Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 09:50 PM EDT

PDB ID	:	2E0W
Title	:	T391A precursor mutant protein of gamma-Glutamyltranspeptidase from Escherichia coli
Authors	:	Okada, T.; Wada, K.; Fukuyama, K.
Deposited on	:	2006-10-16
Resolution	:	2.55 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 ⓘ 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 ⓘ) were used in the production of this report:

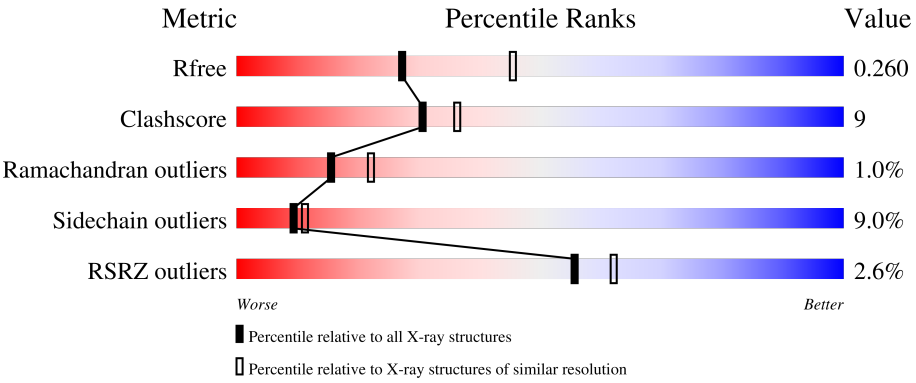
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	556	2% 68% 19% · 11%
1	B	556	3% 70% 18% · 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7468 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 Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3697	2333	620	730	14			
1	B	500	Total	C	N	O	S	0	0	0
			3718	2344	627	732	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	ALA	THR	engineered mutation	UNP P18956
B	391	ALA	THR	engineered mutation	UNP P18956

- Molecule 2 is water.

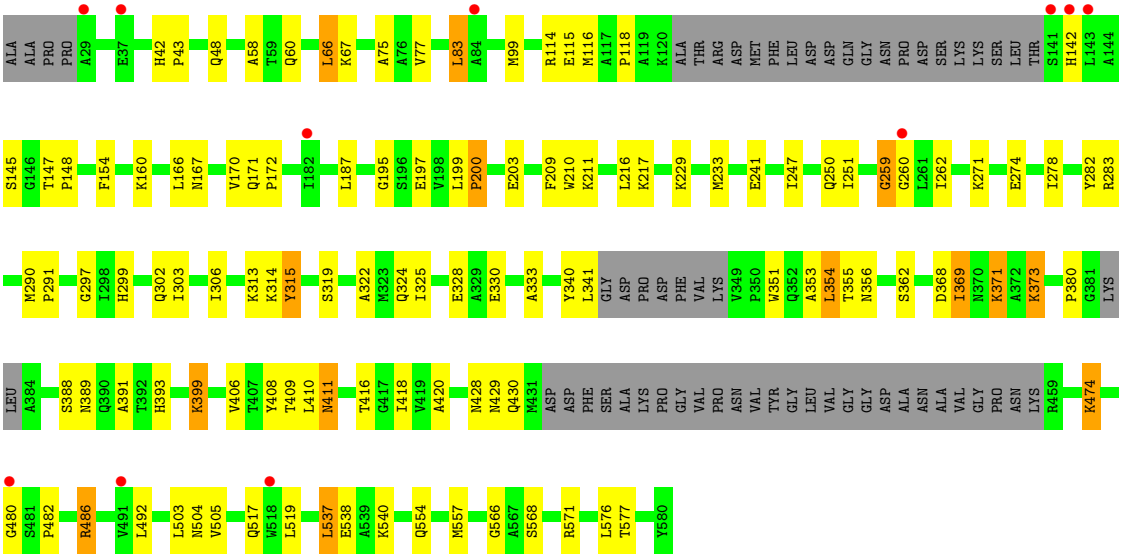
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	28	Total	O	0	0
			28	28		
2	B	25	Total	O	0	0
			25	25		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

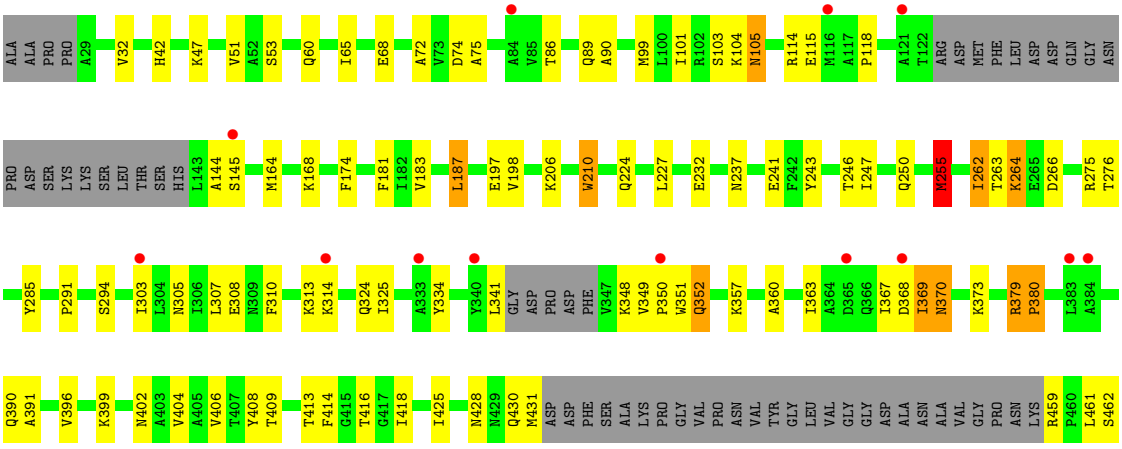
• Molecule 1: Gamma-glutamyltranspeptidase

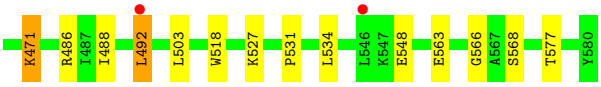
Chain A:



• Molecule 1: Gamma-glutamyltranspeptidase

Chain B:




K471
R486
I487
I488
L492
L503
W518
K527
P531
L534
L546
K547
E548
E563
G566
A567
S568
T577
Y580

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.60Å 134.60Å 118.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 29.17 – 2.55	Depositor EDS
% Data completeness (in resolution range)	92.0 (30.00-2.55) 85.3 (29.17-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.23 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.270 0.211 , 0.260	Depositor DCC
R_{free} test set	1521 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	0.48	0/3767	0.63	1/5112 (0.0%)
1	B	0.47	0/3789	0.63	0/5143
All	All	0.47	0/7556	0.63	1/10255 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	537	LEU	CA-CB-CG	5.54	128.05	115.30

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	3697	0	3627	65	0
1	B	3718	0	3639	72	0
2	A	28	0	0	0	0
2	B	25	0	0	0	0
All	All	7468	0	7266	135	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 9.

All (135) 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:416:THR:HB	1:B:418:ILE:HD12	1.43	1.00
1:B:379:ARG:HB3	1:B:380:PRO:CD	2.06	0.86
1:B:303:ILE:HG21	1:B:492:LEU:HD11	1.57	0.85
1:A:303:ILE:HD11	1:A:333:ALA:HB3	1.57	0.84
1:A:278:ILE:HD13	1:A:291:PRO:HA	1.61	0.82
1:B:74:ASP:HB3	1:B:164:MET:HE2	1.64	0.79
1:A:486:ARG:HH11	1:A:517:GLN:HE22	1.41	0.69
1:B:428:ASN:HD22	1:B:430:GLN:HB2	1.59	0.68
1:A:351:TRP:O	1:A:354:LEU:HD22	1.94	0.68
1:A:58:ALA:HB2	1:A:83:LEU:HD13	1.77	0.67
1:B:74:ASP:HB3	1:B:164:MET:CE	2.23	0.67
1:A:325:ILE:HD11	1:A:369:ILE:HD12	1.75	0.67
1:A:351:TRP:O	1:A:354:LEU:CD2	2.43	0.67
1:A:340:TYR:O	1:A:341:LEU:HB2	1.95	0.67
1:A:58:ALA:CB	1:A:83:LEU:HD13	2.24	0.66
1:B:428:ASN:ND2	1:B:430:GLN:HB2	2.11	0.66
1:A:299:HIS:HE2	1:A:351:TRP:HE1	1.44	0.66
1:A:66:LEU:HD13	1:A:75:ALA:HB2	1.77	0.65
1:A:554:GLN:NE2	1:A:568:SER:OG	2.29	0.65
1:B:416:THR:HB	1:B:418:ILE:CD1	2.22	0.64
1:A:303:ILE:HD11	1:A:333:ALA:CB	2.25	0.64
1:A:314:LYS:O	1:A:315:TYR:CG	2.52	0.62
1:A:195:GLY:O	1:A:200:PRO:HD3	2.00	0.62
1:B:379:ARG:CB	1:B:380:PRO:CD	2.78	0.60
1:A:354:LEU:HD22	1:A:354:LEU:H	1.67	0.59
1:A:302:GLN:O	1:A:306:ILE:HG13	2.02	0.59
1:B:118:PRO:HG3	1:B:262:ILE:HG23	1.84	0.59
1:B:237:ASN:HB2	1:B:241:GLU:HB2	1.85	0.57
1:A:145:SER:HB3	1:A:428:ASN:O	2.04	0.57
1:B:72:ALA:HB1	1:B:404:VAL:HG23	1.84	0.57
1:A:118:PRO:HB3	1:A:262:ILE:HG22	1.87	0.57
1:B:391:ALA:CB	1:B:409:THR:HB	2.35	0.57
1:B:416:THR:CB	1:B:418:ILE:HD12	2.28	0.56
1:B:379:ARG:HB3	1:B:380:PRO:HD3	1.88	0.56
1:A:115:GLU:H	1:A:115:GLU:CD	2.09	0.56
1:B:145:SER:O	1:B:428:ASN:ND2	2.39	0.56
1:A:166:LEU:O	1:A:170:VAL:HG23	2.05	0.55
1:B:369:ILE:HG23	1:B:370:ASN:HD22	1.71	0.55
1:B:379:ARG:HB3	1:B:380:PRO:HD2	1.87	0.55
1:B:247:ILE:HA	1:B:250:GLN:HE21	1.70	0.55
1:B:303:ILE:CG2	1:B:492:LEU:HD11	2.34	0.55
1:B:351:TRP:O	1:B:352:GLN:CB	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:OG1	1:A:410:LEU:O	2.16	0.55
1:A:114:ARG:NH2	1:A:430:GLN:HE22	2.05	0.55
1:A:282:TYR:CZ	1:A:283:ARG:NH1	2.75	0.54
1:B:379:ARG:CB	1:B:380:PRO:HD3	2.38	0.54
1:B:488:ILE:O	1:B:492:LEU:HB2	2.08	0.54
1:A:566:GLY:HA3	1:A:577:THR:HG21	1.90	0.53
1:A:160:LYS:HE2	1:A:274:GLU:OE1	2.09	0.53
1:B:103:SER:HA	1:B:402:ASN:HD22	1.73	0.53
1:A:303:ILE:HG21	1:A:492:LEU:HD21	1.90	0.53
1:B:379:ARG:CG	1:B:380:PRO:HD3	2.39	0.52
1:B:305:ASN:HB3	1:B:360:ALA:CB	2.39	0.52
1:B:65:ILE:HG23	1:B:164:MET:HE2	1.92	0.52
1:A:229:LYS:O	1:A:233:MET:HG2	2.10	0.51
1:B:51:VAL:HG22	1:B:396:VAL:HG22	1.92	0.51
1:B:89:GLN:HB3	1:B:413:THR:HG23	1.91	0.51
1:A:299:HIS:ND1	1:A:302:GLN:NE2	2.59	0.51
1:B:104:LYS:H	1:B:402:ASN:ND2	2.09	0.51
1:B:90:ALA:HB2	1:B:390:GLN:HE21	1.75	0.51
1:A:303:ILE:CD1	1:A:333:ALA:CB	2.90	0.50
1:A:391:ALA:HB3	1:A:482:PRO:HB3	1.93	0.50
1:B:379:ARG:HG2	1:B:380:PRO:HD3	1.93	0.50
1:B:566:GLY:HA3	1:B:577:THR:HG21	1.93	0.50
1:A:505:VAL:HB	1:A:557:MET:HE2	1.93	0.50
1:A:354:LEU:CD2	1:A:354:LEU:H	2.24	0.50
1:A:233:MET:HB3	1:A:241:GLU:HG3	1.94	0.49
1:A:290:MET:O	1:A:297:GLY:HA3	2.12	0.49
1:A:554:GLN:HE22	1:A:568:SER:CB	2.25	0.49
1:B:243:TYR:O	1:B:264:LYS:NZ	2.46	0.49
1:A:315:TYR:HD1	1:A:322:ALA:HB2	1.77	0.48
1:B:324:GLN:HG2	1:B:369:ILE:O	2.13	0.48
1:B:145:SER:HB2	1:B:262:ILE:HD11	1.96	0.47
1:B:197:GLU:HB3	1:B:198:VAL:HG13	1.95	0.47
1:A:393:HIS:CE1	1:A:480:GLY:HA3	2.49	0.47
1:B:99:MET:HG3	1:B:406:VAL:HG22	1.95	0.47
1:B:391:ALA:HB2	1:B:409:THR:HB	1.96	0.47
1:A:99:MET:HG3	1:A:406:VAL:HG22	1.96	0.47
1:A:247:ILE:HA	1:A:250:GLN:HE21	1.79	0.47
1:A:303:ILE:CD1	1:A:330:GLU:HA	2.45	0.47
1:B:255:MET:HE1	1:B:262:ILE:N	2.29	0.47
1:A:209:PHE:O	1:A:216:LEU:HG	2.15	0.46
1:A:299:HIS:O	1:A:303:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HD13	1:A:75:ALA:CB	2.45	0.46
1:B:86:THR:HA	1:B:181:PHE:CZ	2.51	0.46
1:B:72:ALA:CB	1:B:404:VAL:HG23	2.45	0.46
1:B:174:PHE:CE1	1:B:232:GLU:HB2	2.51	0.46
1:A:319:SER:HB3	1:B:531:PRO:HG2	1.97	0.45
1:B:255:MET:HE3	1:B:255:MET:HB3	1.72	0.45
1:A:48:GLN:O	1:A:399:LYS:HA	2.17	0.45
1:B:369:ILE:HG23	1:B:370:ASN:ND2	2.31	0.45
1:B:99:MET:SD	1:B:101:ILE:HD11	2.57	0.44
1:B:348:LYS:HA	1:B:349:VAL:HA	1.61	0.44
1:B:115:GLU:OE1	1:B:430:GLN:NE2	2.51	0.44
1:A:411:ASN:HB3	1:A:429:ASN:OD1	2.18	0.44
1:B:164:MET:HB2	1:B:164:MET:HE3	1.76	0.44
1:A:145:SER:CB	1:A:428:ASN:O	2.66	0.43
1:B:334:TYR:OH	1:B:488:ILE:HB	2.18	0.43
1:A:474:LYS:HB2	1:A:474:LYS:NZ	2.33	0.43
1:A:142:HIS:HA	1:A:259:GLY:HA3	2.01	0.43
1:A:315:TYR:CD1	1:A:322:ALA:HB2	2.54	0.43
1:B:105:ASN:H	1:B:105:ASN:HD22	1.66	0.43
1:A:371:LYS:HE3	1:A:540:LYS:O	2.18	0.43
1:B:75:ALA:HB3	1:B:396:VAL:HG11	2.01	0.43
1:B:183:VAL:HG13	1:B:187:LEU:HB3	2.00	0.43
1:B:114:ARG:CZ	1:B:462:SER:HB2	2.49	0.42
1:B:390:GLN:OE1	1:B:390:GLN:HA	2.19	0.42
1:B:325:ILE:HD11	1:B:369:ILE:HG12	2.01	0.42
1:A:42:HIS:HA	1:A:43:PRO:HD3	1.88	0.42
1:B:308:GLU:OE1	1:B:357:LYS:HE2	2.19	0.42
1:B:47:LYS:HG2	1:B:563:GLU:OE1	2.19	0.42
1:A:303:ILE:HD12	1:A:330:GLU:HA	2.02	0.42
1:A:353:ALA:O	1:A:356:ASN:HB2	2.20	0.42
1:A:251:ILE:HA	1:A:420:ALA:HB1	2.02	0.41
1:A:571:ARG:O	1:B:42:HIS:HE1	2.03	0.41
1:B:285:TYR:CE1	1:B:471:LYS:HB2	2.55	0.41
1:B:263:THR:O	1:B:266:ASP:HB2	2.20	0.41
1:B:413:THR:HG22	1:B:414:PHE:CD2	2.55	0.41
1:B:276:THR:O	1:B:291:PRO:HG3	2.21	0.41
1:A:416:THR:HB	1:A:418:ILE:HD13	2.02	0.41
1:A:504:ASN:OD1	1:A:504:ASN:C	2.59	0.41
1:A:171:GLN:HB3	1:A:172:PRO:HD3	2.02	0.41
1:B:310:PHE:CD1	1:B:325:ILE:HD13	2.54	0.41
1:A:77:VAL:HG13	1:A:154:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:OE1	1:A:373:LYS:HG2	2.21	0.41
1:A:373:LYS:HG2	1:A:373:LYS:H	1.76	0.41
1:B:206:LYS:O	1:B:210:TRP:HB2	2.21	0.41
1:B:380:PRO:HD2	1:B:518:TRP:HH2	1.86	0.41
1:A:368:ASP:H	1:A:373:LYS:NZ	2.19	0.40
1:B:291:PRO:O	1:B:294:SER:HB3	2.20	0.40
1:B:351:TRP:O	1:B:352:GLN:HB2	2.20	0.40
1:B:144:ALA:HB1	1:B:431:MET:HB2	2.03	0.40
1:B:224:GLN:HB3	1:B:227:LEU:HB3	2.03	0.40
1:B:227:LEU:HD13	1:B:425:ILE:HD13	2.03	0.40
1:A:147:THR:HA	1:A:148:PRO:HD3	1.90	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	486/556 (87%)	454 (93%)	27 (6%)	5 (1%)	15	22
1	B	492/556 (88%)	457 (93%)	30 (6%)	5 (1%)	15	22
All	All	978/1112 (88%)	911 (93%)	57 (6%)	10 (1%)	15	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	379	ARG
1	B	380	PRO
1	A	259	GLY
1	A	380	PRO
1	B	350	PRO
1	A	315	TYR
1	A	411	ASN

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Mol	Chain	Res	Type
1	B	255	MET
1	B	352	GLN
1	A	260	GLY

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	385/440 (88%)	351 (91%)	34 (9%)	10 12
1	B	384/440 (87%)	349 (91%)	35 (9%)	9 11
All	All	769/880 (87%)	700 (91%)	69 (9%)	9 11

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	66	LEU
1	A	67	LYS
1	A	83	LEU
1	A	116	MET
1	A	167	ASN
1	A	187	LEU
1	A	197	GLU
1	A	199	LEU
1	A	200	PRO
1	A	203	GLU
1	A	210	TRP
1	A	211	LYS
1	A	217	LYS
1	A	271	LYS
1	A	313	LYS
1	A	324	GLN
1	A	354	LEU
1	A	355	THR
1	A	362	SER

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Mol	Chain	Res	Type
1	A	369	ILE
1	A	371	LYS
1	A	373	LYS
1	A	388	SER
1	A	389	ASN
1	A	399	LYS
1	A	408	TYR
1	A	474	LYS
1	A	486	ARG
1	A	503	LEU
1	A	519	LEU
1	A	537	LEU
1	A	538	GLU
1	A	576	LEU
1	B	32	VAL
1	B	53	SER
1	B	60	GLN
1	B	68	GLU
1	B	105	ASN
1	B	168	LYS
1	B	187	LEU
1	B	210	TRP
1	B	246	THR
1	B	255	MET
1	B	262	ILE
1	B	264	LYS
1	B	275	ARG
1	B	307	LEU
1	B	313	LYS
1	B	314	LYS
1	B	341	LEU
1	B	363	ILE
1	B	367	ILE
1	B	368	ASP
1	B	369	ILE
1	B	370	ASN
1	B	373	LYS
1	B	399	LYS
1	B	408	TYR
1	B	459	ARG
1	B	461	LEU
1	B	471	LYS

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Mol	Chain	Res	Type
1	B	486	ARG
1	B	492	LEU
1	B	503	LEU
1	B	527	LYS
1	B	534	LEU
1	B	548	GLU
1	B	568	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	302	GLN
1	A	324	GLN
1	A	352	GLN
1	A	370	ASN
1	A	430	GLN
1	A	517	GLN
1	A	542	GLN
1	A	554	GLN
1	B	42	HIS
1	B	60	GLN
1	B	105	ASN
1	B	107	ASN
1	B	201	ASN
1	B	250	GLN
1	B	370	ASN
1	B	390	GLN
1	B	402	ASN
1	B	428	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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, 95^{th} 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	496/556 (89%)	0.09	11 (2%)	62	68	29, 42, 55, 60	0
1	B	500/556 (89%)	0.14	15 (3%)	50	57	30, 43, 62, 67	0
All	All	996/1112 (89%)	0.12	26 (2%)	56	62	29, 42, 58, 67	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	SER	7.6
1	A	142	HIS	4.6
1	A	29	ALA	3.7
1	B	383	LEU	3.7
1	B	314	LYS	3.5
1	B	303	ILE	3.3
1	A	37	GLU	3.2
1	A	143	LEU	3.0
1	A	260	GLY	2.8
1	A	84	ALA	2.7
1	B	384	ALA	2.7
1	B	333	ALA	2.6
1	B	121	ALA	2.6
1	B	84	ALA	2.5
1	B	145	SER	2.5
1	A	518	TRP	2.4
1	B	368	ASP	2.4
1	B	365	ASP	2.3
1	B	116	MET	2.1
1	B	350	PRO	2.1
1	A	182	ILE	2.1
1	B	546	LEU	2.1
1	B	340	TYR	2.0
1	A	480	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	2.0
1	B	492	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.