0	0	0
1	D	515	3887	2419	670	778	20	0	0	0
1	E	515	3887	2419	670	778	20	0	0	0
1	F	515	3887	2419	670	778	20	0	0	0
1	G	515	3887	2419	670	778	20	0	0	0
1	H	515	3887	2419	670	778	20	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	CYS	engineered mutation	UNP Q877G8
A	237	GLU	CYS	engineered mutation	UNP Q877G8
A	286	VAL	CYS	engineered mutation	UNP Q877G8
A	304	MET	VAL	engineered mutation	UNP Q877G8
A	359	VAL	CYS	engineered mutation	UNP Q877G8
A	393	SER	CYS	engineered mutation	UNP Q877G8
A	470	TYR	CYS	engineered mutation	UNP Q877G8
A	484	THR	CYS	engineered mutation	UNP Q877G8
B	140	MET	CYS	engineered mutation	UNP Q877G8
B	237	GLU	CYS	engineered mutation	UNP Q877G8
B	286	VAL	CYS	engineered mutation	UNP Q877G8
B	304	MET	VAL	engineered mutation	UNP Q877G8
B	359	VAL	CYS	engineered mutation	UNP Q877G8

Continued on next page...

Continued from previous page...

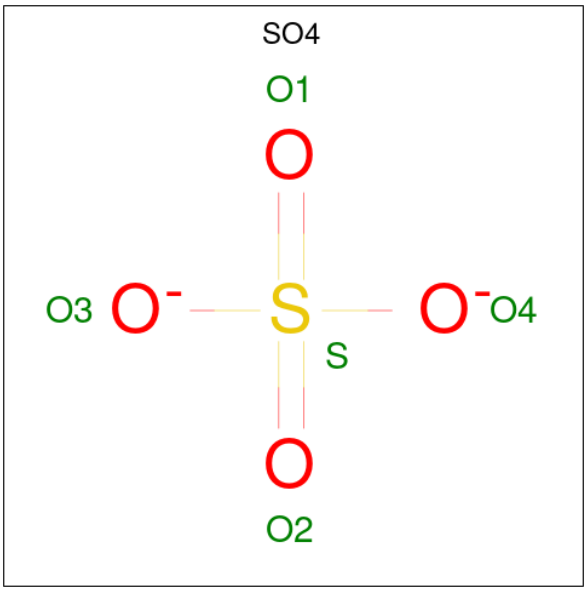
Chain	Residue	Modelled	Actual	Comment	Reference
B	393	SER	CYS	engineered mutation	UNP Q877G8
B	470	TYR	CYS	engineered mutation	UNP Q877G8
B	484	THR	CYS	engineered mutation	UNP Q877G8
C	140	MET	CYS	engineered mutation	UNP Q877G8
C	237	GLU	CYS	engineered mutation	UNP Q877G8
C	286	VAL	CYS	engineered mutation	UNP Q877G8
C	304	MET	VAL	engineered mutation	UNP Q877G8
C	359	VAL	CYS	engineered mutation	UNP Q877G8
C	393	SER	CYS	engineered mutation	UNP Q877G8
C	470	TYR	CYS	engineered mutation	UNP Q877G8
C	484	THR	CYS	engineered mutation	UNP Q877G8
D	140	MET	CYS	engineered mutation	UNP Q877G8
D	237	GLU	CYS	engineered mutation	UNP Q877G8
D	286	VAL	CYS	engineered mutation	UNP Q877G8
D	304	MET	VAL	engineered mutation	UNP Q877G8
D	359	VAL	CYS	engineered mutation	UNP Q877G8
D	393	SER	CYS	engineered mutation	UNP Q877G8
D	470	TYR	CYS	engineered mutation	UNP Q877G8
D	484	THR	CYS	engineered mutation	UNP Q877G8
E	140	MET	CYS	engineered mutation	UNP Q877G8
E	237	GLU	CYS	engineered mutation	UNP Q877G8
E	286	VAL	CYS	engineered mutation	UNP Q877G8
E	304	MET	VAL	engineered mutation	UNP Q877G8
E	359	VAL	CYS	engineered mutation	UNP Q877G8
E	393	SER	CYS	engineered mutation	UNP Q877G8
E	470	TYR	CYS	engineered mutation	UNP Q877G8
E	484	THR	CYS	engineered mutation	UNP Q877G8
F	140	MET	CYS	engineered mutation	UNP Q877G8
F	237	GLU	CYS	engineered mutation	UNP Q877G8
F	286	VAL	CYS	engineered mutation	UNP Q877G8
F	304	MET	VAL	engineered mutation	UNP Q877G8
F	359	VAL	CYS	engineered mutation	UNP Q877G8
F	393	SER	CYS	engineered mutation	UNP Q877G8
F	470	TYR	CYS	engineered mutation	UNP Q877G8
F	484	THR	CYS	engineered mutation	UNP Q877G8
G	140	MET	CYS	engineered mutation	UNP Q877G8
G	237	GLU	CYS	engineered mutation	UNP Q877G8
G	286	VAL	CYS	engineered mutation	UNP Q877G8
G	304	MET	VAL	engineered mutation	UNP Q877G8
G	359	VAL	CYS	engineered mutation	UNP Q877G8
G	393	SER	CYS	engineered mutation	UNP Q877G8
G	470	TYR	CYS	engineered mutation	UNP Q877G8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	484	THR	CYS	engineered mutation	UNP Q877G8
H	140	MET	CYS	engineered mutation	UNP Q877G8
H	237	GLU	CYS	engineered mutation	UNP Q877G8
H	286	VAL	CYS	engineered mutation	UNP Q877G8
H	304	MET	VAL	engineered mutation	UNP Q877G8
H	359	VAL	CYS	engineered mutation	UNP Q877G8
H	393	SER	CYS	engineered mutation	UNP Q877G8
H	470	TYR	CYS	engineered mutation	UNP Q877G8
H	484	THR	CYS	engineered mutation	UNP Q877G8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
2	B	1	5	4	1		0	0
2	C	1	5	4	1		0	0
2	D	1	5	4	1		0	0
2	E	1	5	4	1		0	0
2	F	1	5	4	1		0	0
2	G	1	5	4	1		0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	H	1	5	4	1	0	0

- Molecule 3 is water.

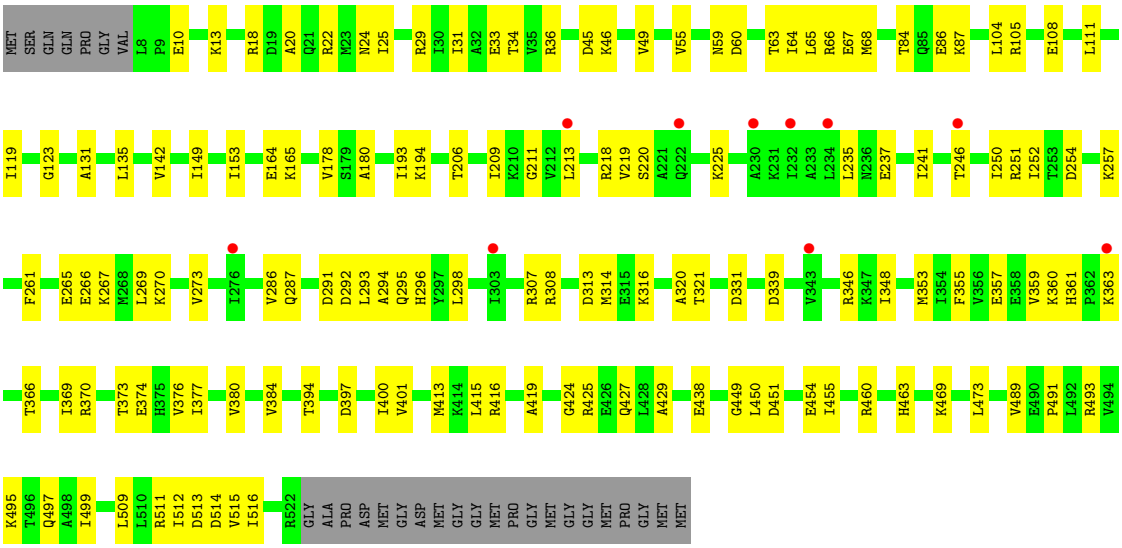
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	1	1	0	0
			Total	O		
3	C	1	1	1	0	0
			Total	O		
3	D	1	1	1	0	0
			Total	O		
3	E	1	1	1	0	0
			Total	O		
3	F	1	1	1	0	0
			Total	O		
3	G	1	1	1	0	0
			Total	O		
3	H	1	1	1	0	0

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.

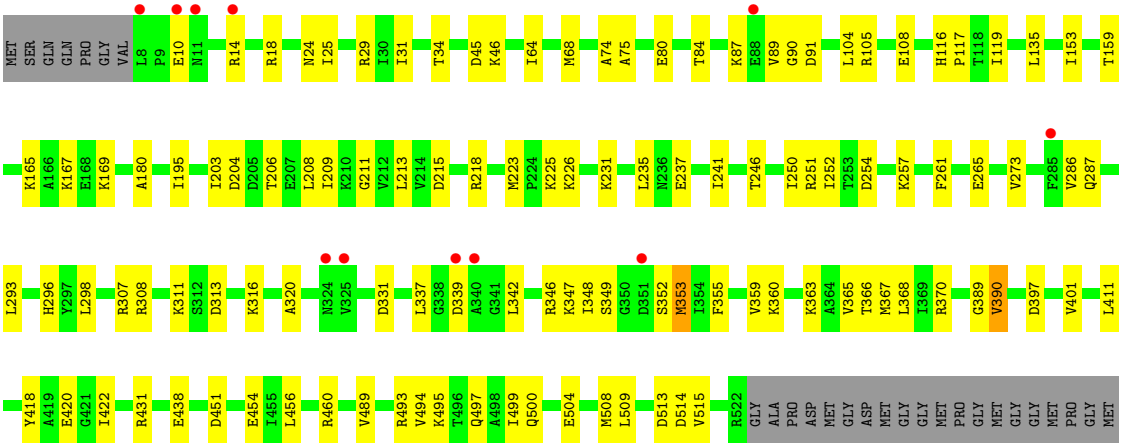
• Molecule 1: Chaperonin

Chain A:



• Molecule 1: Chaperonin

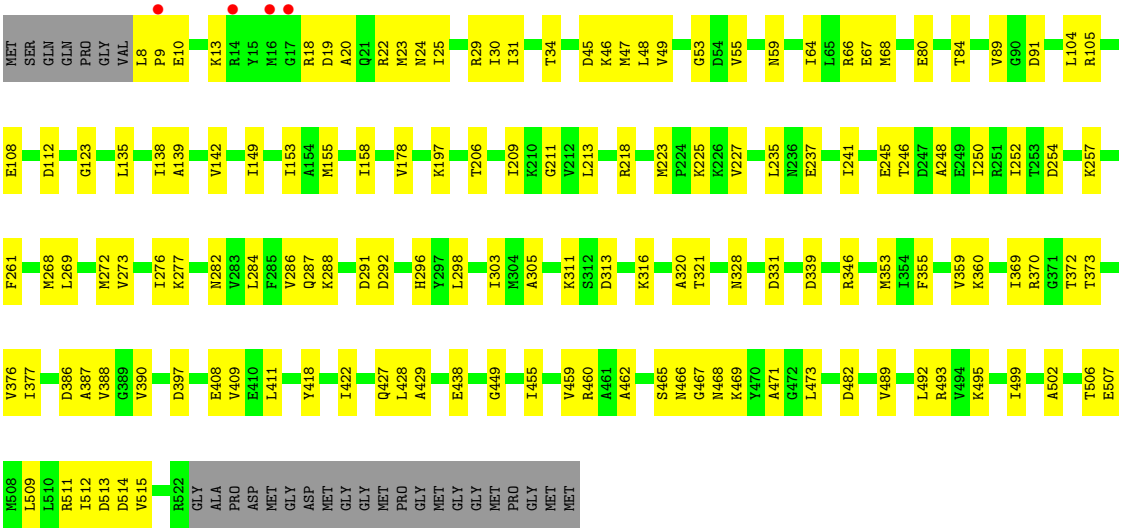
Chain B:



MET

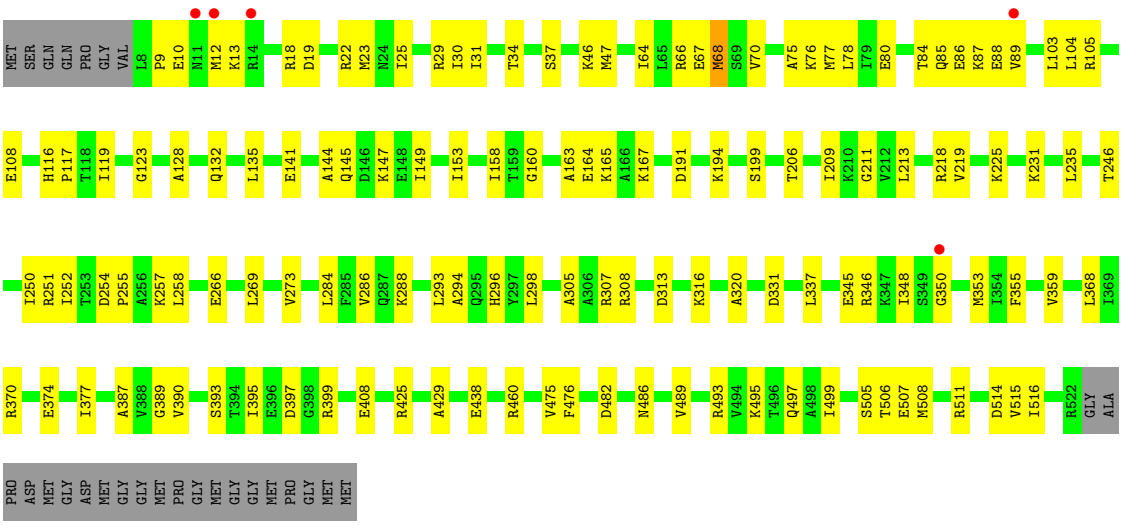
• Molecule 1: Chaperonin

Chain C:



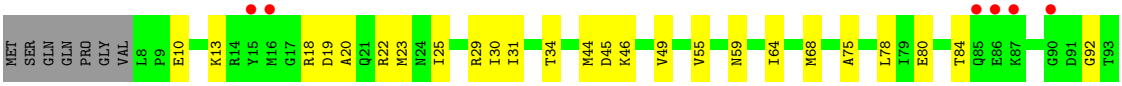
• Molecule 1: Chaperonin

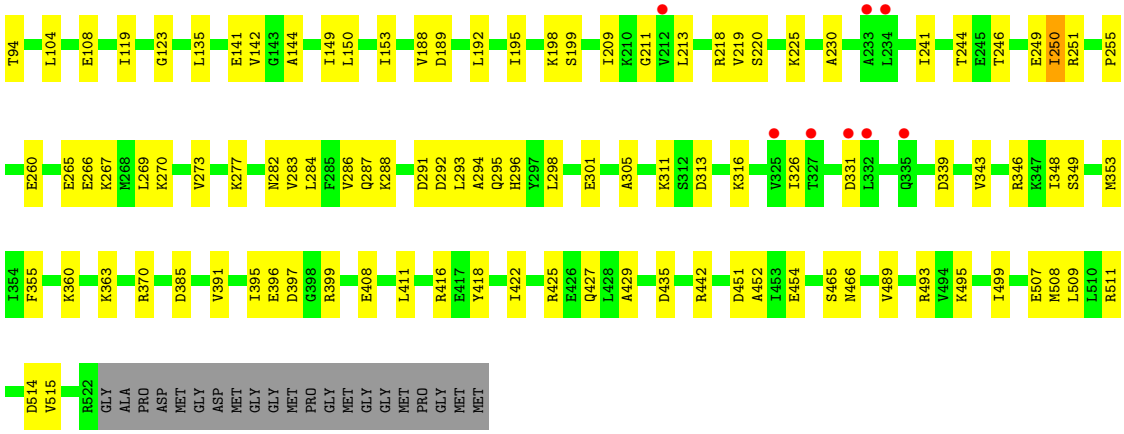
Chain D:



• Molecule 1: Chaperonin

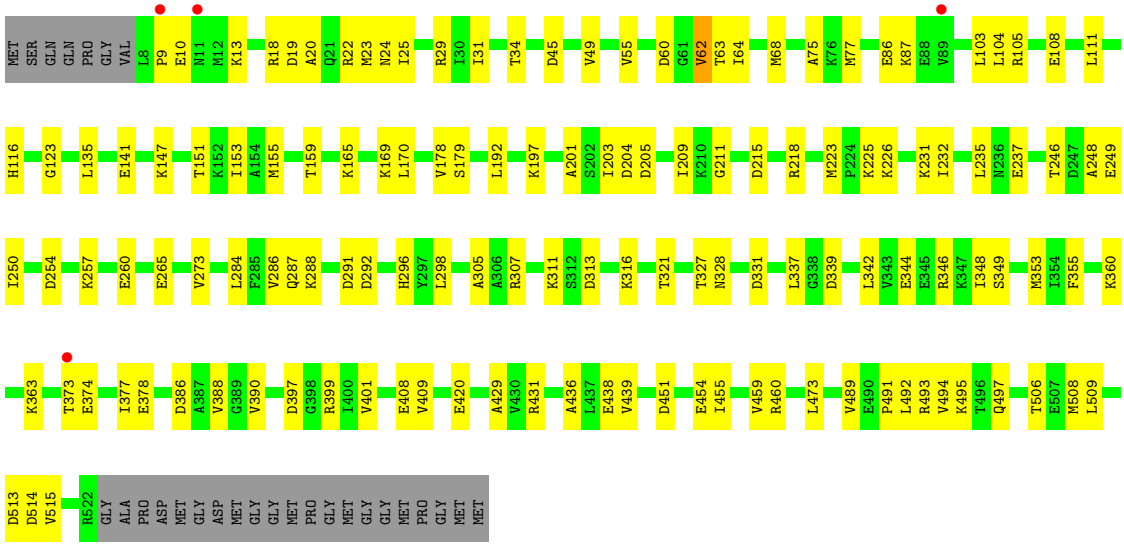
Chain E:





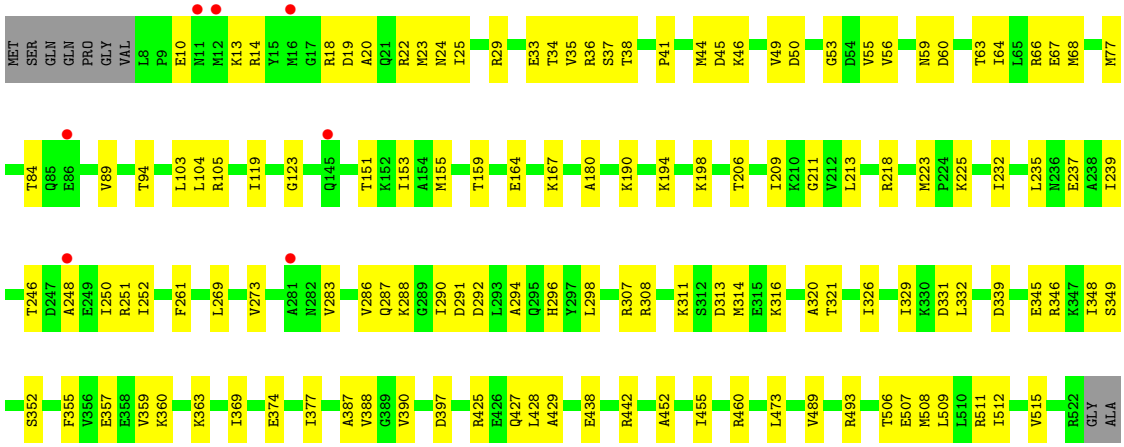
• Molecule 1: Chaperonin

Chain F:



• Molecule 1: Chaperonin

Chain G:



PRO ASP MET GLY ASP MET GLY GLY MET PRO GLY MET GLY GLY MET PRO GLY MET MET

- Molecule 1: Chaperonin

Chain H:

MET SER GLN GLN PRO GLY VAL L8 P9 E10 N11 M12 K13 R14 R18 Q21 R22 M23 N24 I25 R29 I30 T34 D45 K46 V49 V55 N59 I64 L65 R66 E67 M68 K76 E80 T84 Q85 E86 K87 T95 L104 R105 E108 L111

H116 G123 L135 V142 I149 I153 A154 I158 K161 G162 A163 E164 K165 D183 K187 K194 I209 K210 G211 V212 L213 R218 V219 K225 K231 I232 L235 N236 E237 I241 T246 D247 A248 E249 I250 R251 I252 T253 D254 K257 L258

F261 E265 M272 V273 V283 L284 F285 V286 Q287 K288 L293 H296 Y297 L298 M304 R307 R308 V309 K310 K311 S312 D313 M314 E315 K316 A320 T321 N328 D331 L337 E344 E345 R346 K347 I348 S349 M353 I354 F355 V356 E357 E358 V359 K360 H361

T372 T373 I377 V380 A387 V390 D397 V409 E410 L411 I422 S423 G424 Q427 L428 A429 E438 V439 I440 G449 L450 D451 E454 V459 R460 N468 A471 G472 L473 N474 V475 F476 V489 R493 A502 T506 E507 M508 L509 L510 R511 I512

D513 D514 V515 A518 L521 R522 GLY ALA PRO ASP MET GLY ASP MET GLY GLY GLY MET PRO GLY MET GLY GLY MET PRO GLY MET MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.98Å 149.98Å 416.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.24 – 3.12 81.24 – 3.12	Depositor EDS
% Data completeness (in resolution range)	99.0 (81.24-3.12) 99.0 (81.24-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.249 , 0.281 0.249 , 0.281	Depositor DCC
R_{free} test set	4942 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 24.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	31143	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.41	0/3911	0.63	0/5262
1	B	0.39	0/3911	0.61	1/5262 (0.0%)
1	C	0.40	0/3911	0.61	0/5262
1	D	0.42	0/3911	0.63	1/5262 (0.0%)
1	E	0.42	1/3911 (0.0%)	0.61	0/5262
1	F	0.40	0/3911	0.62	0/5262
1	G	0.40	0/3911	0.61	1/5262 (0.0%)
1	H	0.40	0/3911	0.62	1/5262 (0.0%)
All	All	0.40	1/31288 (0.0%)	0.62	4/42096 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	92	GLY	C-O	5.98	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	497	GLN	CA-CB-CG	6.68	128.10	113.40
1	G	59	ASN	CB-CA-C	-6.40	97.60	110.40
1	D	68	MET	CB-CA-C	-5.25	99.89	110.40
1	H	165	LYS	N-CA-C	-5.16	97.08	111.00

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	3887	0	4039	110	0
1	B	3887	0	4040	93	0
1	C	3887	0	4040	102	0
1	D	3887	0	4040	97	0
1	E	3887	0	4040	102	0
1	F	3887	0	4040	96	0
1	G	3887	0	4040	101	0
1	H	3887	0	4040	120	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	1	0
All	All	31143	0	32319	730	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 12.

All (730) 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:D:408:GLU:OE2	1:D:495:LYS:NZ	1.92	1.03
1:H:34:THR:O	1:H:46:LYS:NZ	1.94	1.00
1:H:218:ARG:HH22	1:H:225:LYS:HZ3	1.02	0.97
1:F:344:GLU:OE1	1:F:346:ARG:NH1	1.99	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:GLU:OE2	1:C:495:LYS:NZ	2.01	0.91
1:D:219:VAL:HG23	1:D:307:ARG:HH11	1.35	0.90
1:D:145:GLN:OE1	1:D:147:LYS:NZ	2.05	0.90
1:D:438:GLU:OE2	1:D:460:ARG:NH2	2.03	0.90
1:B:24:ASN:HD22	1:B:74:ALA:HB2	1.36	0.89
1:A:346:ARG:NH2	1:A:357:GLU:OE2	2.10	0.84
1:E:198:LYS:HD2	1:E:348:ILE:HD11	1.59	0.84
1:E:507:GLU:OE2	1:E:511:ARG:NH2	2.11	0.84
1:E:408:GLU:OE2	1:E:495:LYS:NZ	2.10	0.84
1:F:86:GLU:HG3	1:F:497:GLN:HE22	1.42	0.84
1:D:85:GLN:HB3	1:D:497:GLN:HE21	1.44	0.81
1:E:218:ARG:HH22	1:E:225:LYS:HZ1	1.24	0.81
1:G:37:SER:OG	1:G:46:LYS:NZ	2.12	0.81
1:A:86:GLU:HG2	1:H:372:THR:HG21	1.62	0.81
1:A:296:HIS:ND1	1:B:331:ASP:OD1	2.12	0.81
1:D:18:ARG:HH11	1:D:22:ARG:HH11	1.28	0.81
1:D:296:HIS:ND1	1:E:331:ASP:OD1	2.14	0.81
1:C:372:THR:HG21	1:D:86:GLU:HG2	1.63	0.80
1:D:218:ARG:NH1	1:D:345:GLU:OE1	2.13	0.80
1:E:218:ARG:HH12	1:E:225:LYS:HZ3	1.27	0.79
1:E:34:THR:O	1:E:46:LYS:NZ	2.15	0.79
1:A:400:ILE:HD12	1:A:489:VAL:HG21	1.64	0.79
1:C:47:MET:HB3	1:D:515:VAL:HG12	1.66	0.78
1:A:416:ARG:NH2	1:A:438:GLU:OE2	2.17	0.78
1:C:53:GLY:O	1:D:76:LYS:NZ	2.15	0.78
1:H:218:ARG:HH22	1:H:225:LYS:NZ	1.81	0.77
1:B:500:GLN:NE2	1:B:504:GLU:OE2	2.16	0.77
1:H:283:VAL:HG12	1:H:304:MET:HB3	1.66	0.77
1:G:53:GLY:O	1:H:76:LYS:NZ	2.16	0.77
1:B:265:GLU:OE2	1:C:245:GLU:HB3	1.86	0.76
1:H:158:ILE:HD11	1:H:387:ALA:HB2	1.67	0.76
1:A:66:ARG:NH1	1:A:67:GLU:OE2	2.18	0.76
1:F:296:HIS:ND1	1:G:331:ASP:OD1	2.18	0.76
1:A:331:ASP:OD1	1:H:296:HIS:ND1	2.17	0.75
1:H:507:GLU:OE2	1:H:511:ARG:NH2	2.20	0.75
1:D:37:SER:OG	1:D:46:LYS:NZ	2.20	0.74
1:H:218:ARG:NH2	1:H:225:LYS:HZ3	1.83	0.74
1:H:142:VAL:HG11	1:H:149:ILE:HG12	1.69	0.74
1:E:422:ILE:O	1:E:427:GLN:NE2	2.15	0.74
1:A:65:LEU:HD23	1:A:68:MET:HE1	1.69	0.74
1:F:408:GLU:OE2	1:F:495:LYS:NZ	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASP:O	1:D:194:LYS:NZ	2.20	0.73
1:F:86:GLU:O	1:F:497:GLN:NE2	2.21	0.73
1:C:438:GLU:OE2	1:C:460:ARG:NH2	2.16	0.72
1:E:218:ARG:NH1	1:E:225:LYS:HZ3	1.86	0.72
1:G:250:ILE:HG23	1:H:248:ALA:HA	1.71	0.72
1:C:397:ASP:OD2	1:C:493:ARG:HB2	1.89	0.71
1:G:507:GLU:OE2	1:G:511:ARG:NH2	2.22	0.71
1:B:438:GLU:OE2	1:B:460:ARG:NH2	2.23	0.70
1:H:218:ARG:HH12	1:H:225:LYS:HZ2	1.39	0.70
1:B:64:ILE:O	1:B:68:MET:HG3	1.92	0.70
1:H:64:ILE:O	1:H:68:MET:HG3	1.91	0.70
1:G:218:ARG:HH22	1:G:225:LYS:NZ	1.89	0.70
1:H:45:ASP:OD1	1:H:59:ASN:HB3	1.91	0.70
1:H:468:ASN:HB3	1:H:471:ALA:HB2	1.74	0.69
1:G:209:ILE:HG22	1:G:211:GLY:H	1.56	0.69
1:F:209:ILE:HG22	1:F:211:GLY:H	1.58	0.69
1:A:451:ASP:HB3	1:A:454:GLU:HG2	1.75	0.69
1:F:197:LYS:NZ	1:F:378:GLU:OE1	2.25	0.69
1:A:219:VAL:HG23	1:A:307:ARG:HE	1.58	0.69
1:A:246:THR:OG1	1:H:265:GLU:OE2	2.09	0.69
1:B:397:ASP:OD2	1:B:493:ARG:HB2	1.92	0.68
1:B:252:ILE:HB	1:C:250:ILE:HG12	1.76	0.68
1:A:87:LYS:H	1:A:497:GLN:HE22	1.40	0.68
1:H:422:ILE:O	1:H:427:GLN:NE2	2.25	0.68
1:H:287:GLN:HE21	1:H:314:MET:HG3	1.60	0.67
1:A:235:LEU:HB3	1:A:286:VAL:HG12	1.77	0.67
1:H:346:ARG:NH2	1:H:357:GLU:OE2	2.28	0.67
1:F:346:ARG:HH21	1:F:355:PHE:HD2	1.41	0.67
1:B:250:ILE:HG23	1:C:248:ALA:HA	1.76	0.67
1:F:397:ASP:OD2	1:F:493:ARG:HB2	1.95	0.66
1:D:158:ILE:HD11	1:D:387:ALA:HB2	1.77	0.66
1:G:438:GLU:OE2	1:G:460:ARG:NH2	2.29	0.66
1:D:507:GLU:OE2	1:D:511:ARG:NH2	2.28	0.66
1:D:199:SER:OG	1:D:374:GLU:OE2	2.14	0.66
1:B:320:ALA:HB1	1:B:359:VAL:HG21	1.77	0.66
1:G:198:LYS:HG2	1:G:348:ILE:HD13	1.77	0.65
1:A:361:HIS:CE1	1:A:363:LYS:HB2	2.30	0.65
1:D:219:VAL:CG2	1:D:307:ARG:HH11	2.09	0.65
1:G:296:HIS:ND1	1:H:331:ASP:OD1	2.30	0.65
1:C:45:ASP:HB3	1:C:59:ASN:HB3	1.79	0.64
1:E:29:ARG:NH2	1:F:10:GLU:OE2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:VAL:O	1:E:295:GLN:NE2	2.30	0.64
1:D:219:VAL:HG23	1:D:307:ARG:NH1	2.09	0.64
1:A:135:LEU:HD11	1:A:499:ILE:HD12	1.79	0.64
1:C:296:HIS:ND1	1:D:331:ASP:OD1	2.29	0.64
1:H:346:ARG:HH21	1:H:355:PHE:HD2	1.46	0.64
1:A:361:HIS:HE1	1:A:363:LYS:HB2	1.64	0.63
1:E:349:SER:HB2	1:E:370:ARG:HH22	1.61	0.63
1:F:373:THR:HG22	1:G:84:THR:HG21	1.80	0.63
1:E:45:ASP:HB3	1:E:59:ASN:HB3	1.80	0.63
1:B:235:LEU:HB3	1:B:286:VAL:HG12	1.80	0.63
1:H:344:GLU:OE1	1:H:346:ARG:NH1	2.32	0.63
1:C:252:ILE:HB	1:D:250:ILE:HG12	1.80	0.63
1:A:142:VAL:HG11	1:A:149:ILE:HG21	1.80	0.63
1:G:397:ASP:OD1	1:G:493:ARG:NH2	2.32	0.62
1:A:219:VAL:O	1:A:295:GLN:NE2	2.32	0.62
1:B:347:LYS:HA	1:B:352:SER:HB3	1.81	0.62
1:D:141:GLU:HG2	1:D:399:ARG:HG2	1.81	0.62
1:H:18:ARG:NH2	1:H:21:GLN:OE1	2.33	0.62
1:A:313:ASP:HA	1:A:316:LYS:HE2	1.82	0.61
1:C:468:ASN:HB3	1:C:471:ALA:HB2	1.81	0.61
1:A:45:ASP:HB3	1:A:59:ASN:HB3	1.82	0.61
1:A:254:ASP:HB3	1:A:257:LYS:HG2	1.82	0.61
1:C:339:ASP:HB2	1:C:360:LYS:HE2	1.82	0.61
1:A:18:ARG:O	1:A:22:ARG:HG2	1.99	0.61
1:A:320:ALA:HB1	1:A:359:VAL:HG21	1.81	0.61
1:G:287:GLN:HG2	1:G:314:MET:HG3	1.81	0.61
1:G:64:ILE:O	1:G:68:MET:HG3	2.00	0.61
1:B:153:ILE:HD13	1:B:489:VAL:HG23	1.81	0.61
1:H:163:ALA:HB2	1:H:380:VAL:HG22	1.82	0.61
1:E:18:ARG:NH1	1:E:22:ARG:HH11	1.99	0.61
1:E:296:HIS:ND1	1:F:331:ASP:OD1	2.33	0.61
1:F:64:ILE:O	1:F:68:MET:HG3	2.01	0.61
1:E:64:ILE:O	1:E:68:MET:HG3	2.01	0.60
1:G:105:ARG:HH22	1:H:8:LEU:HD23	1.67	0.60
1:D:85:GLN:HB3	1:D:497:GLN:NE2	2.14	0.60
1:D:78:LEU:HD12	1:D:505:SER:HB2	1.83	0.60
1:A:13:LYS:HE2	1:H:34:THR:HG22	1.81	0.60
1:A:60:ASP:OD2	1:A:63:THR:OG1	2.10	0.60
1:G:218:ARG:HH22	1:G:225:LYS:HZ1	1.49	0.60
1:B:508:MET:HG3	1:B:509:LEU:HD22	1.84	0.60
1:E:250:ILE:HG23	1:F:248:ALA:HA	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:ASP:HB3	1:F:454:GLU:HG2	1.82	0.60
1:E:230:ALA:HA	1:E:282:ASN:HD21	1.68	0.59
1:H:209:ILE:HG22	1:H:211:GLY:H	1.67	0.59
1:A:251:ARG:HD2	1:B:251:ARG:HG2	1.84	0.59
1:B:296:HIS:ND1	1:C:331:ASP:OD1	2.34	0.59
1:D:438:GLU:CD	1:D:460:ARG:HH21	2.02	0.59
1:E:18:ARG:O	1:E:22:ARG:HG2	2.00	0.59
1:G:206:THR:HG23	1:G:369:ILE:HA	1.84	0.59
1:C:153:ILE:HD13	1:C:489:VAL:HG23	1.85	0.59
1:B:231:LYS:HB3	1:B:337:LEU:HD13	1.84	0.59
1:F:170:LEU:HD22	1:F:203:ILE:HD11	1.83	0.59
1:D:34:THR:O	1:D:46:LYS:HE2	2.03	0.59
1:C:48:LEU:HD23	1:D:516:ILE:HG13	1.83	0.59
1:A:250:ILE:HD11	1:A:261:PHE:CD1	2.37	0.59
1:E:218:ARG:HH22	1:E:225:LYS:NZ	1.99	0.58
1:E:230:ALA:HA	1:E:282:ASN:ND2	2.18	0.58
1:C:209:ILE:HG22	1:C:211:GLY:H	1.68	0.58
1:E:34:THR:HG22	1:F:13:LYS:HE2	1.86	0.58
1:F:169:LYS:NZ	1:F:204:ASP:O	2.29	0.58
1:G:218:ARG:NH1	1:G:225:LYS:HG2	2.18	0.58
1:H:153:ILE:HD13	1:H:489:VAL:HG23	1.84	0.58
1:A:10:GLU:OE2	1:H:29:ARG:NH2	2.33	0.58
1:A:455:ILE:HG21	1:A:473:LEU:HD22	1.85	0.58
1:D:254:ASP:HB3	1:D:257:LYS:HG2	1.86	0.58
1:A:20:ALA:HB1	1:A:515:VAL:HG12	1.85	0.58
1:A:250:ILE:HD12	1:H:258:LEU:HD21	1.84	0.58
1:F:86:GLU:CG	1:F:497:GLN:HE22	2.12	0.58
1:G:29:ARG:NH2	1:H:10:GLU:OE2	2.37	0.58
1:G:339:ASP:HB2	1:G:360:LYS:HE2	1.85	0.58
1:F:18:ARG:O	1:F:22:ARG:HG2	2.03	0.58
1:B:46:LYS:NZ	1:C:513:ASP:OD1	2.35	0.58
1:C:64:ILE:O	1:C:68:MET:HG3	2.04	0.58
1:E:192:LEU:HD13	1:E:363:LYS:HB3	1.85	0.58
1:F:250:ILE:HG23	1:G:248:ALA:HA	1.86	0.58
1:G:348:ILE:HD12	1:G:349:SER:O	2.04	0.58
1:H:18:ARG:HH11	1:H:22:ARG:HH11	1.52	0.58
1:E:273:VAL:HG13	1:E:298:LEU:HD23	1.86	0.58
1:G:33:GLU:OE1	1:G:36:ARG:HD3	2.04	0.58
1:B:346:ARG:HD2	1:B:355:PHE:CD2	2.39	0.57
1:F:491:PRO:O	1:F:494:VAL:HG12	2.05	0.57
1:B:135:LEU:HD11	1:B:499:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:VAL:HG11	1:E:343:VAL:HG11	1.86	0.57
1:F:22:ARG:HH22	1:F:111:LEU:HB2	1.70	0.57
1:G:66:ARG:NH1	1:G:67:GLU:OE2	2.38	0.57
1:E:25:ILE:HG23	1:E:104:LEU:HB3	1.85	0.57
1:E:209:ILE:HG22	1:E:211:GLY:H	1.70	0.57
1:B:80:GLU:O	1:B:84:THR:HG23	2.04	0.57
1:B:347:LYS:HA	1:B:352:SER:CB	2.35	0.57
1:D:153:ILE:HD13	1:D:489:VAL:HG23	1.87	0.57
1:H:409:VAL:HG11	1:H:459:VAL:HG12	1.87	0.57
1:A:123:GLY:HA3	1:A:429:ALA:HB3	1.85	0.57
1:A:307:ARG:HD3	1:A:308:ARG:HH11	1.70	0.57
1:H:518:ALA:HB3	1:H:521:LEU:HD11	1.85	0.57
1:D:218:ARG:HH12	1:D:225:LYS:HZ3	1.51	0.57
1:G:25:ILE:HG23	1:G:104:LEU:HB3	1.86	0.57
1:C:507:GLU:OE2	1:C:511:ARG:NH2	2.38	0.56
1:D:46:LYS:HD2	1:E:514:ASP:HB3	1.87	0.56
1:F:438:GLU:OE2	1:F:460:ARG:NH2	2.30	0.56
1:A:287:GLN:HG2	1:A:314:MET:HG3	1.87	0.56
1:A:449:GLY:HA3	1:B:119:ILE:HD11	1.86	0.56
1:E:277:LYS:HG2	1:E:301:GLU:OE2	2.05	0.56
1:E:339:ASP:HB2	1:E:360:LYS:HE3	1.87	0.56
1:G:50:ASP:HB3	1:H:521:LEU:HD13	1.86	0.56
1:B:29:ARG:NH2	1:B:105:ARG:HH11	2.03	0.56
1:C:31:ILE:O	1:C:34:THR:OG1	2.22	0.56
1:D:34:THR:HG22	1:E:13:LYS:HE2	1.87	0.56
1:D:160:GLY:N	1:D:164:GLU:OE2	2.36	0.56
1:G:153:ILE:HD13	1:G:489:VAL:HG23	1.85	0.56
1:G:198:LYS:NZ	1:G:348:ILE:HD11	2.20	0.56
1:G:442:ARG:HG3	1:G:452:ALA:HB1	1.88	0.56
1:D:30:ILE:O	1:D:34:THR:HG23	2.06	0.56
1:G:320:ALA:HB1	1:G:359:VAL:HG21	1.87	0.56
1:G:374:GLU:HA	1:G:377:ILE:HG22	1.87	0.56
1:A:10:GLU:OE2	1:H:105:ARG:HD3	2.06	0.56
1:A:119:ILE:HD11	1:H:449:GLY:HA3	1.87	0.56
1:C:197:LYS:HB2	1:C:377:ILE:HG23	1.88	0.56
1:B:273:VAL:HG13	1:B:298:LEU:HD23	1.87	0.56
1:D:64:ILE:O	1:D:68:MET:HG3	2.05	0.56
1:D:209:ILE:HG22	1:D:211:GLY:H	1.70	0.56
1:E:218:ARG:HH12	1:E:225:LYS:NZ	2.02	0.56
1:E:255:PRO:HG3	1:F:260:GLU:HG2	1.87	0.56
1:F:218:ARG:NH1	1:F:225:LYS:HG2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:THR:HG22	1:G:13:LYS:HE2	1.87	0.56
1:A:24:ASN:HB3	1:A:509:LEU:HD22	1.88	0.55
1:E:397:ASP:OD2	1:E:493:ARG:HB2	2.06	0.55
1:H:320:ALA:HB1	1:H:359:VAL:HG21	1.89	0.55
1:A:220:SER:HB2	1:A:295:GLN:HG2	1.89	0.55
1:A:287:GLN:HE21	1:A:314:MET:HG3	1.71	0.55
1:B:209:ILE:HD12	1:B:213:LEU:HD11	1.88	0.55
1:A:194:LYS:HE3	1:A:316:LYS:HB3	1.88	0.55
1:B:235:LEU:O	1:B:286:VAL:HA	2.07	0.55
1:D:119:ILE:HD11	1:D:425:ARG:HH21	1.71	0.55
1:E:153:ILE:HD13	1:E:489:VAL:HG23	1.89	0.55
1:H:29:ARG:NH1	1:H:108:GLU:OE1	2.39	0.55
1:A:514:ASP:HB3	1:H:46:LYS:HD2	1.89	0.55
1:E:451:ASP:HB3	1:E:454:GLU:HG2	1.88	0.55
1:G:151:THR:O	1:G:155:MET:HG2	2.07	0.55
1:C:320:ALA:HB1	1:C:359:VAL:HG21	1.88	0.55
1:F:24:ASN:HB3	1:F:509:LEU:HD12	1.89	0.55
1:B:420:GLU:OE2	1:B:431:ARG:NH2	2.38	0.55
1:E:144:ALA:HB1	1:E:395:ILE:HG23	1.89	0.55
1:E:218:ARG:NH2	1:E:225:LYS:HZ1	2.00	0.55
1:E:141:GLU:HG2	1:E:399:ARG:HG2	1.89	0.54
1:A:194:LYS:HG3	1:A:316:LYS:HD2	1.89	0.54
1:B:105:ARG:HH22	1:C:8:LEU:HD23	1.71	0.54
1:D:286:VAL:HG22	1:D:288:LYS:H	1.73	0.54
1:F:153:ILE:HD13	1:F:489:VAL:HG23	1.90	0.54
1:G:218:ARG:NH1	1:G:345:GLU:OE1	2.38	0.54
1:H:86:GLU:HG2	1:H:87:LYS:HG2	1.89	0.54
1:H:287:GLN:HG2	1:H:314:MET:HG3	1.90	0.54
1:A:250:ILE:HD11	1:A:261:PHE:CE1	2.43	0.54
1:C:22:ARG:NH2	1:C:112:ASP:OD1	2.37	0.54
1:H:194:LYS:HE3	1:H:316:LYS:HB3	1.88	0.54
1:A:348:ILE:HD11	1:A:370:ARG:NH1	2.22	0.54
1:B:397:ASP:OD1	1:B:493:ARG:NH2	2.38	0.54
1:D:307:ARG:HE	1:D:308:ARG:NH2	2.06	0.54
1:F:19:ASP:O	1:F:23:MET:HG2	2.08	0.54
1:A:273:VAL:HG13	1:A:298:LEU:HD23	1.90	0.54
1:C:24:ASN:HB3	1:C:509:LEU:HD12	1.89	0.54
1:G:164:GLU:HA	1:G:167:LYS:HE3	1.90	0.54
1:B:135:LEU:HD21	1:B:411:LEU:HD11	1.90	0.53
1:F:25:ILE:HG23	1:F:104:LEU:HB3	1.90	0.53
1:C:273:VAL:HG13	1:C:298:LEU:HD23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:SER:OG	1:C:466:ASN:N	2.40	0.53
1:F:29:ARG:NH2	1:G:10:GLU:OE2	2.40	0.53
1:A:287:GLN:CG	1:A:314:MET:HG3	2.37	0.53
1:D:252:ILE:HD13	1:D:258:LEU:HD23	1.91	0.53
1:E:49:VAL:HG22	1:E:55:VAL:HG12	1.90	0.53
1:E:189:ASP:HB3	1:E:192:LEU:HD12	1.91	0.53
1:E:346:ARG:HD2	1:E:355:PHE:CE2	2.43	0.53
1:A:209:ILE:HG22	1:A:211:GLY:H	1.73	0.53
1:F:60:ASP:OD2	1:F:62:VAL:HG12	2.09	0.53
1:G:287:GLN:HE22	1:G:311:LYS:HG3	1.74	0.53
1:G:374:GLU:O	1:G:377:ILE:HG22	2.08	0.53
1:H:346:ARG:NH2	1:H:355:PHE:HD2	2.07	0.53
1:G:307:ARG:NH1	1:G:308:ARG:NH2	2.57	0.53
1:B:29:ARG:NH2	1:C:10:GLU:OE2	2.38	0.53
1:H:213:LEU:HD13	1:H:355:PHE:CD1	2.44	0.53
1:B:24:ASN:ND2	1:B:74:ALA:HB2	2.16	0.52
1:C:235:LEU:HG	1:C:237:GLU:H	1.74	0.52
1:D:266:GLU:HG2	1:D:293:LEU:HD21	1.91	0.52
1:G:20:ALA:HB1	1:G:515:VAL:HG12	1.91	0.52
1:A:213:LEU:HD21	1:A:353:MET:HE1	1.90	0.52
1:B:105:ARG:HD2	1:C:10:GLU:OE2	2.08	0.52
1:D:206:THR:HG23	1:D:368:LEU:O	2.10	0.52
1:E:80:GLU:O	1:E:84:THR:HG23	2.09	0.52
1:G:29:ARG:NH2	1:G:105:ARG:HH11	2.07	0.52
1:A:64:ILE:O	1:A:68:MET:HG3	2.09	0.52
1:A:416:ARG:HH12	1:A:460:ARG:CZ	2.22	0.52
1:B:514:ASP:OD1	1:B:515:VAL:N	2.41	0.52
1:E:135:LEU:HD21	1:E:411:LEU:HD11	1.91	0.52
1:A:413:MET:HE1	1:A:463:HIS:HB3	1.92	0.52
1:B:29:ARG:NH1	1:B:108:GLU:OE1	2.43	0.52
1:C:313:ASP:HA	1:C:316:LYS:HE2	1.90	0.52
1:F:29:ARG:NH1	1:F:108:GLU:OE1	2.42	0.52
1:F:123:GLY:HA3	1:F:429:ALA:HB3	1.90	0.52
1:A:401:VAL:HG21	1:A:495:LYS:HG3	1.92	0.52
1:B:209:ILE:HG22	1:B:211:GLY:H	1.74	0.52
1:H:30:ILE:O	1:H:34:THR:HG23	2.10	0.52
1:F:218:ARG:HD2	1:F:223:MET:HB2	1.90	0.52
1:H:348:ILE:HG22	1:H:349:SER:H	1.73	0.52
1:A:424:GLY:O	1:A:427:GLN:HG3	2.10	0.52
1:C:135:LEU:HA	1:C:138:ILE:HG22	1.91	0.52
1:F:265:GLU:OE2	1:G:246:THR:HB	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:ASP:HB3	1:H:454:GLU:HG2	1.91	0.52
1:B:169:LYS:NZ	1:B:204:ASP:O	2.32	0.52
1:F:339:ASP:HB2	1:F:360:LYS:HE2	1.91	0.52
1:H:25:ILE:HG23	1:H:104:LEU:HB3	1.92	0.52
1:F:273:VAL:HG13	1:F:298:LEU:HD23	1.91	0.52
1:G:250:ILE:HD11	1:G:261:PHE:CD1	2.44	0.52
1:C:135:LEU:HD11	1:C:499:ILE:HD12	1.92	0.52
1:E:286:VAL:HG22	1:E:288:LYS:H	1.75	0.51
1:H:123:GLY:HA3	1:H:429:ALA:HB3	1.93	0.51
1:H:286:VAL:HG12	1:H:288:LYS:H	1.75	0.51
1:C:155:MET:HA	1:C:158:ILE:HG22	1.93	0.51
1:E:220:SER:HB2	1:E:295:GLN:HG2	1.91	0.51
1:F:29:ARG:NH2	1:F:105:ARG:HH11	2.08	0.51
1:B:307:ARG:HD2	1:B:308:ARG:NH1	2.25	0.51
1:D:144:ALA:HB1	1:D:395:ILE:HG23	1.92	0.51
1:H:287:GLN:CG	1:H:314:MET:HG3	2.40	0.51
1:H:321:THR:HG22	1:H:359:VAL:HG23	1.93	0.51
1:A:105:ARG:HD2	1:B:10:GLU:OE2	2.10	0.51
1:C:20:ALA:HB1	1:C:515:VAL:HG12	1.92	0.51
1:H:237:GLU:OE1	1:H:328:ASN:HA	2.11	0.51
1:E:241:ILE:HD13	1:E:265:GLU:OE1	2.11	0.51
1:H:235:LEU:HG	1:H:237:GLU:H	1.76	0.51
1:E:250:ILE:HG21	1:F:246:THR:HG23	1.91	0.51
1:H:66:ARG:NH1	1:H:67:GLU:OE2	2.44	0.51
1:A:449:GLY:HA3	1:B:119:ILE:CD1	2.40	0.51
1:E:292:ASP:O	1:E:295:GLN:HB3	2.10	0.51
1:F:60:ASP:O	1:F:64:ILE:HD12	2.10	0.51
1:F:192:LEU:HD13	1:F:363:LYS:HB3	1.93	0.51
1:E:465:SER:OG	1:E:466:ASN:N	2.44	0.51
1:G:123:GLY:HA3	1:G:429:ALA:HB3	1.93	0.51
1:C:29:ARG:NH1	1:C:108:GLU:OE1	2.44	0.50
1:D:66:ARG:NH1	1:D:67:GLU:OE2	2.44	0.50
1:G:346:ARG:HD2	1:G:355:PHE:CD2	2.46	0.50
1:F:286:VAL:HG13	1:F:307:ARG:HA	1.93	0.50
1:H:24:ASN:HB3	1:H:509:LEU:HD12	1.94	0.50
1:C:287:GLN:HE22	1:C:311:LYS:HD2	1.77	0.50
1:G:56:VAL:HG23	1:H:521:LEU:HD23	1.94	0.50
1:G:252:ILE:HG12	1:G:261:PHE:CE2	2.46	0.50
1:H:18:ARG:NH1	1:H:111:LEU:HB3	2.26	0.50
1:A:373:THR:OG1	1:A:376:VAL:HG22	2.12	0.50
1:F:254:ASP:HB3	1:F:257:LYS:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASP:OD1	1:G:292:ASP:N	2.44	0.50
1:H:232:ILE:HG12	1:H:283:VAL:CG2	2.41	0.50
1:A:213:LEU:HB3	1:A:366:THR:HG21	1.93	0.50
1:B:209:ILE:HD13	1:B:213:LEU:HD21	1.93	0.50
1:C:468:ASN:HD21	1:C:482:ASP:HB2	1.75	0.50
1:E:119:ILE:HD13	1:E:425:ARG:HE	1.76	0.50
1:F:235:LEU:HG	1:F:237:GLU:H	1.77	0.50
1:F:237:GLU:HB2	1:F:327:THR:O	2.11	0.50
1:H:218:ARG:NH1	1:H:225:LYS:HZ2	2.08	0.50
1:A:397:ASP:OD2	1:A:493:ARG:HB2	2.11	0.50
1:B:215:ASP:HA	1:B:353:MET:HB2	1.94	0.50
1:B:451:ASP:HB3	1:B:454:GLU:HG2	1.94	0.50
1:C:19:ASP:O	1:C:23:MET:HG2	2.11	0.50
1:D:29:ARG:NH1	1:D:108:GLU:OE1	2.45	0.49
1:D:346:ARG:HD2	1:D:355:PHE:CE2	2.47	0.49
1:F:313:ASP:OD1	1:F:316:LYS:HE2	2.12	0.49
1:H:273:VAL:HG13	1:H:298:LEU:HD23	1.93	0.49
1:A:463:HIS:HE1	1:A:469:LYS:O	1.94	0.49
1:E:442:ARG:HG3	1:E:452:ALA:HB1	1.94	0.49
1:G:239:ILE:HD12	1:G:290:ILE:HG12	1.94	0.49
1:G:287:GLN:NE2	1:G:311:LYS:HG3	2.26	0.49
1:B:339:ASP:HB2	1:B:360:LYS:HE3	1.95	0.49
1:E:30:ILE:O	1:E:34:THR:HG23	2.13	0.49
1:H:231:LYS:HB3	1:H:337:LEU:HD13	1.94	0.49
1:H:348:ILE:HG22	1:H:349:SER:N	2.28	0.49
1:H:397:ASP:OD2	1:H:493:ARG:HB2	2.12	0.49
1:E:346:ARG:HD2	1:E:355:PHE:CD2	2.47	0.49
1:E:326:ILE:HG23	1:E:331:ASP:HB2	1.94	0.49
1:F:284:LEU:O	1:F:305:ALA:HA	2.12	0.49
1:C:218:ARG:HH12	1:C:225:LYS:HZ3	1.60	0.49
1:C:291:ASP:OD1	1:C:292:ASP:N	2.45	0.49
1:F:105:ARG:HD2	1:G:10:GLU:OE2	2.12	0.49
1:C:47:MET:HE1	1:D:77:MET:HG3	1.94	0.49
1:E:416:ARG:NH1	1:E:435:ASP:OD1	2.45	0.49
1:G:34:THR:O	1:G:46:LYS:HE2	2.12	0.49
1:E:267:LYS:HD2	1:E:270:LYS:HE3	1.95	0.49
1:F:409:VAL:HG11	1:F:459:VAL:HG12	1.95	0.49
1:H:502:ALA:O	1:H:506:THR:HG22	2.13	0.49
1:A:33:GLU:OE1	1:A:36:ARG:HD3	2.13	0.48
1:C:237:GLU:OE1	1:C:328:ASN:HA	2.12	0.48
1:C:427:GLN:HG3	1:C:428:LEU:HD12	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:ALA:HB1	1:F:515:VAL:HG12	1.94	0.48
1:G:24:ASN:HB3	1:G:509:LEU:HD12	1.95	0.48
1:G:29:ARG:NH2	1:G:105:ARG:NH1	2.61	0.48
1:H:213:LEU:HD21	1:H:353:MET:HE1	1.95	0.48
1:D:163:ALA:O	1:D:165:LYS:N	2.45	0.48
1:F:49:VAL:HG22	1:F:55:VAL:HG12	1.95	0.48
1:G:250:ILE:HG21	1:H:246:THR:HG23	1.95	0.48
1:H:313:ASP:HA	1:H:316:LYS:HE2	1.95	0.48
1:A:265:GLU:OE2	1:B:246:THR:HB	2.13	0.48
1:C:286:VAL:HG22	1:C:288:LYS:H	1.77	0.48
1:F:286:VAL:HG22	1:F:288:LYS:H	1.78	0.48
1:H:135:LEU:HD21	1:H:411:LEU:HD11	1.95	0.48
1:H:287:GLN:HE22	1:H:311:LYS:HG3	1.78	0.48
1:H:320:ALA:O	1:H:361:HIS:ND1	2.37	0.48
1:B:508:MET:HG3	1:B:509:LEU:N	2.28	0.48
1:E:241:ILE:HG13	1:E:269:LEU:HD11	1.94	0.48
1:C:213:LEU:HD21	1:C:353:MET:HE1	1.96	0.48
1:C:514:ASP:OD1	1:C:515:VAL:N	2.47	0.48
1:F:514:ASP:OD1	1:F:515:VAL:N	2.47	0.48
1:G:18:ARG:O	1:G:22:ARG:HG2	2.13	0.48
1:E:29:ARG:NH1	1:E:108:GLU:OE1	2.47	0.48
1:F:165:LYS:HE3	1:F:203:ILE:HG22	1.95	0.48
1:B:14:ARG:O	1:B:18:ARG:HG3	2.13	0.48
1:B:213:LEU:HD22	1:B:355:PHE:CD1	2.49	0.48
1:F:135:LEU:HB3	1:F:492:LEU:HD11	1.95	0.48
1:H:450:LEU:HD12	1:H:473:LEU:HD21	1.96	0.48
1:H:518:ALA:CB	1:H:521:LEU:HD11	2.44	0.48
1:A:153:ILE:HD13	1:A:489:VAL:HG13	1.96	0.48
1:A:180:ALA:O	1:A:363:LYS:HD2	2.14	0.48
1:B:159:THR:OG1	1:B:167:LYS:NZ	2.40	0.48
1:A:269:LEU:HD23	1:A:294:ALA:N	2.28	0.48
1:B:87:LYS:HB3	1:B:89:VAL:HG22	1.96	0.48
1:C:80:GLU:O	1:C:84:THR:HG23	2.14	0.48
1:F:226:LYS:HE3	1:F:342:LEU:HD11	1.96	0.48
1:B:29:ARG:NH2	1:B:105:ARG:NH1	2.62	0.48
1:C:254:ASP:HB3	1:C:257:LYS:HG2	1.95	0.48
1:C:272:MET:O	1:C:276:ILE:HD12	2.14	0.48
1:E:199:SER:O	1:E:370:ARG:NH2	2.42	0.48
1:F:374:GLU:HA	1:F:377:ILE:HB	1.96	0.48
1:A:31:ILE:O	1:A:34:THR:HG22	2.14	0.47
1:B:438:GLU:HB3	1:B:456:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:424:GLY:O	1:H:427:GLN:HG3	2.14	0.47
1:A:251:ARG:HD2	1:B:251:ARG:CG	2.44	0.47
1:B:346:ARG:O	1:B:352:SER:HB2	2.12	0.47
1:G:60:ASP:OD2	1:G:63:THR:OG1	2.15	0.47
1:G:346:ARG:NH2	1:G:357:GLU:OE1	2.47	0.47
1:C:34:THR:O	1:C:46:LYS:HE3	2.14	0.47
1:F:215:ASP:HB2	1:F:353:MET:HE3	1.96	0.47
1:H:49:VAL:HG22	1:H:55:VAL:HG12	1.97	0.47
1:A:250:ILE:HG13	1:H:252:ILE:HB	1.96	0.47
1:A:374:GLU:HA	1:A:377:ILE:HB	1.95	0.47
1:C:197:LYS:HB2	1:C:377:ILE:CG2	2.44	0.47
1:D:10:GLU:H	1:D:10:GLU:HG2	1.50	0.47
1:D:273:VAL:HG13	1:D:298:LEU:HD23	1.97	0.47
1:F:231:LYS:HB3	1:F:337:LEU:HD13	1.96	0.47
1:G:103:LEU:HB2	1:G:506:THR:HG21	1.95	0.47
1:G:105:ARG:HD2	1:H:10:GLU:OE2	2.14	0.47
1:G:232:ILE:HD13	1:G:283:VAL:HB	1.95	0.47
1:A:513:ASP:OD1	1:A:514:ASP:N	2.48	0.47
1:D:218:ARG:NH1	1:D:225:LYS:HZ3	2.12	0.47
1:D:251:ARG:HA	1:E:249:GLU:O	2.15	0.47
1:D:482:ASP:O	1:D:486:ASN:ND2	2.46	0.47
1:G:194:LYS:HE3	1:G:316:LYS:HB3	1.96	0.47
1:H:211:GLY:HA3	1:H:357:GLU:HA	1.97	0.47
1:D:103:LEU:HB2	1:D:506:THR:HG21	1.96	0.47
1:E:44:MET:CE	1:F:116:HIS:HE1	2.28	0.47
1:A:252:ILE:HG12	1:A:261:PHE:CE2	2.50	0.47
1:B:287:GLN:HE22	1:B:311:LYS:HE2	1.79	0.47
1:B:349:SER:OG	1:B:370:ARG:NH2	2.47	0.47
1:D:25:ILE:HG23	1:D:104:LEU:HB3	1.97	0.47
1:E:218:ARG:NH2	1:E:225:LYS:NZ	2.61	0.47
1:G:313:ASP:OD1	1:G:316:LYS:HE2	2.14	0.47
1:H:252:ILE:HD13	1:H:258:LEU:HD23	1.97	0.47
1:H:284:LEU:HD21	1:H:286:VAL:HG23	1.96	0.47
1:F:10:GLU:H	1:F:10:GLU:HG2	1.51	0.47
1:A:346:ARG:HD2	1:A:355:PHE:CE2	2.50	0.46
1:B:34:THR:O	1:B:46:LYS:HE3	2.15	0.46
1:C:502:ALA:O	1:C:506:THR:HG22	2.14	0.46
1:D:231:LYS:HB3	1:D:337:LEU:HD13	1.97	0.46
1:E:244:THR:HB	1:E:246:THR:HG22	1.97	0.46
1:F:287:GLN:NE2	1:F:311:LYS:HB2	2.30	0.46
1:H:438:GLU:OE2	1:H:460:ARG:NH2	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:VAL:HG22	1:C:388:VAL:HG13	1.97	0.46
1:D:80:GLU:O	1:D:84:THR:HG23	2.16	0.46
1:E:287:GLN:NE2	1:E:311:LYS:HB2	2.30	0.46
1:F:386:ASP:O	1:F:390:VAL:HG23	2.15	0.46
1:G:49:VAL:HG22	1:G:55:VAL:HG12	1.97	0.46
1:G:190:LYS:NZ	1:G:388:VAL:HG12	2.29	0.46
1:D:514:ASP:OD1	1:D:515:VAL:N	2.47	0.46
1:B:250:ILE:HG23	1:C:248:ALA:CA	2.45	0.46
1:E:251:ARG:NH1	1:F:249:GLU:HB2	2.30	0.46
1:E:363:LYS:H	1:E:363:LYS:HD2	1.79	0.46
1:G:46:LYS:HD2	1:H:514:ASP:HB3	1.97	0.46
1:G:251:ARG:HD2	1:H:251:ARG:HG2	1.97	0.46
1:A:266:GLU:HG2	1:A:293:LEU:CD2	2.46	0.46
1:B:165:LYS:HB2	1:B:203:ILE:HD11	1.97	0.46
1:B:213:LEU:HB3	1:B:353:MET:HE1	1.97	0.46
1:G:326:ILE:HD13	1:G:332:LEU:HA	1.96	0.46
1:G:455:ILE:HG21	1:G:473:LEU:HD22	1.97	0.46
1:A:25:ILE:HG23	1:A:104:LEU:HB3	1.97	0.46
1:C:250:ILE:HD12	1:D:246:THR:HG21	1.97	0.46
1:F:87:LYS:HD3	1:F:493:ARG:CZ	2.45	0.46
1:G:269:LEU:HD23	1:G:294:ALA:N	2.31	0.46
1:F:60:ASP:OD2	1:F:63:THR:OG1	2.19	0.46
1:F:344:GLU:CD	1:F:346:ARG:HH11	2.14	0.46
1:G:37:SER:HG	1:G:46:LYS:NZ	2.13	0.46
1:A:213:LEU:HD13	1:A:355:PHE:CD1	2.50	0.46
1:A:450:LEU:HD12	1:A:473:LEU:HD21	1.97	0.46
1:D:123:GLY:HA3	1:D:429:ALA:HB3	1.97	0.46
1:F:178:VAL:HG22	1:F:388:VAL:HG13	1.98	0.46
1:A:86:GLU:HB2	1:A:497:GLN:NE2	2.31	0.46
1:C:138:ILE:HG13	1:C:469:LYS:HD3	1.98	0.46
1:D:370:ARG:C	1:D:377:ILE:HD11	2.36	0.46
1:F:232:ILE:HD12	1:F:321:THR:HG21	1.98	0.46
1:A:46:LYS:HZ3	1:B:513:ASP:CG	2.18	0.46
1:D:164:GLU:HA	1:D:167:LYS:HE3	1.97	0.46
1:D:508:MET:HB3	1:D:508:MET:HE2	1.79	0.46
1:E:46:LYS:HE2	1:F:513:ASP:OD1	2.15	0.46
1:F:31:ILE:HG13	1:F:75:ALA:HB1	1.98	0.46
1:G:29:ARG:NH2	1:H:9:PRO:HD2	2.31	0.46
1:H:218:ARG:NH2	1:H:225:LYS:NZ	2.53	0.46
1:A:22:ARG:HH22	1:A:111:LEU:HB2	1.80	0.45
1:B:34:THR:HG22	1:C:13:LYS:HE2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:LEU:HD23	1:D:294:ALA:N	2.31	0.45
1:H:288:LYS:O	1:H:308:ARG:HG2	2.16	0.45
1:C:139:ALA:HB2	1:C:492:LEU:HD13	1.98	0.45
1:C:438:GLU:CD	1:C:460:ARG:HH21	2.11	0.45
1:D:70:VAL:HG12	1:D:76:LYS:HG3	1.98	0.45
1:E:19:ASP:O	1:E:23:MET:HG2	2.16	0.45
1:E:20:ALA:HB1	1:E:515:VAL:HG22	1.97	0.45
1:B:254:ASP:HB3	1:B:257:LYS:HG2	1.98	0.45
1:D:47:MET:HB3	1:E:515:VAL:HG12	1.98	0.45
1:E:10:GLU:H	1:E:10:GLU:HG2	1.46	0.45
1:E:213:LEU:HD21	1:E:353:MET:HE1	1.98	0.45
1:G:94:THR:HB	2:G:601:SO4:O1	2.16	0.45
1:G:180:ALA:O	1:G:363:LYS:HD2	2.16	0.45
1:G:198:LYS:HZ3	1:G:348:ILE:HD11	1.80	0.45
1:G:273:VAL:HG13	1:G:298:LEU:HD23	1.98	0.45
1:A:416:ARG:HH12	1:A:460:ARG:NH2	2.13	0.45
1:C:370:ARG:C	1:C:377:ILE:HD11	2.36	0.45
1:F:346:ARG:NH2	1:F:355:PHE:HD2	2.11	0.45
1:E:218:ARG:NH1	1:E:225:LYS:HG2	2.32	0.45
1:A:516:ILE:HD11	1:H:64:ILE:HG23	1.98	0.45
1:B:45:ASP:O	1:C:512:ILE:HA	2.17	0.45
1:E:195:ILE:HG13	1:E:385:ASP:OD1	2.16	0.45
1:G:252:ILE:HB	1:H:250:ILE:HG12	1.99	0.45
1:H:218:ARG:NH1	1:H:225:LYS:HG2	2.32	0.45
1:D:199:SER:O	1:D:370:ARG:NH2	2.43	0.45
1:D:235:LEU:O	1:D:286:VAL:HA	2.16	0.45
1:H:80:GLU:O	1:H:84:THR:HG23	2.16	0.45
1:A:49:VAL:HG22	1:A:55:VAL:HG12	1.99	0.45
1:C:449:GLY:O	1:D:425:ARG:NH2	2.46	0.45
1:F:141:GLU:HG2	1:F:399:ARG:HG2	1.98	0.45
1:A:235:LEU:HG	1:A:237:GLU:H	1.82	0.45
1:B:180:ALA:O	1:B:363:LYS:HD2	2.15	0.45
1:G:286:VAL:HG22	1:G:288:LYS:H	1.81	0.45
1:A:291:ASP:OD1	1:A:292:ASP:N	2.50	0.45
1:C:142:VAL:HG21	1:C:149:ILE:HG21	1.99	0.45
1:B:25:ILE:HG23	1:B:104:LEU:HB3	1.98	0.44
1:B:89:VAL:HG12	1:B:389:GLY:HA2	1.98	0.44
1:C:227:VAL:HG11	1:C:282:ASN:HB3	1.99	0.44
1:D:18:ARG:O	1:D:22:ARG:HG2	2.17	0.44
1:E:135:LEU:HD11	1:E:499:ILE:HD12	2.00	0.44
1:E:142:VAL:HG11	1:E:149:ILE:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:ASP:OD1	1:F:292:ASP:N	2.49	0.44
1:G:313:ASP:HA	1:G:316:LYS:HE2	1.99	0.44
1:H:254:ASP:HB3	1:H:257:LYS:HG3	1.99	0.44
1:A:131:ALA:HB1	1:A:499:ILE:HD13	1.98	0.44
1:A:218:ARG:NH1	1:A:225:LYS:HG2	2.32	0.44
1:A:380:VAL:O	1:A:384:VAL:HG23	2.16	0.44
1:B:235:LEU:HG	1:B:237:GLU:H	1.82	0.44
1:E:313:ASP:OD1	1:E:316:LYS:HE2	2.17	0.44
1:H:29:ARG:HH11	1:H:108:GLU:CD	2.20	0.44
1:C:18:ARG:HD2	1:C:22:ARG:HE	1.81	0.44
1:B:195:ILE:HA	1:B:367:MET:HB2	1.98	0.44
1:D:128:ALA:O	1:D:132:GLN:HG2	2.18	0.44
1:H:377:ILE:HD13	1:H:377:ILE:HA	1.83	0.44
1:A:269:LEU:HD21	1:A:291:ASP:OD2	2.18	0.44
1:C:123:GLY:HA3	1:C:429:ALA:HB3	1.98	0.44
1:F:313:ASP:HA	1:F:316:LYS:HE2	1.99	0.44
1:G:14:ARG:O	1:G:18:ARG:HG2	2.17	0.44
1:H:232:ILE:HD12	1:H:321:THR:HG21	2.00	0.44
1:A:119:ILE:HG12	1:A:425:ARG:HD2	1.99	0.44
1:A:511:ARG:O	1:A:511:ARG:HG2	2.17	0.44
1:C:25:ILE:HG23	1:C:104:LEU:HB3	1.98	0.44
1:E:150:LEU:HD22	1:E:391:VAL:HG13	2.00	0.44
1:H:241:ILE:HD13	1:H:241:ILE:HA	1.86	0.44
1:A:178:VAL:HA	1:A:193:ILE:HD11	2.00	0.44
1:A:321:THR:HG22	1:A:359:VAL:HG23	1.99	0.44
1:C:29:ARG:HH11	1:C:108:GLU:CD	2.21	0.44
1:D:19:ASP:O	1:D:23:MET:HG2	2.16	0.44
1:E:119:ILE:CD1	1:E:425:ARG:HE	2.31	0.44
1:G:313:ASP:HA	1:G:316:LYS:HG2	1.99	0.44
1:H:161:LYS:NZ	3:H:701:HOH:O	2.41	0.44
1:F:29:ARG:HH11	1:F:108:GLU:CD	2.21	0.44
1:F:237:GLU:OE1	1:F:328:ASN:HA	2.18	0.44
1:H:514:ASP:OD1	1:H:515:VAL:N	2.51	0.44
1:A:266:GLU:HG2	1:A:293:LEU:HD21	2.00	0.43
1:B:90:GLY:HA2	1:B:494:VAL:HG22	1.99	0.43
1:B:293:LEU:O	1:B:296:HIS:HB3	2.17	0.43
1:C:135:LEU:HD21	1:C:411:LEU:HD11	1.99	0.43
1:C:277:LYS:HD3	1:C:303:ILE:HD11	2.00	0.43
1:E:31:ILE:HG13	1:E:75:ALA:HB1	2.00	0.43
1:E:78:LEU:HB2	1:E:509:LEU:HD21	2.00	0.43
1:F:45:ASP:O	1:G:512:ILE:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ARG:NH1	1:B:225:LYS:HG2	2.34	0.43
1:B:250:ILE:HG21	1:C:246:THR:HG23	2.00	0.43
1:C:218:ARG:HD2	1:C:223:MET:HB2	1.99	0.43
1:B:31:ILE:HG13	1:B:75:ALA:HB1	2.00	0.43
1:D:149:ILE:HD13	1:D:149:ILE:HA	1.88	0.43
1:G:45:ASP:O	1:H:512:ILE:HA	2.19	0.43
1:G:89:VAL:CG1	1:G:190:LYS:HD2	2.48	0.43
1:D:89:VAL:HG22	1:D:393:SER:HB2	2.00	0.43
1:E:218:ARG:NH1	1:E:225:LYS:NZ	2.63	0.43
1:G:213:LEU:HD13	1:G:355:PHE:CD1	2.53	0.43
1:D:29:ARG:NH2	1:E:10:GLU:OE2	2.47	0.43
1:E:123:GLY:HA3	1:E:429:ALA:HB3	2.00	0.43
1:G:508:MET:HE2	1:G:509:LEU:HD22	1.99	0.43
1:H:252:ILE:HG12	1:H:261:PHE:CE2	2.53	0.43
1:A:29:ARG:NH1	1:A:108:GLU:OE1	2.51	0.43
1:A:34:THR:O	1:A:46:LYS:HE3	2.18	0.43
1:A:235:LEU:HD11	1:A:237:GLU:HB3	2.01	0.43
1:A:415:LEU:O	1:A:419:ALA:N	2.49	0.43
1:C:34:THR:HG22	1:D:13:LYS:HE2	2.01	0.43
1:E:266:GLU:HG2	1:E:293:LEU:HD21	1.99	0.43
1:G:35:VAL:O	1:G:38:THR:OG1	2.32	0.43
1:B:218:ARG:HD2	1:B:223:MET:HB2	1.99	0.43
1:B:241:ILE:HD13	1:C:245:GLU:HG2	2.00	0.43
1:B:252:ILE:HG12	1:B:261:PHE:CE2	2.54	0.43
1:C:387:ALA:HA	1:C:390:VAL:HG22	2.00	0.43
1:E:29:ARG:HH11	1:E:108:GLU:CD	2.22	0.43
1:H:219:VAL:HG23	1:H:307:ARG:HD3	2.01	0.43
1:E:219:VAL:HG22	1:E:295:GLN:NE2	2.34	0.43
1:G:44:MET:CE	1:H:116:HIS:HE1	2.32	0.43
1:H:283:VAL:HA	1:H:304:MET:O	2.19	0.43
1:C:18:ARG:O	1:C:22:ARG:HG2	2.18	0.43
1:C:321:THR:HG22	1:C:359:VAL:HG23	2.00	0.43
1:D:89:VAL:HG23	1:D:389:GLY:CA	2.49	0.43
1:D:284:LEU:O	1:D:305:ALA:HA	2.19	0.43
1:D:377:ILE:HD13	1:D:377:ILE:HA	1.74	0.43
1:E:94:THR:HB	2:E:601:SO4:O1	2.19	0.43
1:E:313:ASP:HA	1:E:316:LYS:HE2	2.00	0.43
1:D:135:LEU:HD11	1:D:499:ILE:HD12	2.00	0.42
1:D:348:ILE:HD11	1:D:355:PHE:CZ	2.54	0.42
1:B:208:LEU:HD12	1:B:366:THR:O	2.19	0.42
1:D:293:LEU:O	1:D:296:HIS:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:427:GLN:HG3	1:G:428:LEU:HD12	2.01	0.42
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.89	0.42
1:C:346:ARG:HD2	1:C:355:PHE:CD2	2.54	0.42
1:D:213:LEU:HD21	1:D:353:MET:HE1	2.00	0.42
1:E:514:ASP:OD1	1:E:515:VAL:N	2.51	0.42
1:F:401:VAL:HG21	1:F:495:LYS:HG3	2.01	0.42
1:H:154:ALA:O	1:H:158:ILE:HG12	2.19	0.42
1:A:346:ARG:HD2	1:A:355:PHE:CD2	2.54	0.42
1:C:284:LEU:O	1:C:305:ALA:HA	2.20	0.42
1:D:37:SER:HG	1:D:46:LYS:NZ	2.17	0.42
1:E:284:LEU:O	1:E:305:ALA:HA	2.19	0.42
1:E:291:ASP:OD1	1:E:292:ASP:N	2.52	0.42
1:H:183:ASP:OD1	1:H:187:LYS:N	2.52	0.42
1:A:119:ILE:CD1	1:H:449:GLY:HA3	2.50	0.42
1:C:373:THR:HB	1:C:376:VAL:HG22	2.02	0.42
1:D:266:GLU:HG2	1:D:293:LEU:CD2	2.49	0.42
1:E:29:ARG:NH2	1:F:9:PRO:HD2	2.34	0.42
1:F:201:ALA:HB1	1:F:205:ASP:OD2	2.20	0.42
1:B:116:HIS:CG	1:B:117:PRO:HD2	2.55	0.42
1:B:226:LYS:HE3	1:B:342:LEU:HD11	2.01	0.42
1:B:313:ASP:OD1	1:B:316:LYS:HE2	2.18	0.42
1:C:49:VAL:HG22	1:C:55:VAL:HG12	2.00	0.42
1:C:455:ILE:HG21	1:C:473:LEU:HD13	2.01	0.42
1:G:346:ARG:O	1:G:352:SER:OG	2.21	0.42
1:H:87:LYS:HB3	1:H:493:ARG:NH1	2.35	0.42
1:B:206:THR:HG23	1:B:368:LEU:O	2.20	0.42
1:C:252:ILE:HG12	1:C:261:PHE:CE2	2.55	0.42
1:C:105:ARG:HD2	1:D:10:GLU:OE2	2.20	0.42
1:H:293:LEU:O	1:H:296:HIS:HB3	2.19	0.42
1:A:29:ARG:NH2	1:B:10:GLU:OE2	2.48	0.42
1:A:394:THR:OG1	1:A:491:PRO:HG3	2.20	0.42
1:C:91:ASP:OD1	1:C:386:ASP:HB3	2.20	0.42
1:E:269:LEU:HD23	1:E:294:ALA:N	2.35	0.42
1:F:13:LYS:HD2	1:F:13:LYS:HA	1.89	0.42
1:F:147:LYS:O	1:F:151:THR:HG23	2.20	0.42
1:F:438:GLU:CD	1:F:460:ARG:HH21	2.19	0.42
1:D:320:ALA:HB1	1:D:359:VAL:HG21	2.01	0.42
1:A:84:THR:OG1	1:H:373:THR:HG22	2.20	0.41
1:C:89:VAL:CG2	1:C:493:ARG:HH11	2.33	0.41
1:D:313:ASP:OD1	1:D:316:LYS:HE2	2.20	0.41
1:H:164:GLU:H	1:H:164:GLU:HG2	1.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ASP:OD1	1:H:46:LYS:HE2	2.21	0.41
1:B:208:LEU:HD11	1:B:365:VAL:HG22	2.02	0.41
1:H:95:THR:HG23	1:H:440:ILE:HD12	2.02	0.41
1:C:30:ILE:O	1:C:34:THR:HG23	2.20	0.41
1:C:418:TYR:CZ	1:C:422:ILE:HD11	2.55	0.41
1:F:348:ILE:HG22	1:F:349:SER:N	2.36	0.41
1:G:119:ILE:HD11	1:G:425:ARG:HH21	1.84	0.41
1:G:237:GLU:OE1	1:G:329:ILE:HG13	2.20	0.41
1:B:29:ARG:NH2	1:C:9:PRO:HD2	2.35	0.41
1:C:206:THR:HG23	1:C:369:ILE:HA	2.02	0.41
1:C:313:ASP:OD1	1:C:316:LYS:HE2	2.20	0.41
1:C:409:VAL:HG11	1:C:459:VAL:HG12	2.01	0.41
1:G:218:ARG:HD2	1:G:223:MET:HB2	2.01	0.41
1:H:18:ARG:HA	1:H:18:ARG:HD2	1.74	0.41
1:B:313:ASP:HA	1:B:316:LYS:HG2	2.03	0.41
1:B:418:TYR:CE2	1:B:422:ILE:HD11	2.56	0.41
1:D:255:PRO:HG3	1:E:260:GLU:HB3	2.03	0.41
1:F:313:ASP:HA	1:F:316:LYS:HG2	2.02	0.41
1:G:164:GLU:HA	1:G:167:LYS:HB2	2.01	0.41
1:H:18:ARG:HH12	1:H:111:LEU:HD13	1.86	0.41
1:H:235:LEU:HB3	1:H:286:VAL:HG22	2.01	0.41
1:H:475:VAL:HG23	1:H:476:PHE:CD1	2.55	0.41
1:C:462:ALA:O	1:C:467:GLY:HA3	2.20	0.41
1:D:9:PRO:O	1:D:12:MET:HB3	2.20	0.41
1:E:219:VAL:HG22	1:E:295:GLN:CD	2.41	0.41
1:E:418:TYR:CE2	1:E:422:ILE:HD11	2.55	0.41
1:G:41:PRO:HB3	1:G:159:THR:HG22	2.01	0.41
1:G:321:THR:HG22	1:G:359:VAL:HG23	2.02	0.41
1:F:147:LYS:HE3	1:F:179:SER:OG	2.20	0.41
1:F:377:ILE:HA	1:F:377:ILE:HD13	1.81	0.41
1:G:287:GLN:CG	1:G:314:MET:HG3	2.49	0.41
1:H:508:MET:HE2	1:H:508:MET:HB3	1.86	0.41
1:B:348:ILE:HG13	1:B:348:ILE:O	2.21	0.41
1:B:509:LEU:HD13	1:B:509:LEU:HA	1.92	0.41
1:C:64:ILE:HG23	1:D:516:ILE:HD11	2.03	0.41
1:D:475:VAL:HG23	1:D:476:PHE:CD1	2.56	0.41
1:E:188:VAL:HG12	1:E:396:GLU:OE2	2.21	0.41
1:E:508:MET:HB3	1:E:508:MET:HE2	1.92	0.41
1:F:420:GLU:OE2	1:F:431:ARG:NH2	2.54	0.41
1:F:455:ILE:HG21	1:F:473:LEU:HD22	2.03	0.41
1:G:77:MET:HB3	1:G:508:MET:SD	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:GLU:H	1:H:10:GLU:HG2	1.54	0.41
1:A:164:GLU:O	1:A:165:LYS:C	2.59	0.41
1:A:267:LYS:HD2	1:A:270:LYS:HE3	2.02	0.41
1:C:66:ARG:NH1	1:C:67:GLU:OE2	2.53	0.41
1:C:241:ILE:HD11	1:C:268:MET:SD	2.61	0.41
1:C:269:LEU:HD21	1:C:291:ASP:OD2	2.21	0.41
1:D:397:ASP:OD2	1:D:493:ARG:NE	2.51	0.41
1:F:155:MET:O	1:F:159:THR:OG1	2.31	0.41
1:B:390:VAL:HG12	1:B:494:VAL:HG21	2.02	0.40
1:D:116:HIS:CG	1:D:117:PRO:HD2	2.56	0.40
1:A:206:THR:HG23	1:A:369:ILE:HA	2.03	0.40
1:D:105:ARG:HD3	1:E:10:GLU:OE2	2.21	0.40
1:F:103:LEU:HB2	1:F:506:THR:HG21	2.02	0.40
1:G:19:ASP:O	1:G:23:MET:HG2	2.22	0.40
1:G:387:ALA:HA	1:G:390:VAL:HG22	2.03	0.40
1:A:401:VAL:O	1:A:489:VAL:HG23	2.22	0.40
1:D:31:ILE:HG13	1:D:75:ALA:HB1	2.03	0.40
1:D:87:LYS:O	1:D:89:VAL:N	2.54	0.40
1:D:89:VAL:CG2	1:D:393:SER:HB2	2.51	0.40
1:F:77:MET:HB3	1:F:508:MET:SD	2.61	0.40
1:F:436:ALA:O	1:F:439:VAL:HG12	2.21	0.40
1:C:235:LEU:O	1:C:286:VAL:HA	2.21	0.40
1:C:377:ILE:HD13	1:C:377:ILE:HA	1.75	0.40
1:G:235:LEU:O	1:G:286:VAL:HA	2.21	0.40
1:A:339:ASP:HB2	1:A:360:LYS:HE2	2.04	0.40
1:A:512:ILE:HA	1:H:45:ASP:O	2.21	0.40
1:B:91:ASP:HB3	2:B:601:SO4:O4	2.22	0.40
1:B:401:VAL:HG21	1:B:495:LYS:HG3	2.03	0.40
1:E:18:ARG:HH11	1:E:22:ARG:HH11	1.66	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	513/543 (94%)	501 (98%)	12 (2%)	0	100	100
1	B	513/543 (94%)	499 (97%)	13 (2%)	1 (0%)	47	79
1	C	513/543 (94%)	504 (98%)	9 (2%)	0	100	100
1	D	513/543 (94%)	502 (98%)	9 (2%)	2 (0%)	34	68
1	E	513/543 (94%)	503 (98%)	10 (2%)	0	100	100
1	F	513/543 (94%)	503 (98%)	10 (2%)	0	100	100
1	G	513/543 (94%)	500 (98%)	13 (2%)	0	100	100
1	H	513/543 (94%)	504 (98%)	9 (2%)	0	100	100
All	All	4104/4344 (94%)	4016 (98%)	85 (2%)	3 (0%)	51	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	GLU
1	D	350	GLY
1	B	353	MET

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	416/434 (96%)	416 (100%)	0	100	100
1	B	416/434 (96%)	415 (100%)	1 (0%)	93	97
1	C	416/434 (96%)	416 (100%)	0	100	100
1	D	416/434 (96%)	415 (100%)	1 (0%)	93	97
1	E	416/434 (96%)	415 (100%)	1 (0%)	93	97
1	F	416/434 (96%)	415 (100%)	1 (0%)	93	97
1	G	416/434 (96%)	416 (100%)	0	100	100
1	H	416/434 (96%)	415 (100%)	1 (0%)	93	97
All	All	3328/3472 (96%)	3323 (100%)	5 (0%)	93	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	390	VAL
1	D	390	VAL
1	E	250	ILE
1	F	62	VAL
1	H	390	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	361	HIS
1	A	486	ASN
1	A	497	GLN
1	B	24	ASN
1	B	497	GLN
1	D	497	GLN
1	F	497	GLN
1	H	287	GLN
1	H	486	ASN

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	H	601	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	B	601	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	G	601	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	A	601	1	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	E	601	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	D	601	-	4,4,4	0.16	0	6,6,6	0.05	0
2	SO4	C	601	-	4,4,4	0.25	0	6,6,6	0.14	0
2	SO4	F	601	-	4,4,4	0.16	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	SO4	1	0
2	G	601	SO4	1	0
2	E	601	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 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	515/543 (94%)	0.26	10 (1%)	66	47	39, 59, 93, 102	0
1	B	515/543 (94%)	0.25	11 (2%)	63	43	39, 66, 96, 108	0
1	C	515/543 (94%)	0.13	4 (0%)	86	74	39, 64, 85, 100	0
1	D	515/543 (94%)	0.11	5 (0%)	82	69	36, 61, 83, 94	0
1	E	515/543 (94%)	0.24	14 (2%)	54	31	39, 67, 94, 106	0
1	F	515/543 (94%)	0.11	4 (0%)	86	74	41, 64, 82, 99	0
1	G	515/543 (94%)	0.25	7 (1%)	75	58	43, 68, 87, 100	0
1	H	515/543 (94%)	0.17	11 (2%)	63	43	40, 63, 87, 101	0
All	All	4120/4344 (94%)	0.19	66 (1%)	72	52	36, 64, 91, 108	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	ASN	4.3
1	B	324	ASN	4.0
1	E	234	LEU	3.9
1	E	86	GLU	3.9
1	H	11	ASN	3.8
1	C	9	PRO	3.7
1	B	325	VAL	3.7
1	H	9	PRO	3.4
1	H	14	ARG	3.2
1	A	234	LEU	3.2
1	C	17	GLY	3.2
1	E	327	THR	3.1
1	D	11	ASN	3.0
1	E	233	ALA	2.9
1	F	11	ASN	2.9
1	E	332	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	335	GLN	2.8
1	B	351	ASP	2.8
1	H	235	LEU	2.8
1	B	10	GLU	2.8
1	A	222	GLN	2.8
1	E	90	GLY	2.8
1	H	87	LYS	2.8
1	C	14	ARG	2.8
1	H	12	MET	2.7
1	H	272	MET	2.6
1	A	246	THR	2.6
1	A	363	LYS	2.6
1	H	310	LYS	2.6
1	H	86	GLU	2.5
1	D	89	VAL	2.5
1	G	248	ALA	2.5
1	B	88	GLU	2.5
1	G	281	ALA	2.5
1	G	86	GLU	2.5
1	E	85	GLN	2.4
1	A	343	VAL	2.4
1	E	87	LYS	2.4
1	D	350	GLY	2.4
1	D	12	MET	2.4
1	B	285	PHE	2.4
1	G	11	ASN	2.4
1	A	232	ILE	2.4
1	H	8	LEU	2.3
1	C	16	MET	2.3
1	H	10	GLU	2.3
1	E	16	MET	2.3
1	E	331	ASP	2.2
1	A	213	LEU	2.2
1	A	276	ILE	2.2
1	G	16	MET	2.2
1	E	212	VAL	2.2
1	G	12	MET	2.2
1	G	145	GLN	2.1
1	A	303	ILE	2.1
1	B	339	ASP	2.1
1	B	8	LEU	2.1
1	F	89	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	373	THR	2.1
1	E	15	TYR	2.1
1	D	14	ARG	2.1
1	F	9	PRO	2.1
1	B	14	ARG	2.0
1	E	325	VAL	2.0
1	A	230	ALA	2.0
1	B	340	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	G	601	5/5	0.78	0.27	71,72,72,73	0
2	SO4	E	601	5/5	0.81	0.22	77,78,79,79	0
2	SO4	B	601	5/5	0.84	0.25	73,74,75,76	0
2	SO4	H	601	5/5	0.85	0.23	84,84,85,85	0
2	SO4	D	601	5/5	0.89	0.23	75,76,77,77	0
2	SO4	A	601	5/5	0.91	0.18	59,59,60,60	0
2	SO4	F	601	5/5	0.93	0.14	67,67,69,69	0
2	SO4	C	601	5/5	0.95	0.17	61,62,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.