



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:58 PM UTC

PDB ID : 3N50 / pdb_00003n50
Title : Human Early B-cell factor 3 (EBF3) IPT/TIG and HLHLH domains
Authors : Lehtio, L.; Siponen, M.I.; Arrowsmith, C.H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Schuler, H.; Schutz, P.; Svensson, L.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Wahlberg, E.; Weigelt, J.; Welin, M.; Wisniewska, M.; Berglund, H.; Structural Genomics Consortium (SGC)
Deposited on : 2010-05-24
Resolution : 3.10 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:

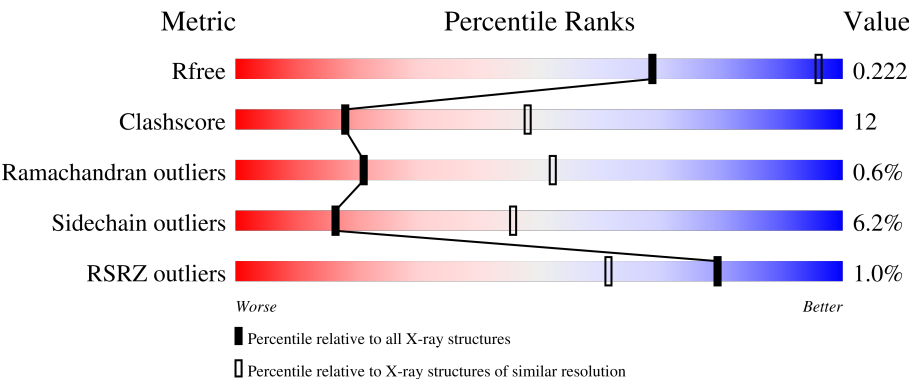
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	159	53%30%•16%
1	B	159	% 75%19%...
1	C	159	2% 58%32%•8%
1	D	159	% 70%25%..

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Mol	Chain	Length	Quality of chain
1	E	159	% 56% 33% • 8%
1	F	159	% 72% 22% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6892 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 Transcription factor COE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1038	673	177	184	4			
1	B	154	Total	C	N	O	S	0	0	0
			1199	774	206	215	4			
1	C	146	Total	C	N	O	S	0	0	0
			1127	729	192	202	4			
1	D	154	Total	C	N	O	S	0	0	0
			1199	774	206	215	4			
1	E	146	Total	C	N	O	S	0	0	0
			1130	733	193	200	4			
1	F	154	Total	C	N	O	S	0	0	0
			1199	774	206	215	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	-	expression tag	UNP Q9H4W6
A	249	MET	-	expression tag	UNP Q9H4W6
A	250	SER	-	expression tag	UNP Q9H4W6
A	251	GLU	-	expression tag	UNP Q9H4W6
B	248	SER	-	expression tag	UNP Q9H4W6
B	249	MET	-	expression tag	UNP Q9H4W6
B	250	SER	-	expression tag	UNP Q9H4W6
B	251	GLU	-	expression tag	UNP Q9H4W6
C	248	SER	-	expression tag	UNP Q9H4W6
C	249	MET	-	expression tag	UNP Q9H4W6
C	250	SER	-	expression tag	UNP Q9H4W6
C	251	GLU	-	expression tag	UNP Q9H4W6
D	248	SER	-	expression tag	UNP Q9H4W6
D	249	MET	-	expression tag	UNP Q9H4W6
D	250	SER	-	expression tag	UNP Q9H4W6
D	251	GLU	-	expression tag	UNP Q9H4W6
E	248	SER	-	expression tag	UNP Q9H4W6

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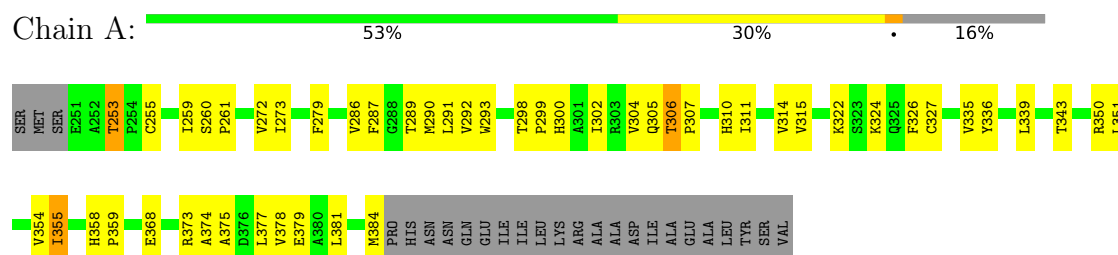
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Chain	Residue	Modelled	Actual	Comment	Reference
E	249	MET	-	expression tag	UNP Q9H4W6
E	250	SER	-	expression tag	UNP Q9H4W6
E	251	GLU	-	expression tag	UNP Q9H4W6
F	248	SER	-	expression tag	UNP Q9H4W6
F	249	MET	-	expression tag	UNP Q9H4W6
F	250	SER	-	expression tag	UNP Q9H4W6
F	251	GLU	-	expression tag	UNP Q9H4W6

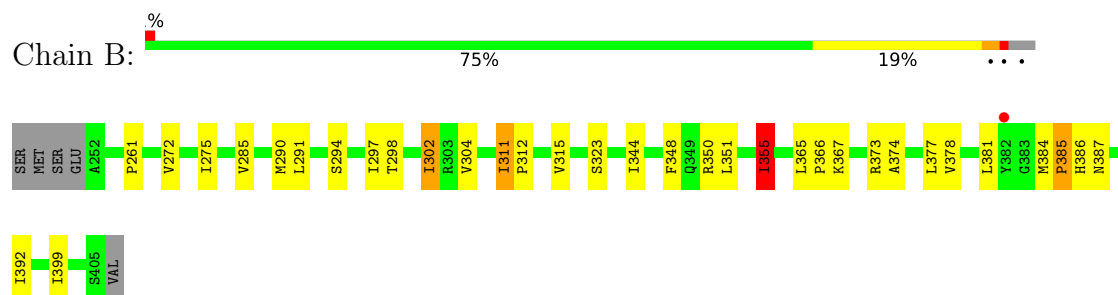
3 Residue-property plots

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.

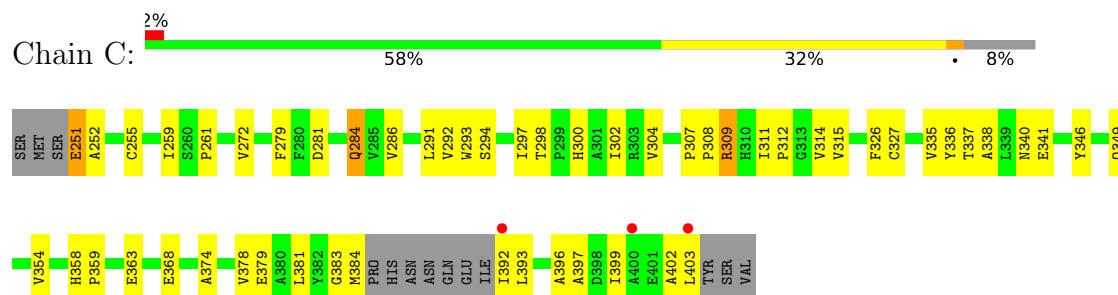
• Molecule 1: Transcription factor COE3



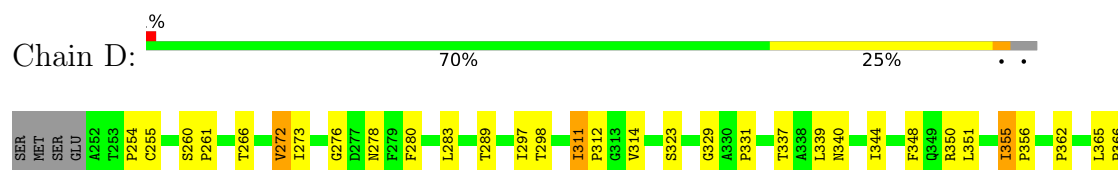
• Molecule 1: Transcription factor COE3



• Molecule 1: Transcription factor COE3

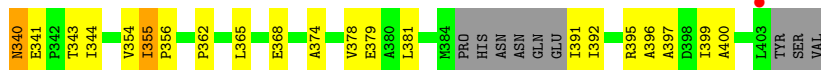
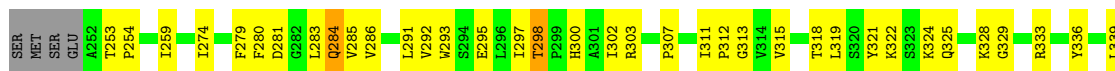


• Molecule 1: Transcription factor COE3

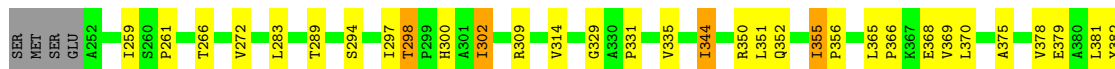




• Molecule 1: Transcription factor COE3



• Molecule 1: Transcription factor COE3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	229.64Å 229.64Å 229.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 3.10 19.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.84-3.10) 99.1 (19.84-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.188 , 0.227 0.185 , 0.222	Depositor DCC
R_{free} test set	2001 reflections (5.53%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6892	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.35	0/1066	0.85	5/1453 (0.3%)
1	B	0.36	0/1230	0.80	2/1676 (0.1%)
1	C	0.37	0/1154	0.82	0/1571
1	D	0.37	0/1230	0.82	0/1676
1	E	0.37	0/1157	0.85	5/1574 (0.3%)
1	F	0.34	0/1230	0.80	0/1676
All	All	0.36	0/7067	0.82	12/9626 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ILE	CA-C-N	5.99	125.75	119.76
1	B	355	ILE	C-N-CA	5.99	125.75	119.76
1	E	311	ILE	CA-C-N	5.73	127.00	119.84
1	E	311	ILE	C-N-CA	5.73	127.00	119.84
1	A	253	THR	CA-C-N	5.50	125.50	119.89
1	A	253	THR	C-N-CA	5.50	125.50	119.89
1	E	355	ILE	CA-C-N	5.27	125.27	119.90
1	E	355	ILE	C-N-CA	5.27	125.27	119.90
1	A	306	THR	CA-C-N	5.06	125.59	120.38
1	A	306	THR	C-N-CA	5.06	125.59	120.38
1	A	355	ILE	N-CA-C	5.06	112.98	108.63
1	E	311	ILE	N-CA-C	5.01	112.82	107.76

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	1038	0	1055	37	0
1	B	1199	0	1218	25	0
1	C	1127	0	1147	42	0
1	D	1199	0	1218	23	0
1	E	1130	0	1163	42	0
1	F	1199	0	1218	33	0
All	All	6892	0	7019	169	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 12.

All (169) 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:E:292:VAL:HG12	1:E:307:PRO:HG3	1.62	0.81
1:C:307:PRO:HD2	1:C:336:TYR:OH	1.88	0.72
1:E:297:ILE:HG22	1:E:298:THR:HG23	1.72	0.72
1:E:399:ILE:HD12	1:F:356:PRO:HG3	1.71	0.71
1:D:386:HIS:HA	1:D:389:GLN:HB2	1.72	0.71
1:F:297:ILE:HG22	1:F:298:THR:HG23	1.76	0.68
1:C:392:ILE:HG23	1:C:393:LEU:H	1.59	0.66
1:A:307:PRO:HD2	1:A:336:TYR:OH	1.97	0.64
1:C:399:ILE:HD12	1:D:356:PRO:HG3	1.79	0.64
1:D:351:LEU:HD22	1:D:355:ILE:HD13	1.78	0.64
1:E:354:VAL:HG12	1:F:378:VAL:HG12	1.79	0.64
1:E:280:PHE:CE1	1:E:283:LEU:HB2	2.33	0.64
1:C:349:GLN:OE1	1:E:333:ARG:HD2	1.99	0.63
1:A:255:CYS:HA	1:A:327:CYS:SG	2.40	0.62
1:E:368:GLU:HG3	1:F:344:ILE:HG13	1.80	0.62
1:D:261:PRO:HD2	1:D:272:VAL:HG22	1.82	0.62
1:B:294:SER:HB2	1:B:302:ILE:HG23	1.83	0.61
1:A:314:VAL:HG22	1:A:335:VAL:HG22	1.83	0.61
1:C:297:ILE:HG22	1:C:298:THR:HG23	1.83	0.60
1:E:379:GLU:OE2	1:F:350:ARG:NH2	2.35	0.60
1:C:381:LEU:HD23	1:D:392:ILE:HD13	1.84	0.60
1:A:261:PRO:HD2	1:A:272:VAL:HG22	1.83	0.59
1:A:377:LEU:O	1:A:381:LEU:HG	2.03	0.59
1:C:354:VAL:HG12	1:D:378:VAL:HG12	1.84	0.59
1:C:255:CYS:HA	1:C:327:CYS:SG	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:LEU:HD22	1:F:355:ILE:HD13	1.85	0.58
1:E:279:PHE:CD2	1:E:302:ILE:HG13	2.38	0.58
1:E:307:PRO:HD2	1:E:336:TYR:OH	2.04	0.58
1:F:386:HIS:HA	1:F:389:GLN:HB2	1.84	0.58
1:A:259:ILE:HG22	1:A:261:PRO:O	2.04	0.57
1:C:358:HIS:HB3	1:C:359:PRO:HD2	1.86	0.57
1:A:354:VAL:HG12	1:B:378:VAL:HG12	1.86	0.56
1:A:351:LEU:O	1:A:355:ILE:HG12	2.04	0.56
1:F:329:GLY:C	1:F:331:PRO:HD3	2.31	0.56
1:B:351:LEU:HD22	1:B:355:ILE:HD13	1.88	0.56
1:A:381:LEU:HD21	1:B:381:LEU:HD12	1.86	0.56
1:A:374:ALA:O	1:A:378:VAL:HG23	2.05	0.55
1:A:379:GLU:OE2	1:B:399:ILE:HD13	2.06	0.55
1:A:381:LEU:CD2	1:B:392:ILE:HD13	2.36	0.55
1:C:396:ALA:O	1:C:397:ALA:HB3	2.08	0.53
1:F:261:PRO:HD2	1:F:272:VAL:HG22	1.90	0.53
1:C:279:PHE:CD2	1:C:302:ILE:HG13	2.43	0.53
1:C:312:PRO:HG3	1:C:338:ALA:HB2	1.90	0.52
1:E:392:ILE:HG23	1:E:392:ILE:O	2.08	0.52
1:C:261:PRO:HD2	1:C:272:VAL:HG22	1.91	0.52
1:A:339:LEU:HD11	1:B:344:ILE:HD13	1.90	0.52
1:C:368:GLU:HG3	1:D:344:ILE:HG13	1.92	0.52
1:C:379:GLU:OE2	1:D:350:ARG:NH2	2.42	0.52
1:C:292:VAL:HG12	1:C:307:PRO:HG3	1.92	0.52
1:E:344:ILE:HG13	1:F:368:GLU:HG2	1.91	0.52
1:F:314:VAL:HG22	1:F:335:VAL:HG22	1.92	0.52
1:E:391:ILE:HG22	1:E:391:ILE:O	2.09	0.52
1:A:273:ILE:HG21	1:B:275:ILE:HD11	1.91	0.52
1:D:348:PHE:CE1	1:D:367:LYS:HB3	2.45	0.52
1:E:280:PHE:HD1	1:E:281:ASP:O	1.93	0.51
1:F:366:PRO:HD2	1:F:369:VAL:HG21	1.92	0.51
1:C:286:VAL:HG22	1:C:291:LEU:HD23	1.92	0.51
1:E:381:LEU:HD23	1:F:392:ILE:HD13	1.92	0.51
1:C:381:LEU:CD2	1:D:392:ILE:HD13	2.40	0.50
1:A:298:THR:C	1:A:300:HIS:H	2.19	0.50
1:C:392:ILE:HG23	1:C:393:LEU:N	2.26	0.50
1:A:350:ARG:O	1:A:354:VAL:HG23	2.11	0.50
1:A:292:VAL:HG12	1:A:307:PRO:HG3	1.93	0.50
1:F:294:SER:HB2	1:F:302:ILE:HG23	1.93	0.50
1:F:385:PRO:C	1:F:387:ASN:H	2.19	0.50
1:E:396:ALA:O	1:E:397:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:GLY:C	1:D:331:PRO:HD3	2.36	0.49
1:E:399:ILE:HD12	1:F:356:PRO:CG	2.42	0.49
1:C:383:GLY:O	1:C:384:MET:HE2	2.12	0.49
1:C:358:HIS:HB3	1:C:359:PRO:CD	2.42	0.49
1:C:340:ASN:O	1:C:341:GLU:C	2.55	0.49
1:C:307:PRO:HD2	1:C:336:TYR:HH	1.76	0.49
1:A:368:GLU:HG3	1:B:344:ILE:HG13	1.94	0.49
1:A:381:LEU:HD23	1:B:392:ILE:HD13	1.95	0.49
1:C:259:ILE:HG22	1:C:261:PRO:O	2.12	0.49
1:C:326:PHE:O	1:C:327:CYS:HB2	2.12	0.48
1:B:373:ARG:O	1:B:377:LEU:HG	2.13	0.48
1:D:385:PRO:C	1:D:387:ASN:H	2.21	0.48
1:E:328:LYS:HD3	1:E:328:LYS:HA	1.68	0.48
1:F:259:ILE:HG22	1:F:261:PRO:O	2.13	0.48
1:E:374:ALA:O	1:E:378:VAL:HG23	2.14	0.48
1:E:293:TRP:CZ2	1:E:295:GLU:HG3	2.50	0.47
1:C:251:GLU:HG2	1:C:252:ALA:H	1.79	0.47
1:B:297:ILE:HG22	1:B:298:THR:HG23	1.95	0.47
1:F:382:TYR:C	1:F:384:MET:H	2.21	0.47
1:E:283:LEU:HD11	1:E:319:LEU:HB3	1.96	0.47
1:D:374:ALA:O	1:D:378:VAL:HG23	2.15	0.47
1:E:259:ILE:HD12	1:E:274:ILE:HG12	1.97	0.47
1:D:366:PRO:HD2	1:D:369:VAL:HG21	1.96	0.47
1:C:309:ARG:NH1	1:C:311:ILE:O	2.49	0.46
1:A:290:MET:HE2	1:C:308:PRO:HD3	1.96	0.46
1:A:384:MET:HG2	1:B:392:ILE:HD11	1.97	0.46
1:E:285:VAL:O	1:E:292:VAL:HG22	2.15	0.46
1:A:286:VAL:HG22	1:A:291:LEU:HD23	1.97	0.46
1:A:293:TRP:HE1	1:C:284:GLN:HG2	1.81	0.46
1:C:251:GLU:CG	1:C:252:ALA:H	2.28	0.46
1:A:311:ILE:N	1:A:311:ILE:HD12	2.31	0.46
1:A:326:PHE:O	1:A:327:CYS:HB2	2.15	0.46
1:B:261:PRO:HD2	1:B:272:VAL:HG22	1.97	0.46
1:E:391:ILE:O	1:E:392:ILE:HG22	2.16	0.46
1:F:375:ALA:O	1:F:379:GLU:HG3	2.16	0.46
1:A:322:LYS:C	1:A:324:LYS:H	2.23	0.45
1:F:298:THR:C	1:F:300:HIS:H	2.23	0.45
1:C:368:GLU:H	1:C:368:GLU:CD	2.24	0.45
1:C:298:THR:C	1:C:300:HIS:H	2.25	0.45
1:C:314:VAL:HG22	1:C:335:VAL:HG22	1.97	0.45
1:F:385:PRO:O	1:F:386:HIS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ILE:HG22	1:D:298:THR:HG23	1.99	0.45
1:D:365:LEU:HA	1:D:366:PRO:HD3	1.82	0.45
1:F:283:LEU:HD23	1:F:302:ILE:CD1	2.47	0.45
1:E:298:THR:C	1:E:300:HIS:H	2.25	0.44
1:E:292:VAL:CG1	1:E:307:PRO:HG3	2.39	0.44
1:A:305:GLN:NE2	1:C:291:LEU:H	2.15	0.44
1:A:305:GLN:HE22	1:C:291:LEU:H	1.65	0.44
1:F:266:THR:HB	1:F:309:ARG:O	2.17	0.44
1:B:290:MET:HE2	1:B:290:MET:HB3	1.91	0.44
1:D:311:ILE:HA	1:D:312:PRO:HD3	1.80	0.44
1:B:285:VAL:HG21	1:B:304:VAL:HG11	2.00	0.44
1:F:297:ILE:HG22	1:F:298:THR:CG2	2.47	0.44
1:F:352:GLN:NE2	1:F:370:LEU:HD11	2.33	0.44
1:A:358:HIS:HB3	1:A:359:PRO:HD2	2.00	0.44
1:F:384:MET:C	1:F:386:HIS:H	2.26	0.44
1:C:311:ILE:HG13	1:E:312:PRO:HG2	1.99	0.43
1:C:340:ASN:HB3	1:E:313:GLY:HA3	2.00	0.43
1:E:368:GLU:H	1:E:368:GLU:CD	2.27	0.43
1:B:351:LEU:HD22	1:B:355:ILE:CD1	2.49	0.43
1:A:291:LEU:HD13	1:C:293:TRP:CE2	2.54	0.43
1:F:378:VAL:O	1:F:381:LEU:HB3	2.19	0.43
1:A:306:THR:HA	1:A:307:PRO:HD3	1.75	0.43
1:E:253:THR:HA	1:E:254:PRO:HD3	1.86	0.42
1:E:333:ARG:HH11	1:E:333:ARG:HG3	1.83	0.42
1:A:358:HIS:HD2	1:A:373:ARG:NH2	2.17	0.42
1:E:355:ILE:HA	1:E:356:PRO:HD3	1.94	0.42
1:A:279:PHE:CD2	1:A:302:ILE:HG13	2.54	0.42
1:A:298:THR:C	1:A:300:HIS:N	2.77	0.42
1:B:348:PHE:CE1	1:B:367:LYS:HB3	2.55	0.42
1:D:266:THR:HG23	1:D:337:THR:O	2.20	0.42
1:D:368:GLU:H	1:D:368:GLU:HG3	1.59	0.42
1:E:321:TYR:CZ	1:E:322:LYS:HE3	2.54	0.42
1:E:340:ASN:O	1:E:341:GLU:C	2.62	0.42
1:E:307:PRO:HD2	1:E:336:TYR:HH	1.83	0.42
1:E:399:ILE:O	1:E:400:ALA:C	2.63	0.42
1:D:254:PRO:HA	1:D:278:ASN:HB2	2.01	0.42
1:F:366:PRO:HB2	1:F:369:VAL:HG23	2.01	0.41
1:C:363:GLU:HG2	1:E:329:GLY:HA2	2.02	0.41
1:A:287:PHE:CD1	1:A:292:VAL:HG11	2.55	0.41
1:E:284:GLN:CG	1:E:291:LEU:HD22	2.50	0.41
1:E:322:LYS:O	1:E:324:LYS:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:LEU:HD11	1:F:344:ILE:HD13	2.02	0.41
1:B:374:ALA:O	1:B:378:VAL:HG23	2.20	0.41
1:A:375:ALA:CB	1:B:350:ARG:HG2	2.51	0.41
1:B:365:LEU:HA	1:B:366:PRO:HD3	1.92	0.41
1:B:384:MET:C	1:B:386:HIS:H	2.29	0.41
1:B:385:PRO:C	1:B:387:ASN:H	2.27	0.41
1:C:402:ALA:O	1:C:403:LEU:C	2.63	0.41
1:D:280:PHE:CZ	1:D:283:LEU:HD13	2.56	0.41
1:E:297:ILE:HD11	1:E:303:ARG:CZ	2.51	0.41
1:F:365:LEU:HA	1:F:366:PRO:HD3	1.93	0.41
1:F:395:ARG:O	1:F:399:ILE:HG13	2.21	0.41
1:D:355:ILE:HA	1:D:356:PRO:HD3	1.82	0.41
1:E:322:LYS:C	1:E:324:LYS:H	2.27	0.40
1:A:310:HIS:HB2	1:A:311:ILE:HD12	2.02	0.40
1:B:367:LYS:H	1:B:367:LYS:HG2	1.69	0.40
1:F:355:ILE:HA	1:F:356:PRO:HD3	1.91	0.40
1:B:311:ILE:HA	1:B:312:PRO:HD3	1.81	0.40
1:C:374:ALA:O	1:C:378:VAL:HG23	2.21	0.40
1:C:346:TYR:O	1:C:349:GLN:HB2	2.21	0.40
1:F:366:PRO:C	1:F:368:GLU:H	2.28	0.40
1:D:255:CYS:O	1:D:276:GLY:HA3	2.22	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	132/159 (83%)	123 (93%)	8 (6%)	1 (1%)	16	47
1	B	152/159 (96%)	142 (93%)	9 (6%)	1 (1%)	18	49
1	C	142/159 (89%)	128 (90%)	14 (10%)	0	100	100
1	D	152/159 (96%)	144 (95%)	7 (5%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	142/159 (89%)	126 (89%)	15 (11%)	1 (1%)	18	49
1	F	152/159 (96%)	144 (95%)	7 (5%)	1 (1%)	18	49
All	All	872/954 (91%)	807 (92%)	60 (7%)	5 (1%)	21	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	385	PRO
1	B	385	PRO
1	D	362	PRO
1	E	362	PRO
1	A	299	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/134 (84%)	106 (95%)	6 (5%)	20	50
1	B	129/134 (96%)	123 (95%)	6 (5%)	23	55
1	C	120/134 (90%)	112 (93%)	8 (7%)	15	43
1	D	129/134 (96%)	118 (92%)	11 (8%)	10	35
1	E	121/134 (90%)	111 (92%)	10 (8%)	10	35
1	F	129/134 (96%)	124 (96%)	5 (4%)	28	60
All	All	740/804 (92%)	694 (94%)	46 (6%)	16	46

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	THR
1	A	260	SER
1	A	289	THR
1	A	304	VAL
1	A	315	VAL

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Mol	Chain	Res	Type
1	A	343	THR
1	B	291	LEU
1	B	302	ILE
1	B	311	ILE
1	B	315	VAL
1	B	323	SER
1	B	355	ILE
1	C	251	GLU
1	C	281	ASP
1	C	284	GLN
1	C	294	SER
1	C	304	VAL
1	C	309	ARG
1	C	315	VAL
1	C	337	THR
1	D	260	SER
1	D	272	VAL
1	D	273	ILE
1	D	289	THR
1	D	311	ILE
1	D	314	VAL
1	D	323	SER
1	D	339	LEU
1	D	340	ASN
1	D	355	ILE
1	D	381	LEU
1	E	284	GLN
1	E	286	VAL
1	E	298	THR
1	E	315	VAL
1	E	318	THR
1	E	325	GLN
1	E	340	ASN
1	E	343	THR
1	E	365	LEU
1	E	395	ARG
1	F	289	THR
1	F	298	THR
1	F	302	ILE
1	F	344	ILE
1	F	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	340	ASN
1	A	358	HIS
1	B	389	GLN
1	D	389	GLN
1	E	310	HIS
1	E	340	ASN
1	F	284	GLN
1	F	310	HIS
1	F	349	GLN
1	F	358	HIS
1	F	389	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 oligosaccharides 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](#)

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, 95th 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	134/159 (84%)	-0.43	0 100 100	52, 81, 132, 144	0
1	B	154/159 (96%)	-0.42	1 (0%) 85 70	53, 73, 140, 162	0
1	C	146/159 (91%)	-0.39	3 (2%) 63 42	52, 72, 113, 143	0
1	D	154/159 (96%)	-0.54	2 (1%) 75 56	52, 69, 119, 139	0
1	E	146/159 (91%)	-0.14	1 (0%) 84 68	52, 88, 119, 133	0
1	F	154/159 (96%)	-0.39	2 (1%) 75 56	52, 78, 132, 153	0
All	All	888/954 (93%)	-0.39	9 (1%) 79 61	52, 76, 126, 162	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	403	LEU	4.9
1	C	403	LEU	4.7
1	D	405	SER	3.7
1	B	382	TYR	3.0
1	F	405	SER	2.9
1	D	385	PRO	2.8
1	C	392	ILE	2.7
1	F	385	PRO	2.4
1	C	400	ALA	2.1

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 oligosaccharides 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.