Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:14 PM EDT

PDB ID	:	1G7R
Title	:	X-RAY STRUCTURE OF TRANSLATION INITIATION FACTOR IF2/EIF5B
Authors	:	Roll-Mecak, A.; Cao, C.; Dever, T.E.; Burley, S.K.
Deposited on	:	2000-11-14
Resolution	:	2.20 Å(reported)

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

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

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

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

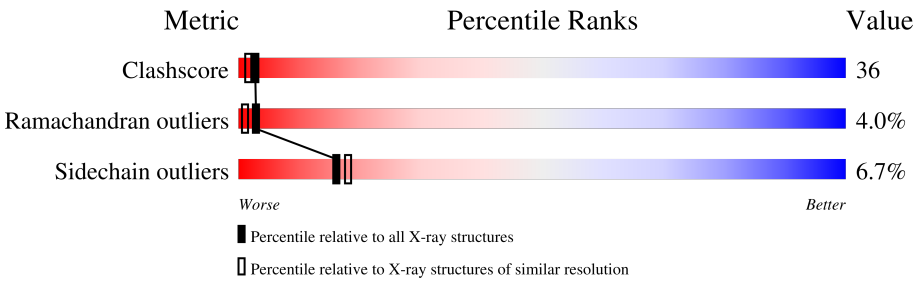
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	594	45% 43% 6% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4539 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 TRANSLATION INITIATION FACTOR IF2/EIF5B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	559	4274	2721	717	818	1	17	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O26359
A	49	MSE	MET	modified residue	UNP O26359
A	120	MSE	MET	modified residue	UNP O26359
A	147	MSE	MET	modified residue	UNP O26359
A	211	MSE	MET	modified residue	UNP O26359
A	213	MSE	MET	modified residue	UNP O26359
A	247	MSE	MET	modified residue	UNP O26359
A	266	MSE	MET	modified residue	UNP O26359
A	267	MSE	MET	modified residue	UNP O26359
A	289	MSE	MET	modified residue	UNP O26359
A	319	MSE	MET	modified residue	UNP O26359
A	373	MSE	MET	modified residue	UNP O26359
A	438	MSE	MET	modified residue	UNP O26359
A	457	MSE	MET	modified residue	UNP O26359
A	498	MSE	MET	modified residue	UNP O26359
A	511	MSE	MET	modified residue	UNP O26359
A	529	MSE	MET	modified residue	UNP O26359
A	574	MSE	MET	modified residue	UNP O26359
A	590	MSE	MET	modified residue	UNP O26359

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	265	265	265	0	0

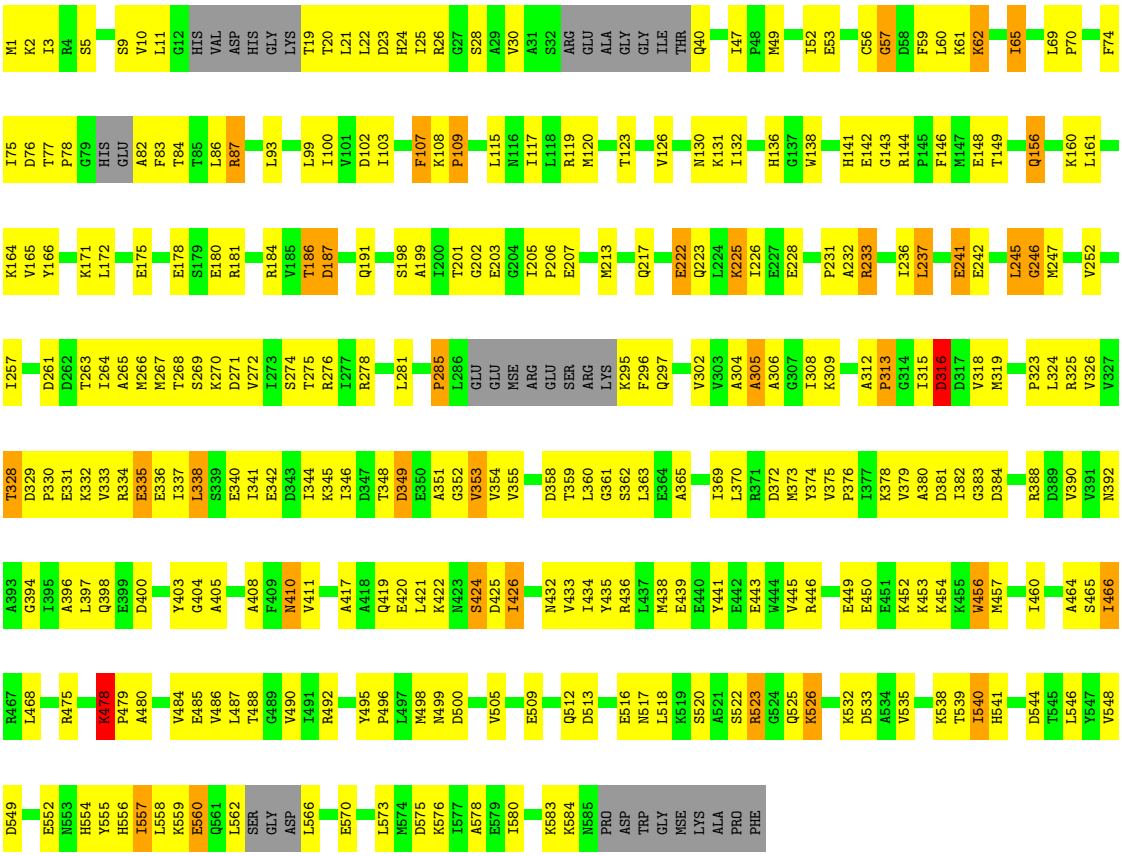
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: TRANSLATION INITIATION FACTOR IF2/EIF5B

Chain A: 45% 43% 6% 6%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.32Å 54.35Å 90.98Å 104.90° 101.33° 98.75°	Depositor
Resolution (Å)	22.00 – 2.20	Depositor
% Data completeness (in resolution range)	92.0 (22.00-2.20)	Depositor
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4539	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

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	0.56	2/4316 (0.0%)	0.76	4/5809 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	GLU	CB-CG	-5.24	1.42	1.52
1	A	222	GLU	CB-CG	-5.22	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	LYS	C-N-CD	7.09	143.28	128.40
1	A	313	PRO	N-CA-C	6.15	128.09	112.10
1	A	478	LYS	N-CA-C	-5.50	96.16	111.00
1	A	480	ALA	N-CA-C	-5.38	96.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Sidechain

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	4274	0	4296	305	0
2	A	265	0	0	26	0
All	All	4539	0	4296	305	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 36.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:HG21	1:A:203:GLU:OE2	1.60	1.01
1:A:20:THR:HA	1:A:23:ASP:HB2	1.45	0.97
1:A:478:LYS:CG	1:A:479:PRO:HD3	1.93	0.97
1:A:268:THR:HG22	1:A:271:ASP:H	1.29	0.95
1:A:338:LEU:O	1:A:342:GLU:HG2	1.67	0.95
1:A:186:THR:H	1:A:191:GLN:HE22	1.00	0.94
1:A:278:ARG:HD3	2:A:713:HOH:O	1.70	0.91
1:A:267:MSE:HE2	1:A:337:ILE:HG22	1.55	0.89
1:A:268:THR:HG23	1:A:270:LYS:H	1.37	0.88
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.39	0.88
1:A:223:GLN:HG3	2:A:706:HOH:O	1.73	0.87
1:A:268:THR:CG2	1:A:271:ASP:H	1.88	0.86
1:A:475:ARG:HE	1:A:478:LYS:HB3	1.40	0.86
1:A:186:THR:H	1:A:191:GLN:NE2	1.76	0.84
1:A:186:THR:O	1:A:191:GLN:NE2	2.10	0.84
1:A:231:PRO:HB3	1:A:326:VAL:HG23	1.59	0.84
1:A:65:ILE:HG13	1:A:217:GLN:OE1	1.79	0.82
1:A:267:MSE:HE3	1:A:341:ILE:HG13	1.62	0.81
1:A:233:ARG:HG3	1:A:233:ARG:NH1	1.94	0.81
1:A:558:LEU:HD12	1:A:559:LYS:N	1.96	0.81
1:A:370:LEU:HD23	1:A:438:MSE:HE1	1.61	0.81
1:A:478:LYS:CG	1:A:479:PRO:CD	2.57	0.81
1:A:490:VAL:HG22	1:A:522:SER:HB3	1.62	0.81
1:A:117:ILE:HA	1:A:120:MSE:HE3	1.62	0.80
1:A:397:LEU:HD12	1:A:426:ILE:HG23	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLN:HA	1:A:422:LYS:NZ	1.99	0.77
1:A:580:ILE:HA	1:A:583:LYS:HE2	1.65	0.77
1:A:237:LEU:HD21	1:A:252:VAL:HG23	1.66	0.76
1:A:131:LYS:HE3	2:A:877:HOH:O	1.84	0.76
1:A:484:VAL:O	1:A:526:LYS:HA	1.87	0.75
1:A:267:MSE:CE	1:A:337:ILE:HG22	2.16	0.75
1:A:144:ARG:HD3	1:A:148:GLU:OE2	1.87	0.74
1:A:373:MSE:SE	1:A:438:MSE:HE3	2.38	0.73
1:A:164:LYS:HG2	2:A:730:HOH:O	1.87	0.73
1:A:86:LEU:HG	1:A:93:LEU:HB3	1.71	0.71
1:A:201:THR:HG22	1:A:203:GLU:H	1.55	0.71
1:A:21:LEU:HD22	1:A:100:ILE:HD11	1.71	0.70
1:A:268:THR:HG22	1:A:271:ASP:N	2.06	0.70
1:A:233:ARG:HG2	2:A:868:HOH:O	1.90	0.70
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.05	0.70
1:A:245:LEU:O	1:A:246:GLY:O	2.09	0.69
1:A:201:THR:CG2	1:A:203:GLU:HG3	2.22	0.69
1:A:315:ILE:O	1:A:316:ASP:HB2	1.93	0.69
1:A:156:GLN:H	1:A:156:GLN:NE2	1.92	0.68
1:A:449:GLU:O	1:A:452:LYS:CG	2.42	0.68
1:A:156:GLN:H	1:A:156:GLN:HE21	1.42	0.67
1:A:26:ARG:O	1:A:30:VAL:HG23	1.94	0.67
1:A:452:LYS:CG	1:A:453:LYS:H	2.08	0.67
1:A:52:ILE:HG22	1:A:60:LEU:HD11	1.77	0.67
1:A:107:PHE:CG	1:A:171:LYS:HG2	2.30	0.66
1:A:505:VAL:HG11	1:A:540:ILE:HG13	1.78	0.66
1:A:231:PRO:HB3	1:A:326:VAL:CG2	2.23	0.66
1:A:49:MSE:CE	1:A:69:LEU:HB2	2.26	0.66
1:A:82:ALA:C	1:A:84:THR:H	2.00	0.65
1:A:267:MSE:HE2	1:A:337:ILE:CG2	2.25	0.65
1:A:351:ALA:HB1	1:A:376:PRO:HB2	1.77	0.65
1:A:60:LEU:HD21	1:A:213:MSE:HG3	1.78	0.65
1:A:452:LYS:CG	1:A:453:LYS:N	2.59	0.65
1:A:475:ARG:HH21	1:A:478:LYS:CG	2.10	0.64
1:A:354:VAL:HG22	1:A:379:VAL:HB	1.78	0.64
1:A:390:VAL:HG13	1:A:426:ILE:HD12	1.79	0.64
1:A:268:THR:HG21	2:A:888:HOH:O	1.98	0.63
1:A:384:ASP:HA	1:A:411:VAL:HG22	1.79	0.63
1:A:345:LYS:O	1:A:380:ALA:HB3	1.98	0.63
1:A:488:THR:OG1	1:A:573:LEU:HD22	1.98	0.63
1:A:130:ASN:HD21	1:A:199:ALA:H	1.47	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:CD2	1:A:438:MSE:HE1	2.29	0.62
1:A:397:LEU:HD11	1:A:425:ASP:HB3	1.80	0.62
1:A:466:ILE:HD12	1:A:486:VAL:HA	1.81	0.62
1:A:130:ASN:ND2	1:A:131:LYS:H	1.98	0.62
1:A:22:LEU:HB3	1:A:26:ARG:NH1	2.15	0.62
1:A:419:GLN:HA	1:A:422:LYS:HZ3	1.63	0.62
1:A:275:THR:CG2	1:A:313:PRO:HD2	2.30	0.61
1:A:404:GLY:O	1:A:426:ILE:HA	1.99	0.61
1:A:201:THR:HG21	1:A:203:GLU:HG3	1.81	0.61
1:A:369:ILE:O	1:A:372:ASP:HB3	2.00	0.61
1:A:441:TYR:O	1:A:445:VAL:HG23	2.01	0.61
1:A:557:ILE:HG22	1:A:557:ILE:O	2.00	0.61
1:A:464:ALA:HB3	1:A:548:VAL:CG2	2.31	0.60
1:A:486:VAL:O	1:A:523:ARG:O	2.20	0.60
1:A:198:SER:O	1:A:201:THR:O	2.20	0.60
1:A:352:GLY:O	1:A:353:VAL:HB	2.01	0.60
1:A:304:ALA:O	1:A:305:ALA:CB	2.49	0.60
1:A:329:ASP:O	1:A:333:VAL:HG23	2.02	0.60
1:A:77:THR:HG22	1:A:82:ALA:N	2.17	0.60
1:A:419:GLN:HA	1:A:422:LYS:HZ2	1.66	0.60
1:A:315:ILE:O	1:A:316:ASP:CB	2.50	0.60
1:A:516:GLU:HG3	2:A:912:HOH:O	2.02	0.60
1:A:539:THR:HG21	2:A:949:HOH:O	2.02	0.60
1:A:21:LEU:O	1:A:25:ILE:HG13	2.03	0.59
1:A:119:ARG:HG3	1:A:120:MSE:N	2.18	0.59
1:A:226:ILE:HD13	1:A:304:ALA:HB3	1.83	0.59
1:A:408:ALA:HB1	1:A:411:VAL:HG12	1.84	0.59
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.67	0.58
1:A:328:THR:HG22	1:A:329:ASP:N	2.17	0.58
1:A:9:SER:HG	1:A:83:PHE:HD1	1.51	0.58
1:A:505:VAL:HG13	1:A:539:THR:HG22	1.85	0.58
1:A:359:THR:HG23	1:A:362:SER:H	1.69	0.58
1:A:82:ALA:HB1	1:A:84:THR:HG22	1.86	0.58
1:A:513:ASP:HB2	1:A:518:LEU:HD11	1.84	0.58
1:A:22:LEU:HA	1:A:25:ILE:HB	1.84	0.58
1:A:225:LYS:HD2	1:A:225:LYS:C	2.23	0.58
1:A:365:ALA:O	1:A:369:ILE:HG13	2.03	0.58
1:A:84:THR:O	1:A:87:ARG:HG2	2.04	0.58
1:A:160:LYS:HE3	2:A:853:HOH:O	2.03	0.57
1:A:363:LEU:HD21	1:A:380:ALA:HB1	1.84	0.57
1:A:499:ASN:OD1	1:A:500:ASP:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:O	1:A:26:ARG:HG3	2.04	0.57
1:A:267:MSE:HE3	1:A:341:ILE:CG1	2.31	0.57
1:A:344:ILE:HG22	1:A:344:ILE:O	2.03	0.57
1:A:419:GLN:O	1:A:422:LYS:HG2	2.05	0.56
1:A:268:THR:HG23	1:A:269:SER:N	2.19	0.56
1:A:47:ILE:HD13	1:A:74:PHE:CD1	2.41	0.56
1:A:82:ALA:O	1:A:84:THR:N	2.32	0.56
1:A:349:ASP:O	1:A:378:LYS:HE2	2.06	0.56
1:A:522:SER:O	1:A:525:GLN:HB2	2.06	0.56
1:A:108:LYS:HB3	1:A:109:PRO:CD	2.36	0.56
1:A:424:SER:O	1:A:425:ASP:HB2	2.06	0.56
1:A:237:LEU:HD21	1:A:252:VAL:CG2	2.34	0.55
1:A:358:ASP:HB3	1:A:410:ASN:O	2.06	0.55
1:A:457:MSE:HA	1:A:460:ILE:HD12	1.89	0.55
1:A:558:LEU:O	1:A:562:LEU:HB2	2.07	0.55
1:A:268:THR:HG23	1:A:270:LYS:N	2.15	0.55
1:A:47:ILE:HD13	1:A:74:PHE:CE1	2.42	0.55
1:A:161:LEU:HD23	1:A:161:LEU:C	2.26	0.55
1:A:540:ILE:HD11	1:A:546:LEU:HD11	1.88	0.55
1:A:187:ASP:HB2	2:A:787:HOH:O	2.06	0.54
1:A:509:GLU:OE1	1:A:532:LYS:HB2	2.07	0.54
1:A:466:ILE:CD1	1:A:486:VAL:HA	2.37	0.54
1:A:445:VAL:O	1:A:449:GLU:HB2	2.06	0.54
1:A:496:PRO:HB2	1:A:549:ASP:HB3	1.89	0.54
1:A:464:ALA:HB3	1:A:548:VAL:HG21	1.89	0.54
1:A:465:SER:O	1:A:466:ILE:HD12	2.08	0.54
1:A:241:GLU:HG3	1:A:242:GLU:H	1.73	0.54
1:A:65:ILE:HD13	1:A:213:MSE:HE3	1.90	0.53
1:A:486:VAL:HB	1:A:523:ARG:O	2.08	0.53
1:A:275:THR:HG22	1:A:313:PRO:HD2	1.89	0.53
1:A:285:PRO:HD3	1:A:297:GLN:NE2	2.24	0.53
1:A:82:ALA:HB1	1:A:84:THR:CG2	2.39	0.53
1:A:141:HIS:HB2	1:A:149:THR:HG23	1.90	0.53
1:A:228:GLU:HG2	2:A:728:HOH:O	2.08	0.53
1:A:475:ARG:NE	1:A:478:LYS:HB3	2.18	0.53
1:A:40:GLN:N	2:A:858:HOH:O	2.41	0.53
1:A:226:ILE:CD1	1:A:304:ALA:HB3	2.37	0.53
1:A:302:VAL:HG13	1:A:306:ALA:CB	2.38	0.53
1:A:492:ARG:HB2	1:A:495:TYR:CE2	2.44	0.53
1:A:276:ARG:NH2	2:A:867:HOH:O	2.41	0.53
1:A:345:LYS:O	1:A:380:ALA:O	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:CG	1:A:454:LYS:N	2.72	0.53
1:A:435:TYR:O	1:A:439:GLU:HG3	2.09	0.52
1:A:25:ILE:HA	1:A:28:SER:OG	2.09	0.52
1:A:47:ILE:N	1:A:47:ILE:HD12	2.24	0.52
1:A:186:THR:N	1:A:191:GLN:HE22	1.85	0.52
1:A:236:ILE:HD13	1:A:318:VAL:HG11	1.90	0.52
1:A:62:LYS:NZ	1:A:62:LYS:HB3	2.25	0.52
1:A:419:GLN:C	1:A:421:LEU:H	2.13	0.52
1:A:505:VAL:CG1	1:A:540:ILE:HG13	2.40	0.52
1:A:466:ILE:HG22	1:A:546:LEU:HB2	1.91	0.52
1:A:201:THR:HG22	1:A:203:GLU:N	2.21	0.51
1:A:143:GLY:HA2	1:A:202:GLY:HA3	1.91	0.51
1:A:378:LYS:HD2	1:A:396:ALA:HB2	1.93	0.51
1:A:24:HIS:HB3	2:A:873:HOH:O	2.11	0.51
1:A:492:ARG:NH1	1:A:520:SER:HB2	2.25	0.51
1:A:75:ILE:HG13	1:A:86:LEU:CD2	2.41	0.50
1:A:268:THR:HG22	1:A:271:ASP:O	2.12	0.50
1:A:82:ALA:C	1:A:84:THR:N	2.65	0.50
1:A:178:GLU:HA	1:A:178:GLU:OE1	2.11	0.50
1:A:233:ARG:HD2	1:A:325:ARG:HE	1.75	0.50
1:A:475:ARG:HH21	1:A:478:LYS:CB	2.25	0.50
1:A:381:ASP:OD1	1:A:382:ILE:N	2.40	0.50
1:A:241:GLU:HG3	1:A:242:GLU:N	2.26	0.50
1:A:443:GLU:O	1:A:446:ARG:HB3	2.12	0.50
1:A:201:THR:HG21	1:A:203:GLU:CG	2.42	0.50
1:A:156:GLN:HE21	1:A:156:GLN:N	2.09	0.49
1:A:82:ALA:O	1:A:84:THR:HG22	2.12	0.49
1:A:86:LEU:CG	1:A:93:LEU:HB3	2.42	0.49
1:A:146:PHE:N	1:A:207:GLU:OE2	2.46	0.49
1:A:468:LEU:HD23	1:A:484:VAL:HG22	1.95	0.49
1:A:453:LYS:CG	1:A:454:LYS:H	2.26	0.49
1:A:580:ILE:O	1:A:583:LYS:HG2	2.13	0.49
1:A:25:ILE:O	1:A:28:SER:HB2	2.13	0.49
1:A:86:LEU:CD1	1:A:93:LEU:HD23	2.43	0.49
1:A:86:LEU:HD12	1:A:93:LEU:HD23	1.95	0.48
1:A:205:ILE:N	1:A:206:PRO:CD	2.76	0.48
1:A:369:ILE:HG22	1:A:438:MSE:HE2	1.95	0.48
1:A:453:LYS:O	1:A:456:TRP:HD1	1.96	0.48
1:A:264:ILE:HB	1:A:324:LEU:HD11	1.94	0.48
1:A:242:GLU:OE1	1:A:295:LYS:HE3	2.13	0.48
1:A:556:HIS:C	1:A:558:LEU:H	2.16	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HG13	1:A:309:LYS:N	2.28	0.48
1:A:335:GLU:HB2	2:A:806:HOH:O	2.13	0.48
1:A:201:THR:HG22	1:A:203:GLU:HG3	1.95	0.47
1:A:222:GLU:HB2	2:A:811:HOH:O	2.14	0.47
1:A:466:ILE:HG13	1:A:484:VAL:CG1	2.45	0.47
1:A:319:MSE:CE	1:A:360:LEU:HD22	2.45	0.47
1:A:424:SER:O	1:A:425:ASP:CB	2.63	0.47
1:A:304:ALA:O	1:A:305:ALA:HB3	2.13	0.47
1:A:345:LYS:NZ	2:A:855:HOH:O	2.48	0.47
1:A:485:GLU:HG3	1:A:526:LYS:CG	2.45	0.47
1:A:352:GLY:O	1:A:353:VAL:CB	2.62	0.47
1:A:120:MSE:SE	1:A:369:ILE:HG12	2.65	0.47
1:A:202:GLY:HA2	1:A:205:ILE:HD12	1.97	0.47
1:A:265:ALA:C	1:A:266:MSE:HG3	2.34	0.47
1:A:559:LYS:O	1:A:560:GLU:CB	2.63	0.46
1:A:201:THR:HG22	1:A:202:GLY:N	2.30	0.46
1:A:397:LEU:HD11	1:A:425:ASP:CB	2.44	0.46
1:A:323:PRO:HG3	1:A:340:GLU:OE2	2.16	0.46
1:A:24:HIS:O	1:A:24:HIS:ND1	2.48	0.46
1:A:498:MSE:SE	1:A:549:ASP:OD1	2.83	0.46
1:A:11:LEU:N	1:A:11:LEU:HD12	2.31	0.46
1:A:231:PRO:CB	1:A:326:VAL:CG2	2.94	0.46
1:A:264:ILE:O	1:A:274:SER:HA	2.15	0.46
1:A:457:MSE:SE	1:A:460:ILE:HD12	2.66	0.46
1:A:1:MSE:SE	1:A:225:LYS:HD3	2.65	0.46
1:A:107:PHE:HZ	1:A:115:LEU:CD1	2.29	0.46
1:A:397:LEU:O	1:A:397:LEU:HD23	2.16	0.45
1:A:478:LYS:O	1:A:479:PRO:C	2.51	0.45
1:A:465:SER:HB3	1:A:487:LEU:HB2	1.99	0.45
1:A:2:LYS:CG	1:A:3:ILE:N	2.80	0.45
1:A:388:ARG:O	1:A:392:ASN:ND2	2.50	0.45
1:A:93:LEU:O	1:A:93:LEU:HD12	2.16	0.45
1:A:369:ILE:CG2	1:A:438:MSE:HE2	2.47	0.45
1:A:485:GLU:CD	1:A:526:LYS:HE2	2.37	0.45
1:A:143:GLY:HA2	1:A:202:GLY:CA	2.47	0.44
1:A:87:ARG:HB3	2:A:900:HOH:O	2.17	0.44
1:A:541:HIS:O	1:A:544:ASP:HB2	2.18	0.44
1:A:21:LEU:O	1:A:25:ILE:CG1	2.64	0.44
1:A:53:GLU:HA	1:A:60:LEU:HD12	2.00	0.44
1:A:75:ILE:HG13	1:A:86:LEU:HD22	2.00	0.44
1:A:241:GLU:HG2	2:A:930:HOH:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:HE2	1:A:309:LYS:HB2	1.80	0.44
1:A:373:MSE:SE	1:A:438:MSE:CE	3.14	0.44
1:A:49:MSE:HE2	1:A:69:LEU:HB2	1.98	0.44
1:A:432:ASN:OD1	1:A:433:VAL:HG23	2.18	0.44
1:A:460:ILE:HG23	1:A:554:HIS:ND1	2.33	0.44
1:A:434:ILE:O	1:A:438:MSE:HG2	2.18	0.44
1:A:77:THR:CG2	1:A:82:ALA:N	2.81	0.43
1:A:180:GLU:CG	1:A:184:ARG:HB2	2.48	0.43
1:A:566:LEU:HB3	1:A:570:GLU:HB2	1.99	0.43
1:A:86:LEU:CD1	1:A:93:LEU:HB3	2.48	0.43
1:A:236:ILE:HD11	1:A:266:MSE:SE	2.68	0.43
1:A:576:LYS:O	1:A:580:ILE:HG13	2.18	0.43
1:A:233:ARG:HD2	1:A:325:ARG:NE	2.33	0.43
1:A:403:TYR:O	1:A:405:ALA:N	2.46	0.43
1:A:464:ALA:HB3	1:A:548:VAL:HG23	1.99	0.43
1:A:232:ALA:HB2	1:A:257:ILE:C	2.39	0.43
1:A:247:MSE:HG2	1:A:316:ASP:HA	2.00	0.43
1:A:312:ALA:HA	1:A:313:PRO:HD3	1.67	0.43
1:A:359:THR:OG1	1:A:360:LEU:N	2.51	0.43
1:A:452:LYS:O	1:A:453:LYS:C	2.57	0.43
1:A:558:LEU:HD12	1:A:558:LEU:C	2.38	0.43
1:A:47:ILE:HG22	1:A:52:ILE:HG13	2.00	0.43
1:A:419:GLN:CG	1:A:420:GLU:N	2.82	0.43
1:A:180:GLU:HG3	1:A:181:ARG:N	2.34	0.43
1:A:281:LEU:O	1:A:308:ILE:HD12	2.19	0.43
1:A:332:LYS:HG2	1:A:336:GLU:OE2	2.19	0.43
1:A:272:VAL:HG21	1:A:338:LEU:HD12	2.00	0.43
1:A:450:GLU:C	1:A:452:LYS:H	2.21	0.43
1:A:146:PHE:H	1:A:207:GLU:CD	2.22	0.43
1:A:454:LYS:O	1:A:457:MSE:HB2	2.19	0.43
1:A:136:HIS:HB2	2:A:796:HOH:O	2.18	0.42
1:A:355:VAL:O	1:A:380:ALA:HA	2.19	0.42
1:A:76:ASP:HA	2:A:715:HOH:O	2.18	0.42
1:A:512:GLN:HA	1:A:516:GLU:O	2.19	0.42
1:A:132:ILE:HD12	1:A:138:TRP:CZ2	2.54	0.42
1:A:261:ASP:O	1:A:276:ARG:NE	2.51	0.42
1:A:56:CYS:O	1:A:57:GLY:O	2.37	0.42
1:A:532:LYS:O	1:A:533:ASP:HB2	2.20	0.42
1:A:5:SER:OG	1:A:70:PRO:HB2	2.18	0.42
1:A:575:ASP:O	1:A:578:ALA:HB3	2.19	0.42
1:A:19:THR:C	1:A:21:LEU:N	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:HIS:CE1	2:A:866:HOH:O	2.72	0.42
1:A:84:THR:OG1	1:A:361:GLY:C	2.58	0.41
1:A:120:MSE:SE	1:A:369:ILE:CG1	3.18	0.41
1:A:325:ARG:NE	2:A:789:HOH:O	2.53	0.41
1:A:383:GLY:C	1:A:411:VAL:HG21	2.41	0.41
1:A:408:ALA:HB1	1:A:411:VAL:CG1	2.48	0.41
1:A:552:GLU:O	1:A:555:TYR:HB3	2.19	0.41
1:A:130:ASN:HD22	1:A:131:LYS:H	1.67	0.41
1:A:373:MSE:O	1:A:375:VAL:N	2.53	0.41
1:A:485:GLU:HG3	1:A:526:LYS:HG3	2.01	0.41
1:A:556:HIS:O	1:A:558:LEU:N	2.49	0.41
1:A:69:LEU:HA	1:A:70:PRO:HD3	1.82	0.41
1:A:10:VAL:O	1:A:78:PRO:HA	2.21	0.41
1:A:186:THR:N	1:A:191:GLN:NE2	2.56	0.41
1:A:56:CYS:HB2	1:A:60:LEU:HD12	2.02	0.41
1:A:325:ARG:HH11	1:A:325:ARG:CG	2.32	0.41
1:A:102:ASP:OD2	1:A:131:LYS:HD2	2.20	0.41
1:A:120:MSE:CE	1:A:369:ILE:HD11	2.51	0.41
1:A:263:THR:OG1	1:A:276:ARG:HD3	2.21	0.41
1:A:352:GLY:HA3	1:A:403:TYR:HB3	2.03	0.41
1:A:517:ASN:CG	2:A:745:HOH:O	2.59	0.41
1:A:76:ASP:CA	2:A:715:HOH:O	2.69	0.41
1:A:296:PHE:CZ	1:A:309:LYS:HE3	2.56	0.41
1:A:330:PRO:O	1:A:334:ARG:HB2	2.21	0.41
1:A:180:GLU:HG3	1:A:184:ARG:HB2	2.02	0.40
1:A:268:THR:CG2	1:A:270:LYS:H	2.19	0.40
1:A:275:THR:HG21	1:A:312:ALA:HB1	2.03	0.40
1:A:103:ILE:HD11	1:A:165:VAL:HG23	2.03	0.40
1:A:19:THR:C	1:A:21:LEU:H	2.24	0.40
1:A:325:ARG:HD2	2:A:788:HOH:O	2.21	0.40
1:A:394:GLY:O	1:A:397:LEU:N	2.55	0.40
1:A:417:ALA:O	1:A:421:LEU:HB2	2.22	0.40
1:A:261:ASP:O	1:A:276:ARG:CZ	2.70	0.40
1:A:424:SER:HB3	1:A:425:ASP:H	1.75	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	547/594 (92%)	479 (88%)	46 (8%)	22 (4%)	3 1

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLY
1	A	305	ALA
1	A	316	ASP
1	A	374	TYR
1	A	424	SER
1	A	523	ARG
1	A	584	LYS
1	A	57	GLY
1	A	142	GLU
1	A	285	PRO
1	A	348	THR
1	A	353	VAL
1	A	478	LYS
1	A	557	ILE
1	A	61	LYS
1	A	346	ILE
1	A	526	LYS
1	A	538	LYS
1	A	187	ASP
1	A	560	GLU
1	A	398	GLN
1	A	109	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	450/488 (92%)	420 (93%)	30 (7%)	16 18

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PHE
1	A	62	LYS
1	A	65	ILE
1	A	87	ARG
1	A	99	LEU
1	A	107	PHE
1	A	123	THR
1	A	126	VAL
1	A	156	GLN
1	A	172	LEU
1	A	175	GLU
1	A	186	THR
1	A	225	LYS
1	A	233	ARG
1	A	237	LEU
1	A	241	GLU
1	A	245	LEU
1	A	316	ASP
1	A	328	THR
1	A	331	GLU
1	A	338	LEU
1	A	349	ASP
1	A	400	ASP
1	A	410	ASN
1	A	426	ILE
1	A	436	ARG
1	A	456	TRP
1	A	466	ILE
1	A	535	VAL
1	A	540	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	141	HIS
1	A	156	GLN
1	A	191	GLN
1	A	223	GLN
1	A	297	GLN
1	A	392	ASN
1	A	410	ASN
1	A	512	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.