Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:58 PM 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 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 (i) symbol.

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

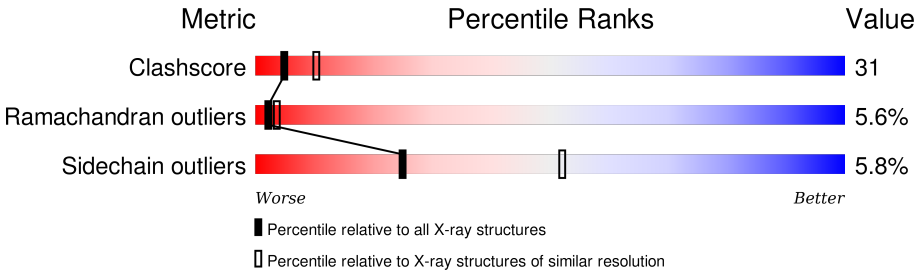
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	432	57% 37% 5%
1	B	432	47% 43% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6860 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 TRIGGER FACTOR.

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

- Molecule 2 is water.

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

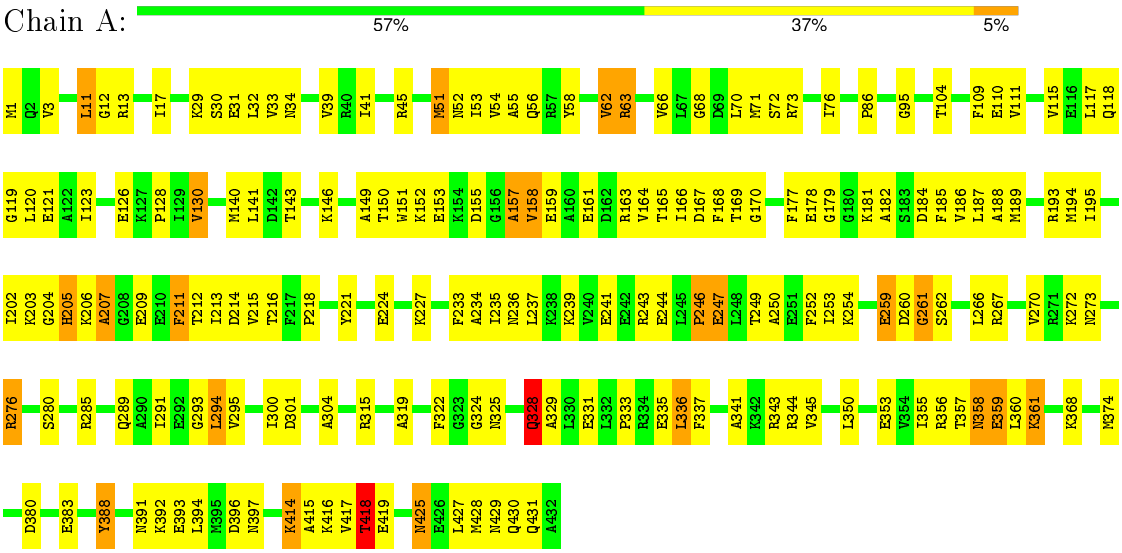
3 Residue-property plots (i)

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

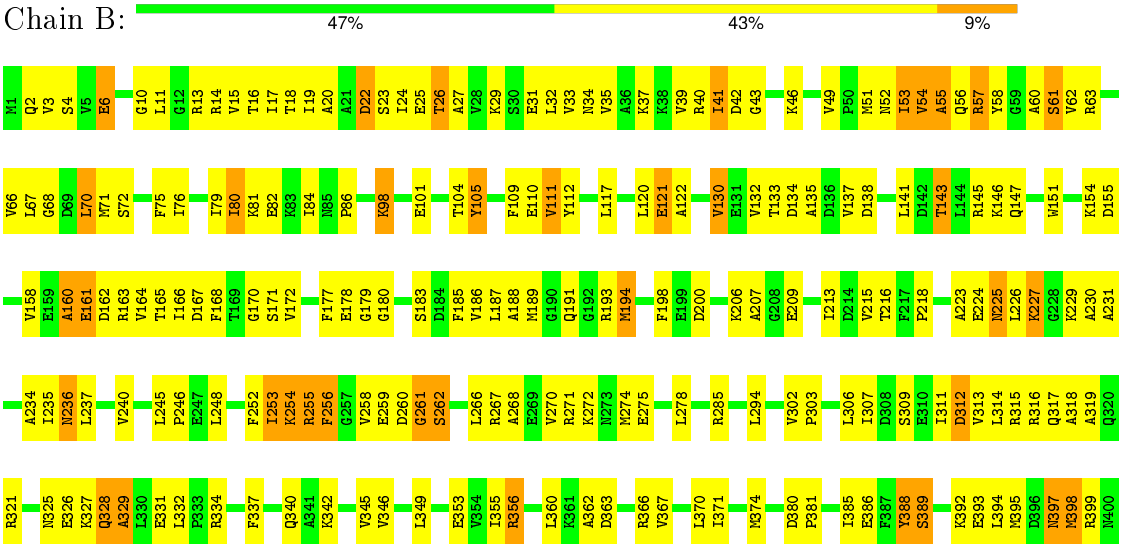
- Molecule 1: TRIGGER FACTOR

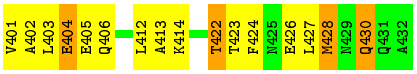
Chain A:



- Molecule 1: TRIGGER FACTOR

Chain B:




V401
A402
L403
E404
E405
Q406
L412
A413
K414
T422
T423
F424
N425
E426
L427
M428
N429
Q430
Q431
A432

4 Data and refinement statistics (i)

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, α, β, γ	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^2)	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(^{o})	Ideal(^{o})
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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 31.

All (425) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG3	1:A:45:ARG:HH11	1.54	0.71
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	3	6
1	B	430/432 (100%)	339 (79%)	62 (14%)	29 (7%)	1	2
All	All	860/864 (100%)	707 (82%)	105 (12%)	48 (6%)	2	3

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLY
1	A	247	GLU
1	A	261	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	55	ALA
1	B	227	LYS
1	B	218	PRO

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	359/348 (103%)	339 (94%)	20 (6%)	26	54
1	B	359/348 (103%)	337 (94%)	22 (6%)	23	49
All	All	718/696 (103%)	676 (94%)	42 (6%)	25	52

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	406	GLN
1	B	429	ASN

5.3.3 RNA

There are no RNA molecules 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.