Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2024 – 02:52 PM EST

PDB ID	:	1EFU
Title	:	ELONGATION FACTOR COMPLEX EF-TU/EF-TS FROM ESCHERICHIA COLI
Authors	:	Kawashima, T.; Berthet-Colominas, C.; Wulff, M.; Cusack, S.; Leberman, R.
Deposited on	:	1996-07-09
Resolution	:	2.50 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:

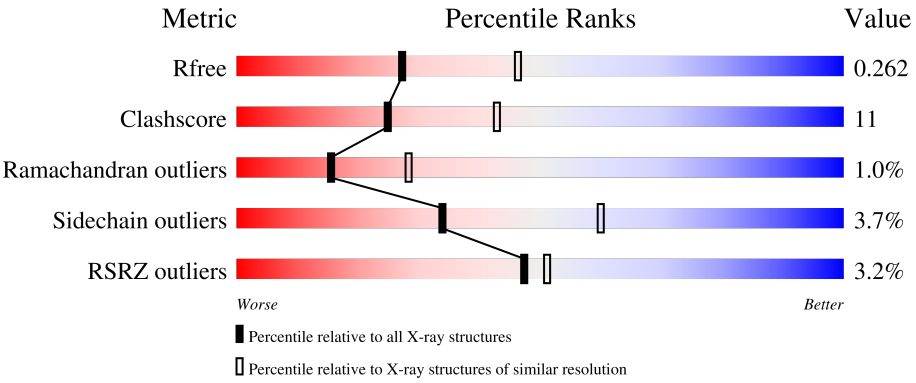
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	385	2% 68% 24% • 5%
1	C	385	6% 66% 26% • 5%
2	B	282	% 79% 19% •
2	D	282	3% 76% 23% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11023 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 ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	1
			2798	1772	479	534	13			
1	C	364	Total	C	N	O	S	0	0	1
			2798	1772	479	534	13			

- Molecule 2 is a protein called ELONGATION FACTOR TS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	S	0	0	0
			2122	1331	363	417	11			
2	D	282	Total	C	N	O	S	0	0	0
			2122	1331	363	417	11			

- Molecule 3 is water.

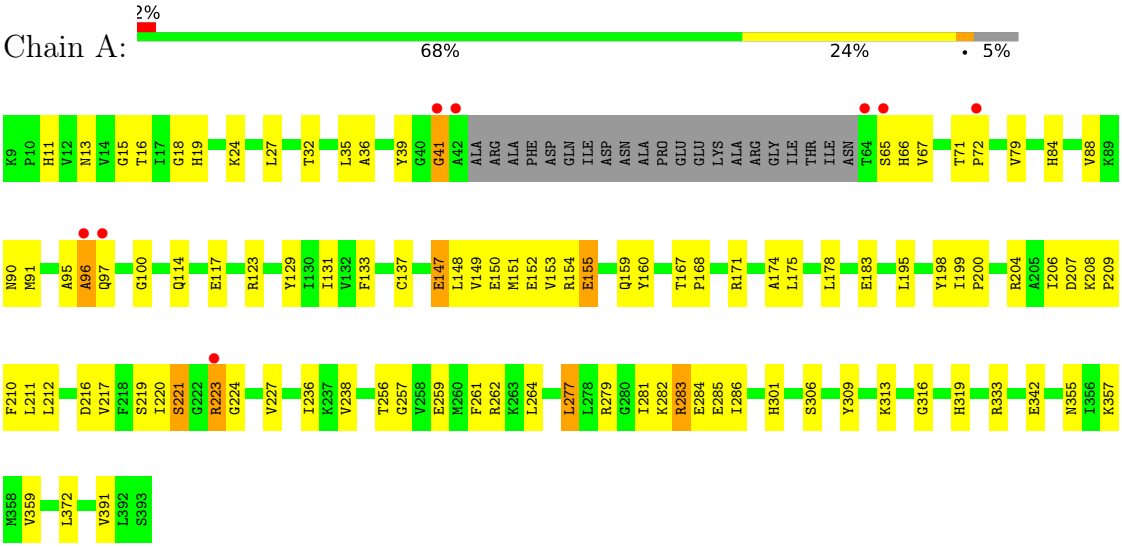
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	278	Total	O	0	0
			278	278		
3	B	342	Total	O	0	0
			342	342		
3	C	258	Total	O	0	0
			258	258		
3	D	305	Total	O	0	0
			305	305		

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.

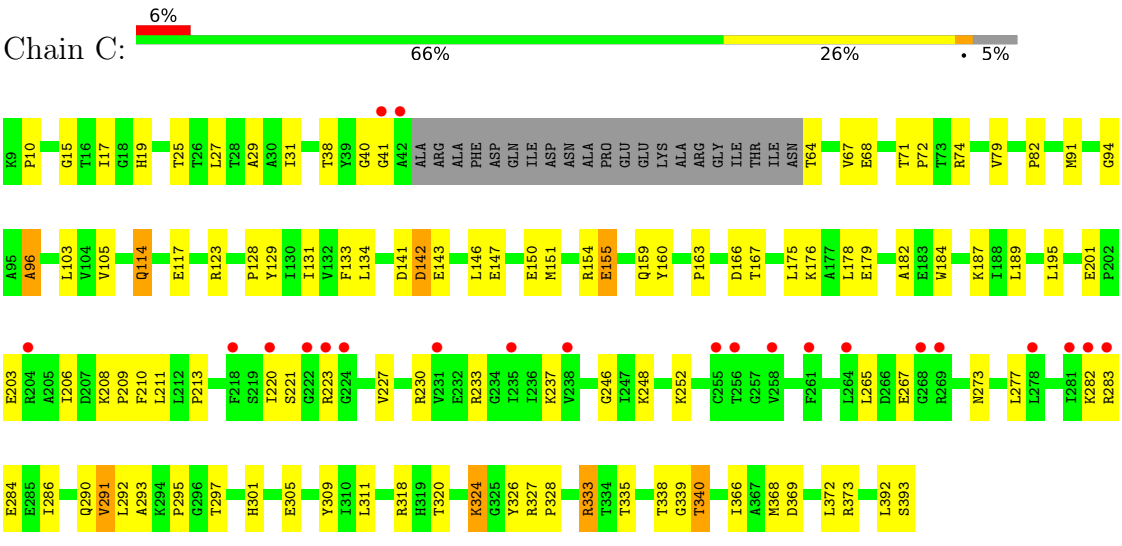
• Molecule 1: ELONGATION FACTOR TU

Chain A:



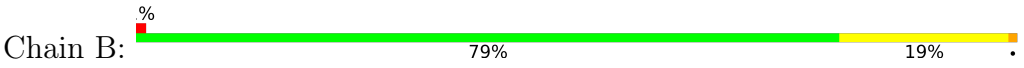
• Molecule 1: ELONGATION FACTOR TU

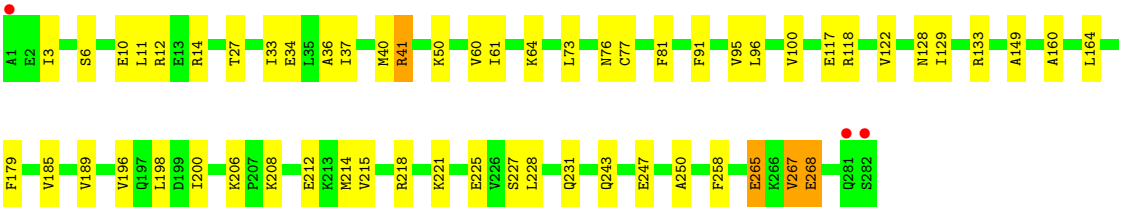
Chain C:



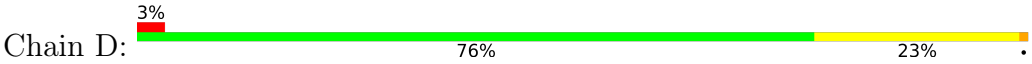
• Molecule 2: ELONGATION FACTOR TS

Chain B:





• Molecule 2: ELONGATION FACTOR TS



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.53Å 108.54Å 194.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 43.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 99.4 (43.66-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	9.91 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , 0.283 0.169 , 0.262	Depositor DCC
R_{free} test set	2749 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 129.0	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	0.95	EDS
Total number of atoms	11023	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.39	0/2850	0.69	0/3858
1	C	0.37	0/2850	0.66	0/3858
2	B	0.38	0/2143	0.66	1/2875 (0.0%)
2	D	0.38	0/2143	0.63	0/2875
All	All	0.38	0/9986	0.66	1/13466 (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})
2	B	265	GLU	N-CA-C	5.15	124.92	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	2798	0	2813	68	0
1	C	2798	0	2813	70	0
2	B	2122	0	2170	36	0
2	D	2122	0	2170	52	0
3	A	278	0	0	2	0
3	B	342	0	0	5	0
3	C	258	0	0	8	0
3	D	305	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11023	0	9966	213	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 11.

All (213) 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:C:114:GLN:H	1:C:114:GLN:HE21	1.24	0.85
2:D:3:ILE:HD12	2:D:26:LEU:HB3	1.68	0.76
1:C:178:LEU:HG	2:D:281:GLN:HB2	1.70	0.72
2:D:150:ARG:HH11	2:D:150:ARG:HG3	1.56	0.69
2:D:1:ALA:HB3	2:D:31:GLY:HA3	1.74	0.68
1:C:163:PRO:HB2	1:C:166:ASP:HB2	1.76	0.68
1:C:150:GLU:O	1:C:154:ARG:HG3	1.93	0.67
2:D:246:LYS:HE2	2:D:246:LYS:HA	1.75	0.67
2:D:222:PHE:O	2:D:225:GLU:HG2	1.94	0.67
2:D:11:LEU:HD13	2:D:33:ILE:HG13	1.77	0.67
1:C:25:THR:HG21	2:D:274:GLU:HG2	1.77	0.66
1:C:64:THR:HA	3:C:441:HOH:O	1.94	0.66
1:A:155:GLU:O	1:A:159:GLN:HG3	1.96	0.66
1:A:223:ARG:HG2	1:A:224:GLY:H	1.62	0.65
2:B:200:ILE:HG23	2:D:179:PHE:CE1	2.31	0.65
1:A:282:LYS:HB2	1:A:285:GLU:HG3	1.79	0.64
1:C:91:MET:HA	1:C:96:ALA:HB3	1.80	0.64
1:A:220:ILE:HG21	1:A:223:ARG:HD3	1.79	0.64
2:B:61:ILE:HD12	2:B:258:PHE:HB3	1.81	0.63
1:A:261:PHE:O	1:A:262:ARG:HG2	1.99	0.63
1:C:324:LYS:HD3	1:C:324:LYS:H	1.63	0.63
1:C:123:ARG:HD2	1:C:160:TYR:O	2.00	0.62
1:A:281:ILE:HG21	1:A:286:ILE:HD11	1.81	0.62
1:C:10:PRO:HB2	1:C:74:ARG:HG2	1.80	0.62
1:C:209:PRO:O	1:C:233:ARG:HG3	2.00	0.61
1:C:175:LEU:O	1:C:179:GLU:HG3	2.01	0.61
1:C:29:ALA:HB2	2:D:278:MET:HB2	1.83	0.61
1:A:71:THR:HB	1:A:72:PRO:HD2	1.82	0.61
1:C:209:PRO:HB3	1:C:297:THR:HG21	1.83	0.61
2:B:227:SER:O	2:B:231:GLN:HG3	2.00	0.60
2:B:198:LEU:HA	2:B:215:VAL:HG21	1.84	0.59
2:D:209:GLU:O	2:D:213:LYS:HG3	2.02	0.59
2:B:36:ALA:O	2:B:40:MET:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:LYS:HE2	2:B:214:MET:SD	2.43	0.58
1:C:19:HIS:HD2	3:D:342:HOH:O	1.85	0.58
1:C:19:HIS:HE1	3:C:450:HOH:O	1.85	0.58
1:C:176:LYS:HZ3	1:C:184:TRP:HE1	1.48	0.58
1:C:327:ARG:HH11	1:C:338:THR:HG21	1.68	0.58
2:D:107:VAL:HG22	3:D:491:HOH:O	2.04	0.57
1:C:27:LEU:O	1:C:31:ILE:HG13	2.04	0.57
2:D:269:THR:HA	3:D:537:HOH:O	2.03	0.57
1:C:94:GLY:HA2	1:C:373:ARG:CZ	2.34	0.57
2:B:117:GLU:HG3	3:B:613:HOH:O	2.03	0.57
1:C:210:PHE:HA	1:C:233:ARG:O	2.04	0.56
2:B:3:ILE:HG13	2:B:27:THR:HA	1.88	0.56
1:A:91:MET:HA	1:A:96:ALA:O	2.06	0.56
1:C:71:THR:HB	1:C:72:PRO:HD2	1.88	0.55
2:B:41:ARG:HB3	2:B:41:ARG:NH1	2.21	0.55
1:C:25:THR:HG22	2:D:278:MET:HG3	1.88	0.55
1:A:220:ILE:O	1:A:221:SER:HB2	2.07	0.55
2:B:14:ARG:HH11	2:B:14:ARG:HG2	1.72	0.55
2:D:61:ILE:HG12	2:D:260:VAL:HG23	1.88	0.55
1:C:114:GLN:H	1:C:114:GLN:NE2	2.00	0.55
1:A:227:VAL:HG11	1:A:286:ILE:HG21	1.89	0.54
1:C:208:LYS:HB2	1:C:233:ARG:HB2	1.89	0.54
2:B:12:ARG:NH2	3:B:1083:HOH:O	2.40	0.54
1:A:210:PHE:CE1	1:A:236:ILE:HB	2.42	0.54
2:B:267:VAL:O	2:B:268:GLU:HB2	2.07	0.54
1:C:114:GLN:HE21	1:C:114:GLN:N	2.01	0.54
1:A:18:GLY:N	1:A:24:LYS:HD3	2.23	0.54
1:A:15:GLY:HA2	1:A:79:VAL:O	2.08	0.54
1:A:84:HIS:O	1:A:88:VAL:HG23	2.08	0.54
1:C:147:GLU:O	1:C:151:MET:HG2	2.08	0.54
1:C:213:PRO:HA	1:C:291:VAL:HG23	1.88	0.54
1:A:217:VAL:HG22	1:A:227:VAL:HG12	1.91	0.53
1:C:211:LEU:HA	1:C:292:LEU:O	2.09	0.53
1:A:211:LEU:HD23	1:A:212:LEU:N	2.24	0.53
3:B:1053:HOH:O	2:D:188:GLU:HB3	2.09	0.53
1:C:155:GLU:O	1:C:159:GLN:HG3	2.08	0.53
1:A:131:ILE:HD12	1:A:195:LEU:HD23	1.91	0.53
1:C:220:ILE:O	1:C:221:SER:HB3	2.08	0.53
1:C:237:LYS:HG2	1:C:267:GLU:HB3	1.91	0.53
1:A:123:ARG:HD2	1:A:160:TYR:O	2.09	0.52
1:C:230:ARG:HA	1:C:273:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:HG2	2:B:81:PHE:O	2.10	0.52
2:B:185:VAL:HG12	2:B:189:VAL:CG2	2.40	0.52
2:D:107:VAL:HG11	2:D:133:ARG:HA	1.92	0.52
2:B:179:PHE:CE1	2:D:200:ILE:HG23	2.44	0.51
1:A:66:HIS:HB3	1:A:79:VAL:HG12	1.92	0.51
2:B:11:LEU:HD13	2:B:33:ILE:HG23	1.92	0.51
1:A:11:HIS:HE1	1:A:13:ASN:ND2	2.07	0.51
1:A:95:ALA:O	1:A:96:ALA:HB2	2.11	0.51
1:C:146:LEU:O	1:C:150:GLU:HG3	2.11	0.50
1:C:227:VAL:HG11	1:C:286:ILE:HG21	1.92	0.50
1:C:282:LYS:HG2	1:C:284:GLU:HG2	1.93	0.50
2:D:192:LYS:O	2:D:196:VAL:HG23	2.12	0.49
1:C:318:ARG:NH1	1:C:320:THR:O	2.44	0.49
2:B:185:VAL:HG12	2:B:189:VAL:HG23	1.94	0.49
2:B:243:GLN:O	2:B:247:GLU:HG2	2.12	0.49
1:A:206:ILE:HD12	3:A:596:HOH:O	2.13	0.48
2:D:227:SER:O	2:D:231:GLN:HG3	2.12	0.48
2:D:154:LEU:O	2:D:255:PHE:HA	2.13	0.48
1:C:29:ALA:CB	2:D:278:MET:HB2	2.42	0.48
1:C:178:LEU:O	2:D:281:GLN:HB3	2.13	0.48
2:D:11:LEU:HD22	2:D:26:LEU:HG	1.95	0.48
2:D:150:ARG:HG3	2:D:150:ARG:NH1	2.20	0.48
2:D:233:PHE:CE2	2:D:235:MET:HB2	2.48	0.48
1:C:252:LYS:HE2	1:C:295:PRO:HB3	1.96	0.48
1:A:36:ALA:HA	1:A:41:GLY:N	2.29	0.47
1:A:100:GLY:HA3	1:A:199:ILE:HD13	1.97	0.47
1:A:313:LYS:HG3	1:A:319:HIS:CD2	2.49	0.47
1:A:301:HIS:CD2	1:A:391:VAL:HG11	2.49	0.47
2:B:179:PHE:HE1	2:D:200:ILE:HG23	1.79	0.47
1:A:223:ARG:NH1	1:A:277:LEU:HD11	2.29	0.47
2:D:168:ILE:O	2:D:172:VAL:HG23	2.15	0.47
2:D:23:LYS:HG3	2:D:24:LYS:HE2	1.97	0.47
1:A:91:MET:HG3	1:A:97:GLN:OE1	2.14	0.47
1:A:204:ARG:HB2	1:A:207:ASP:OD2	2.14	0.47
2:B:160:ALA:HB2	2:B:250:ALA:HB1	1.96	0.47
1:C:176:LYS:NZ	1:C:184:TRP:HE1	2.12	0.47
1:A:223:ARG:HG3	1:A:277:LEU:HD21	1.96	0.47
2:B:73:LEU:HD12	2:B:133:ARG:O	2.15	0.47
2:B:34:GLU:HG3	3:B:1181:HOH:O	2.14	0.47
1:A:11:HIS:HE1	1:A:13:ASN:HD21	1.62	0.46
2:B:60:VAL:HG12	2:B:149:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:CYS:SG	1:A:171:ARG:HB3	2.56	0.46
1:C:114:GLN:HA	1:C:117:GLU:OE1	2.15	0.46
1:A:129:TYR:CE2	1:A:200:PRO:HD2	2.50	0.46
2:D:91:PHE:O	2:D:95:VAL:HG23	2.16	0.46
2:B:221:LYS:O	2:B:225:GLU:HG3	2.16	0.46
1:A:39:TYR:CE1	1:A:72:PRO:HD3	2.50	0.46
1:A:174:ALA:O	1:A:178:LEU:HB2	2.16	0.46
1:A:220:ILE:HD12	1:A:223:ARG:HH11	1.80	0.46
1:C:223:ARG:HG3	1:C:277:LEU:HD11	1.98	0.46
1:A:316:GLY:HA2	2:D:237:PRO:HB2	1.98	0.46
2:B:208:LYS:O	2:B:212:GLU:HG3	2.16	0.46
2:D:80:ASP:O	2:D:84:LYS:HG3	2.16	0.46
2:D:246:LYS:HE2	2:D:246:LYS:CA	2.45	0.46
1:C:340:THR:HG22	3:C:502:HOH:O	2.16	0.46
1:A:19:HIS:HD2	1:A:114:GLN:HE21	1.63	0.45
2:D:23:LYS:HG3	2:D:24:LYS:CE	2.47	0.45
2:D:24:LYS:HE2	2:D:24:LYS:HA	1.98	0.45
1:A:256:THR:CG2	1:A:279:ARG:HB2	2.46	0.45
1:C:203:GLU:HA	3:C:587:HOH:O	2.16	0.45
1:A:220:ILE:HD12	1:A:223:ARG:NH1	2.31	0.45
1:C:248:LYS:HB3	1:C:248:LYS:NZ	2.32	0.45
1:C:27:LEU:HD22	1:C:133:PHE:CD2	2.52	0.45
1:A:147:GLU:O	1:A:151:MET:SD	2.74	0.45
1:C:213:PRO:HG3	1:C:333:ARG:HD3	1.98	0.45
1:A:284:GLU:H	1:A:284:GLU:CD	2.21	0.44
2:B:91:PHE:O	2:B:95:VAL:HG23	2.16	0.44
2:B:218:ARG:HD3	3:B:696:HOH:O	2.17	0.44
2:D:194:TYR:CE1	2:D:198:LEU:HD22	2.52	0.44
1:A:256:THR:HG23	1:A:279:ARG:HB2	2.00	0.44
1:C:326:TYR:HB3	3:C:551:HOH:O	2.17	0.44
2:D:61:ILE:HD12	2:D:258:PHE:HB3	1.99	0.44
1:C:141:ASP:O	1:C:142:ASP:HB2	2.17	0.44
2:D:150:ARG:HA	2:D:150:ARG:HD2	1.80	0.44
1:A:281:ILE:HG21	1:A:286:ILE:CD1	2.48	0.44
2:B:33:ILE:O	2:B:37:ILE:HG13	2.18	0.44
2:D:176:LYS:HE2	2:D:257:ARG:NH2	2.33	0.44
1:C:206:ILE:HG12	3:C:403:HOH:O	2.18	0.44
2:D:132:ARG:NH2	2:D:262:GLU:O	2.49	0.44
2:D:107:VAL:HG13	2:D:134:VAL:HG12	1.99	0.44
1:A:198:TYR:O	1:A:200:PRO:HD3	2.18	0.43
1:C:67:VAL:HG12	1:C:68:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:GLY:O	1:C:290:GLN:HG2	2.17	0.43
1:C:206:ILE:HG23	3:C:403:HOH:O	2.19	0.43
2:D:122:VAL:HG13	2:D:127:GLU:O	2.18	0.43
1:A:259:GLU:HB3	1:A:264:LEU:HD13	2.00	0.43
1:C:10:PRO:HB3	1:C:201:GLU:HG3	2.00	0.43
2:B:196:VAL:HG22	2:D:192:LYS:HB3	2.01	0.43
1:A:309:TYR:HD1	1:A:355:ASN:OD1	2.02	0.43
2:B:50:LYS:HE3	2:B:50:LYS:HB2	1.64	0.43
2:B:76:ASN:O	2:B:129:ILE:HA	2.19	0.43
1:A:238:VAL:HG22	1:A:257:GLY:HA2	2.01	0.42
1:A:90:ASN:O	1:A:95:ALA:N	2.53	0.42
1:C:154:ARG:NH2	1:C:167:THR:O	2.53	0.42
2:B:64:LYS:HB3	2:B:100:VAL:HG21	2.02	0.42
1:C:210:PHE:O	1:C:293:ALA:HA	2.19	0.42
1:C:305:GLU:HG3	1:C:392:LEU:HD21	2.02	0.42
2:D:3:ILE:HG23	2:D:26:LEU:HD13	2.02	0.42
1:C:38:THR:HG21	1:C:189:LEU:HD11	2.02	0.42
1:A:35:LEU:HD22	1:A:39:TYR:HE2	1.85	0.42
1:A:150:GLU:O	1:A:154:ARG:HG3	2.20	0.42
1:A:27:LEU:HD13	1:A:133:PHE:CE2	2.55	0.41
1:A:223:ARG:HG2	1:A:224:GLY:N	2.31	0.41
1:A:306:SER:O	1:A:357:LYS:HA	2.20	0.41
1:A:149:VAL:O	1:A:153:VAL:HG23	2.20	0.41
1:A:282:LYS:HB3	1:A:284:GLU:OE2	2.21	0.41
2:B:14:ARG:HG2	2:B:14:ARG:NH1	2.36	0.41
2:D:166:LYS:HE3	3:D:408:HOH:O	2.20	0.41
2:B:118:ARG:O	2:B:122:VAL:HG23	2.20	0.41
1:C:15:GLY:HA2	1:C:79:VAL:O	2.20	0.41
1:C:17:ILE:O	1:C:103:LEU:HD12	2.20	0.41
2:D:194:TYR:HE1	2:D:198:LEU:HD22	1.86	0.41
1:A:219:SER:HB3	1:A:283:ARG:HB2	2.03	0.41
2:B:200:ILE:HG23	2:D:179:PHE:HE1	1.81	0.41
1:C:366:ILE:HG22	1:C:368:MET:CE	2.51	0.41
1:A:32:THR:HG21	1:A:67:VAL:HG11	2.03	0.41
1:A:208:LYS:HB3	1:A:209:PRO:HD2	2.03	0.41
1:C:82:PRO:HD2	3:C:444:HOH:O	2.21	0.41
1:C:105:VAL:O	1:C:134:LEU:HA	2.20	0.41
1:C:309:TYR:HE2	1:C:311:LEU:HD23	1.86	0.41
1:C:338:THR:HG22	1:C:339:GLY:N	2.35	0.41
1:A:129:TYR:HB3	1:A:198:TYR:CE2	2.55	0.41
1:A:216:ASP:HA	3:A:602:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:HB2	1:A:359:VAL:HB	2.03	0.41
2:B:77:CYS:HA	2:B:128:ASN:O	2.21	0.41
2:D:198:LEU:O	2:D:202:MET:HG2	2.21	0.41
1:A:148:LEU:O	1:A:152:GLU:HG3	2.21	0.40
1:C:128:PRO:HB2	1:C:129:TYR:CE1	2.55	0.40
1:C:187:LYS:HD3	1:C:187:LYS:HA	1.90	0.40
2:D:70:GLY:O	2:D:136:ALA:HA	2.21	0.40
1:A:219:SER:HB3	1:A:283:ARG:HG3	2.03	0.40
1:A:167:THR:HA	1:A:168:PRO:HD3	1.86	0.40
1:A:257:GLY:O	1:A:277:LEU:HB2	2.21	0.40
1:A:282:LYS:N	1:A:282:LYS:HD2	2.37	0.40
1:C:131:ILE:HD12	1:C:195:LEU:HD23	2.03	0.40
2:D:60:VAL:HG21	2:D:62:LYS:HE2	2.03	0.40
2:D:64:LYS:HB3	2:D:100:VAL:HG21	2.03	0.40
2:D:259:GLU:HB3	2:D:262:GLU:HG3	2.04	0.40
1:C:301:HIS:HB3	1:C:393:SER:OXT	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	360/385 (94%)	340 (94%)	15 (4%)	5 (1%)	11 20
1	C	360/385 (94%)	336 (93%)	18 (5%)	6 (2%)	9 16
2	B	280/282 (99%)	272 (97%)	6 (2%)	2 (1%)	22 39
2	D	280/282 (99%)	270 (96%)	10 (4%)	0	100 100
All	All	1280/1334 (96%)	1218 (95%)	49 (4%)	13 (1%)	15 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	96	ALA
1	A	333	ARG
1	C	96	ALA
1	C	182	ALA
1	C	40	GLY
1	C	41	GLY
1	C	142	ASP
1	C	333	ARG
2	B	268	GLU
1	A	41	GLY
1	A	221	SER
2	B	267	VAL

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	302/318 (95%)	293 (97%)	9 (3%)	41	68
1	C	302/318 (95%)	290 (96%)	12 (4%)	31	56
2	B	219/219 (100%)	212 (97%)	7 (3%)	39	65
2	D	219/219 (100%)	208 (95%)	11 (5%)	24	46
All	All	1042/1074 (97%)	1003 (96%)	39 (4%)	34	60

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	147	GLU
1	A	155	GLU
1	A	175	LEU
1	A	183	GLU
1	A	223	ARG
1	A	277	LEU
1	A	283	ARG
1	A	372	LEU

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Mol	Chain	Res	Type
2	B	6	SER
2	B	10	GLU
2	B	41	ARG
2	B	96	LEU
2	B	164	LEU
2	B	228	LEU
2	B	265	GLU
1	C	114	GLN
1	C	143	GLU
1	C	155	GLU
1	C	265	LEU
1	C	283	ARG
1	C	291	VAL
1	C	324	LYS
1	C	328	PRO
1	C	335	THR
1	C	340	THR
1	C	369	ASP
1	C	372	LEU
2	D	10	GLU
2	D	96	LEU
2	D	107	VAL
2	D	150	ARG
2	D	153	VAL
2	D	164	LEU
2	D	183	GLU
2	D	191	GLU
2	D	208	LYS
2	D	228	LEU
2	D	268	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	13	ASN
1	A	19	HIS
1	A	84	HIS
1	C	13	ASN
1	C	19	HIS
1	C	75	HIS
1	C	114	GLN

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Mol	Chain	Res	Type
2	D	39	ASN
2	D	281	GLN

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 monosaccharides 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

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	364/385 (94%)	-0.35	8 (2%) 62 65	9, 31, 74, 152	0
1	C	364/385 (94%)	0.13	22 (6%) 21 22	9, 36, 95, 153	0
2	B	282/282 (100%)	-0.30	3 (1%) 80 82	8, 25, 62, 183	0
2	D	282/282 (100%)	-0.13	8 (2%) 53 56	10, 26, 76, 144	0
All	All	1292/1334 (96%)	-0.16	41 (3%) 47 51	8, 30, 86, 183	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	282	SER	15.7
1	C	42	ALA	14.4
2	D	282	SER	11.2
1	A	42	ALA	7.5
2	D	281	GLN	6.7
1	C	41	GLY	6.1
2	D	1	ALA	6.0
1	C	261	PHE	5.6
1	C	224	GLY	4.7
2	D	280	LYS	4.0
2	D	2	GLU	4.0
1	C	281	ILE	3.8
1	C	220	ILE	3.7
1	C	282	LYS	3.7
1	A	97	GLN	3.6
1	A	223	ARG	3.6
1	A	64	THR	3.4
1	C	256	THR	3.2
1	A	41	GLY	3.2
2	D	3	ILE	3.1
1	C	268	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	3.1
2	B	1	ALA	2.8
1	C	278	LEU	2.7
1	C	231	VAL	2.7
1	A	65	SER	2.6
1	C	269	ARG	2.4
1	C	238	VAL	2.4
1	C	204	ARG	2.4
2	D	7	LEU	2.4
1	C	283	ARG	2.2
1	C	223	ARG	2.2
2	D	279	SER	2.2
1	C	255	CYS	2.1
1	C	235	ILE	2.1
1	C	258	VAL	2.1
1	C	218	PHE	2.1
1	C	264	LEU	2.1
1	C	222	GLY	2.0
1	A	72	PRO	2.0
2	B	281	GLN	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.