



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:47 AM GMT

PDB ID : 1W26  
Title : TRIGGER FACTOR IN COMPLEX WITH THE RIBOSOME FORMS A  
MOLECULAR CRADLE FOR NASCENT PROTEINS  
Authors : Ferbitz, L.; Maier, T.; Patzelt, H.; Bukau, B.; Deuerling, E.; Ban, N.  
Deposited on : 2004-06-28  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

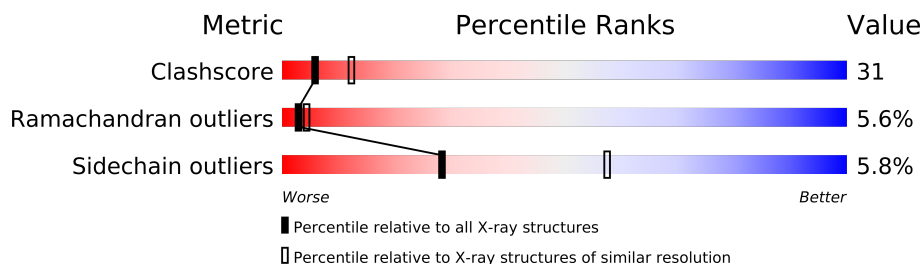
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 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))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	
1	B	432	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6860 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TRIGGER FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total 3386	C 2119	N 582	O 674	Se 11	0	0	0
1	B	432	Total 3386	C 2119	N 582	O 674	Se 11	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total 55	O 55	0	0
2	B	33	Total 33	O 33	0	0

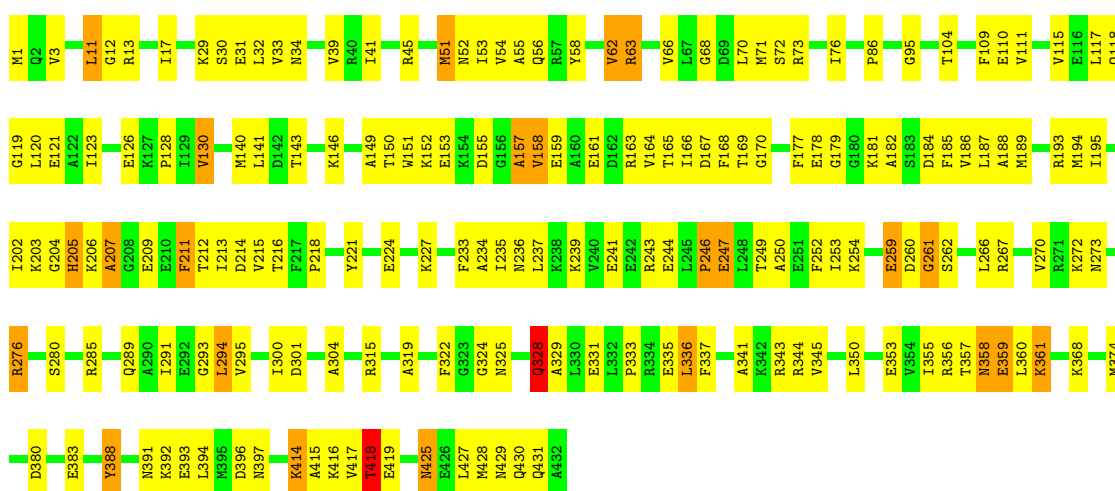
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

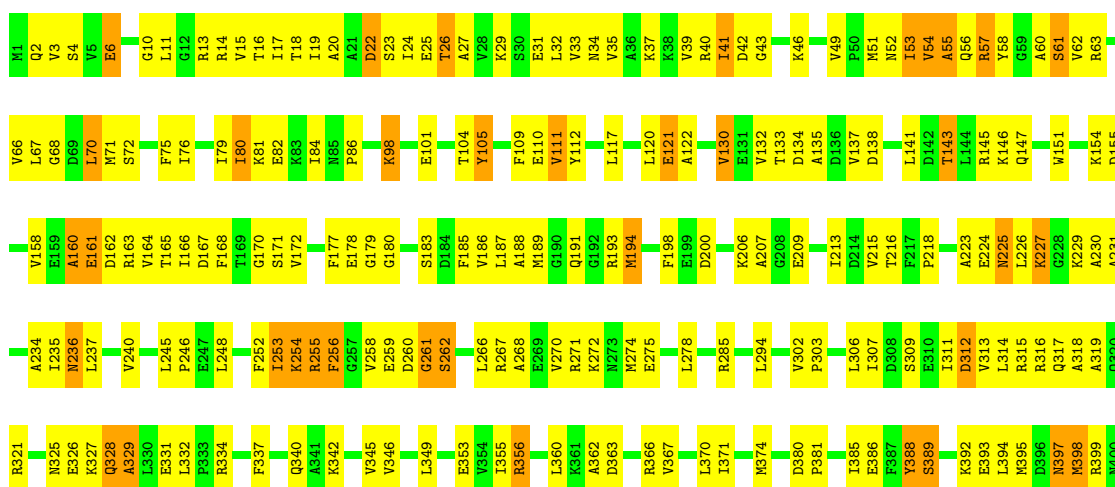
#### • Molecule 1: TRIGGER FACTOR

Chain A:



#### • Molecule 1: TRIGGER FACTOR

Chain B:



V401	L412	T422
A402	A413	T423
L403	K414	F424
E404		M425
E405		E426
Q406		L427
		M428
		M429
		Q430
		Q431
		A432

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.25Å 47.41Å 114.83Å 90.00° 113.66° 90.00°	Depositor
Resolution (Å)	45.91 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (45.91-2.70)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.241 , 0.324	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/3416	0.64	2/4575 (0.0%)
1	B	0.37	0/3416	0.61	0/4575
All	All	0.38	0/6832	0.63	2/9150 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	GLY	N-CA-C	-5.30	99.86	113.10
1	A	328	GLN	N-CA-C	-5.13	97.14	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3386	0	3403	182	0
1	B	3386	0	3403	243	0
2	A	55	0	0	3	0
2	B	33	0	0	3	0
All	All	6860	0	6806	425	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (425) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:53:ILE:HG21	1:B:58:TYR:CB	1.89	1.02
1:B:53:ILE:HG21	1:B:58:TYR:HB3	1.00	0.99
1:B:53:ILE:CG2	1:B:58:TYR:HB3	1.93	0.98
1:B:133:THR:HG22	1:B:135:ALA:H	1.28	0.97
1:A:168:PHE:H	1:A:182:ALA:HB3	1.28	0.96
1:B:32:LEU:HD13	1:B:53:ILE:HG23	1.44	0.95
1:B:355:ILE:HA	1:B:360:LEU:HD12	1.52	0.91
1:A:140:MSE:HE3	1:A:143:THR:HB	1.53	0.90
1:B:146:LYS:HG2	1:B:245:LEU:HD11	1.51	0.90
1:A:425:ASN:HD22	1:A:425:ASN:N	1.77	0.82
1:A:164:VAL:HG11	1:A:237:LEU:HD11	1.62	0.82
1:A:152:LYS:HG2	1:A:153:GLU:H	1.43	0.81
1:B:39:VAL:HG21	1:B:46:LYS:HD3	1.61	0.81
1:B:133:THR:HG22	1:B:135:ALA:N	1.95	0.80
1:A:164:VAL:HG13	1:A:239:LYS:O	1.81	0.80
1:B:194:MSE:HA	1:B:194:MSE:HE2	1.61	0.80
1:B:207:ALA:HA	1:B:237:LEU:HG	1.63	0.80
1:A:167:ASP:HB2	1:A:236:ASN:HB2	1.64	0.80
1:B:158:VAL:CG1	1:B:189:MSE:HE2	2.13	0.79
1:B:158:VAL:HG11	1:B:189:MSE:HE2	1.63	0.79
1:B:18:THR:HG23	1:B:104:THR:HG22	1.64	0.79
1:B:363:ASP:H	1:B:406:GLN:HE22	1.27	0.79
1:A:361:LYS:HD2	1:A:361:LYS:O	1.83	0.78
1:B:366:ARG:HD3	1:B:405:GLU:OE1	1.83	0.78
1:A:187:LEU:HA	1:A:193:ARG:HH21	1.48	0.78
1:B:6:GLU:HG3	1:B:14:ARG:HB3	1.66	0.77
1:B:386:GLU:O	1:B:389:SER:HB3	1.84	0.77
1:A:193:ARG:O	1:A:194:MSE:HE2	1.84	0.77
1:A:358:ASN:N	1:A:358:ASN:HD22	1.80	0.77
1:B:254:LYS:HG3	1:B:255:ARG:H	1.50	0.76
1:B:303:PRO:HG2	1:B:306:LEU:HD12	1.68	0.76
1:B:342:LYS:O	1:B:346:VAL:HG23	1.87	0.75
1:B:215:VAL:HG12	1:B:216:THR:H	1.52	0.75
1:A:260:ASP:O	1:A:262:SER:N	2.20	0.74
1:B:326:GLU:HG3	1:B:327:LYS:N	2.02	0.74
1:B:49:VAL:HG11	1:B:54:VAL:HG13	1.69	0.74
1:B:2:GLN:HB2	1:B:18:THR:HB	1.68	0.73
1:A:73:ARG:HH11	1:A:73:ARG:HB3	1.53	0.72
1:A:150:THR:HA	2:A:2027:HOH:O	1.88	0.72
1:A:250:ALA:O	1:A:254:LYS:HG2	1.90	0.72
1:A:335:GLU:CD	1:A:335:GLU:H	1.94	0.71
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.54	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60:ALA:C	1:B:62:VAL:H	1.94	0.71
1:B:63:ARG:HB2	1:B:63:ARG:HH11	1.54	0.71
1:B:168:PHE:HA	1:B:234:ALA:O	1.91	0.71
1:B:32:LEU:HD12	1:B:53:ILE:HD12	1.71	0.70
1:B:207:ALA:HB2	1:B:240:VAL:HG23	1.73	0.70
1:B:4:SER:HB2	2:B:2001:HOH:O	1.92	0.70
1:B:120:LEU:C	1:B:122:ALA:H	1.95	0.70
1:A:13:ARG:HH11	1:A:13:ARG:HG3	1.56	0.70
1:B:49:VAL:CG1	1:B:54:VAL:HG22	2.22	0.69
1:A:130:VAL:HG21	1:A:427:LEU:HD22	1.72	0.69
1:A:118:GLN:O	1:A:120:LEU:N	2.25	0.69
1:B:164:VAL:HG12	1:B:166:ILE:HG23	1.74	0.69
1:B:311:ILE:O	1:B:315:ARG:HG2	1.92	0.69
1:B:60:ALA:O	1:B:62:VAL:N	2.23	0.69
1:A:206:LYS:O	1:A:237:LEU:HD23	1.92	0.69
1:A:187:LEU:HA	1:A:193:ARG:NH2	2.08	0.69
1:A:51:MSE:SE	1:A:54:VAL:HG21	2.43	0.69
1:A:164:VAL:HG11	1:A:237:LEU:CD1	2.23	0.68
1:B:6:GLU:CD	1:B:14:ARG:HD2	2.14	0.68
1:A:62:VAL:HG13	1:A:66:VAL:CG2	2.23	0.68
1:B:41:ILE:HD11	1:B:46:LYS:HD3	1.75	0.68
1:B:31:GLU:O	1:B:35:VAL:HG23	1.93	0.67
1:B:312:ASP:HB3	1:B:316:ARG:HH12	1.59	0.67
1:A:357:THR:HG22	1:A:358:ASN:ND2	2.09	0.67
1:A:325:ASN:O	1:A:328:GLN:HB2	1.94	0.67
1:B:32:LEU:CD1	1:B:53:ILE:HD12	2.24	0.67
1:B:145:ARG:HD3	1:B:248:LEU:HD21	1.77	0.67
1:B:206:LYS:O	1:B:209:GLU:HG2	1.93	0.67
1:B:76:ILE:O	1:B:79:ILE:HG12	1.94	0.67
1:B:389:SER:HA	1:B:395:MSE:HE3	1.77	0.66
1:B:253:ILE:HD12	1:B:266:LEU:HD12	1.76	0.66
1:A:388:TYR:CE1	1:A:394:LEU:HD23	2.30	0.66
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.59	0.66
1:B:171:SER:O	1:B:231:ALA:HB1	1.95	0.66
1:A:291:ILE:O	1:A:295:VAL:HG23	1.96	0.66
1:A:425:ASN:HD22	1:A:425:ASN:H	1.44	0.66
1:A:357:THR:HG22	1:A:358:ASN:HD22	1.60	0.65
1:B:178:GLU:HG2	1:B:179:GLY:N	2.12	0.65
1:B:371:ILE:HD13	1:B:395:MSE:HE1	1.78	0.65
1:B:80:ILE:O	1:B:80:ILE:HG22	1.95	0.65
1:A:213:ILE:HD12	1:A:214:ASP:H	1.61	0.65
1:B:254:LYS:HG3	1:B:255:ARG:N	2.10	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:49:VAL:HG11	1:B:54:VAL:HG22	1.78	0.65
1:A:166:ILE:HG21	1:A:235:ILE:HG23	1.79	0.65
1:A:1:MSE:HE3	1:A:3:VAL:HG11	1.79	0.65
1:A:149:ALA:HA	1:A:246:PRO:CD	2.27	0.65
1:A:165:THR:HG22	1:A:186:VAL:HG12	1.77	0.64
1:B:397:ASN:O	1:B:401:VAL:HG23	1.97	0.64
1:B:41:ILE:C	1:B:43:GLY:H	2.00	0.64
1:A:72:SER:O	1:A:76:ILE:HG22	1.97	0.64
1:B:253:ILE:HG23	1:B:266:LEU:HD12	1.80	0.63
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.12	0.63
1:B:17:ILE:HB	1:B:105:TYR:CE2	2.34	0.63
1:B:193:ARG:O	1:B:194:MSE:HE3	1.99	0.63
1:B:120:LEU:HD21	1:B:294:LEU:HD13	1.81	0.63
1:A:41:ILE:HG22	1:A:41:ILE:O	1.98	0.63
1:B:389:SER:CA	1:B:395:MSE:HE3	2.29	0.62
1:B:141:LEU:O	1:B:145:ARG:HG3	1.99	0.62
1:B:430:GLN:OE1	1:B:430:GLN:HA	1.98	0.62
1:A:62:VAL:HG13	1:A:66:VAL:HG21	1.81	0.62
1:A:165:THR:OG1	1:A:239:LYS:HB2	1.99	0.62
1:B:303:PRO:CG	1:B:306:LEU:HD12	2.29	0.62
1:A:168:PHE:N	1:A:182:ALA:HB3	2.09	0.61
1:A:272:LYS:HE2	1:A:276:ARG:NH2	2.14	0.61
1:B:254:LYS:HZ2	1:B:255:ARG:HG3	1.66	0.60
1:A:195:ILE:HD11	1:A:221:TYR:HE1	1.65	0.60
1:A:168:PHE:HA	1:A:234:ALA:O	2.02	0.60
1:A:315:ARG:HG2	1:A:337:PHE:CE1	2.37	0.60
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.67	0.60
1:A:253:ILE:HG21	1:A:261:GLY:O	2.02	0.60
1:A:355:ILE:HA	1:A:360:LEU:HD12	1.84	0.60
1:B:53:ILE:HG22	1:B:53:ILE:O	2.01	0.59
1:B:328:GLN:O	1:B:332:LEU:HD13	2.02	0.59
1:B:252:PHE:O	1:B:254:LYS:HG2	2.02	0.59
1:A:146:LYS:HE2	1:A:243:ARG:HH11	1.68	0.59
1:A:166:ILE:HG22	1:A:167:ASP:N	2.16	0.59
1:A:126:GLU:HA	1:A:418:THR:HG23	1.83	0.59
1:B:194:MSE:CE	1:B:194:MSE:HA	2.32	0.59
1:A:368:LYS:HE3	2:A:2040:HOH:O	2.01	0.59
1:B:326:GLU:HG3	1:B:327:LYS:H	1.66	0.58
1:B:54:VAL:C	1:B:56:GLN:H	2.05	0.58
1:A:325:ASN:OD1	1:A:328:GLN:HG3	2.04	0.58
1:B:63:ARG:O	1:B:67:LEU:HB2	2.03	0.58
1:B:112:TYR:CE2	1:B:306:LEU:HD11	2.38	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:198:PHE:CD1	1:B:213:ILE:HD11	2.38	0.58
1:A:429:ASN:HA	1:A:431:GLN:HE22	1.69	0.58
1:B:66:VAL:O	1:B:70:LEU:HD13	2.03	0.58
1:A:166:ILE:CG2	1:A:167:ASP:N	2.67	0.57
1:A:68:GLY:HA2	1:A:71:MSE:HE2	1.85	0.57
1:B:13:ARG:HH11	1:B:13:ARG:HG3	1.69	0.57
1:A:333:PRO:O	1:A:336:LEU:HB2	2.04	0.57
1:B:401:VAL:O	1:B:404:GLU:HG3	2.04	0.57
1:B:307:ILE:O	1:B:311:ILE:HG23	2.05	0.57
1:A:188:ALA:H	1:A:193:ARG:NH2	2.02	0.57
1:B:198:PHE:HD1	1:B:213:ILE:HD11	1.70	0.57
1:B:68:GLY:O	1:B:71:MSE:HB2	2.05	0.57
1:B:325:ASN:OD1	1:B:328:GLN:HG2	2.05	0.57
1:B:40:ARG:O	1:B:42:ASP:N	2.35	0.57
1:A:361:LYS:HD2	1:A:361:LYS:C	2.25	0.57
1:B:55:ALA:HA	1:B:58:TYR:CD2	2.40	0.56
1:B:15:VAL:HG21	1:B:75:PHE:HE1	1.70	0.56
1:B:137:VAL:HG11	1:B:267:ARG:HG3	1.87	0.56
1:B:34:ASN:O	1:B:37:LYS:HG3	2.04	0.56
1:B:172:VAL:HG11	1:B:229:LYS:HD3	1.86	0.56
1:A:31:GLU:HG3	1:A:62:VAL:CG2	2.36	0.56
1:B:23:SER:O	1:B:27:ALA:HB2	2.06	0.56
1:B:315:ARG:HB3	1:B:337:PHE:CE2	2.40	0.56
1:B:120:LEU:HD21	1:B:294:LEU:CD1	2.36	0.56
1:A:54:VAL:HG23	1:A:55:ALA:N	2.20	0.55
1:A:425:ASN:N	1:A:425:ASN:ND2	2.49	0.55
1:B:13:ARG:HG3	1:B:13:ARG:NH1	2.22	0.55
1:A:30:SER:O	1:A:33:VAL:HG12	2.07	0.55
1:A:358:ASN:ND2	1:A:358:ASN:N	2.49	0.55
1:B:427:LEU:O	1:B:430:GLN:HG2	2.07	0.55
1:B:40:ARG:HG3	1:B:40:ARG:O	2.07	0.55
1:B:22:ASP:O	1:B:26:THR:HG23	2.07	0.55
1:B:29:LYS:HG2	1:B:53:ILE:HD11	1.88	0.55
1:B:392:LYS:NZ	1:B:393:GLU:HG3	2.21	0.55
1:B:271:ARG:O	1:B:275:GLU:HG3	2.07	0.55
1:B:68:GLY:HA2	1:B:71:MSE:HE3	1.89	0.55
1:B:172:VAL:HG23	1:B:177:PHE:CD2	2.42	0.55
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.21	0.54
1:A:205:HIS:HB2	1:A:237:LEU:HD22	1.89	0.54
1:B:302:VAL:HG23	1:B:307:ILE:HD11	1.89	0.54
1:A:428:MSE:HE3	1:A:430:GLN:HG3	1.89	0.54
1:A:3:VAL:HG12	1:A:17:ILE:HG12	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:396:ASP:OD1	1:A:397:ASN:N	2.41	0.54
1:B:254:LYS:HZ2	1:B:255:ARG:CG	2.21	0.54
1:B:41:ILE:HG22	1:B:41:ILE:O	2.08	0.53
1:B:165:THR:HA	1:B:185:PHE:O	2.08	0.53
1:B:327:LYS:C	1:B:329:ALA:H	2.12	0.53
1:B:423:THR:OG1	1:B:426:GLU:HB2	2.08	0.53
1:A:45:ARG:NH1	1:A:45:ARG:HG3	2.23	0.53
1:A:428:MSE:HE1	1:A:430:GLN:HE21	1.72	0.53
1:B:309:SER:O	1:B:313:VAL:HG23	2.07	0.53
1:B:39:VAL:O	1:B:39:VAL:HG13	2.08	0.53
1:A:140:MSE:HG2	1:A:270:VAL:HG13	1.90	0.53
1:B:164:VAL:CG1	1:B:166:ILE:HG23	2.37	0.53
1:B:266:LEU:O	1:B:270:VAL:HG23	2.09	0.53
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.24	0.53
1:B:198:PHE:CE1	1:B:235:ILE:HD11	2.43	0.53
1:B:11:LEU:HD22	1:B:111:VAL:O	2.08	0.53
1:A:153:GLU:HG2	1:A:241:GLU:HG2	1.91	0.53
1:A:151:TRP:CH2	1:A:163:ARG:HB2	2.45	0.53
1:B:353:GLU:OE1	1:B:356:ARG:HD3	2.08	0.53
1:B:268:ALA:O	1:B:272:LYS:HG3	2.09	0.53
1:A:29:LYS:HB2	1:A:29:LYS:HZ2	1.72	0.52
1:B:61:SER:HA	2:B:2010:HOH:O	2.09	0.52
1:B:362:ALA:N	1:B:403:LEU:HD21	2.24	0.52
1:A:418:THR:OG1	1:A:419:GLU:N	2.42	0.52
1:B:189:MSE:O	1:B:191:GLN:HG3	2.10	0.52
1:B:60:ALA:O	1:B:62:VAL:HG13	2.10	0.52
1:A:126:GLU:HB3	1:A:289:GLN:HE22	1.75	0.52
1:B:198:PHE:HE1	1:B:235:ILE:HD11	1.75	0.52
1:B:363:ASP:N	1:B:406:GLN:HE22	2.02	0.52
1:A:13:ARG:HG3	1:A:13:ARG:NH1	2.19	0.52
1:B:57:ARG:O	1:B:57:ARG:HG3	2.10	0.52
1:B:302:VAL:HG22	1:B:342:LYS:HE3	1.91	0.52
1:B:24:ILE:O	1:B:27:ALA:HB3	2.09	0.52
1:A:31:GLU:HG3	1:A:62:VAL:HG22	1.92	0.52
1:A:62:VAL:HG13	1:A:66:VAL:HG23	1.92	0.52
1:B:60:ALA:C	1:B:62:VAL:N	2.63	0.52
1:A:300:ILE:HG13	1:A:301:ASP:N	2.25	0.52
1:B:3:VAL:HG12	1:B:4:SER:H	1.75	0.51
1:B:143:THR:O	1:B:147:GLN:HG2	2.09	0.51
1:A:253:ILE:HG13	1:A:266:LEU:HB2	1.92	0.51
1:A:429:ASN:HA	1:A:431:GLN:NE2	2.26	0.51
1:B:3:VAL:HG12	1:B:4:SER:N	2.25	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:166:ILE:HD13	1:A:235:ILE:CG2	2.41	0.51
1:B:215:VAL:HG12	1:B:216:THR:N	2.21	0.51
1:A:224:GLU:HA	1:A:227:LYS:HD2	1.92	0.51
1:A:141:LEU:HD11	1:A:267:ARG:HG2	1.92	0.51
1:B:345:VAL:O	1:B:349:LEU:HD13	2.10	0.51
1:B:39:VAL:HG22	1:B:41:ILE:HG12	1.93	0.51
1:A:253:ILE:HD13	1:A:261:GLY:O	2.10	0.51
1:B:327:LYS:O	1:B:331:GLU:HG2	2.10	0.51
1:A:149:ALA:HA	1:A:246:PRO:HD3	1.93	0.51
1:B:41:ILE:C	1:B:43:GLY:N	2.63	0.51
1:B:158:VAL:HG22	1:B:240:VAL:HG11	1.93	0.51
1:B:120:LEU:O	1:B:122:ALA:N	2.44	0.51
1:A:157:ALA:O	1:A:159:GLU:N	2.45	0.50
1:A:165:THR:HA	1:A:185:PHE:O	2.11	0.50
1:A:167:ASP:HB2	1:A:236:ASN:CB	2.40	0.50
1:A:358:ASN:O	1:A:359:GLU:C	2.49	0.50
1:B:76:ILE:O	1:B:79:ILE:CG1	2.59	0.50
1:A:425:ASN:H	1:A:425:ASN:ND2	2.07	0.50
1:A:29:LYS:HG3	1:A:51:MSE:HG3	1.93	0.50
1:B:224:GLU:O	1:B:226:LEU:N	2.45	0.50
1:B:31:GLU:OE1	1:B:31:GLU:HA	2.12	0.50
1:B:172:VAL:HG23	1:B:177:PHE:CE2	2.46	0.50
1:B:374:MSE:HE2	1:B:398:MSE:SE	2.61	0.50
1:A:167:ASP:OD1	1:A:184:ASP:N	2.35	0.50
1:B:254:LYS:CG	1:B:255:ARG:H	2.23	0.50
1:A:202:ILE:HG22	1:A:202:ILE:O	2.12	0.50
1:A:260:ASP:C	1:A:262:SER:H	2.14	0.49
1:A:221:TYR:O	1:A:227:LYS:HE3	2.12	0.49
1:A:246:PRO:O	1:A:247:GLU:O	2.30	0.49
1:A:294:LEU:HD22	1:A:350:LEU:HD13	1.93	0.49
1:A:152:LYS:HG2	1:A:153:GLU:N	2.20	0.49
1:B:302:VAL:CG2	1:B:307:ILE:HD11	2.43	0.49
1:B:388:TYR:C	1:B:395:MSE:CE	2.81	0.49
1:B:62:VAL:HG23	1:B:63:ARG:N	2.28	0.49
1:A:319:ALA:HB2	1:A:329:ALA:HB2	1.95	0.49
1:B:172:VAL:CG1	1:B:229:LYS:HD3	2.42	0.49
1:A:1:MSE:HE3	1:A:3:VAL:CG1	2.42	0.49
1:B:25:GLU:HG2	2:B:2005:HOH:O	2.13	0.49
1:A:374:MSE:HE1	1:A:388:TYR:CE1	2.48	0.49
1:A:249:THR:O	1:A:253:ILE:HG22	2.12	0.48
1:A:73:ARG:HB3	1:A:73:ARG:NH1	2.26	0.48
1:A:117:LEU:HG	1:A:353:GLU:HG2	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:285:ARG:O	1:B:285:ARG:HD2	2.13	0.48
1:A:322:PHE:O	1:A:322:PHE:CG	2.65	0.48
1:B:20:ALA:O	1:B:24:ILE:HG13	2.13	0.48
1:A:328:GLN:O	1:A:331:GLU:HB3	2.13	0.48
1:A:272:LYS:CE	1:A:276:ARG:NH2	2.77	0.48
1:A:170:GLY:HA3	1:A:177:PHE:CZ	2.49	0.48
1:B:170:GLY:N	1:B:180:GLY:O	2.45	0.48
1:A:39:VAL:O	1:A:39:VAL:HG12	2.12	0.48
1:B:76:ILE:HG22	1:B:80:ILE:HD12	1.96	0.48
1:A:146:LYS:CE	1:A:243:ARG:HH11	2.26	0.48
1:B:313:VAL:O	1:B:317:GLN:HG3	2.14	0.48
1:A:115:VAL:HG12	1:A:353:GLU:HG2	1.96	0.48
1:A:52:ASN:OD1	1:A:53:ILE:HG13	2.14	0.48
1:B:133:THR:CG2	1:B:135:ALA:H	2.12	0.48
1:B:428:MSE:O	1:B:430:GLN:N	2.44	0.48
1:B:120:LEU:C	1:B:122:ALA:N	2.62	0.47
1:A:169:THR:OG1	1:A:234:ALA:HB3	2.13	0.47
1:B:253:ILE:CD1	1:B:266:LEU:HD12	2.43	0.47
1:B:363:ASP:H	1:B:406:GLN:NE2	2.04	0.47
1:A:243:ARG:HG3	1:A:243:ARG:O	2.13	0.47
1:B:52:ASN:O	1:B:53:ILE:HG12	2.14	0.47
1:B:253:ILE:HG22	1:B:258:VAL:HB	1.97	0.47
1:A:428:MSE:HA	1:A:428:MSE:HE3	1.97	0.47
1:B:388:TYR:CD2	1:B:394:LEU:HB3	2.50	0.47
1:B:253:ILE:O	1:B:254:LYS:C	2.53	0.47
1:A:272:LYS:NZ	1:A:276:ARG:NH2	2.63	0.47
1:A:155:ASP:HA	1:A:207:ALA:HB2	1.97	0.47
1:A:168:PHE:CE1	1:A:182:ALA:HB2	2.50	0.47
1:A:333:PRO:HG2	1:A:336:LEU:HG	1.96	0.47
1:B:398:MSE:HA	1:B:398:MSE:HE3	1.97	0.47
1:A:341:ALA:O	1:A:345:VAL:HG23	2.15	0.47
1:B:53:ILE:C	1:B:55:ALA:H	2.18	0.46
1:A:32:LEU:CD1	1:A:55:ALA:HA	2.44	0.46
1:B:110:GLU:HB3	1:B:303:PRO:HB3	1.96	0.46
1:B:325:ASN:CG	1:B:328:GLN:HG2	2.36	0.46
1:A:117:LEU:HG	1:A:353:GLU:CG	2.45	0.46
1:B:33:VAL:HG23	1:B:51:MSE:SE	2.66	0.46
1:A:41:ILE:CG2	1:A:41:ILE:O	2.64	0.46
1:A:123:ILE:HG23	1:A:293:GLY:HA3	1.98	0.46
1:B:355:ILE:CD1	1:B:403:LEU:HB3	2.46	0.46
1:B:254:LYS:O	1:B:256:PHE:N	2.49	0.46
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:19:ILE:HD13	1:B:70:LEU:HB3	1.97	0.46
1:A:391:ASN:OD1	1:A:393:GLU:HB3	2.16	0.46
1:A:429:ASN:HB3	1:A:431:GLN:OE1	2.16	0.45
1:A:195:ILE:HG23	1:A:218:PRO:HD3	1.98	0.45
1:A:380:ASP:OD2	1:A:383:GLU:HB3	2.15	0.45
1:A:168:PHE:CZ	1:A:182:ALA:HB2	2.52	0.45
1:B:254:LYS:CG	1:B:255:ARG:N	2.79	0.45
1:B:52:ASN:O	1:B:53:ILE:HB	2.17	0.45
1:B:133:THR:CG2	1:B:134:ASP:N	2.79	0.45
1:B:105:TYR:N	1:B:105:TYR:CD2	2.85	0.45
1:A:205:HIS:CE1	1:A:211:PHE:HB3	2.52	0.45
1:A:244:GLU:O	1:A:246:PRO:HD3	2.16	0.45
1:B:22:ASP:OD1	1:B:22:ASP:N	2.42	0.45
1:A:272:LYS:HE3	1:A:272:LYS:HB2	1.68	0.45
1:A:259:GLU:H	1:A:259:GLU:CD	2.20	0.45
1:A:415:ALA:O	1:A:417:VAL:HG23	2.17	0.45
1:B:223:ALA:O	1:B:227:LYS:HB2	2.16	0.45
1:B:371:ILE:CD1	1:B:395:MSE:HE1	2.45	0.45
1:A:12:GLY:O	1:A:13:ARG:HG3	2.16	0.45
1:A:253:ILE:HG23	1:A:261:GLY:HA2	1.98	0.45
1:A:121:GLU:HA	1:A:414:LYS:O	2.17	0.45
1:A:206:LYS:H	1:A:209:GLU:HG2	1.82	0.44
1:A:158:VAL:HG21	1:A:237:LEU:HD21	1.97	0.44
1:B:388:TYR:CE2	1:B:394:LEU:HB3	2.52	0.44
1:A:151:TRP:CZ2	1:A:163:ARG:HB2	2.52	0.44
1:B:84:ILE:HG22	1:B:86:PRO:HD3	1.99	0.44
1:B:404:GLU:HG3	1:B:405:GLU:H	1.82	0.44
1:B:216:THR:HA	1:B:230:ALA:HA	2.00	0.44
1:A:128:PRO:CG	1:A:427:LEU:HD21	2.47	0.44
1:B:52:ASN:O	1:B:53:ILE:CB	2.65	0.44
1:B:258:VAL:C	1:B:260:ASP:H	2.21	0.44
1:B:328:GLN:HA	1:B:331:GLU:HG3	2.00	0.44
1:A:29:LYS:CB	1:A:29:LYS:NZ	2.80	0.44
1:A:272:LYS:HG3	1:A:273:ASN:N	2.32	0.44
1:A:272:LYS:HZ3	1:A:276:ARG:HH22	1.65	0.44
1:B:138:ASP:OD1	1:B:267:ARG:NH2	2.51	0.44
1:A:319:ALA:HA	1:A:322:PHE:HB3	2.00	0.44
1:A:86:PRO:HB3	1:A:109:PHE:CD1	2.52	0.44
1:B:160:ALA:O	1:B:162:ASP:N	2.51	0.44
1:A:178:GLU:O	1:A:181:LYS:HE3	2.17	0.44
1:B:367:VAL:HA	1:B:370:LEU:HD12	2.00	0.44
1:B:245:LEU:HA	1:B:246:PRO:HD3	1.81	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:381:PRO:O	1:B:385:ILE:HG13	2.16	0.44
1:A:17:ILE:O	1:A:104:THR:HG23	2.17	0.44
1:B:19:ILE:HG22	1:B:20:ALA:N	2.33	0.44
1:B:54:VAL:C	1:B:56:GLN:N	2.70	0.43
1:B:314:LEU:HD21	1:B:340:GLN:NE2	2.33	0.43
1:B:41:ILE:O	1:B:43:GLY:N	2.47	0.43
1:A:195:ILE:HD11	1:A:221:TYR:CE1	2.50	0.43
1:B:392:LYS:HZ2	1:B:393:GLU:HG3	1.83	0.43
1:B:254:LYS:HE3	1:B:255:ARG:NH1	2.33	0.43
1:B:312:ASP:HB3	1:B:316:ARG:NH1	2.30	0.43
1:A:126:GLU:H	1:A:289:GLN:NE2	2.15	0.43
1:A:11:LEU:HG	1:A:111:VAL:O	2.19	0.43
1:B:121:GLU:O	1:B:121:GLU:HG2	2.18	0.43
1:B:35:VAL:C	1:B:37:LYS:H	2.22	0.43
1:B:332:LEU:N	1:B:332:LEU:HD12	2.33	0.43
1:B:137:VAL:CG1	1:B:267:ARG:HG3	2.48	0.43
1:B:167:ASP:HB2	1:B:236:ASN:HB2	2.01	0.43
1:B:32:LEU:O	1:B:35:VAL:HB	2.18	0.43
1:B:371:ILE:HD11	1:B:395:MSE:SE	2.69	0.43
1:B:49:VAL:HG11	1:B:54:VAL:CG1	2.46	0.43
1:B:75:PHE:O	1:B:76:ILE:C	2.57	0.43
1:B:79:ILE:HG13	1:B:80:ILE:N	2.34	0.43
1:B:117:LEU:HG	1:B:353:GLU:CG	2.48	0.43
1:B:117:LEU:HG	1:B:353:GLU:HG3	2.01	0.42
1:B:261:GLY:O	1:B:262:SER:C	2.57	0.42
1:A:272:LYS:NZ	1:A:276:ARG:HH22	2.17	0.42
1:B:51:MSE:C	1:B:53:ILE:H	2.23	0.42
1:B:53:ILE:O	1:B:53:ILE:CG2	2.67	0.42
1:B:72:SER:O	1:B:75:PHE:N	2.50	0.42
1:B:261:GLY:O	1:B:262:SER:O	2.36	0.42
1:B:161:GLU:N	1:B:189:MSE:HB2	2.35	0.42
1:A:45:ARG:CG	1:A:45:ARG:HH11	2.28	0.42
1:B:4:SER:HB3	1:B:16:THR:HB	2.01	0.42
1:A:110:GLU:OE1	1:A:304:ALA:N	2.46	0.42
1:B:58:TYR:C	1:B:60:ALA:H	2.22	0.42
1:B:121:GLU:HA	1:B:414:LYS:O	2.19	0.42
1:B:151:TRP:CZ3	1:B:163:ARG:HB2	2.55	0.42
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.85	0.42
1:A:39:VAL:CG1	1:A:39:VAL:O	2.67	0.42
1:B:399:ARG:O	1:B:402:ALA:HB3	2.20	0.42
1:B:51:MSE:HE3	1:B:53:ILE:HD13	2.02	0.41
1:A:233:PHE:HB3	1:A:235:ILE:HD11	2.01	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:247:GLU:HB3	1:A:252:PHE:HB2	2.02	0.41
1:A:153:GLU:HA	1:A:241:GLU:HA	2.01	0.41
1:A:253:ILE:HD11	1:A:262:SER:O	2.19	0.41
1:B:380:ASP:O	1:B:381:PRO:C	2.58	0.41
1:A:54:VAL:CG2	1:A:55:ALA:N	2.84	0.41
1:A:128:PRO:HG3	1:A:427:LEU:HD21	2.03	0.41
1:A:319:ALA:O	1:A:322:PHE:N	2.53	0.41
1:B:82:GLU:OE1	1:B:82:GLU:N	2.54	0.41
1:B:187:LEU:HD12	1:B:188:ALA:N	2.35	0.41
1:B:388:TYR:C	1:B:395:MSE:HE2	2.41	0.41
1:B:254:LYS:NZ	1:B:255:ARG:CZ	2.83	0.41
1:B:315:ARG:HA	1:B:318:ALA:HB3	2.03	0.41
1:B:327:LYS:C	1:B:329:ALA:N	2.74	0.41
1:B:54:VAL:O	1:B:56:GLN:N	2.54	0.41
1:A:344:ARG:HH11	1:A:344:ARG:HG2	1.86	0.41
1:A:427:LEU:N	1:A:427:LEU:HD12	2.35	0.41
1:B:274:MSE:HE2	1:B:424:PHE:CE2	2.56	0.41
1:B:39:VAL:HB	1:B:46:LYS:HZ3	1.85	0.41
1:B:164:VAL:HG13	1:B:237:LEU:CD1	2.51	0.41
1:B:311:ILE:HD13	1:B:334:ARG:HD3	2.03	0.41
1:A:68:GLY:HA2	1:A:71:MSE:CE	2.50	0.41
1:B:63:ARG:HB2	1:B:63:ARG:NH1	2.27	0.41
1:B:325:ASN:OD1	1:B:327:LYS:HB2	2.21	0.41
1:A:30:SER:O	1:A:34:ASN:ND2	2.54	0.41
1:A:215:VAL:HG12	1:A:216:THR:N	2.35	0.41
1:A:140:MSE:O	1:A:143:THR:HB	2.21	0.41
1:B:168:PHE:CD1	1:B:168:PHE:C	2.94	0.41
1:A:374:MSE:HE1	1:A:388:TYR:CD1	2.56	0.41
1:A:368:LYS:CE	2:A:2040:HOH:O	2.66	0.41
1:B:167:ASP:HB2	1:B:236:ASN:CB	2.51	0.41
1:B:319:ALA:C	1:B:321:ARG:H	2.24	0.41
1:B:105:TYR:H	1:B:105:TYR:HD2	1.67	0.41
1:A:237:LEU:HD12	1:A:237:LEU:HA	1.91	0.40
1:B:17:ILE:HG22	1:B:18:THR:N	2.35	0.40
1:B:98:LYS:HE3	1:B:101:GLU:OE1	2.21	0.40
1:A:62:VAL:O	1:A:66:VAL:HG23	2.21	0.40
1:A:212:THR:HA	1:A:233:PHE:O	2.21	0.40
1:A:427:LEU:C	1:A:429:ASN:H	2.24	0.40
1:A:54:VAL:O	1:A:58:TYR:N	2.50	0.40
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.90	0.40
1:B:130:VAL:HG13	1:B:422:THR:O	2.21	0.40
1:B:75:PHE:HZ	1:B:109:PHE:CE2	2.39	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:66:VAL:HG12	1:B:70:LEU:HD22	2.03	0.40
1:B:167:ASP:OD1	1:B:183:SER:HA	2.21	0.40
1:B:132:VAL:HG23	1:B:278:LEU:HD23	2.02	0.40
1:A:179:GLY:O	1:A:181:LYS:HG3	2.21	0.40
1:B:412:LEU:C	1:B:414:LYS:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/432 (100%)	368 (86%)	43 (10%)	19 (4%)	4	8
1	B	430/432 (100%)	339 (79%)	62 (14%)	29 (7%)	2	2
All	All	860/864 (100%)	707 (82%)	105 (12%)	48 (6%)	3	4

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLY
1	A	247	GLU
1	A	261	GLY
1	B	53	ILE
1	B	54	VAL
1	B	61	SER
1	B	161	GLU
1	B	253	ILE
1	B	254	LYS
1	B	255	ARG
1	B	262	SER
1	B	329	ALA
1	A	158	VAL
1	A	189	MSE
1	B	10	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	41	ILE
1	B	121	GLU
1	B	154	LYS
1	B	225	ASN
1	B	259	GLU
1	B	261	GLY
1	B	389	SER
1	B	413	ALA
1	A	205	HIS
1	A	207	ALA
1	A	414	LYS
1	A	416	LYS
1	B	57	ARG
1	B	155	ASP
1	A	259	GLU
1	A	324	GLY
1	A	392	LYS
1	A	418	THR
1	B	80	ILE
1	B	81	LYS
1	B	160	ALA
1	B	328	GLN
1	B	356	ARG
1	A	157	ALA
1	A	203	LYS
1	A	204	GLY
1	A	359	GLU
1	B	98	LYS
1	A	63	ARG
1	A	246	PRO
1	B	55	ALA
1	B	227	LYS
1	B	218	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/348 (103%)	339 (94%)	20 (6%)	30	59
1	B	359/348 (103%)	337 (94%)	22 (6%)	26	54
All	All	718/696 (103%)	676 (94%)	42 (6%)	28	57

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	51	MSE
1	A	56	GLN
1	A	62	VAL
1	A	63	ARG
1	A	130	VAL
1	A	161	GLU
1	A	211	PHE
1	A	276	ARG
1	A	280	SER
1	A	285	ARG
1	A	294	LEU
1	A	328	GLN
1	A	336	LEU
1	A	343	ARG
1	A	358	ASN
1	A	361	LYS
1	A	388	TYR
1	A	418	THR
1	A	425	ASN
1	B	6	GLU
1	B	22	ASP
1	B	26	THR
1	B	70	LEU
1	B	105	TYR
1	B	111	VAL
1	B	130	VAL
1	B	143	THR
1	B	186	VAL
1	B	194	MSE
1	B	200	ASP
1	B	225	ASN
1	B	236	ASN
1	B	256	PHE
1	B	312	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	388	TYR
1	B	397	ASN
1	B	398	MSE
1	B	404	GLU
1	B	422	THR
1	B	428	MSE
1	B	430	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	34	ASN
1	A	56	GLN
1	A	205	HIS
1	A	225	ASN
1	A	236	ASN
1	A	289	GLN
1	A	328	GLN
1	A	358	ASN
1	A	400	ASN
1	A	425	ASN
1	B	289	GLN
1	B	298	ASN
1	B	340	GLN
1	B	358	ASN
1	B	397	ASN
1	B	406	GLN
1	B	429	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.