



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2025 – 10:11 AM EDT

PDB ID : 9Y55 / pdb_00009y55
Title : A crystal structure of DUSP10 loop mutant I445A
Authors : Manjula, R.; Lolis, E.J.; Bennett, A.
Deposited on : 2025-09-04
Resolution : 3.50 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	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

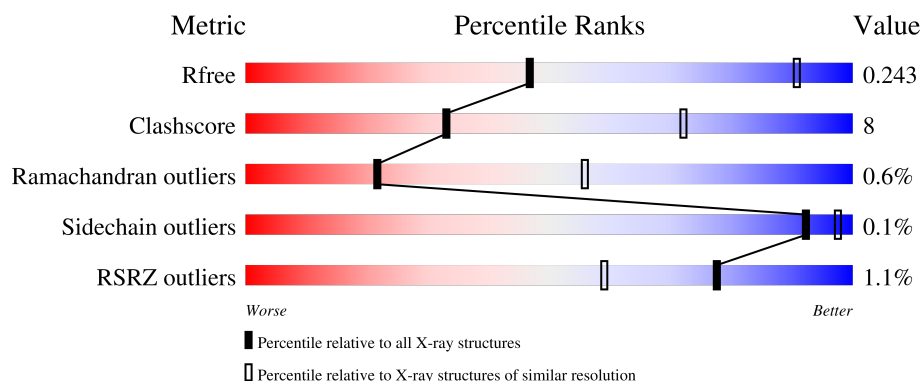
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	148	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 85%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 14% .. </div> </div>
1	B	148	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 83%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 83% 16% . </div> </div>
1	C	148	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 24%, green 74%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 74% 24% .. </div> </div>
1	D	148	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 17% .. </div> </div>
1	E	148	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 81%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 81% 18% .. </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	148	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>79%</div><div>19%</div><div>••</div></div></div>
1	G	148	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>84%</div><div>15%</div><div>•</div></div></div>
1	H	148	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>13%</div><div>•</div></div></div>
1	I	148	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>91%</div><div>9%</div><div>•</div></div></div>
1	J	148	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>84%</div><div>16%</div><div>•</div></div></div>
1	K	148	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>72%</div><div>24%</div><div>••</div></div></div>
1	L	148	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>86%</div><div>14%</div><div>•</div></div></div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 28121 atoms, of which 13944 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 Dual specificity protein phosphatase 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	B	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	C	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	D	147	Total	C	H	N	O	S	0	0	0
			2335	752	1158	200	218	7			
1	E	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	F	147	Total	C	H	N	O	S	0	0	0
			2316	752	1143	196	218	7			
1	G	147	Total	C	H	N	O	S	0	0	0
			2338	756	1158	200	218	6			
1	H	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	I	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	J	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	K	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			
1	L	147	Total	C	H	N	O	S	0	0	0
			2348	758	1165	200	218	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	319	MET	-	initiating methionine	UNP Q9Y6W6
A	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
B	319	MET	-	initiating methionine	UNP Q9Y6W6
B	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
C	319	MET	-	initiating methionine	UNP Q9Y6W6

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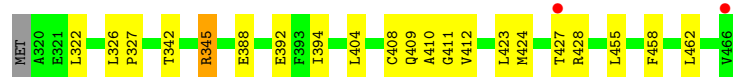
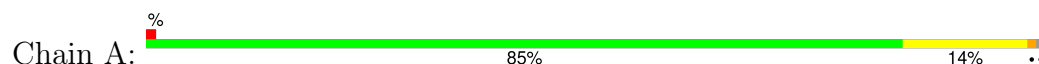
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Chain	Residue	Modelled	Actual	Comment	Reference
C	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
D	319	MET	-	initiating methionine	UNP Q9Y6W6
D	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
E	319	MET	-	initiating methionine	UNP Q9Y6W6
E	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
F	319	MET	-	initiating methionine	UNP Q9Y6W6
F	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
G	319	MET	-	initiating methionine	UNP Q9Y6W6
G	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
H	319	MET	-	initiating methionine	UNP Q9Y6W6
H	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
I	319	MET	-	initiating methionine	UNP Q9Y6W6
I	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
J	319	MET	-	initiating methionine	UNP Q9Y6W6
J	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
K	319	MET	-	initiating methionine	UNP Q9Y6W6
K	445	ALA	ILE	engineered mutation	UNP Q9Y6W6
L	319	MET	-	initiating methionine	UNP Q9Y6W6
L	445	ALA	ILE	engineered mutation	UNP Q9Y6W6

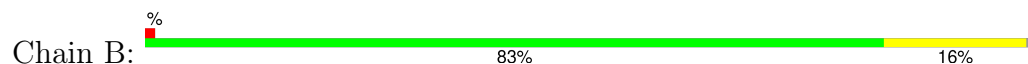
3 Residue-property plots [i](#)

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.

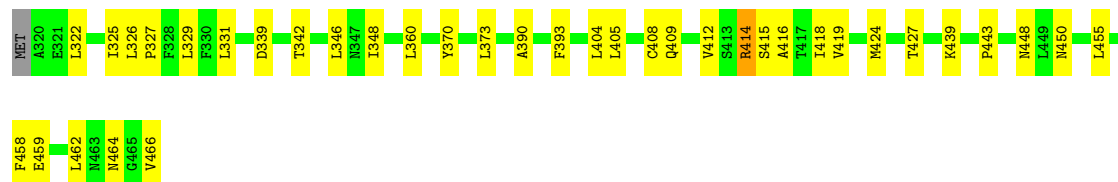
- Molecule 1: Dual specificity protein phosphatase 10



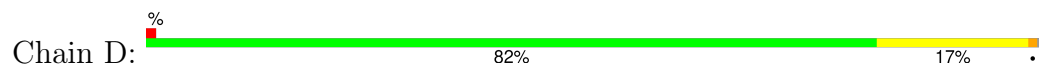
- Molecule 1: Dual specificity protein phosphatase 10



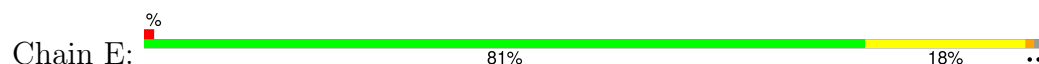
- Molecule 1: Dual specificity protein phosphatase 10



- Molecule 1: Dual specificity protein phosphatase 10

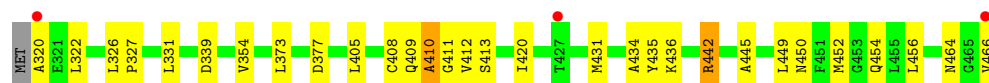
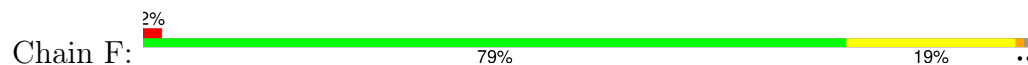


- Molecule 1: Dual specificity protein phosphatase 10

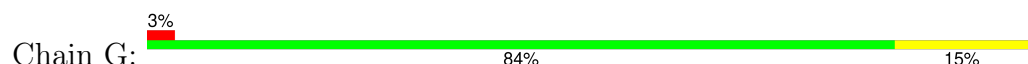




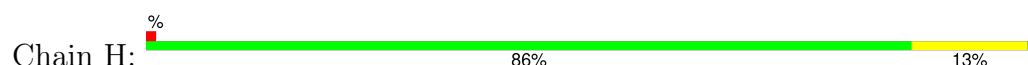
- Molecule 1: Dual specificity protein phosphatase 10



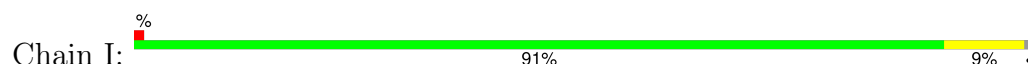
- Molecule 1: Dual specificity protein phosphatase 10



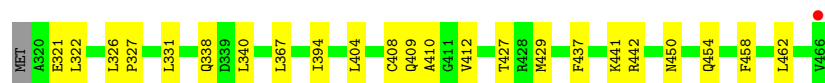
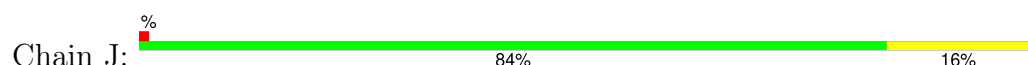
- Molecule 1: Dual specificity protein phosphatase 10



- Molecule 1: Dual specificity protein phosphatase 10

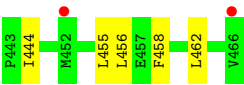


- Molecule 1: Dual specificity protein phosphatase 10

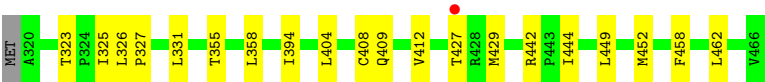
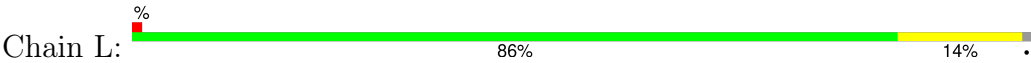


- Molecule 1: Dual specificity protein phosphatase 10





● Molecule 1: Dual specificity protein phosphatase 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.40Å 110.05Å 166.23Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	166.23 – 3.50 166.23 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (166.23-3.50) 95.9 (166.23-3.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.211 , 0.245 0.213 , 0.243	Depositor DCC
R_{free} test set	2176 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l 0.044 for k,h,-l 0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28121	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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	0.15	0/1209	0.36	0/1634
1	B	0.14	0/1209	0.33	0/1634
1	C	0.13	0/1209	0.33	0/1634
1	D	0.14	0/1202	0.31	0/1625
1	E	0.13	0/1209	0.34	0/1634
1	F	0.13	0/1199	0.33	0/1623
1	G	0.12	0/1206	0.32	0/1631
1	H	0.13	0/1209	0.32	0/1634
1	I	0.18	0/1209	0.33	0/1634
1	J	0.13	0/1209	0.34	0/1634
1	K	0.15	0/1209	0.37	0/1634
1	L	0.15	0/1209	0.32	0/1634
All	All	0.14	0/14488	0.33	0/19585

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	2
1	C	0	1
1	F	0	1
1	K	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	ARG	Sidechain
1	A	428	ARG	Sidechain
1	C	414	ARG	Sidechain
1	F	442	ARG	Sidechain
1	K	372	ARG	Sidechain
1	K	442	ARG	Sidechain

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	1183	1165	1165	15	0
1	B	1183	1165	1165	20	0
1	C	1183	1165	1165	25	0
1	D	1177	1158	1158	23	0
1	E	1183	1165	1165	18	0
1	F	1173	1143	1143	23	0
1	G	1180	1158	1158	14	0
1	H	1183	1165	1165	13	0
1	I	1183	1165	1165	9	0
1	J	1183	1165	1165	22	0
1	K	1183	1165	1165	37	0
1	L	1183	1165	1165	15	0
All	All	14177	13944	13944	217	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 8.

All (217) 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:F:377:ASP:OD2	1:F:413:SER:OG	1.89	0.89
1:J:327:PRO:HB3	1:K:431:MET:HE2	1.58	0.85
1:F:431:MET:HE1	1:H:327:PRO:HD3	1.63	0.80
1:G:408:CYS:SG	1:G:409:GLN:N	2.55	0.79
1:J:427:THR:HG21	1:J:429:MET:HE2	1.63	0.79
1:D:408:CYS:SG	1:D:409:GLN:N	2.56	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:CYS:SG	1:H:409:GLN:N	2.56	0.78
1:K:408:CYS:SG	1:K:409:GLN:N	2.58	0.77
1:K:348:ILE:HD13	1:K:405:LEU:HD22	1.67	0.76
1:K:343:MET:HE3	1:K:405:LEU:HD23	1.67	0.76
1:K:431:MET:HE1	1:K:456:LEU:CD1	2.17	0.74
1:E:408:CYS:SG	1:E:409:GLN:N	2.63	0.71
1:A:345:ARG:HH11	1:A:345:ARG:HB2	1.54	0.71
1:C:464:ASN:HB2	1:C:466:VAL:HG23	1.72	0.71
1:C:408:CYS:SG	1:C:409:GLN:N	2.66	0.68
1:F:449:LEU:HD11	1:H:422:TYR:OH	1.93	0.68
1:B:464:ASN:HB2	1:B:466:VAL:HG23	1.77	0.67
1:K:412:VAL:HG11	1:K:442:ARG:HH11	1.59	0.67
1:L:408:CYS:SG	1:L:409:GLN:N	2.64	0.67
1:I:408:CYS:SG	1:I:409:GLN:N	2.66	0.67
1:J:321:GLU:O	1:J:442:ARG:NH2	2.27	0.67
1:A:408:CYS:SG	1:A:409:GLN:N	2.68	0.66
1:J:408:CYS:SG	1:J:409:GLN:N	2.65	0.66
1:C:414:ARG:O	1:C:418:ILE:HD12	1.95	0.65
1:K:331:LEU:HD23	1:K:442:ARG:HD2	1.76	0.65
1:K:404:LEU:HD23	1:K:405:LEU:N	2.12	0.65
1:C:412:VAL:HG13	1:C:415:SER:OG	1.97	0.65
1:H:331:LEU:HD23	1:H:442:ARG:HD2	1.78	0.64
1:B:431:MET:HE1	1:C:327:PRO:HD3	1.81	0.63
1:E:464:ASN:HB2	1:E:466:VAL:HG23	1.81	0.62
1:K:404:LEU:HD23	1:K:406:ILE:N	2.14	0.62
1:A:427:THR:HG22	1:D:427:THR:HG23	1.81	0.61
1:D:346:LEU:HD12	1:D:348:ILE:HD11	1.82	0.61
1:A:427:THR:CG2	1:D:427:THR:HG23	2.31	0.61
1:F:322:LEU:HD23	1:F:405:LEU:HD13	1.82	0.61
1:F:408:CYS:SG	1:F:409:GLN:N	2.66	0.60
1:D:326:LEU:HD12	1:D:329:LEU:HD22	1.84	0.60
1:B:327:PRO:HD3	1:D:431:MET:HE1	1.84	0.59
1:J:327:PRO:HG2	1:K:432:THR:HA	1.84	0.58
1:J:331:LEU:HD23	1:J:442:ARG:HD2	1.85	0.58
1:K:323:THR:HG23	1:K:441:LYS:HB3	1.85	0.58
1:D:464:ASN:HB2	1:D:466:VAL:HG23	1.86	0.57
1:L:331:LEU:HD23	1:L:442:ARG:HD2	1.87	0.57
1:K:431:MET:HE1	1:K:456:LEU:HD12	1.86	0.56
1:K:343:MET:HA	1:K:348:ILE:HD12	1.86	0.56
1:F:412:VAL:HG11	1:F:442:ARG:HH11	1.71	0.56
1:D:423:LEU:O	1:D:427:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:323:THR:HG21	1:L:442:ARG:HB2	1.87	0.55
1:E:409:GLN:O	1:E:411:GLY:N	2.40	0.55
1:B:437:PHE:CZ	1:D:456:LEU:HD22	2.43	0.54
1:K:340:LEU:HD11	1:K:367:LEU:HD12	1.89	0.54
1:C:412:VAL:HG12	1:C:416:ALA:HB2	1.89	0.54
1:F:431:MET:HE2	1:F:456:LEU:HD13	1.87	0.54
1:K:323:THR:HG23	1:K:441:LYS:CB	2.37	0.54
1:B:339:ASP:OD2	1:B:342:THR:OG1	2.26	0.54
1:D:394:ILE:HA	1:D:404:LEU:HD13	1.89	0.53
1:B:331:LEU:HD23	1:B:442:ARG:HD2	1.89	0.53
1:E:331:LEU:HD23	1:E:442:ARG:HD2	1.91	0.53
1:C:346:LEU:HD12	1:C:348:ILE:HD11	1.91	0.52
1:E:412:VAL:HG23	1:E:445:ALA:HA	1.90	0.52
1:C:373:LEU:HD11	1:C:390:ALA:HB2	1.90	0.52
1:F:320:ALA:HB3	1:F:339:ASP:OD2	2.09	0.52
1:L:427:THR:HG21	1:L:429:MET:HE2	1.91	0.52
1:K:330:PHE:CE2	1:K:346:LEU:HD13	2.45	0.52
1:K:323:THR:HG22	1:K:323:THR:O	2.09	0.52
1:L:358:LEU:HD11	1:L:409:GLN:HG2	1.91	0.52
1:L:325:ILE:O	1:L:326:LEU:HD23	2.10	0.52
1:E:373:LEU:HD11	1:E:390:ALA:HB2	1.92	0.51
1:B:373:LEU:HD21	1:B:390:ALA:HB2	1.91	0.51
1:A:423:LEU:O	1:A:427:THR:HB	2.11	0.51
1:B:427:THR:HG23	1:D:453:GLY:HA2	1.93	0.50
1:J:326:LEU:HD21	1:K:436:LYS:HZ3	1.77	0.50
1:E:322:LEU:HD13	1:E:342:THR:HG21	1.94	0.50
1:K:373:LEU:HD11	1:K:390:ALA:HB2	1.94	0.49
1:C:458:PHE:CD2	1:C:462:LEU:HD11	2.47	0.49
1:E:339:ASP:OD2	1:E:342:THR:OG1	2.30	0.49
1:E:431:MET:SD	1:E:456:LEU:HD12	2.53	0.49
1:B:431:MET:HE2	1:B:456:LEU:HD13	1.93	0.49
1:C:458:PHE:CE2	1:C:462:LEU:HD11	2.48	0.49
1:C:322:LEU:HD13	1:C:342:THR:HG21	1.95	0.49
1:F:435:TYR:CE2	1:F:452:MET:HE2	2.48	0.49
1:J:394:ILE:HA	1:J:404:LEU:HD13	1.95	0.49
1:C:339:ASP:OD2	1:C:342:THR:OG1	2.31	0.48
1:A:424:MET:HE1	1:A:455:LEU:O	2.14	0.48
1:G:412:VAL:HG23	1:G:445:ALA:HA	1.95	0.48
1:H:427:THR:O	1:H:427:THR:HG22	2.14	0.48
1:K:322:LEU:O	1:K:323:THR:C	2.56	0.48
1:B:464:ASN:CB	1:B:466:VAL:HG23	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:437:PHE:CE1	1:J:441:LYS:HD2	2.50	0.47
1:D:322:LEU:N	1:D:322:LEU:HD12	2.29	0.47
1:C:427:THR:O	1:C:427:THR:HG22	2.15	0.47
1:C:448:ASN:OD1	1:C:450:ASN:N	2.48	0.47
1:J:427:THR:HG21	1:J:429:MET:CE	2.38	0.47
1:B:326:LEU:CD2	1:D:456:LEU:HD11	2.44	0.47
1:K:412:VAL:HG11	1:K:442:ARG:NH1	2.26	0.47
1:A:458:PHE:CZ	1:A:462:LEU:HD11	2.50	0.47
1:L:408:CYS:HG	1:L:409:GLN:H	1.61	0.47
1:E:342:THR:O	1:E:346:LEU:HD23	2.15	0.47
1:K:404:LEU:HD23	1:K:406:ILE:H	1.77	0.47
1:B:427:THR:HG23	1:D:453:GLY:CA	2.45	0.46
1:I:322:LEU:N	1:I:322:LEU:HD12	2.30	0.46
1:J:437:PHE:CD1	1:J:437:PHE:C	2.89	0.46
1:I:340:LEU:HD11	1:I:367:LEU:HD13	1.98	0.46
1:C:322:LEU:HD23	1:C:405:LEU:HD13	1.97	0.46
1:F:431:MET:HE2	1:F:456:LEU:CD1	2.46	0.46
1:D:323:THR:HG21	1:D:442:ARG:HB2	1.98	0.46
1:H:340:LEU:HD11	1:H:367:LEU:HD13	1.97	0.46
1:C:360:LEU:HD13	1:C:370:TYR:HB3	1.98	0.45
1:H:452:MET:O	1:H:456:LEU:HD13	2.16	0.45
1:F:408:CYS:SG	1:F:412:VAL:HA	2.57	0.45
1:H:408:CYS:SG	1:H:412:VAL:HA	2.56	0.45
1:K:427:THR:HG22	1:K:427:THR:O	2.16	0.45
1:J:340:LEU:HD11	1:J:367:LEU:HD13	1.98	0.45
1:K:352:ILE:CD1	1:K:404:LEU:HD11	2.46	0.45
1:K:352:ILE:HD12	1:K:404:LEU:HD11	1.98	0.45
1:L:427:THR:HG22	1:L:427:THR:O	2.17	0.45
1:G:425:LYS:O	1:G:428:ARG:NH1	2.50	0.45
1:L:394:ILE:HA	1:L:404:LEU:HD13	1.98	0.45
1:G:394:ILE:HA	1:G:404:LEU:HD13	1.99	0.45
1:K:429:MET:HB3	1:K:433:ASP:HB2	1.99	0.45
1:A:408:CYS:SG	1:A:412:VAL:HA	2.57	0.45
1:B:447:PRO:O	1:B:452:MET:HE3	2.16	0.45
1:A:427:THR:HG22	1:A:427:THR:O	2.16	0.45
1:F:331:LEU:HD23	1:F:442:ARG:HD2	1.98	0.44
1:A:388:GLU:O	1:A:392:GLU:HG3	2.17	0.44
1:C:393:PHE:CD2	1:C:404:LEU:HD11	2.52	0.44
1:E:448:ASN:OD1	1:E:450:ASN:N	2.50	0.44
1:I:331:LEU:HD23	1:I:442:ARG:HD2	2.00	0.44
1:D:333:ASN:HD22	1:D:442:ARG:HH22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:ARG:O	1:E:418:ILE:HD12	2.17	0.44
1:E:450:ASN:O	1:E:454:GLN:HG3	2.17	0.44
1:F:412:VAL:HG23	1:F:445:ALA:HA	1.99	0.44
1:I:427:THR:HG22	1:I:427:THR:O	2.16	0.44
1:K:431:MET:SD	1:K:455:LEU:HB3	2.57	0.44
1:I:406:ILE:HG23	1:I:406:ILE:O	2.18	0.44
1:D:408:CYS:HG	1:D:409:GLN:H	1.63	0.44
1:E:431:MET:SD	1:E:456:LEU:CD1	3.05	0.44
1:J:322:LEU:N	1:J:322:LEU:HD12	2.33	0.44
1:A:394:ILE:HA	1:A:404:LEU:HD13	2.00	0.44
1:C:424:MET:HE1	1:C:455:LEU:O	2.18	0.44
1:L:355:THR:OG1	1:L:358:LEU:HB2	2.18	0.44
1:A:458:PHE:CE2	1:A:462:LEU:HD11	2.53	0.44
1:B:320:ALA:HB1	1:B:336:ASP:HA	2.00	0.44
1:G:331:LEU:HD23	1:G:442:ARG:HD2	1.99	0.44
1:G:391:PHE:O	1:G:395:GLU:HG2	2.18	0.43
1:F:326:LEU:HB3	1:F:327:PRO:CD	2.49	0.43
1:J:338:GLN:O	1:J:340:LEU:N	2.51	0.43
1:F:450:ASN:O	1:F:454:GLN:HG3	2.18	0.43
1:K:326:LEU:HD21	1:K:423:LEU:HD21	2.00	0.43
1:L:444:ILE:O	1:L:444:ILE:HG22	2.18	0.43
1:I:338:GLN:O	1:I:340:LEU:N	2.51	0.43
1:J:437:PHE:CE1	1:K:439:LYS:CD	3.01	0.43
1:C:326:LEU:HB3	1:C:327:PRO:CD	2.49	0.43
1:C:331:LEU:HD13	1:C:419:VAL:HG21	2.01	0.43
1:D:331:LEU:HD23	1:D:442:ARG:HD3	2.00	0.43
1:J:427:THR:O	1:J:427:THR:HG22	2.17	0.43
1:D:332:GLY:O	1:D:412:VAL:HG12	2.19	0.43
1:K:372:ARG:HG2	1:K:374:PRO:HD3	2.01	0.43
1:A:326:LEU:HB3	1:A:327:PRO:CD	2.49	0.43
1:J:437:PHE:CD1	1:K:439:LYS:HD2	2.53	0.43
1:F:409:GLN:O	1:F:410:ALA:C	2.62	0.42
1:B:449:LEU:O	1:B:449:LEU:HD23	2.19	0.42
1:G:412:VAL:HG11	1:G:442:ARG:HD3	2.00	0.42
1:K:386:TYR:O	1:K:387:PHE:C	2.62	0.42
1:K:458:PHE:O	1:K:462:LEU:HG	2.19	0.42
1:H:444:ILE:O	1:H:444:ILE:HG22	2.19	0.42
1:H:322:LEU:HD12	1:H:322:LEU:N	2.34	0.42
1:F:412:VAL:HG21	1:F:442:ARG:HD3	2.02	0.42
1:G:322:LEU:N	1:G:322:LEU:HD12	2.34	0.42
1:G:326:LEU:HB3	1:G:327:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:ILE:HG22	1:I:444:ILE:O	2.19	0.42
1:C:459:GLU:HA	1:C:462:LEU:HD12	2.01	0.42
1:D:326:LEU:HB3	1:D:327:PRO:CD	2.49	0.42
1:E:427:THR:O	1:E:427:THR:HG22	2.19	0.42
1:F:420:ILE:HG23	1:F:434:ALA:HB3	2.01	0.42
1:J:450:ASN:O	1:J:454:GLN:HG3	2.19	0.42
1:B:326:LEU:HB3	1:B:327:PRO:CD	2.50	0.42
1:C:412:VAL:HG12	1:C:412:VAL:O	2.19	0.42
1:E:393:PHE:CD2	1:E:404:LEU:HD11	2.55	0.42
1:G:449:LEU:HD23	1:G:449:LEU:O	2.20	0.42
1:B:379:ASN:HD22	1:B:379:ASN:C	2.17	0.41
1:F:464:ASN:HB2	1:F:466:VAL:HG23	2.02	0.41
1:J:437:PHE:CE1	1:K:439:LYS:HD2	2.56	0.41
1:K:375:ALA:HB1	1:K:381:GLN:HG2	2.02	0.41
1:L:458:PHE:O	1:L:462:LEU:HG	2.20	0.41
1:F:409:GLN:O	1:F:411:GLY:N	2.53	0.41
1:F:354:VAL:HG13	1:F:373:LEU:HB2	2.02	0.41
1:G:396:GLU:O	1:G:400:CYS:HB3	2.19	0.41
1:H:326:LEU:HB3	1:H:327:PRO:CD	2.50	0.41
1:C:393:PHE:HD2	1:C:404:LEU:HD11	1.86	0.41
1:B:424:MET:HE1	1:B:455:LEU:O	2.20	0.41
1:C:325:ILE:HB	1:C:329:LEU:HD23	2.02	0.41
1:D:409:GLN:O	1:D:411:GLY:N	2.54	0.41
1:A:411:GLY:O	1:A:412:VAL:HG22	2.20	0.41
1:F:354:VAL:HG22	1:F:373:LEU:HD12	2.02	0.41
1:H:430:THR:HB	1:H:459:GLU:OE2	2.21	0.41
1:A:322:LEU:HD13	1:A:342:THR:HG21	2.03	0.41
1:B:333:ASN:ND2	1:B:336:ASP:OD2	2.54	0.41
1:E:373:LEU:HD22	1:E:386:TYR:HB3	2.02	0.41
1:J:408:CYS:SG	1:J:412:VAL:HA	2.60	0.41
1:L:412:VAL:HG11	1:L:442:ARG:HD3	2.02	0.41
1:G:340:LEU:HD11	1:G:367:LEU:HD13	2.03	0.40
1:I:321:GLU:O	1:I:442:ARG:NH2	2.54	0.40
1:K:444:ILE:O	1:K:444:ILE:HG22	2.21	0.40
1:D:408:CYS:SG	1:D:412:VAL:HA	2.60	0.40
1:E:409:GLN:O	1:E:410:ALA:C	2.64	0.40
1:F:449:LEU:HD23	1:F:449:LEU:O	2.21	0.40
1:G:333:ASN:ND2	1:G:336:ASP:OD2	2.54	0.40
1:L:326:LEU:HB3	1:L:327:PRO:CD	2.51	0.40
1:D:409:GLN:O	1:D:410:ALA:C	2.63	0.40
1:J:458:PHE:O	1:J:462:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:449:LEU:HD23	1:L:452:MET:HE3	2.02	0.40
1:B:444:ILE:HG22	1:B:444:ILE:O	2.21	0.40
1:C:439:LYS:HE2	1:C:443:PRO:O	2.22	0.40
1:G:322:LEU:HG	1:G:336:ASP:HB3	2.03	0.40
1:H:325:ILE:O	1:H:326:LEU:HD23	2.22	0.40
1:J:437:PHE:CZ	1:K:439:LYS:HD3	2.57	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	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	19	53
1	B	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
1	C	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
1	D	145/148 (98%)	136 (94%)	7 (5%)	2 (1%)	9	40
1	E	145/148 (98%)	137 (94%)	7 (5%)	1 (1%)	19	53
1	F	145/148 (98%)	134 (92%)	9 (6%)	2 (1%)	9	40
1	G	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
1	H	145/148 (98%)	137 (94%)	7 (5%)	1 (1%)	19	53
1	I	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	19	53
1	J	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	19	53
1	K	145/148 (98%)	127 (88%)	17 (12%)	1 (1%)	19	53
1	L	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
All	All	1740/1776 (98%)	1629 (94%)	101 (6%)	10 (1%)	22	56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	410	ALA
1	F	410	ALA
1	F	436	LYS
1	J	410	ALA
1	D	410	ALA
1	A	410	ALA
1	H	410	ALA
1	I	410	ALA
1	K	323	THR
1	D	354	VAL

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	127/129 (98%)	127 (100%)	0	100	100
1	B	127/129 (98%)	127 (100%)	0	100	100
1	C	127/129 (98%)	127 (100%)	0	100	100
1	D	126/129 (98%)	126 (100%)	0	100	100
1	E	127/129 (98%)	127 (100%)	0	100	100
1	F	125/129 (97%)	125 (100%)	0	100	100
1	G	126/129 (98%)	126 (100%)	0	100	100
1	H	127/129 (98%)	127 (100%)	0	100	100
1	I	127/129 (98%)	127 (100%)	0	100	100
1	J	127/129 (98%)	127 (100%)	0	100	100
1	K	127/129 (98%)	126 (99%)	1 (1%)	79	88
1	L	127/129 (98%)	127 (100%)	0	100	100
All	All	1520/1548 (98%)	1519 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	439	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	450	ASN
1	B	333	ASN
1	B	344	GLN
1	C	338	GLN
1	C	407	HIS
1	D	379	ASN
1	D	407	HIS
1	E	338	GLN
1	E	464	ASN
1	F	338	GLN
1	F	362	HIS
1	F	407	HIS
1	G	407	HIS
1	G	409	GLN
1	H	379	ASN
1	I	347	ASN
1	J	344	GLN
1	J	407	HIS
1	K	347	ASN
1	K	381	GLN
1	L	379	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 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

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, 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	147/148 (99%)	-0.24	2 (1%) 73 53	60, 89, 126, 163	0
1	B	147/148 (99%)	-0.32	1 (0%) 84 69	52, 87, 123, 157	0
1	C	147/148 (99%)	-0.34	0 100 100	63, 89, 123, 153	0
1	D	147/148 (99%)	-0.28	1 (0%) 84 69	67, 97, 136, 156	0
1	E	147/148 (99%)	-0.26	1 (0%) 84 69	65, 95, 130, 164	0
1	F	147/148 (99%)	-0.20	3 (2%) 64 45	70, 97, 135, 154	0
1	G	147/148 (99%)	-0.16	4 (2%) 56 38	74, 105, 142, 159	0
1	H	147/148 (99%)	-0.24	1 (0%) 84 69	73, 104, 142, 164	0
1	I	147/148 (99%)	-0.14	2 (1%) 73 53	77, 110, 144, 183	0
1	J	147/148 (99%)	-0.05	1 (0%) 84 69	77, 116, 158, 174	0
1	K	147/148 (99%)	0.09	3 (2%) 64 45	85, 120, 151, 179	0
1	L	147/148 (99%)	-0.09	1 (0%) 84 69	85, 121, 157, 216	0
All	All	1764/1776 (99%)	-0.19	20 (1%) 77 59	52, 102, 146, 216	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	THR	3.8
1	A	427	THR	3.0
1	G	427	THR	3.0
1	I	334	GLU	2.8
1	F	320	ALA	2.6
1	A	466	VAL	2.6
1	F	427	THR	2.5
1	I	452	MET	2.5
1	H	427	THR	2.5
1	G	466	VAL	2.5
1	L	427	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	466	VAL	2.4
1	K	466	VAL	2.4
1	K	452	MET	2.3
1	E	466	VAL	2.2
1	G	429	MET	2.2
1	B	466	VAL	2.1
1	K	427	THR	2.1
1	G	337	ALA	2.1
1	J	466	VAL	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 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.