



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:34 PM GMT

PDB ID : 4FCC
Title : Glutamate dehydrogenase from E. coli
Authors : Bilokapic, S.; Schwartz, T.U.
Deposited on : 2012-05-24
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

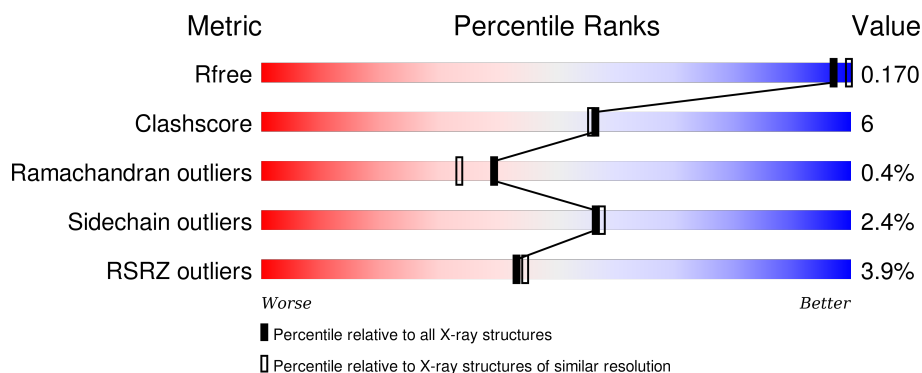
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div>5%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	450	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	C	450	<div> <div>11%</div> <div>80%</div> <div>16%</div> <div>..</div> </div>
1	D	450	<div> <div>3%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	E	450	<div> <div>%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	450	<div><div></div><div>87%</div><div>11%</div><div>••</div></div>
1	G	450	<div><div>%</div><div></div><div>88%</div><div>10%</div><div>••</div></div>
1	H	450	<div><div>7%</div><div></div><div>79%</div><div>18%</div><div>•</div></div>
1	I	450	<div><div>15%</div><div></div><div>82%</div><div>14%</div><div>••</div></div>
1	J	450	<div><div>%</div><div></div><div>86%</div><div>12%</div><div>•</div></div>
1	K	450	<div><div>%</div><div></div><div>84%</div><div>13%</div><div>••</div></div>
1	L	450	<div><div>%</div><div></div><div>89%</div><div>9%</div><div>••</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 44159 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	B	442	Total	C	N	O	S	0	1	0
			3370	2122	594	633	21			
1	C	435	Total	C	N	O	S	0	1	0
			3318	2094	582	621	21			
1	D	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	E	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	F	442	Total	C	N	O	S	0	1	0
			3373	2124	596	632	21			
1	G	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	H	438	Total	C	N	O	S	0	0	0
			3337	2104	587	625	21			
1	I	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	J	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	K	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			
1	L	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
A	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
A	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
B	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
B	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
C	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
C	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
C	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
D	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
D	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
D	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
E	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
E	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
E	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
F	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
F	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
F	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
G	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
G	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
G	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
H	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
H	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
H	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
I	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
I	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
I	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
J	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
J	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
J	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
K	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
K	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
K	0	SER	-	EXPRESSION TAG	UNP Q8XDW9
L	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
L	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
L	0	SER	-	EXPRESSION TAG	UNP Q8XDW9

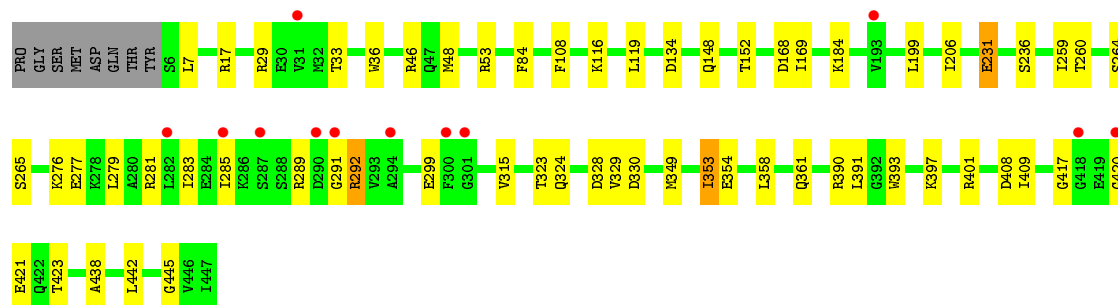
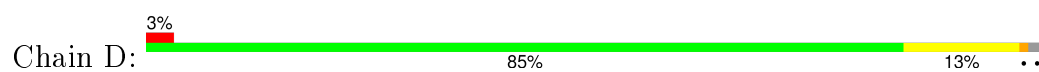
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	409	Total O 409 409	0	0
2	B	277	Total O 277 277	0	0
2	C	300	Total O 300 300	0	0
2	D	254	Total O 254 254	0	0

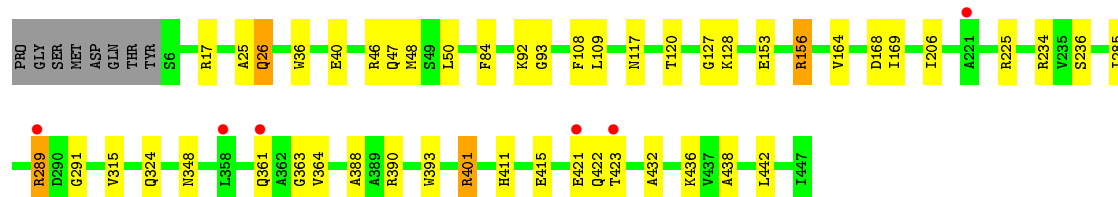
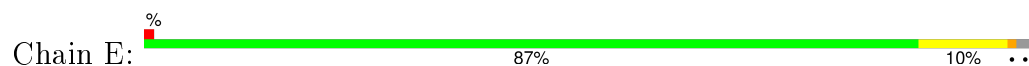
Continued on next page...

Continued from previous page...

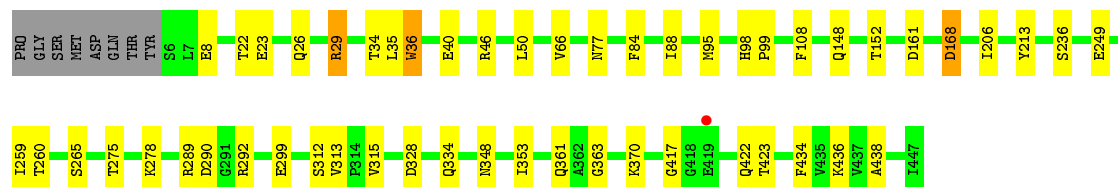
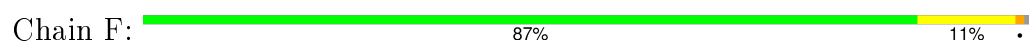
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	351	Total 351	O 351	0	0
2	F	323	Total 323	O 323	0	0
2	G	370	Total 370	O 370	0	0
2	H	288	Total 288	O 288	0	0
2	I	276	Total 276	O 276	0	0
2	J	325	Total 325	O 325	0	0
2	K	335	Total 335	O 335	0	0
2	L	325	Total 325	O 325	0	0



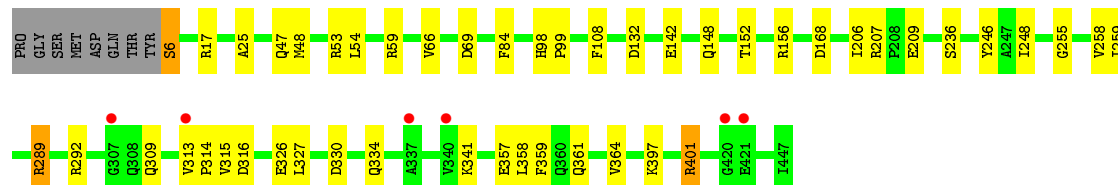
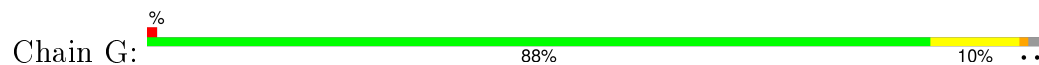
- Molecule 1: Glutamate dehydrogenase



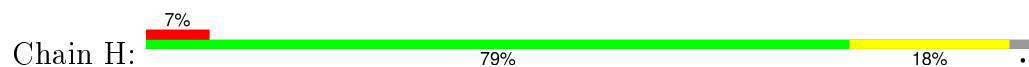
- Molecule 1: Glutamate dehydrogenase

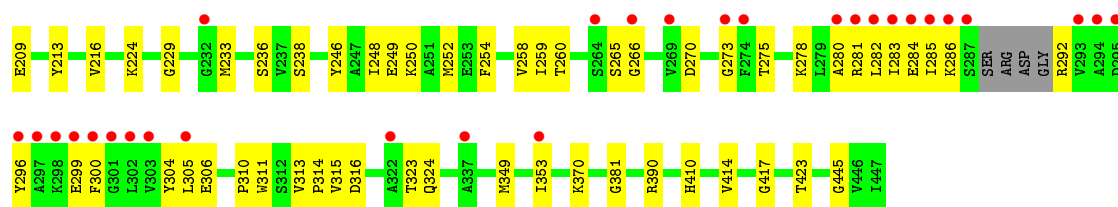


- Molecule 1: Glutamate dehydrogenase

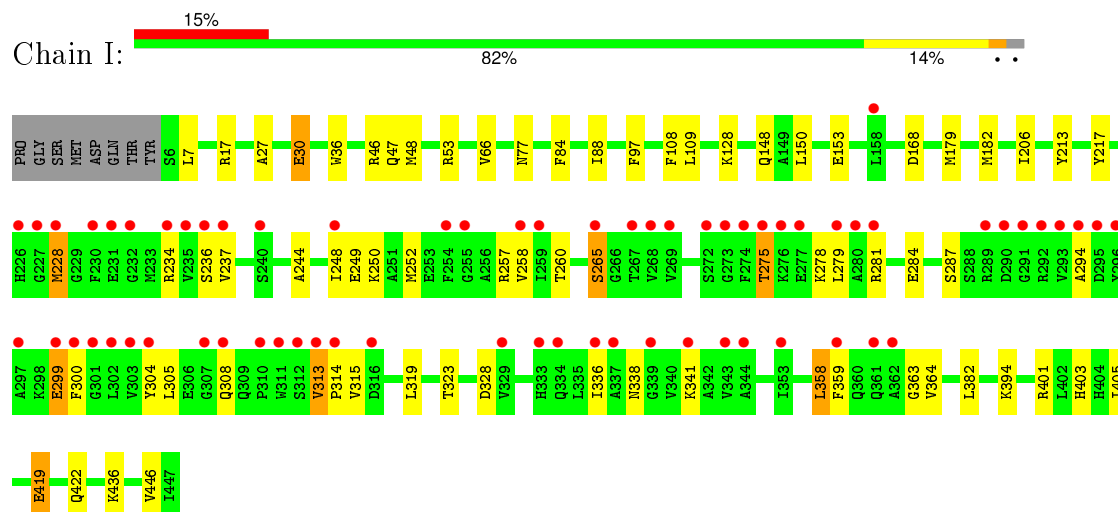


- Molecule 1: Glutamate dehydrogenase

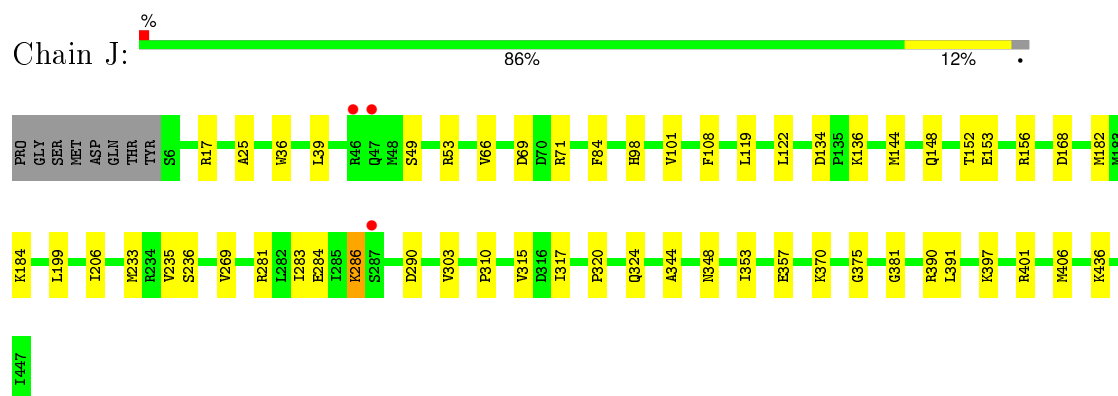




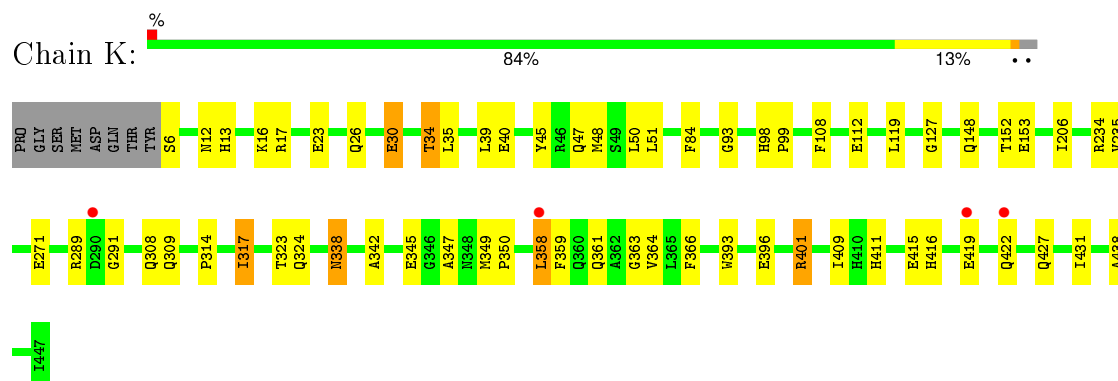
• Molecule 1: Glutamate dehydrogenase



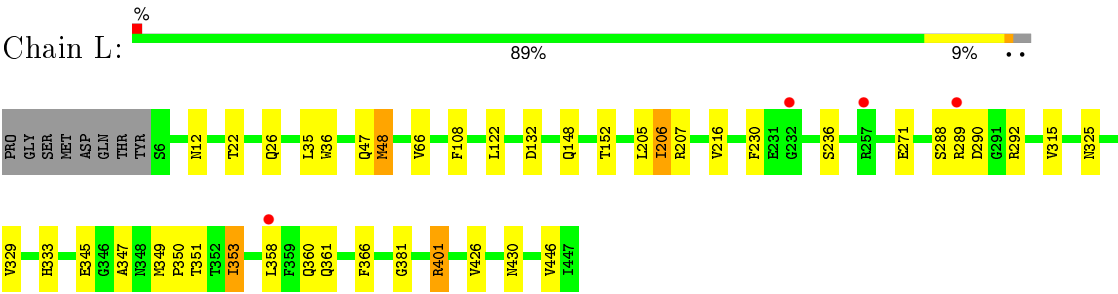
• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase



● Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.22Å 176.26Å 150.25Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	49.65 – 2.00 49.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.65-2.00) 99.0 (49.67-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.181 , 0.229 0.141 , 0.170	Depositor DCC
R_{free} test set	3641 reflections (1.00%)	DCC
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.1	EDS
Estimated twinning fraction	0.346 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 364176 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	44159	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/3431	0.53	0/4630
1	B	0.35	0/3438	0.52	0/4640
1	C	0.38	0/3386	0.53	0/4571
1	D	0.35	0/3431	0.51	0/4630
1	E	0.39	0/3431	0.52	0/4630
1	F	0.38	0/3442	0.51	0/4645
1	G	0.41	0/3431	0.54	0/4630
1	H	0.36	0/3401	0.52	1/4589 (0.0%)
1	I	0.36	0/3431	0.50	0/4630
1	J	0.38	0/3431	0.52	0/4630
1	K	0.38	0/3431	0.54	0/4630
1	L	0.38	0/3431	0.51	0/4630
All	All	0.38	0/41115	0.52	1/55485 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	59	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3366	0	3324	37	0
1	B	3370	0	3331	49	0
1	C	3318	0	3274	55	0
1	D	3366	0	3324	43	0
1	E	3366	0	3324	30	0
1	F	3373	0	3331	37	0
1	G	3366	0	3324	32	0
1	H	3337	0	3298	59	0
1	I	3366	0	3324	48	0
1	J	3366	0	3324	46	0
1	K	3366	0	3324	41	0
1	L	3366	0	3324	32	0
2	A	409	0	0	16	0
2	B	277	0	0	14	0
2	C	300	0	0	12	0
2	D	254	0	0	18	0
2	E	351	0	0	8	0
2	F	323	0	0	12	0
2	G	370	0	0	10	0
2	H	288	0	0	16	0
2	I	276	0	0	4	0
2	J	325	0	0	14	0
2	K	335	0	0	11	0
2	L	325	0	0	12	0
All	All	44159	0	39826	485	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 6.

All (485) 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:H:151:MET:SD	2:H:508:HOH:O	2.07	1.10
1:C:179:MET:SD	2:C:639:HOH:O	2.17	1.01
1:H:153:GLU:O	1:H:156:ARG:NH1	1.93	1.00
1:J:153:GLU:O	1:J:156:ARG:NH1	1.98	0.96
1:J:406:MET:SD	2:J:542:HOH:O	2.23	0.95
1:I:46:ARG:NH2	2:I:715:HOH:O	2.01	0.93
1:B:153:GLU:O	1:B:156:ARG:NH1	2.06	0.89
1:B:34:THR:O	2:B:646:HOH:O	1.92	0.88
1:C:48:MET:SD	2:F:691:HOH:O	2.32	0.86
1:G:6:SER:N	2:G:815:HOH:O	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:PHE:O	2:C:727:HOH:O	1.97	0.83
1:H:156:ARG:NE	2:H:700:HOH:O	2.05	0.82
1:C:257:ARG:NH2	2:C:725:HOH:O	2.13	0.82
1:H:324:GLN:HG3	1:H:349:MET:HG3	1.63	0.81
1:B:153:GLU:HA	1:B:156:ARG:HH12	1.46	0.81
1:L:347:ALA:HB3	1:L:350:PRO:HG3	1.63	0.80
1:J:153:GLU:HA	1:J:156:ARG:HH12	1.46	0.79
1:A:207:ARG:NH2	2:A:801:HOH:O	2.08	0.79
1:F:299:GLU:OE1	2:F:649:HOH:O	2.01	0.79
1:D:168:ASP:OD1	1:D:169:ILE:N	2.16	0.78
1:H:270:ASP:OD2	1:H:278:LYS:NZ	2.16	0.78
1:J:156:ARG:NE	2:J:775:HOH:O	2.08	0.78
1:A:144:MET:SD	2:A:719:HOH:O	2.42	0.77
1:I:248:ILE:HG13	1:I:258:VAL:HG11	1.66	0.77
1:H:254:PHE:O	2:H:722:HOH:O	2.01	0.76
1:L:12:ASN:ND2	2:L:748:HOH:O	2.08	0.76
1:A:292:ARG:NH2	2:A:651:HOH:O	2.17	0.76
1:F:23:GLU:OE2	2:F:525:HOH:O	2.02	0.76
1:D:134:ASP:OD2	2:D:744:HOH:O	2.03	0.76
1:H:153:GLU:HA	1:H:156:ARG:HH12	1.51	0.76
1:A:401:ARG:NH1	2:A:858:HOH:O	2.18	0.76
1:D:199:LEU:O	2:D:555:HOH:O	2.03	0.76
1:B:114[A]:THR:HG22	1:B:126:GLY:HA3	1.67	0.75
1:L:360:GLN:O	2:L:795:HOH:O	2.03	0.75
1:G:255:GLY:O	2:G:754:HOH:O	2.03	0.75
1:A:224:LYS:NZ	2:A:774:HOH:O	2.19	0.75
1:G:47:GLN:HG3	1:G:48:MET:HG2	1.69	0.75
1:D:116:LYS:NZ	2:D:728:HOH:O	2.18	0.75
1:B:302:LEU:O	2:B:753:HOH:O	2.05	0.75
1:I:228:MET:SD	1:I:341:LYS:NZ	2.59	0.74
1:E:401:ARG:NH1	2:E:759:HOH:O	2.18	0.74
1:H:116:LYS:NZ	2:H:742:HOH:O	2.19	0.74
1:L:333:HIS:ND1	2:L:792:HOH:O	2.20	0.74
1:B:156:ARG:NE	2:B:767:HOH:O	2.07	0.74
1:K:317:ILE:HG22	1:K:342:ALA:HB3	1.69	0.73
1:C:270:ASP:OD2	1:C:278:LYS:NZ	2.22	0.73
1:H:151:MET:HE1	1:H:154:LEU:HD23	1.70	0.72
1:I:109:LEU:HB3	1:I:128:LYS:HE3	1.69	0.72
1:C:314:PRO:HA	1:C:338:ASN:HB3	1.72	0.71
1:L:288:SER:O	2:L:805:HOH:O	2.08	0.71
1:K:347:ALA:HB3	1:K:350:PRO:HG3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:47:GLN:HG3	1:I:48:MET:HG2	1.72	0.71
1:H:156:ARG:NH2	2:H:700:HOH:O	2.24	0.70
1:J:156:ARG:NH2	2:J:775:HOH:O	2.24	0.70
1:B:245:GLN:OE1	2:B:718:HOH:O	2.08	0.70
1:C:46:ARG:NH1	2:C:660:HOH:O	2.20	0.70
1:A:66:VAL:HG11	1:C:53:ARG:HD3	1.72	0.70
1:F:8:GLU:OE2	1:F:29:ARG:NH2	2.23	0.70
1:L:292:ARG:NH1	2:L:772:HOH:O	2.25	0.70
1:K:345:GLU:OE1	2:K:780:HOH:O	2.09	0.70
1:B:151:MET:HE1	1:B:154:LEU:HD23	1.74	0.70
1:J:390:ARG:NH1	2:J:579:HOH:O	2.20	0.69
1:D:46:ARG:O	2:D:622:HOH:O	2.10	0.69
1:D:231:GLU:OE1	2:D:732:HOH:O	2.09	0.69
1:J:233:MET:SD	2:J:759:HOH:O	2.50	0.69
1:L:325:ASN:OD1	2:L:824:HOH:O	2.11	0.68
1:K:419:GLU:OE2	2:K:705:HOH:O	2.11	0.68
1:G:66:VAL:HG11	1:I:53:ARG:HD3	1.75	0.68
1:J:375:GLY:HA2	1:J:406:MET:CE	2.23	0.68
1:I:394:LYS:HG3	2:I:771:HOH:O	1.92	0.68
1:J:370:LYS:HD3	2:J:551:HOH:O	1.93	0.67
1:I:47:GLN:NE2	2:I:721:HOH:O	2.27	0.67
1:D:46:ARG:NH1	2:D:702:HOH:O	2.28	0.67
1:H:34:THR:O	2:H:579:HOH:O	2.12	0.67
1:C:50:LEU:HD21	1:C:438:ALA:HB1	1.77	0.67
1:J:199:LEU:O	2:J:670:HOH:O	2.12	0.67
1:C:363:GLY:HA2	1:C:422:GLN:HE22	1.59	0.66
1:C:254:PHE:O	2:C:577:HOH:O	2.13	0.66
1:C:47:GLN:HG3	1:C:48:MET:HG2	1.78	0.66
1:L:47:GLN:HG3	1:L:48:MET:HG2	1.77	0.66
1:D:328:ASP:OD1	2:D:625:HOH:O	2.13	0.66
1:F:312:SER:HA	1:F:334:GLN:HG2	1.78	0.66
1:J:324:GLN:NE2	2:J:773:HOH:O	2.28	0.66
1:B:6:SER:N	2:B:738:HOH:O	2.28	0.66
1:E:225:ARG:NH2	1:E:423:THR:OG1	2.29	0.65
1:K:13:HIS:HA	1:K:16:LYS:HE2	1.76	0.65
1:E:324:GLN:OE1	1:E:324:GLN:N	2.28	0.65
1:D:408:ASP:OD2	2:D:718:HOH:O	2.15	0.65
1:H:156:ARG:CZ	2:H:700:HOH:O	2.43	0.65
1:K:47:GLN:HG2	1:K:48:MET:HG2	1.77	0.65
1:F:328:ASP:HB2	2:F:820:HOH:O	1.95	0.65
1:L:271:GLU:OE2	2:L:822:HOH:O	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ALA:HA	1:B:283:ILE:HD12	1.79	0.65
1:B:316:ASP:HB3	1:B:341:LYS:HE3	1.79	0.65
1:F:348:ASN:ND2	2:F:779:HOH:O	2.30	0.65
1:E:234:ARG:NH1	2:E:760:HOH:O	2.30	0.65
1:J:69:ASP:OD2	1:J:71:ARG:NH2	2.31	0.64
1:H:265:SER:O	1:H:304:TYR:OH	2.16	0.64
1:J:156:ARG:CZ	2:J:775:HOH:O	2.45	0.64
1:A:306:GLU:OE2	2:A:870:HOH:O	2.15	0.64
1:J:153:GLU:CA	1:J:156:ARG:HH12	2.10	0.64
1:H:259:ILE:HG13	1:H:260:THR:HG23	1.79	0.64
1:K:12:ASN:ND2	2:K:662:HOH:O	2.30	0.63
1:H:284:GLU:OE1	2:H:785:HOH:O	2.15	0.63
1:J:119:LEU:HD22	1:J:370:LYS:HE2	1.81	0.63
1:H:281:ARG:NH2	2:H:635:HOH:O	2.31	0.63
1:F:40:GLU:OE2	1:F:46:ARG:NH2	2.32	0.63
1:D:329:VAL:HG23	1:D:358:LEU:HD22	1.81	0.62
1:L:345:GLU:OE2	1:L:351:THR:HG22	1.98	0.62
1:E:47:GLN:HG3	1:E:48:MET:HG2	1.80	0.62
1:I:236:SER:HB3	1:I:315:VAL:HG11	1.80	0.62
1:D:276:LYS:NZ	1:D:277:GLU:OE2	2.32	0.62
1:G:132:ASP:OD2	1:I:17:ARG:HD3	1.99	0.62
1:C:293:VAL:N	2:C:757:HOH:O	2.32	0.62
1:K:6:SER:N	2:K:797:HOH:O	2.32	0.62
1:H:59:ARG:HD3	1:K:153:GLU:OE2	2.00	0.62
1:H:153:GLU:CA	1:H:156:ARG:HH12	2.13	0.62
1:B:216:VAL:HG21	1:B:250:LYS:HG3	1.80	0.62
1:A:53:ARG:HD3	1:C:66:VAL:HG11	1.82	0.62
1:I:265:SER:OG	1:I:304:TYR:OH	2.18	0.61
1:D:29:ARG:NE	2:D:703:HOH:O	2.31	0.61
1:F:36:TRP:O	1:F:40:GLU:HG2	2.00	0.61
1:B:156:ARG:NH2	2:B:767:HOH:O	2.30	0.61
1:J:53:ARG:HD3	1:L:66:VAL:HG11	1.81	0.61
1:G:334:GLN:NE2	2:G:837:HOH:O	2.34	0.61
1:E:117:ASN:O	1:E:120:THR:OG1	2.18	0.61
1:G:289:ARG:NH2	2:G:818:HOH:O	2.20	0.61
1:J:281:ARG:NH2	1:J:284:GLU:OE1	2.33	0.61
1:B:41:GLN:NE2	2:B:642:HOH:O	2.21	0.60
1:B:363:GLY:O	1:B:422:GLN:NE2	2.34	0.60
1:A:46:ARG:NH2	2:A:610:HOH:O	2.34	0.60
1:B:422:GLN:O	2:B:689:HOH:O	2.15	0.60
1:D:390:ARG:NH1	2:D:561:HOH:O	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:GLU:HA	2:K:732:HOH:O	2.01	0.60
1:B:394:LYS:NZ	2:B:750:HOH:O	2.34	0.60
1:D:265:SER:OG	1:D:292:ARG:NH1	2.35	0.59
1:E:17:ARG:NH2	2:E:693:HOH:O	2.33	0.59
1:K:23:GLU:O	1:K:26:GLN:HG2	2.02	0.59
1:B:426:VAL:O	1:B:430:ASN:ND2	2.33	0.59
1:C:215:LEU:HD21	1:C:319:LEU:HD22	1.84	0.59
1:B:153:GLU:CA	1:B:156:ARG:HH12	2.14	0.59
1:I:234:ARG:NH1	1:I:314:PRO:O	2.27	0.59
1:C:236:SER:HB3	1:C:315:VAL:HG21	1.83	0.59
1:H:95:MET:HE1	1:H:154:LEU:HD21	1.85	0.59
1:H:132:ASP:OD2	1:K:17:ARG:HD3	2.02	0.59
1:J:17:ARG:HD3	1:L:132:ASP:OD2	2.03	0.58
1:E:361:GLN:N	1:E:361:GLN:OE1	2.35	0.58
1:H:233:MET:HE3	1:H:316:ASP:HB3	1.85	0.58
1:B:265:SER:OG	1:B:292:ARG:NH2	2.36	0.58
1:I:305:LEU:HB3	1:I:308:GLN:HB2	1.85	0.58
1:F:370:LYS:NZ	2:F:655:HOH:O	2.35	0.58
1:A:405:ILE:HG13	2:A:850:HOH:O	2.03	0.58
1:J:375:GLY:HA2	1:J:406:MET:HE1	1.84	0.58
1:G:359:PHE:O	1:G:364:VAL:HG12	2.04	0.57
1:C:269:VAL:HB	1:C:303:VAL:HB	1.86	0.57
1:C:334:GLN:O	1:C:338:ASN:ND2	2.26	0.57
1:G:316:ASP:OD1	1:G:341:LYS:NZ	2.31	0.57
1:C:281:ARG:NH2	1:C:284:GLU:OE1	2.34	0.56
1:D:390:ARG:HH11	1:E:388:ALA:HB2	1.68	0.56
1:K:50:LEU:HD21	1:K:438:ALA:HB1	1.87	0.56
1:J:375:GLY:HA2	1:J:406:MET:HE3	1.87	0.56
1:A:234:ARG:NH1	1:A:314:PRO:O	2.38	0.56
1:C:109:LEU:HD13	1:C:128:LYS:NZ	2.21	0.56
1:C:186:LEU:O	1:E:156:ARG:NH2	2.37	0.56
1:D:390:ARG:NE	2:D:721:HOH:O	2.16	0.56
1:G:292:ARG:NH1	2:G:750:HOH:O	2.37	0.56
1:K:422:GLN:NE2	2:K:710:HOH:O	2.38	0.56
1:I:328:ASP:HB3	2:I:776:HOH:O	2.06	0.56
1:B:156:ARG:CZ	2:B:767:HOH:O	2.48	0.56
1:I:213:TYR:OH	1:I:249:GLU:OE2	2.20	0.55
1:J:436:LYS:HE3	2:J:730:HOH:O	2.06	0.55
1:C:390:ARG:NH2	2:C:685:HOH:O	2.31	0.55
1:D:134:ASP:OD1	2:D:700:HOH:O	2.18	0.55
1:K:235:VAL:HG22	1:K:317:ILE:HG13	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:GLU:O	1:K:34:THR:HG22	2.07	0.55
1:G:357:GLU:OE2	1:G:361:GLN:NE2	2.40	0.55
1:I:27:ALA:O	1:I:30:GLU:HG3	2.07	0.55
1:G:54:LEU:HD12	2:G:648:HOH:O	2.05	0.55
1:I:148:GLN:CG	1:I:182:MET:HE3	2.37	0.55
1:K:35:LEU:HD23	1:K:431:ILE:HD13	1.89	0.54
1:F:290:ASP:N	2:F:583:HOH:O	2.09	0.54
1:C:122:LEU:HD13	1:C:381:GLY:HA3	1.89	0.54
1:B:119:LEU:HD12	1:B:370:LYS:HE2	1.90	0.54
1:J:25:ALA:HB2	2:J:601:HOH:O	2.06	0.54
1:J:49:SER:O	1:J:53:ARG:HG3	2.07	0.54
1:A:234:ARG:HH12	1:A:314:PRO:HB2	1.72	0.54
1:I:148:GLN:HG2	1:I:182:MET:HE3	1.88	0.54
1:D:7:LEU:HD11	1:D:33:THR:HA	1.90	0.54
1:B:110:GLY:O	1:B:114[A]:THR:HG23	2.07	0.54
1:G:207:ARG:NH1	2:G:697:HOH:O	2.40	0.54
1:C:275:THR:HG23	1:C:278:LYS:HE3	1.88	0.54
1:F:363:GLY:HA2	1:F:422:GLN:HE22	1.73	0.54
1:A:209:GLU:HG3	1:A:246:TYR:CD1	2.42	0.54
1:D:353:ILE:HD12	1:D:354:GLU:H	1.73	0.54
1:B:39:LEU:HD13	1:B:51:LEU:HD21	1.90	0.53
1:E:50:LEU:HD21	1:E:438:ALA:HB1	1.91	0.53
1:E:348:ASN:HB2	2:E:781:HOH:O	2.07	0.53
1:H:299:GLU:HB3	2:H:786:HOH:O	2.08	0.53
1:A:132:ASP:OD2	1:C:17:ARG:HD3	2.09	0.53
1:H:236:SER:HB2	1:H:315:VAL:HG11	1.91	0.53
1:I:217:TYR:OH	1:I:250:LYS:HE3	2.07	0.53
1:K:366:PHE:O	2:K:625:HOH:O	2.19	0.53
1:K:234:ARG:HH12	1:K:271:GLU:HG2	1.73	0.53
1:I:419:GLU:CD	1:I:419:GLU:H	2.12	0.53
1:H:151:MET:HE2	1:H:179:MET:SD	2.49	0.52
1:K:396:GLU:OE2	2:K:805:HOH:O	2.18	0.52
1:L:329:VAL:HG12	1:L:333:HIS:CD2	2.44	0.52
1:A:304:TYR:CE2	1:A:306:GLU:HG2	2.43	0.52
1:I:314:PRO:HA	1:I:338:ASN:HB3	1.91	0.52
1:D:361:GLN:NE2	2:D:689:HOH:O	2.37	0.52
1:L:329:VAL:HG13	1:L:358:LEU:HD22	1.92	0.52
1:D:53:ARG:HD3	1:F:66:VAL:HG11	1.92	0.52
1:H:213:TYR:OH	1:H:249:GLU:OE2	2.17	0.52
1:D:393:TRP:CG	1:D:397:LYS:HD2	2.45	0.52
1:J:320:PRO:HD2	1:J:344:ALA:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ILE:HG13	1:F:260:THR:HG23	1.92	0.52
1:B:250:LYS:NZ	2:B:567:HOH:O	2.43	0.52
1:H:281:ARG:HD2	1:H:300:PHE:CE2	2.45	0.51
1:A:304:TYR:HE2	1:A:306:GLU:HG2	1.74	0.51
1:C:225:ARG:HE	1:C:423:THR:CG2	2.22	0.51
1:G:259:ILE:HD11	1:G:315:VAL:HG12	1.93	0.51
1:B:270:ASP:OD2	1:B:278:LYS:NZ	2.38	0.51
1:C:109:LEU:HD13	1:C:128:LYS:HZ2	1.75	0.51
1:F:35:LEU:HD21	1:F:434:PHE:CG	2.46	0.51
1:H:153:GLU:C	1:H:156:ARG:HH12	2.13	0.51
1:I:97:PHE:HZ	1:I:179:MET:HE3	1.75	0.51
1:J:286:LYS:NZ	2:J:583:HOH:O	2.44	0.51
1:A:46:ARG:HG3	2:A:852:HOH:O	2.11	0.51
1:A:234:ARG:HD3	2:A:853:HOH:O	2.10	0.51
1:I:150:LEU:HD22	1:I:179:MET:HE2	1.93	0.51
1:H:248:ILE:HG12	1:H:258:VAL:HG11	1.91	0.51
1:A:236:SER:HB3	1:A:315:VAL:HG11	1.92	0.51
1:K:427:GLN:O	1:K:431:ILE:HG12	2.11	0.50
1:H:390:ARG:NH2	2:H:518:HOH:O	2.44	0.50
1:G:148:GLN:O	1:G:152:THR:HG23	2.11	0.50
1:G:401:ARG:NH1	2:G:665:HOH:O	2.43	0.50
1:J:283:ILE:HG13	1:J:284:GLU:N	2.26	0.50
1:B:59:ARG:HD3	1:E:153:GLU:OE2	2.10	0.50
1:L:345:GLU:OE2	1:L:350:PRO:HD2	2.11	0.50
1:D:231:GLU:OE1	2:D:698:HOH:O	2.20	0.50
1:A:348:ASN:ND2	2:A:724:HOH:O	2.21	0.50
1:A:217:TYR:CE1	1:A:250:LYS:HD3	2.46	0.50
1:D:420:GLY:O	2:D:688:HOH:O	2.19	0.50
1:F:290:ASP:HB3	2:F:791:HOH:O	2.12	0.50
1:K:338:ASN:OD1	2:K:796:HOH:O	2.19	0.49
1:C:275:THR:H	1:C:278:LYS:HG2	1.76	0.49
1:K:411:HIS:O	1:K:415:GLU:HG2	2.11	0.49
1:J:397:LYS:O	1:J:401:ARG:HG2	2.12	0.49
1:C:422:GLN:NE2	2:C:785:HOH:O	2.46	0.49
1:H:304:TYR:CE2	1:H:306:GLU:HB3	2.47	0.49
1:J:153:GLU:C	1:J:156:ARG:HH12	2.16	0.49
1:C:275:THR:OG1	2:C:735:HOH:O	2.20	0.49
1:L:401:ARG:NH2	2:L:692:HOH:O	2.44	0.49
1:A:148:GLN:O	1:A:152:THR:HG23	2.12	0.49
1:F:22:THR:HG22	2:F:567:HOH:O	2.12	0.49
1:C:148:GLN:CG	1:C:182:MET:HE3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD21	1:B:434:PHE:CD1	2.48	0.49
1:L:207:ARG:NH1	2:L:768:HOH:O	2.45	0.48
1:F:363:GLY:HA2	1:F:422:GLN:NE2	2.28	0.48
1:J:235:VAL:HG22	1:J:317:ILE:HB	1.94	0.48
1:H:280:ALA:HA	1:H:283:ILE:HD12	1.95	0.48
1:G:209:GLU:HG3	1:G:246:TYR:CD1	2.48	0.48
1:D:48:MET:CB	1:D:53:ARG:HH21	2.27	0.48
1:K:148:GLN:O	1:K:152:THR:HG23	2.13	0.48
1:A:330:ASP:O	1:A:334:GLN:HG3	2.14	0.48
1:J:375:GLY:CA	1:J:406:MET:HE3	2.43	0.48
1:B:216:VAL:HG21	1:B:250:LYS:CG	2.44	0.48
1:D:324:GLN:HG3	1:D:349:MET:HB2	1.96	0.48
1:D:17:ARG:NH2	1:F:77:ASN:HA	2.29	0.48
1:J:184:LYS:NZ	2:J:656:HOH:O	2.14	0.48
1:H:310:PRO:O	2:H:569:HOH:O	2.19	0.48
1:I:248:ILE:HG22	1:I:279:LEU:HD22	1.95	0.48
1:F:275:THR:CG2	1:F:278:LYS:H	2.27	0.48
1:F:275:THR:HG23	1:F:278:LYS:H	1.78	0.48
1:H:285:ILE:HD12	1:H:296:TYR:HB2	1.95	0.48
1:I:275:THR:H	1:I:278:LYS:HG3	1.78	0.48
1:C:274:PHE:HA	1:C:278:LYS:HD2	1.95	0.47
1:D:48:MET:HB2	1:D:53:ARG:HH21	1.79	0.47
1:L:401:ARG:HG2	2:L:749:HOH:O	2.14	0.47
1:J:122:LEU:HD13	1:J:381:GLY:HA3	1.96	0.47
1:E:93:GLY:HA3	1:E:127:GLY:O	2.14	0.47
1:E:168:ASP:OD1	1:E:169:ILE:N	2.42	0.47
1:C:273:GLY:O	1:C:278:LYS:NZ	2.37	0.47
1:F:50:LEU:HD21	1:F:438:ALA:HB1	1.96	0.47
1:L:236:SER:HB3	1:L:315:VAL:HG11	1.96	0.47
1:I:237:VAL:HG22	1:I:319:LEU:HB2	1.96	0.47
1:I:359:PHE:HB3	1:I:364:VAL:HG22	1.95	0.47
1:C:353:ILE:O	1:C:357:GLU:HG2	2.14	0.47
1:H:41:GLN:NE2	2:H:775:HOH:O	2.45	0.47
1:G:248:ILE:HG12	1:G:258:VAL:HG11	1.95	0.47
1:E:363:GLY:O	1:E:422:GLN:NE2	2.48	0.47
1:I:237:VAL:H	1:I:260:THR:HG23	1.79	0.47
1:L:22:THR:O	1:L:26:GLN:NE2	2.47	0.47
1:D:184:LYS:NZ	2:D:725:HOH:O	2.47	0.47
1:I:250:LYS:HD2	1:I:250:LYS:HA	1.70	0.47
1:C:148:GLN:HG2	1:C:182:MET:HE3	1.96	0.47
1:H:98:HIS:CG	1:H:99:PRO:HD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:OD1	1:E:390:ARG:NH2	2.46	0.47
1:D:259:ILE:HG13	1:D:260:THR:HG23	1.96	0.47
1:D:391:LEU:HD11	1:E:393:TRP:HH2	1.79	0.47
1:H:39:LEU:HD13	1:H:51:LEU:HD21	1.96	0.47
1:K:112:GLU:OE1	2:K:621:HOH:O	2.20	0.47
1:H:410:HIS:O	1:H:414:VAL:HG23	2.15	0.46
1:E:46:ARG:NH1	2:E:799:HOH:O	2.49	0.46
1:B:397:LYS:O	1:B:401:ARG:HG2	2.16	0.46
1:E:92:LYS:HD2	1:E:164:VAL:O	2.15	0.46
1:D:29:ARG:NH1	2:D:674:HOH:O	2.05	0.46
1:G:313:VAL:HG12	1:G:315:VAL:HG13	1.97	0.46
1:E:109:LEU:HD13	1:E:128:LYS:HE2	1.97	0.46
1:C:359:PHE:O	1:C:364:VAL:HG13	2.16	0.46
1:B:10:PHE:O	1:B:14:VAL:HG23	2.14	0.46
1:K:98:HIS:CG	1:K:99:PRO:HD2	2.51	0.46
1:E:26:GLN:OE1	2:E:605:HOH:O	2.20	0.46
1:D:148:GLN:O	1:D:152:THR:HG23	2.16	0.46
1:L:351:THR:HG21	1:L:366:PHE:CZ	2.51	0.46
1:F:363:GLY:CA	1:F:422:GLN:HE22	2.29	0.46
1:A:34:THR:HG21	2:A:906:HOH:O	2.15	0.46
1:H:445:GLY:HA2	2:H:591:HOH:O	2.15	0.46
1:L:349:MET:HG3	2:L:824:HOH:O	2.16	0.46
1:B:294:ALA:HB2	1:B:304:TYR:CZ	2.51	0.46
1:H:229:GLY:O	1:H:233:MET:HG3	2.16	0.45
1:I:249:GLU:HA	1:I:252:MET:HE2	1.99	0.45
1:G:53:ARG:HD3	1:I:66:VAL:HG11	1.99	0.45
1:L:349:MET:N	1:L:350:PRO:HD3	2.31	0.45
1:F:361:GLN:NE2	2:F:806:HOH:O	2.45	0.45
1:A:30:GLU:HG3	2:A:840:HOH:O	2.16	0.45
1:C:324:GLN:HG3	1:C:348:ASN:O	2.16	0.45
1:G:66:VAL:HG12	1:I:446:VAL:HG13	1.99	0.45
1:A:217:TYR:CZ	1:A:250:LYS:HD3	2.51	0.45
1:J:236:SER:HB3	1:J:315:VAL:HG11	1.99	0.45
1:H:353:ILE:HD12	1:H:353:ILE:H	1.81	0.45
1:I:313:VAL:HG22	1:I:314:PRO:HD2	1.99	0.45
1:B:46:ARG:HD2	2:B:770:HOH:O	2.16	0.45
1:B:315:VAL:HG13	1:B:317:ILE:N	2.32	0.45
1:B:353:ILE:HD12	1:B:354:GLU:N	2.32	0.45
1:C:326:GLU:N	1:C:350:PRO:O	2.50	0.45
1:D:279:LEU:O	1:D:283:ILE:HG13	2.17	0.45
1:A:93:GLY:HA3	1:A:127:GLY:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:345:GLU:CD	1:K:350:PRO:HD2	2.36	0.45
1:C:262:SER:HB2	1:C:266:GLY:O	2.17	0.45
1:A:238:SER:OG	1:A:320:PRO:HA	2.17	0.45
1:C:277:GLU:N	2:C:735:HOH:O	2.27	0.45
1:C:44:LYS:HE3	1:C:45:TYR:CE2	2.52	0.45
1:H:151:MET:HE3	1:H:194:PHE:HZ	1.82	0.45
1:C:53:ARG:HD2	2:C:521:HOH:O	2.16	0.45
1:L:353:ILE:HG22	2:L:767:HOH:O	2.17	0.45
1:E:236:SER:HB3	1:E:315:VAL:HG11	1.99	0.45
1:G:309:GLN:NE2	1:G:326:GLU:O	2.49	0.45
1:H:275:THR:HG23	1:H:278:LYS:HD3	1.99	0.45
1:G:236:SER:HB3	1:G:315:VAL:HG11	1.99	0.45
1:D:285:ILE:O	1:D:291:GLY:HA3	2.16	0.45
1:I:244:ALA:O	1:I:248:ILE:HD13	2.16	0.44
1:F:8:GLU:CD	1:F:29:ARG:HH22	2.15	0.44
1:E:285:ILE:O	1:E:291:GLY:HA3	2.17	0.44
1:B:148:GLN:O	1:B:152:THR:HG23	2.16	0.44
1:I:7:LEU:HD23	1:I:36:TRP:CE3	2.52	0.44
1:L:345:GLU:CD	1:L:350:PRO:HD2	2.37	0.44
1:J:324:GLN:HG3	1:J:348:ASN:O	2.17	0.44
1:F:26:GLN:OE1	2:F:770:HOH:O	2.20	0.44
1:K:93:GLY:HA3	1:K:127:GLY:O	2.18	0.44
1:K:416:HIS:ND1	2:K:686:HOH:O	2.36	0.44
1:F:313:VAL:HG23	1:F:315:VAL:HG13	1.99	0.44
1:E:289:ARG:HA	1:E:289:ARG:HD3	1.75	0.44
1:H:281:ARG:HD2	1:H:300:PHE:CZ	2.53	0.44
1:D:417:GLY:HA3	1:D:423:THR:HG23	1.98	0.44
1:K:235:VAL:HG22	1:K:317:ILE:CG1	2.47	0.44
1:C:45:TYR:O	1:C:50:LEU:HD23	2.18	0.44
1:C:262:SER:OG	2:C:630:HOH:O	2.21	0.44
1:J:66:VAL:HG12	1:L:446:VAL:HG13	1.99	0.44
1:I:363:GLY:HA2	1:I:422:GLN:OE1	2.17	0.44
1:D:236:SER:HB3	1:D:315:VAL:HG11	1.99	0.44
1:I:336:ILE:HD12	1:I:358:LEU:HD13	1.99	0.44
1:E:421:GLU:N	2:E:643:HOH:O	2.51	0.44
1:C:343:VAL:HG21	1:C:359:PHE:CE2	2.53	0.43
1:C:39:LEU:HD13	1:C:51:LEU:HD11	1.99	0.43
1:B:397:LYS:HE3	1:B:401:ARG:NH2	2.33	0.43
1:G:25:ALA:HB2	2:G:556:HOH:O	2.17	0.43
1:H:323:THR:OG1	1:H:324:GLN:N	2.52	0.43
1:J:290:ASP:N	1:J:290:ASP:OD1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:GLU:HB3	1:I:300:PHE:CD1	2.54	0.43
1:F:265:SER:CB	1:F:292:ARG:HH21	2.30	0.43
1:G:341:LYS:C	1:G:364:VAL:HG23	2.39	0.43
1:A:318:ALA:HB3	1:A:343:VAL:HG22	2.00	0.43
1:B:390:ARG:NH2	1:F:161:ASP:OD1	2.51	0.43
1:L:216:VAL:HG13	1:L:230:PHE:CE2	2.53	0.43
1:D:328:ASP:OD1	1:D:330:ASP:HB3	2.18	0.43
1:F:236:SER:HB3	1:F:315:VAL:HG11	2.01	0.43
1:H:122:LEU:HD13	1:H:381:GLY:HA3	2.00	0.43
1:B:329:VAL:HG22	1:B:354:GLU:OE2	2.18	0.43
1:B:98:HIS:CG	1:B:99:PRO:HD2	2.54	0.43
1:H:29:ARG:NH1	2:H:757:HOH:O	2.52	0.43
1:H:209:GLU:HG3	1:H:246:TYR:CD1	2.54	0.43
1:I:401:ARG:HD3	1:I:401:ARG:HA	1.83	0.43
1:K:314:PRO:HB3	1:K:338:ASN:HB2	2.00	0.43
1:F:353:ILE:HG22	2:F:801:HOH:O	2.19	0.43
1:E:432:ALA:O	1:E:436:LYS:HG3	2.19	0.43
1:C:97:PHE:HZ	1:C:179:MET:HE3	1.84	0.42
1:B:213:TYR:OH	1:B:249:GLU:OE2	2.30	0.42
1:K:358:LEU:HD23	1:K:359:PHE:N	2.34	0.42
1:F:213:TYR:OH	1:F:249:GLU:OE2	2.33	0.42
1:B:15:GLN:NE2	2:B:675:HOH:O	2.48	0.42
1:J:148:GLN:CG	1:J:182:MET:HE3	2.48	0.42
1:L:148:GLN:O	1:L:152:THR:HG23	2.18	0.42
1:H:266:GLY:HA3	1:H:304:TYR:OH	2.20	0.42
1:I:236:SER:HA	1:I:260:THR:HG22	2.01	0.42
1:H:10:PHE:O	1:H:14:VAL:HG23	2.19	0.42
1:I:294:ALA:HB2	1:I:304:TYR:CZ	2.53	0.42
1:G:17:ARG:NH2	1:I:77:ASN:HA	2.34	0.42
1:J:391:LEU:HD11	1:K:393:TRP:HH2	1.85	0.42
1:L:289:ARG:NH2	1:L:290:ASP:OD2	2.53	0.42
1:J:269:VAL:HB	1:J:303:VAL:HB	2.02	0.42
1:K:39:LEU:HD13	1:K:51:LEU:HD11	2.02	0.42
1:C:315:VAL:HG12	1:C:317:ILE:H	1.85	0.42
1:C:275:THR:H	1:C:278:LYS:CG	2.33	0.42
1:B:370:LYS:HD3	2:B:706:HOH:O	2.20	0.42
1:K:119:LEU:HG	1:K:409:ILE:HG23	2.02	0.42
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.83	0.42
1:L:426:VAL:O	1:L:430:ASN:ND2	2.53	0.42
1:C:363:GLY:CA	1:C:422:GLN:HE22	2.27	0.42
1:J:353:ILE:O	1:J:357:GLU:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:349:MET:N	1:K:350:PRO:HD3	2.34	0.41
1:B:9:SER:O	1:B:13:HIS:ND1	2.43	0.41
1:D:323:THR:OG1	1:D:324:GLN:N	2.53	0.41
1:H:417:GLY:HA3	1:H:423:THR:HG23	2.02	0.41
1:K:401:ARG:HA	1:K:401:ARG:HD2	1.74	0.41
1:H:238:SER:HB3	1:H:311:TRP:CH2	2.55	0.41
1:C:278:LYS:HD3	1:C:296:TYR:OH	2.20	0.41
1:E:50:LEU:HD22	1:E:442:LEU:HD21	2.03	0.41
1:J:310:PRO:HD3	2:J:734:HOH:O	2.19	0.41
1:J:134:ASP:OD1	1:J:136:LYS:HG2	2.20	0.41
1:C:336:ILE:HD12	1:C:358:LEU:HG	2.02	0.41
1:H:250:LYS:HA	1:H:250:LYS:HD3	1.89	0.41
1:G:313:VAL:HA	1:G:314:PRO:HD3	1.93	0.41
1:H:151:MET:CE	1:H:179:MET:SD	3.09	0.41
1:B:151:MET:HE3	1:B:194:PHE:CZ	2.55	0.41
1:B:151:MET:HE3	1:B:194:PHE:HZ	1.85	0.41
1:A:53:ARG:HD2	2:A:701:HOH:O	2.21	0.41
1:H:248:ILE:O	1:H:252:MET:HG3	2.20	0.41
1:A:17:ARG:NH2	1:C:77:ASN:HA	2.36	0.41
1:I:88:ILE:HD11	1:I:436:LYS:HG2	2.03	0.41
1:A:26:GLN:NE2	2:A:611:HOH:O	2.52	0.41
1:I:281:ARG:HD2	1:I:281:ARG:HA	1.88	0.41
1:F:98:HIS:CG	1:F:99:PRO:HD2	2.56	0.41
1:L:122:LEU:HD13	1:L:381:GLY:HA3	2.02	0.41
1:G:98:HIS:CG	1:G:99:PRO:HD2	2.56	0.41
1:D:281:ARG:NE	1:D:299:GLU:OE2	2.54	0.41
1:H:273:GLY:O	1:H:278:LYS:NZ	2.54	0.41
1:J:370:LYS:O	1:J:370:LYS:HD2	2.21	0.41
1:K:45:TYR:O	1:K:50:LEU:HD23	2.21	0.41
1:K:363:GLY:HA2	1:K:422:GLN:OE1	2.21	0.41
1:F:417:GLY:HA3	1:F:423:THR:HG23	2.03	0.41
1:B:248:ILE:O	1:B:252:MET:HG3	2.21	0.41
1:K:308:GLN:CD	1:K:309:GLN:H	2.24	0.41
1:F:148:GLN:O	1:F:152:THR:HG23	2.21	0.41
1:L:205:LEU:O	1:L:206:ILE:HB	2.21	0.41
1:H:282:LEU:O	1:H:286:LYS:HG2	2.21	0.41
1:F:88:ILE:CD1	1:F:436:LYS:HD2	2.51	0.41
1:H:370:LYS:HE3	2:H:537:HOH:O	2.19	0.41
1:C:393:TRP:HB3	1:C:397:LYS:HG2	2.03	0.41
1:A:401:ARG:NE	2:A:850:HOH:O	2.13	0.41
1:H:313:VAL:HA	1:H:314:PRO:HD3	1.97	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LEU:HG	1:D:409:ILE:HG23	2.03	0.41
1:G:330:ASP:O	1:G:334:GLN:HG3	2.22	0.40
1:C:237:VAL:H	1:C:260:THR:HG23	1.86	0.40
1:D:445:GLY:HA2	2:D:738:HOH:O	2.21	0.40
1:I:382:LEU:HD21	1:I:405:ILE:HD11	2.03	0.40
1:H:36:TRP:O	1:H:40:GLU:HG3	2.22	0.40
1:A:109:LEU:HD13	1:A:128:LYS:HE2	2.03	0.40
1:E:411:HIS:O	1:E:415:GLU:HG2	2.21	0.40
1:B:153:GLU:CD	1:B:156:ARG:NH1	2.75	0.40
1:J:144:MET:O	1:J:148:GLN:HG3	2.22	0.40
1:J:148:GLN:O	1:J:152:THR:HG23	2.21	0.40
1:I:88:ILE:CD1	1:I:436:LYS:HG2	2.51	0.40
1:G:59:ARG:HD3	1:I:153:GLU:OE2	2.22	0.40
1:K:323:THR:OG1	1:K:324:GLN:N	2.55	0.40
1:D:438:ALA:O	1:D:442:LEU:HG	2.22	0.40
1:B:250:LYS:HA	1:B:250:LYS:HD3	1.80	0.40
1:F:35:LEU:HD21	1:F:434:PHE:CD1	2.56	0.40
1:A:12:ASN:OD1	1:A:16:LYS:NZ	2.54	0.40
1:I:284:GLU:O	1:I:287:SER:HB3	2.22	0.40
1:F:95:MET:O	1:F:168:ASP:HB3	2.20	0.40
1:J:98:HIS:HB3	1:J:101:VAL:HG23	2.04	0.40
1:G:397:LYS:NZ	2:G:869:HOH:O	2.54	0.40
1:E:25:ALA:HB2	2:E:812:HOH:O	2.22	0.40
1:G:69:ASP:HB2	1:G:142:GLU:OE2	2.21	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	440/450 (98%)	433 (98%)	6 (1%)	1 (0%)	52 48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	441/450 (98%)	427 (97%)	12 (3%)	2 (0%)	34	26
1	C	432/450 (96%)	420 (97%)	11 (2%)	1 (0%)	52	48
1	D	440/450 (98%)	421 (96%)	15 (3%)	4 (1%)	21	13
1	E	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	52	48
1	F	441/450 (98%)	429 (97%)	10 (2%)	2 (0%)	34	26
1	G	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	34	26
1	H	434/450 (96%)	418 (96%)	15 (4%)	1 (0%)	52	48
1	I	440/450 (98%)	429 (98%)	9 (2%)	2 (0%)	34	26
1	J	440/450 (98%)	428 (97%)	10 (2%)	2 (0%)	34	26
1	K	440/450 (98%)	430 (98%)	8 (2%)	2 (0%)	34	26
1	L	440/450 (98%)	431 (98%)	8 (2%)	1 (0%)	52	48
All	All	5268/5400 (98%)	5127 (97%)	120 (2%)	21 (0%)	39	33

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	B	206	ILE
1	C	206	ILE
1	D	206	ILE
1	E	206	ILE
1	F	206	ILE
1	G	206	ILE
1	H	206	ILE
1	I	206	ILE
1	J	206	ILE
1	K	206	ILE
1	L	206	ILE
1	D	264	SER
1	D	289	ARG
1	K	291	GLY
1	B	168	ASP
1	F	168	ASP
1	G	168	ASP
1	I	168	ASP
1	J	168	ASP
1	D	231	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/354 (98%)	340 (98%)	7 (2%)	63	65
1	B	348/354 (98%)	340 (98%)	8 (2%)	58	60
1	C	342/354 (97%)	331 (97%)	11 (3%)	46	44
1	D	347/354 (98%)	340 (98%)	7 (2%)	63	65
1	E	347/354 (98%)	338 (97%)	9 (3%)	54	54
1	F	348/354 (98%)	342 (98%)	6 (2%)	68	71
1	G	347/354 (98%)	339 (98%)	8 (2%)	58	60
1	H	344/354 (97%)	336 (98%)	8 (2%)	58	60
1	I	347/354 (98%)	334 (96%)	13 (4%)	41	38
1	J	347/354 (98%)	342 (99%)	5 (1%)	74	77
1	K	347/354 (98%)	336 (97%)	11 (3%)	46	44
1	L	347/354 (98%)	340 (98%)	7 (2%)	63	65
All	All	4158/4248 (98%)	4058 (98%)	100 (2%)	57	58

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	36	TRP
1	A	84	PHE
1	A	108	PHE
1	A	231	GLU
1	A	250	LYS
1	A	401	ARG
1	B	6	SER
1	B	84	PHE
1	B	108	PHE
1	B	216	VAL
1	B	288	SER
1	B	290	ASP
1	B	313	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	315	VAL
1	C	47	GLN
1	C	84	PHE
1	C	108	PHE
1	C	168	ASP
1	C	271	GLU
1	C	353	ILE
1	C	364	VAL
1	C	401	ARG
1	C	403	HIS
1	C	419	GLU
1	C	423	THR
1	D	36	TRP
1	D	84	PHE
1	D	108	PHE
1	D	292	ARG
1	D	353	ILE
1	D	401	ARG
1	D	421	GLU
1	E	26	GLN
1	E	36	TRP
1	E	40	GLU
1	E	84	PHE
1	E	108	PHE
1	E	156	ARG
1	E	289	ARG
1	E	364	VAL
1	E	401	ARG
1	F	29	ARG
1	F	34	THR
1	F	36	TRP
1	F	84	PHE
1	F	108	PHE
1	F	289	ARG
1	G	6	SER
1	G	84	PHE
1	G	108	PHE
1	G	156	ARG
1	G	289	ARG
1	G	327	LEU
1	G	358	LEU
1	G	401	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	29	ARG
1	H	71	ARG
1	H	84	PHE
1	H	108	PHE
1	H	216	VAL
1	H	224	LYS
1	H	292	ARG
1	H	305	LEU
1	I	30	GLU
1	I	84	PHE
1	I	108	PHE
1	I	228	MET
1	I	257	ARG
1	I	265	SER
1	I	275	THR
1	I	299	GLU
1	I	313	VAL
1	I	323	THR
1	I	358	LEU
1	I	403	HIS
1	I	419	GLU
1	J	36	TRP
1	J	39	LEU
1	J	84	PHE
1	J	108	PHE
1	J	286	LYS
1	K	30	GLU
1	K	34	THR
1	K	84	PHE
1	K	108	PHE
1	K	289	ARG
1	K	317	ILE
1	K	338	ASN
1	K	358	LEU
1	K	361	GLN
1	K	364	VAL
1	K	401	ARG
1	L	35	LEU
1	L	36	TRP
1	L	48	MET
1	L	108	PHE
1	L	353	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	361	GLN
1	L	401	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	422	GLN
1	F	422	GLN
1	L	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/450 (98%)	-0.05	1 (0%) 95 95	15, 26, 45, 79	0
1	B	442/450 (98%)	0.20	24 (5%) 29 31	17, 32, 68, 129	0
1	C	435/450 (96%)	0.49	49 (11%) 7 7	14, 31, 78, 104	0
1	D	442/450 (98%)	0.11	12 (2%) 58 58	17, 33, 59, 108	0
1	E	442/450 (98%)	0.01	6 (1%) 78 78	15, 28, 49, 80	0
1	F	442/450 (98%)	-0.11	1 (0%) 95 95	15, 28, 47, 69	0
1	G	442/450 (98%)	0.01	6 (1%) 78 78	14, 26, 48, 69	0
1	H	438/450 (97%)	0.29	30 (6%) 20 22	17, 32, 75, 111	0
1	I	442/450 (98%)	0.59	66 (14%) 3 3	14, 33, 81, 132	0
1	J	442/450 (98%)	-0.14	3 (0%) 89 89	15, 26, 48, 86	0
1	K	442/450 (98%)	0.02	4 (0%) 85 86	15, 28, 50, 68	0
1	L	442/450 (98%)	0.07	4 (0%) 85 86	14, 29, 54, 77	0
All	All	5293/5400 (98%)	0.12	206 (3%) 43 45	14, 29, 62, 132	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	290	ASP	7.7
1	H	281	ARG	7.6
1	B	289	ARG	7.1
1	B	269	VAL	6.4
1	H	282	LEU	5.7
1	I	269	VAL	5.4
1	I	290	ASP	5.3
1	I	289	ARG	5.2
1	D	291	GLY	5.2
1	I	268	VAL	5.2
1	I	303	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	337	ALA	5.1
1	C	280	ALA	5.0
1	C	296	TYR	5.0
1	C	265	SER	5.0
1	C	274	PHE	4.7
1	J	46	ARG	4.5
1	I	300	PHE	4.5
1	I	274	PHE	4.5
1	H	273	GLY	4.4
1	B	279	LEU	4.4
1	I	293	VAL	4.3
1	C	354	GLU	4.3
1	C	237	VAL	4.3
1	H	302	LEU	4.2
1	I	230	PHE	4.1
1	I	291	GLY	4.1
1	C	340	VAL	4.1
1	I	294	ALA	4.1
1	I	301	GLY	4.0
1	I	279	LEU	3.9
1	I	304	TYR	3.8
1	H	284	GLU	3.8
1	C	300	PHE	3.8
1	C	336	ILE	3.7
1	B	307	GLY	3.7
1	B	273	GLY	3.7
1	C	304	TYR	3.7
1	I	302	LEU	3.7
1	C	273	GLY	3.7
1	H	300	PHE	3.7
1	I	259	ILE	3.5
1	D	287	SER	3.5
1	C	281	ARG	3.5
1	D	285	ILE	3.5
1	H	299	GLU	3.5
1	B	302	LEU	3.4
1	I	296	TYR	3.4
1	H	232	GLY	3.4
1	D	282	LEU	3.4
1	H	298	LYS	3.3
1	L	358	LEU	3.3
1	I	280	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	234	ARG	3.2
1	C	335	LEU	3.2
1	G	307	GLY	3.2
1	I	299	GLU	3.2
1	C	235	VAL	3.2
1	I	273	GLY	3.2
1	H	305	LEU	3.2
1	C	337	ALA	3.1
1	C	311	TRP	3.1
1	I	297	ALA	3.1
1	I	310	PRO	3.1
1	I	308	GLN	3.1
1	K	290	ASP	3.1
1	I	336	ILE	3.1
1	K	358	LEU	3.0
1	C	261	ALA	3.0
1	I	254	PHE	3.0
1	C	358	LEU	3.0
1	G	313	VAL	3.0
1	I	237	VAL	3.0
1	I	334	GLN	3.0
1	I	339	GLY	3.0
1	H	269	VAL	3.0
1	H	296	TYR	3.0
1	I	343	VAL	3.0
1	C	307	GLY	2.9
1	I	312	SER	2.9
1	I	344	ALA	2.9
1	E	423	THR	2.9
1	C	262	SER	2.9
1	E	358	LEU	2.9
1	C	234	ARG	2.9
1	I	258	VAL	2.9
1	C	295	ASP	2.9
1	B	290	ASP	2.8
1	I	227	GLY	2.8
1	C	305	LEU	2.8
1	B	303	VAL	2.8
1	C	260	THR	2.8
1	B	295	ASP	2.8
1	C	308	GLN	2.8
1	C	259	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	302	LEU	2.8
1	C	293	VAL	2.8
1	I	265	SER	2.7
1	I	359	PHE	2.7
1	I	353	ILE	2.7
1	I	329	VAL	2.7
1	I	333	HIS	2.7
1	B	420	GLY	2.7
1	D	418	GLY	2.7
1	C	318	ALA	2.7
1	I	277	GLU	2.7
1	B	285	ILE	2.7
1	G	340	VAL	2.7
1	H	303	VAL	2.7
1	I	228	MET	2.7
1	I	307	GLY	2.7
1	I	276	LYS	2.6
1	D	31	VAL	2.6
1	B	291	GLY	2.6
1	C	327	LEU	2.6
1	H	294	ALA	2.6
1	J	287	SER	2.6
1	H	301	GLY	2.6
1	E	221	ALA	2.6
1	H	274	PHE	2.5
1	I	236	SER	2.5
1	I	240	SER	2.5
1	C	275	THR	2.5
1	I	316	ASP	2.5
1	C	303	VAL	2.5
1	I	314	PRO	2.5
1	B	421	GLU	2.5
1	H	297	ALA	2.5
1	C	276	LYS	2.5
1	D	300	PHE	2.5
1	E	361	GLN	2.5
1	H	353	ILE	2.5
1	I	281	ARG	2.5
1	I	313	VAL	2.4
1	G	421	GLU	2.4
1	I	275	THR	2.4
1	E	421	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	341	LYS	2.4
1	C	264	SER	2.4
1	L	232	GLY	2.4
1	C	252	MET	2.4
1	C	267	THR	2.4
1	G	337	ALA	2.4
1	H	280	ALA	2.4
1	C	266	GLY	2.4
1	I	267	THR	2.4
1	B	329	VAL	2.3
1	C	279	LEU	2.3
1	H	287	SER	2.3
1	L	289	ARG	2.3
1	C	230	PHE	2.3
1	I	362	ALA	2.3
1	C	362	ALA	2.3
1	H	285	ILE	2.3
1	I	158	LEU	2.3
1	I	232	GLY	2.2
1	I	292	ARG	2.2
1	I	295	ASP	2.2
1	B	287	SER	2.2
1	I	311	TRP	2.2
1	K	419	GLU	2.2
1	J	47	GLN	2.2
1	B	341	LYS	2.2
1	H	266	GLY	2.2
1	C	334	GLN	2.2
1	I	361	GLN	2.2
1	H	295	ASP	2.2
1	H	264	SER	2.2
1	C	277	GLU	2.2
1	F	419	GLU	2.2
1	C	268	VAL	2.2
1	I	248	ILE	2.2
1	C	422	GLN	2.1
1	G	420	GLY	2.1
1	I	255	GLY	2.1
1	H	286	LYS	2.1
1	I	226	HIS	2.1
1	I	231	GLU	2.1
1	A	328	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	339	GLY	2.1
1	C	158	LEU	2.1
1	B	274	PHE	2.1
1	B	270	ASP	2.1
1	I	272	SER	2.1
1	D	294	ALA	2.1
1	D	193	VAL	2.1
1	D	420	GLY	2.1
1	B	419	GLU	2.1
1	C	285	ILE	2.1
1	K	422	GLN	2.1
1	B	266	GLY	2.1
1	H	283	ILE	2.1
1	H	158	LEU	2.1
1	C	284	GLU	2.1
1	L	257	ARG	2.1
1	D	301	GLY	2.1
1	B	296	TYR	2.1
1	H	293	VAL	2.1
1	C	310	PRO	2.0
1	C	238	SER	2.0
1	B	275	THR	2.0
1	B	158	LEU	2.0
1	H	322	ALA	2.0
1	H	337	ALA	2.0
1	E	289	ARG	2.0
1	I	235	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.