



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:01 AM UTC

PDB ID : 7TRJ / pdb_00007trj
EMDB ID : EMD-26098
Title : The eukaryotic translation initiation factor 2B from Homo sapiens with a H160D mutation in the beta subunit
Authors : Wang, L.; Schoof, M.; Lawrence, R.; Boone, M.; Frost, A.; Walter, P.
Deposited on : 2022-01-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

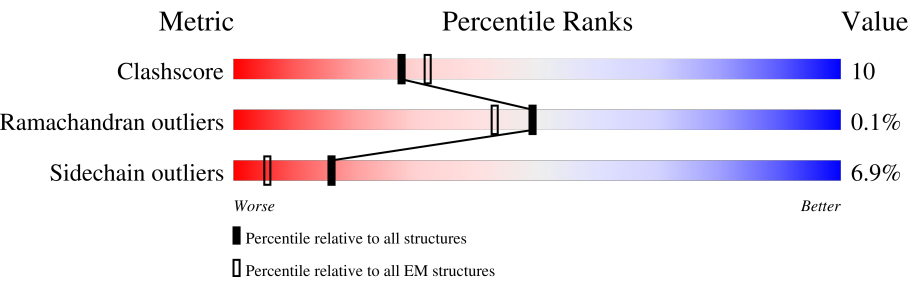
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	721	44% 12% . 43%
1	B	721	45% 12% . 43%
2	C	351	68% 25% . 6%
2	D	351	67% 26% . 6%
3	E	523	51% 15% . 33%
3	F	523	51% 15% . 33%
4	G	305	64% 27% . 7%
4	H	305	65% 26% . 7%
5	I	452	37% 13% . 48%

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Mol	Chain	Length	Quality of chain
5	J	452	37% 13% 48%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25190 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3210	2030	570	595	15		
1	B	414	Total	C	N	O	S	0	0
			3210	2030	570	595	15		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	329	Total	C	N	O	S	0	0
			2571	1629	450	477	15		
2	C	329	Total	C	N	O	S	0	0
			2571	1629	450	477	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	160	ASP	HIS	engineered mutation	UNP P49770
C	160	ASP	HIS	engineered mutation	UNP P49770

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	353	Total	C	N	O	S	0	0
			2750	1741	490	505	14		
3	F	353	Total	C	N	O	S	0	0
			2750	1741	490	505	14		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	285	Total	C	N	O	S	0	0
			2203	1419	364	409	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	285	Total	C	N	O	S	0	0
			2203	1419	364	409	11		

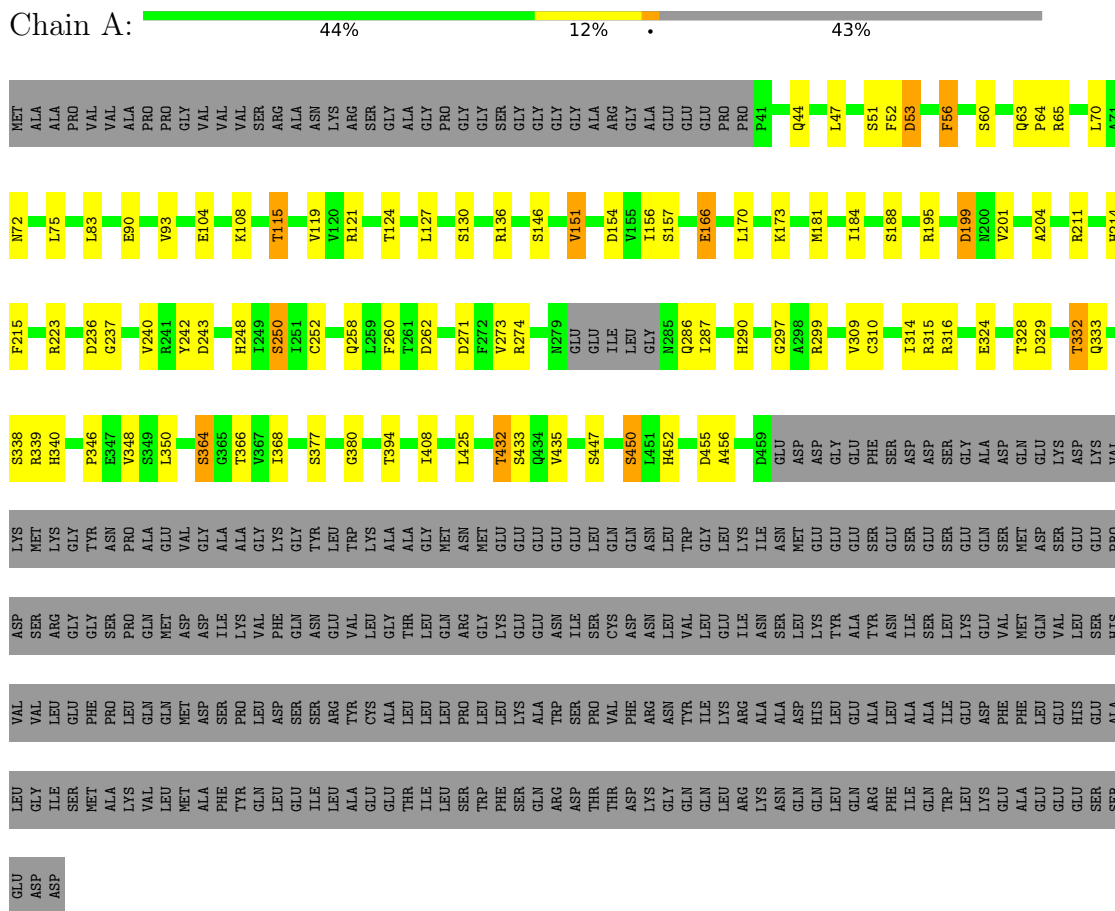
- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	236	Total	C	N	O	S	0	0
			1861	1212	312	321	16		
5	J	236	Total	C	N	O	S	0	0
			1861	1212	312	321	16		

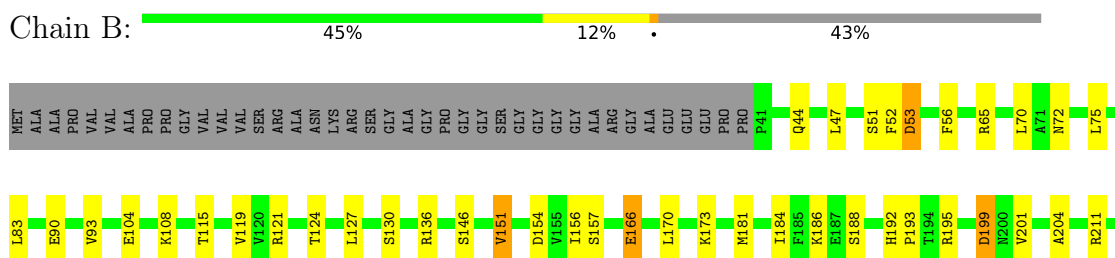
3 Residue-property plots

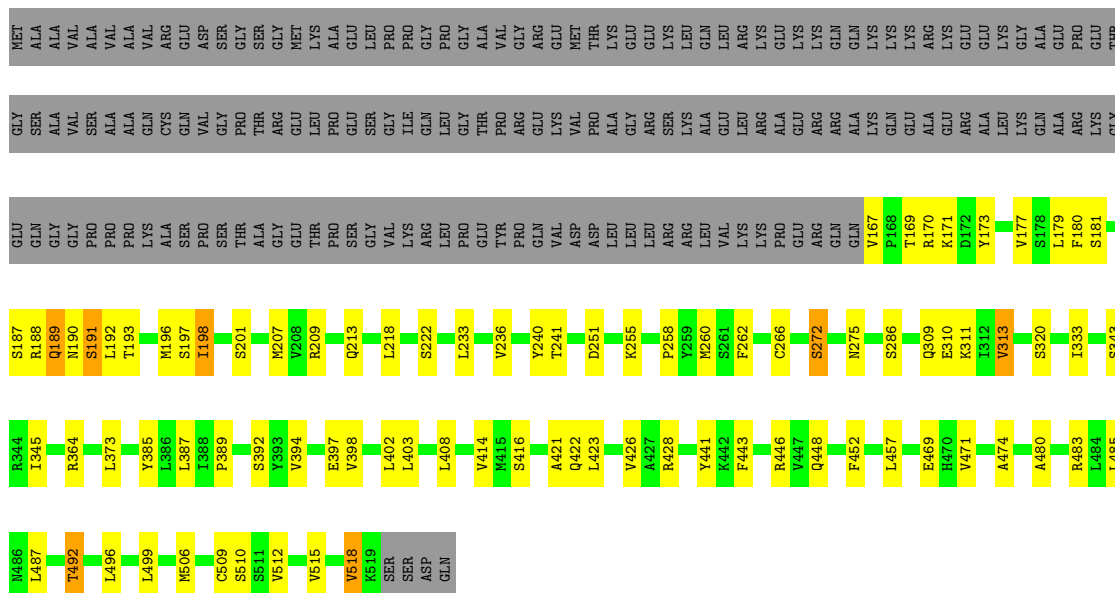
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Translation initiation factor eIF-2B subunit epsilon

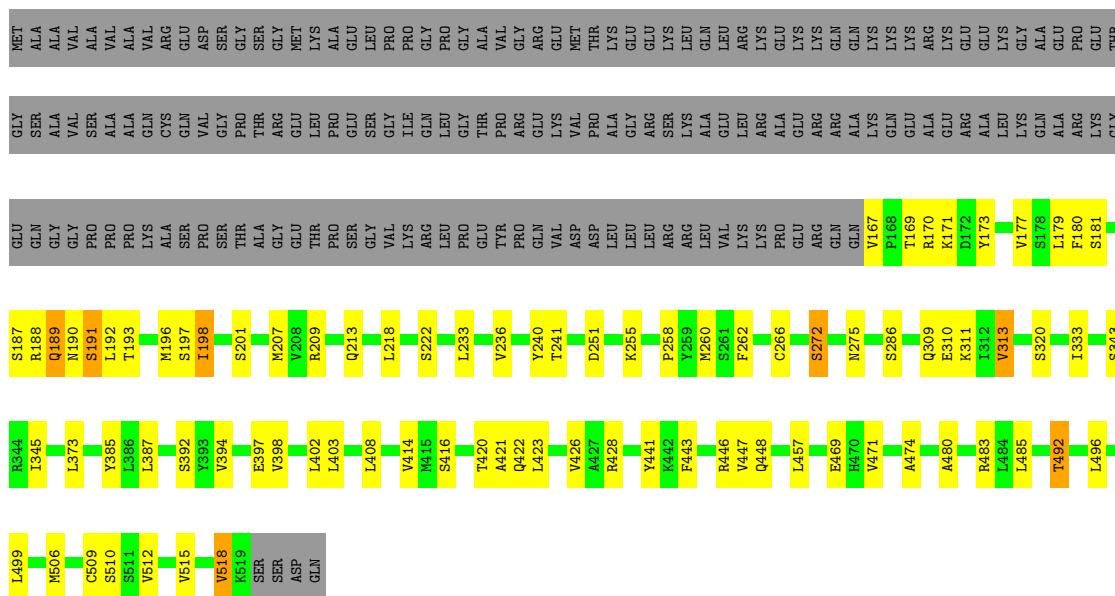


- Molecule 1: Translation initiation factor eIF-2B subunit epsilon

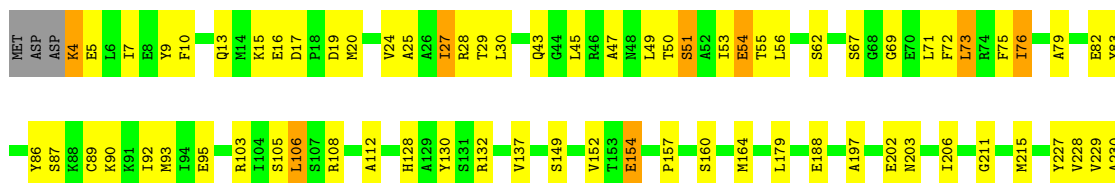




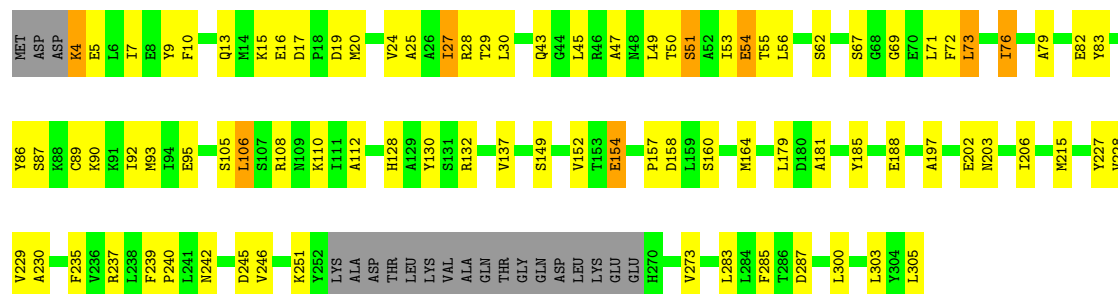
- Molecule 3: Translation initiation factor eIF-2B subunit delta



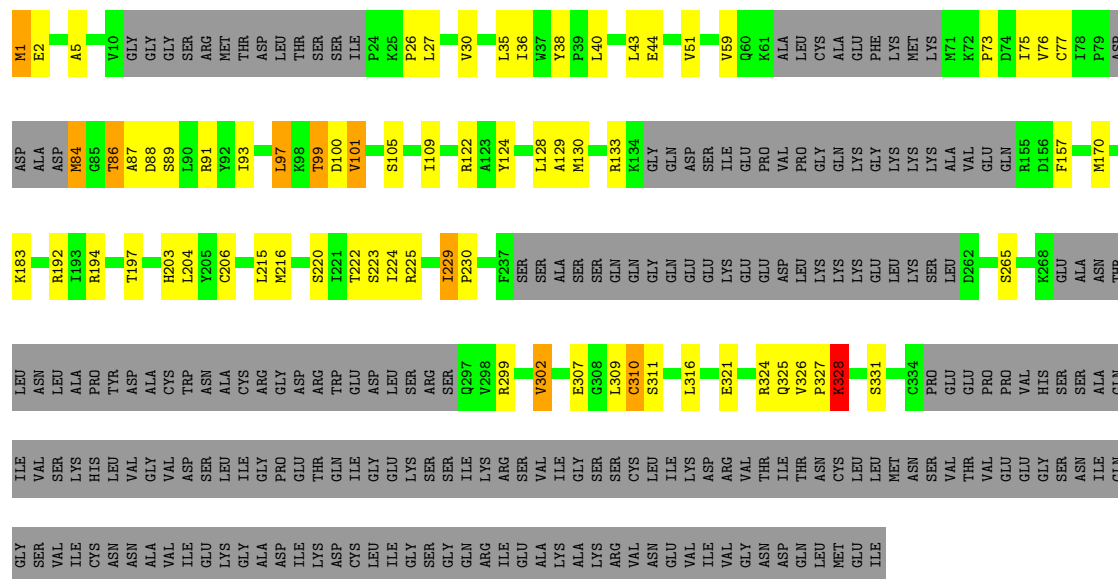
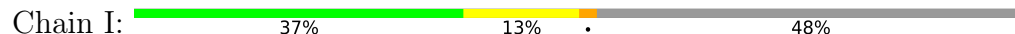
- Molecule 4: Translation initiation factor eIF-2B subunit alpha



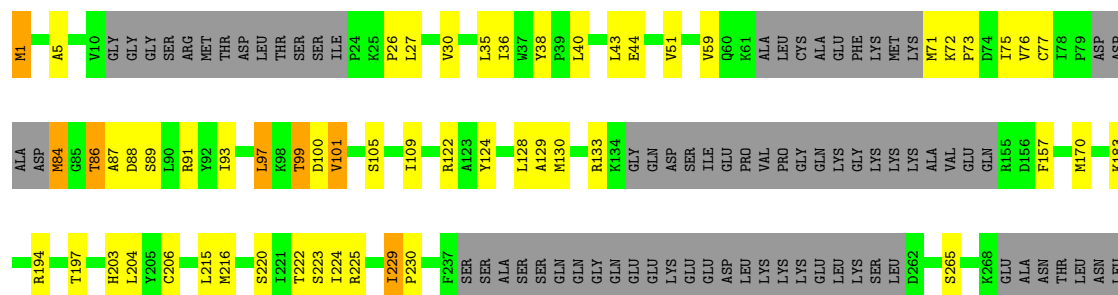
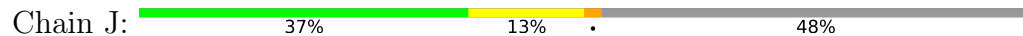
- Molecule 4: Translation initiation factor eIF-2B subunit alpha



- Molecule 5: Translation initiation factor eIF-2B subunit gamma



- Molecule 5: Translation initiation factor eIF-2B subunit gamma



ALA	PRO	TYR	ASP	ALA	CYS	TRP	ASN	ALA	CYS	ARG	GLY	ASP	ARG	TRP	GLU	ASP	LEU	SER	ARG	SER	Q297	V298	R299	V302	E307	G308	L309	C310	S311	L316	E321	R324	Q325	V326	P327	K328	S331	C334	PRO	GLU	GLU	PRO	PRO	VAL	HIS	SER	SER	ALA	GLN	ILE	VAL	SER				
LYS	HIS	LEU	VAL	GLY	VAL	ASP	SER	LEU	ILE	GLY	PRO	GLU	THR	GLN	ILE	GLY	LYS	SER	SER	ILE	LYS	ARG	SER	VAL	ILE	GLY	SER	SER	CYS	LEU	ILE	LYS	ASP	ARG	THR	ILE	THR	ASN	CYS	LEU	LEU	MET	ASN	SER	VAL	THR	VAL	GLU	GLY	SER	ASN	ILE	GLN	GLY	SER	VAL
ILE	CYS	ASN	ALA	VAL	ILE	GLU	LYS	GLY	ALA	ASP	ILE	LYS	ASP	CYS	LEU	ILE	GLY	SER	GLY	GLN	ARG	ILE	GLU	ALA	LYS	ALA	LYS	ARG	VAL	ASN	GLU	VAL	ILE	VAL	GLY	ASN	ASP	GLN	LEU	MET	GLU	ILE														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	0.6	Depositor
Maximum defocus (nm)	2.0	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.16	0/3277	0.52	1/4465 (0.0%)
1	B	0.16	0/3277	0.52	1/4465 (0.0%)
2	C	0.15	0/2619	0.48	0/3540
2	D	0.15	0/2619	0.47	0/3540
3	E	0.16	0/2802	0.44	0/3808
3	F	0.16	0/2802	0.44	0/3808
4	G	0.17	0/2239	0.52	0/3027
4	H	0.18	0/2239	0.52	0/3027
5	I	0.25	1/1890 (0.1%)	0.59	1/2546 (0.0%)
5	J	0.25	1/1890 (0.1%)	0.59	1/2546 (0.0%)
All	All	0.18	2/25654 (0.0%)	0.51	4/34772 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	229	ILE	CA-CB	-7.71	1.50	1.54
5	I	229	ILE	CA-CB	-7.62	1.50	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	328	LYS	CA-CB-CG	5.53	125.16	114.10
5	I	328	LYS	CA-CB-CG	5.52	125.15	114.10
1	B	56	PHE	N-CA-C	-5.19	102.65	110.70
1	A	56	PHE	N-CA-C	-5.16	102.71	110.70

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	3210	0	3160	54	0
1	B	3210	0	3160	50	0
2	C	2571	0	2581	60	0
2	D	2571	0	2581	60	0
3	E	2750	0	2816	53	0
3	F	2750	0	2816	53	0
4	G	2203	0	2271	59	0
4	H	2203	0	2271	58	0
5	I	1861	0	1924	46	0
5	J	1861	0	1924	45	0
All	All	25190	0	25504	491	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 10.

All (491) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD1	1:A:274:ARG:NH2	2.08	0.85
1:B:271:ASP:OD1	1:B:274:ARG:NH2	2.08	0.85
4:H:303:LEU:HD23	4:H:305:LEU:HD22	1.61	0.82
4:G:303:LEU:HD23	4:G:305:LEU:HD22	1.61	0.82
3:F:193:THR:HA	3:F:196:MET:HE3	1.63	0.81
3:E:193:THR:HA	3:E:196:MET:HE3	1.63	0.79
4:G:235:PHE:HB3	4:G:300:LEU:HD21	1.66	0.77
5:J:124:TYR:O	5:J:299:ARG:NH1	2.18	0.77
4:H:235:PHE:HB3	4:H:300:LEU:HD21	1.66	0.77
1:A:223:ARG:HG3	5:I:183:LYS:HA	1.67	0.76
5:I:124:TYR:O	5:I:299:ARG:NH1	2.18	0.76
3:E:189:GLN:OE1	3:E:189:GLN:N	2.22	0.72
3:F:189:GLN:N	3:F:189:GLN:OE1	2.22	0.71
1:B:236:ASP:O	5:J:194:ARG:NH1	2.24	0.71
1:A:199:ASP:N	1:A:199:ASP:OD1	2.23	0.70
2:C:54:ALA:HB3	2:C:122:PHE:HB3	1.72	0.70
2:D:54:ALA:HB3	2:D:122:PHE:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:OD1	1:B:199:ASP:N	2.23	0.69
2:D:32:GLU:OE2	2:D:36:ARG:NH2	2.25	0.69
3:F:198:ILE:O	5:J:122:ARG:NH2	2.26	0.69
1:B:44:GLN:NE2	1:B:90:GLU:OE1	2.27	0.67
1:B:156:ILE:HD13	1:B:309:VAL:HG11	1.75	0.67
1:B:204:ALA:HB3	1:B:214:HIS:HB3	1.76	0.67
1:A:44:GLN:NE2	1:A:90:GLU:OE1	2.27	0.66
1:A:204:ALA:HB3	1:A:214:HIS:HB3	1.76	0.66
3:F:421:ALA:HA	3:F:492:THR:HG23	1.77	0.66
4:G:69:GLY:O	4:G:73:LEU:HD13	1.96	0.66
5:I:88:ASP:OD1	5:I:91:ARG:NH1	2.28	0.66
5:J:88:ASP:OD1	5:J:91:ARG:NH1	2.28	0.66
1:A:156:ILE:HD13	1:A:309:VAL:HG11	1.75	0.66
3:F:499:LEU:HD11	3:F:506:MET:HB3	1.78	0.66
2:C:238:THR:HG22	2:C:246:ARG:HB3	1.77	0.66
2:C:228:ARG:HH11	3:F:179:LEU:HD23	1.62	0.65
4:H:69:GLY:O	4:H:73:LEU:HD13	1.96	0.65
3:E:421:ALA:HA	3:E:492:THR:HG23	1.77	0.65
3:E:499:LEU:HD11	3:E:506:MET:HB3	1.78	0.65
2:C:274:LEU:HD22	2:C:340:MET:HE1	1.79	0.65
1:B:223:ARG:HG3	5:J:183:LYS:HA	1.79	0.65
2:D:30:SER:OG	2:D:33:GLU:OE1	2.14	0.64
2:D:238:THR:HG22	2:D:246:ARG:HB3	1.77	0.64
4:G:9:TYR:HD1	4:G:29:THR:HG22	1.62	0.64
2:C:32:GLU:OE2	2:C:36:ARG:NH2	2.25	0.64
4:H:9:TYR:HD1	4:H:29:THR:HG22	1.62	0.64
5:J:1:MET:SD	5:J:1:MET:N	2.68	0.64
2:D:274:LEU:HD22	2:D:340:MET:HE1	1.79	0.64
3:E:198:ILE:O	5:I:122:ARG:NH2	2.31	0.64
1:A:70:LEU:HD13	1:A:75:LEU:HD21	1.80	0.63
5:I:86:THR:OG1	5:I:224:ILE:HG12	1.98	0.63
2:C:30:SER:OG	2:C:33:GLU:OE1	2.14	0.63
5:J:86:THR:OG1	5:J:224:ILE:HG12	1.98	0.63
2:D:113:LEU:HD12	4:H:303:LEU:HD11	1.80	0.63
3:F:275:ASN:ND2	3:F:441:TYR:O	2.32	0.62
1:B:70:LEU:HD13	1:B:75:LEU:HD21	1.80	0.62
3:E:275:ASN:ND2	3:E:441:TYR:O	2.32	0.62
2:D:14:ARG:NH1	2:D:44:GLN:OE1	2.33	0.62
5:I:133:ARG:HD2	5:I:310:CYS:HB3	1.82	0.61
4:H:246:VAL:HB	4:H:251:LYS:HE2	1.83	0.61
4:G:246:VAL:HB	4:G:251:LYS:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:133:ARG:HD2	5:J:310:CYS:HB3	1.82	0.61
5:J:328:LYS:H	5:J:328:LYS:HD3	1.65	0.61
2:D:143:GLU:O	2:D:147:THR:HG23	2.01	0.61
3:E:408:LEU:HD12	3:E:443:PHE:CE1	2.36	0.61
4:H:49:LEU:O	4:H:53:ILE:HG23	2.01	0.61
3:E:191:SER:OG	3:E:193:THR:HG22	2.01	0.61
1:A:236:ASP:O	5:I:194:ARG:NH1	2.33	0.60
3:F:408:LEU:HD12	3:F:443:PHE:CE1	2.36	0.60
4:G:49:LEU:O	4:G:53:ILE:HG23	2.01	0.60
2:C:143:GLU:O	2:C:147:THR:HG23	2.01	0.60
5:I:328:LYS:H	5:I:328:LYS:HD3	1.65	0.60
3:F:191:SER:OG	3:F:193:THR:HG22	2.01	0.60
2:C:14:ARG:NH1	2:C:44:GLN:OE1	2.33	0.60
5:I:321:GLU:OE2	5:I:324:ARG:NH2	2.35	0.59
5:J:170:MET:HE2	5:J:230:PRO:HG3	1.84	0.59
4:G:179:LEU:HD13	4:H:157:PRO:HG3	1.83	0.59
3:F:309:GLN:HA	3:F:313:VAL:HG13	1.85	0.59
1:A:315:ARG:NH1	2:D:303:LEU:O	2.33	0.59
5:I:170:MET:HE2	5:I:230:PRO:HG3	1.84	0.59
3:F:469:GLU:N	3:F:469:GLU:OE1	2.36	0.59
2:C:278:PHE:O	2:C:280:ASN:N	2.35	0.59
5:J:321:GLU:OE2	5:J:324:ARG:NH2	2.36	0.59
5:I:97:LEU:HD21	5:I:101:VAL:HG23	1.84	0.59
5:I:129:ALA:HB3	5:I:206:CYS:HB2	1.85	0.58
3:E:309:GLN:HA	3:E:313:VAL:HG13	1.85	0.58
3:E:469:GLU:OE1	3:E:469:GLU:N	2.36	0.58
1:B:408:ILE:HG12	1:B:425:LEU:HD13	1.85	0.58
1:A:195:ARG:NH1	1:A:242:TYR:O	2.30	0.58
5:I:1:MET:SD	5:I:1:MET:N	2.68	0.58
3:F:320:SER:HA	3:F:345:ILE:HG12	1.86	0.58
1:B:366:THR:OG1	1:B:380:GLY:O	2.22	0.58
1:A:90:GLU:OE2	1:A:121:ARG:NH1	2.37	0.58
2:D:228:ARG:HH11	3:E:179:LEU:HD23	1.69	0.58
1:B:90:GLU:OE2	1:B:121:ARG:NH1	2.37	0.58
1:A:366:THR:OG1	1:A:380:GLY:O	2.22	0.57
1:A:408:ILE:HG12	1:A:425:LEU:HD13	1.85	0.57
4:G:86:TYR:HA	4:G:89:CYS:HB3	1.85	0.57
5:J:97:LEU:HD21	5:J:101:VAL:HG23	1.84	0.57
5:J:129:ALA:HB3	5:J:206:CYS:HB2	1.85	0.57
1:A:432:THR:HG22	1:A:433:SER:H	1.70	0.57
1:B:316:ARG:HH12	1:B:324:GLU:HG2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:LEU:HD11	3:F:447:VAL:HG11	1.87	0.57
1:A:316:ARG:HH12	1:A:324:GLU:HG2	1.70	0.57
4:G:30:LEU:HD21	4:G:53:ILE:HG22	1.85	0.57
4:H:30:LEU:HD21	4:H:53:ILE:HG22	1.86	0.56
2:D:165:ILE:HD13	2:D:231:LYS:HB3	1.86	0.56
2:D:278:PHE:O	2:D:280:ASN:N	2.35	0.56
1:B:432:THR:HG22	1:B:433:SER:H	1.70	0.56
4:H:86:TYR:HA	4:H:89:CYS:HB3	1.85	0.56
3:E:320:SER:HA	3:E:345:ILE:HG12	1.86	0.56
2:C:165:ILE:HD13	2:C:231:LYS:HB3	1.87	0.56
1:B:258:GLN:NE2	1:B:262:ASP:OD2	2.39	0.56
5:J:325:GLN:HB3	5:J:328:LYS:NZ	2.21	0.55
5:I:325:GLN:HB3	5:I:328:LYS:NZ	2.21	0.55
1:B:53:ASP:O	1:B:65:ARG:NH2	2.39	0.55
4:G:73:LEU:O	4:G:76:ILE:HG13	2.07	0.55
1:A:53:ASP:O	1:A:65:ARG:NH2	2.39	0.55
4:G:72:PHE:O	4:G:76:ILE:HG23	2.07	0.55
2:C:195:ALA:HB1	3:F:387:LEU:HD13	1.88	0.55
4:H:72:PHE:O	4:H:76:ILE:HG23	2.07	0.55
5:J:99:THR:HG22	5:J:100:ASP:H	1.72	0.55
3:F:213:GLN:HG2	3:F:218:LEU:HD12	1.89	0.54
5:I:99:THR:HG22	5:I:100:ASP:H	1.72	0.54
1:B:184:ILE:HD13	1:B:290:HIS:HB3	1.90	0.54
3:E:213:GLN:HG2	3:E:218:LEU:HD12	1.89	0.54
3:F:408:LEU:HD12	3:F:443:PHE:HE1	1.73	0.54
4:H:73:LEU:O	4:H:76:ILE:HG13	2.07	0.54
4:G:197:ALA:HB3	4:G:230:ALA:HB2	1.90	0.54
1:A:258:GLN:NE2	1:A:262:ASP:OD2	2.39	0.54
1:A:184:ILE:HD13	1:A:290:HIS:HB3	1.90	0.54
3:E:187:SER:HB3	3:E:190:ASN:OD1	2.08	0.54
3:E:333:ILE:HG21	3:E:402:LEU:HD12	1.90	0.54
2:C:52:SER:N	2:C:56:GLU:OE2	2.31	0.53
4:H:197:ALA:HB3	4:H:230:ALA:HB2	1.89	0.53
2:D:52:SER:N	2:D:56:GLU:OE2	2.31	0.53
4:G:17:ASP:OD2	4:G:17:ASP:N	2.42	0.53
2:D:92:GLU:O	2:D:96:LEU:HD12	2.09	0.53
2:C:241:ALA:HA	2:C:340:MET:HE3	1.91	0.53
4:H:53:ILE:HD13	4:H:73:LEU:HD11	1.91	0.53
3:E:408:LEU:HD12	3:E:443:PHE:HE1	1.73	0.53
4:G:157:PRO:HG3	4:H:179:LEU:HD13	1.90	0.53
3:F:187:SER:HB3	3:F:190:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:128:LEU:HD21	5:J:229:ILE:HG23	1.91	0.53
2:D:241:ALA:HA	2:D:340:MET:HE3	1.91	0.53
5:J:27:LEU:HD21	5:J:59:VAL:HG13	1.91	0.53
2:D:53:ASN:ND2	2:D:123:SER:O	2.42	0.52
4:G:53:ILE:HD13	4:G:73:LEU:HD11	1.91	0.52
2:C:92:GLU:O	2:C:96:LEU:HD12	2.09	0.52
2:C:128:GLN:OE1	2:C:128:GLN:N	2.32	0.52
4:H:4:LYS:HB2	4:H:4:LYS:NZ	2.25	0.52
4:H:17:ASP:OD2	4:H:17:ASP:N	2.42	0.52
3:E:222:SER:HG	3:E:272:SER:HG	1.57	0.52
4:G:203:ASN:HB3	4:G:239:PHE:CZ	2.44	0.52
2:C:53:ASN:ND2	2:C:123:SER:O	2.42	0.52
4:H:203:ASN:HB3	4:H:239:PHE:CZ	2.44	0.52
4:G:4:LYS:NZ	4:G:4:LYS:HB2	2.25	0.52
4:G:108:ARG:HD3	4:G:132:ARG:HG3	1.91	0.52
5:I:128:LEU:HD21	5:I:229:ILE:HG23	1.91	0.52
3:F:333:ILE:HG21	3:F:402:LEU:HD12	1.90	0.52
5:I:87:ALA:HB2	5:I:224:ILE:HG23	1.91	0.52
3:F:403:LEU:HD21	3:F:423:LEU:HD23	1.92	0.52
4:G:229:VAL:HG12	4:G:285:PHE:HB2	1.91	0.52
3:F:209:ARG:HH21	5:J:122:ARG:HA	1.75	0.52
4:H:10:PHE:HA	4:H:29:THR:HG21	1.92	0.51
1:A:83:LEU:HD21	1:A:151:VAL:HG21	1.92	0.51
3:E:403:LEU:HD21	3:E:423:LEU:HD23	1.92	0.51
5:I:203:HIS:ND1	5:I:225:ARG:HD3	2.25	0.51
1:B:83:LEU:HD21	1:B:151:VAL:HG21	1.92	0.51
2:C:130:GLN:O	2:C:134:ILE:HG12	2.11	0.51
2:D:89:ILE:HA	2:D:133:ILE:HD11	1.93	0.51
5:I:27:LEU:HD21	5:I:59:VAL:HG13	1.91	0.51
5:J:203:HIS:ND1	5:J:225:ARG:HD3	2.25	0.51
1:A:237:GLY:HA2	5:I:194:ARG:NH1	2.25	0.51
2:D:59:GLU:HA	2:D:59:GLU:OE1	2.10	0.51
5:J:87:ALA:HB2	5:J:224:ILE:HG23	1.91	0.51
2:D:130:GLN:O	2:D:134:ILE:HG12	2.10	0.51
3:E:509:CYS:O	3:E:512:VAL:HG23	2.11	0.51
5:I:328:LYS:O	5:I:331:SER:OG	2.29	0.51
1:B:195:ARG:NH1	1:B:242:TYR:O	2.30	0.51
2:C:59:GLU:OE1	2:C:59:GLU:HA	2.10	0.51
3:F:196:MET:HE1	3:F:262:PHE:CE1	2.46	0.51
3:F:428:ARG:HE	3:F:496:LEU:HA	1.76	0.51
4:H:229:VAL:HG12	4:H:285:PHE:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLN:OE1	2:D:128:GLN:N	2.32	0.51
3:E:196:MET:HE1	3:E:262:PHE:CE1	2.46	0.51
4:H:108:ARG:HD3	4:H:132:ARG:HG3	1.91	0.51
2:C:43:ARG:NH2	2:C:138:ASN:OD1	2.41	0.51
1:A:338:SER:OG	1:A:339:ARG:N	2.45	0.50
3:E:428:ARG:HE	3:E:496:LEU:HA	1.76	0.50
1:B:338:SER:OG	1:B:339:ARG:N	2.45	0.50
2:D:43:ARG:NH2	2:D:138:ASN:OD1	2.41	0.50
4:G:13:GLN:HE22	4:G:28:ARG:HB3	1.77	0.50
2:C:89:ILE:HA	2:C:133:ILE:HD11	1.93	0.50
3:F:180:PHE:HB3	3:F:457:LEU:HD11	1.93	0.50
3:E:209:ARG:HH21	5:I:122:ARG:HA	1.76	0.50
1:B:340:HIS:NE2	3:F:397:GLU:OE2	2.45	0.50
3:F:509:CYS:O	3:F:512:VAL:HG23	2.11	0.50
4:H:67:SER:O	4:H:71:LEU:HD13	2.12	0.50
1:A:315:ARG:HH12	2:D:304:GLU:HA	1.77	0.50
4:G:75:PHE:HB2	2:C:113:LEU:HB3	1.93	0.50
4:G:10:PHE:HA	4:G:29:THR:HG21	1.92	0.50
4:G:242:ASN:HB2	4:H:188:GLU:OE1	2.10	0.50
1:B:450:SER:OG	1:B:455:ASP:OD2	2.21	0.50
2:C:131:SER:O	2:C:135:GLU:HG2	2.12	0.50
4:H:13:GLN:HE22	4:H:28:ARG:HB3	1.77	0.50
1:A:47:LEU:HD23	1:A:93:VAL:HG13	1.93	0.49
3:E:180:PHE:HB3	3:E:457:LEU:HD11	1.93	0.49
5:J:328:LYS:O	5:J:331:SER:OG	2.29	0.49
4:G:79:ALA:HB3	4:G:93:MET:HE2	1.94	0.49
1:A:201:VAL:HG11	1:A:215:PHE:CZ	2.48	0.49
2:D:90:ARG:NH2	2:D:348:ASP:OD1	2.44	0.49
4:G:211:GLY:CA	4:H:181:ALA:HB1	2.42	0.49
2:D:284:SER:O	2:D:284:SER:OG	2.29	0.49
1:B:250:SER:HG	1:B:252:CYS:HG	1.60	0.49
3:F:310:GLU:HG3	3:F:311:LYS:HD2	1.95	0.49
4:H:300:LEU:HD22	4:H:305:LEU:HD21	1.95	0.49
1:B:47:LEU:HD23	1:B:93:VAL:HG13	1.93	0.49
3:F:240:TYR:OH	3:F:251:ASP:OD2	2.22	0.49
4:H:79:ALA:HB3	4:H:93:MET:HE2	1.94	0.49
1:A:452:HIS:HB2	1:A:455:ASP:OD2	2.12	0.49
4:G:300:LEU:HD22	4:G:305:LEU:HD21	1.95	0.49
3:E:173:TYR:CG	3:E:187:SER:HB2	2.48	0.49
4:G:67:SER:O	4:G:71:LEU:HD13	2.12	0.49
2:D:131:SER:O	2:D:135:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:HIS:HB2	1:B:455:ASP:OD2	2.12	0.49
1:B:455:ASP:OD1	1:B:456:ALA:N	2.45	0.49
1:A:450:SER:OG	1:A:455:ASP:OD2	2.21	0.48
3:E:446:ARG:HH12	3:E:448:GLN:HE21	1.61	0.48
2:D:43:ARG:HG2	2:D:134:ILE:HD12	1.95	0.48
3:F:173:TYR:CG	3:F:187:SER:HB2	2.47	0.48
3:F:446:ARG:HH12	3:F:448:GLN:HE21	1.60	0.48
3:F:233:LEU:HD21	3:F:260:MET:HE1	1.95	0.48
3:F:471:VAL:HB	3:F:474:ALA:HB2	1.96	0.48
3:E:480:ALA:O	3:E:483:ARG:NH2	2.46	0.48
2:C:43:ARG:HG2	2:C:134:ILE:HD12	1.94	0.48
2:C:284:SER:O	2:C:284:SER:OG	2.29	0.48
2:D:97:HIS:ND1	2:D:126:TYR:OH	2.46	0.48
3:E:471:VAL:HB	3:E:474:ALA:HB2	1.96	0.48
3:F:222:SER:HG	3:F:272:SER:HG	1.60	0.48
4:G:188:GLU:OE1	4:H:242:ASN:HB2	2.13	0.48
1:B:201:VAL:HG11	1:B:215:PHE:CZ	2.48	0.48
3:F:480:ALA:O	3:F:483:ARG:NH2	2.46	0.48
1:A:72:ASN:HD21	1:A:380:GLY:HA2	1.78	0.48
4:H:50:THR:O	4:H:53:ILE:HG12	2.14	0.48
2:C:90:ARG:NH2	2:C:348:ASP:OD1	2.44	0.48
2:C:234:ILE:HD11	2:C:265:LEU:HD21	1.94	0.48
4:H:51:SER:O	4:H:54:GLU:HG3	2.14	0.48
2:D:195:ALA:HB1	3:E:387:LEU:HD13	1.95	0.48
3:E:310:GLU:HG3	3:E:311:LYS:HD2	1.95	0.48
4:G:51:SER:O	4:G:54:GLU:HG3	2.14	0.48
5:I:5:ALA:HB1	5:I:43:LEU:HD13	1.96	0.48
2:C:245:LEU:HD11	2:C:267:VAL:HG21	1.95	0.48
2:D:234:ILE:HD11	2:D:265:LEU:HD21	1.95	0.48
4:G:203:ASN:OD1	4:G:203:ASN:N	2.46	0.48
1:B:315:ARG:NH1	2:C:303:LEU:O	2.47	0.47
2:C:65:GLY:HA2	2:C:68:MET:HE3	1.96	0.47
1:A:166:GLU:OE2	1:A:166:GLU:HA	2.15	0.47
2:D:306:VAL:HG11	3:E:373:LEU:HD21	1.96	0.47
4:G:50:THR:O	4:G:53:ILE:HG12	2.14	0.47
5:J:26:PRO:O	5:J:35:LEU:HB3	2.15	0.47
1:A:455:ASP:OD1	1:A:456:ALA:N	2.46	0.47
3:E:233:LEU:HD21	3:E:260:MET:HE1	1.95	0.47
5:I:130:MET:HG3	5:I:302:VAL:HG23	1.97	0.47
1:B:72:ASN:HD21	1:B:380:GLY:HA2	1.78	0.47
2:D:245:LEU:HD11	2:D:267:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:287:ASP:OD1	4:G:287:ASP:N	2.47	0.47
5:I:84:MET:HE2	5:I:89:SER:HA	1.96	0.47
5:I:325:GLN:HB3	5:I:328:LYS:HZ2	1.78	0.47
2:C:72:GLN:HE22	2:C:287:LYS:HD2	1.80	0.47
4:H:287:ASP:OD1	4:H:287:ASP:N	2.47	0.47
5:J:5:ALA:HB1	5:J:43:LEU:HD13	1.96	0.47
5:J:26:PRO:HA	5:J:35:LEU:HD23	1.96	0.47
2:D:274:LEU:O	2:D:344:TYR:OH	2.29	0.47
1:B:192:HIS:CD2	2:C:303:LEU:HD12	2.49	0.47
2:D:65:GLY:HA2	2:D:68:MET:HE3	1.96	0.47
2:D:72:GLN:HE22	2:D:287:LYS:HD2	1.80	0.47
4:G:47:ALA:O	4:G:51:SER:OG	2.31	0.46
1:A:340:HIS:NE2	3:E:397:GLU:OE2	2.47	0.46
3:E:188:ARG:NH1	3:E:188:ARG:HB2	2.30	0.46
3:E:198:ILE:HD13	3:E:198:ILE:HA	1.72	0.46
4:G:130:TYR:HB3	4:G:160:SER:OG	2.16	0.46
4:H:56:LEU:HA	4:H:56:LEU:HD23	1.67	0.46
4:G:27:ILE:HD11	4:G:72:PHE:HB2	1.97	0.46
4:G:112:ALA:HA	4:G:137:VAL:HG22	1.98	0.46
5:I:26:PRO:O	5:I:35:LEU:HB3	2.15	0.46
4:H:112:ALA:HA	4:H:137:VAL:HG22	1.98	0.46
3:E:422:GLN:O	3:E:426:VAL:HG23	2.15	0.46
5:J:84:MET:HE2	5:J:89:SER:HA	1.96	0.46
5:J:97:LEU:HD21	5:J:101:VAL:CG2	2.46	0.46
5:I:26:PRO:HB2	5:I:36:ILE:HD11	1.98	0.46
5:I:40:LEU:O	5:I:44:GLU:N	2.44	0.46
4:H:130:TYR:HB3	4:H:160:SER:OG	2.16	0.46
4:G:303:LEU:HD11	2:C:113:LEU:HD12	1.97	0.46
5:I:157:PHE:HD1	5:I:197:THR:HG22	1.81	0.46
1:A:201:VAL:HG11	1:A:215:PHE:CE2	2.51	0.46
1:A:248:HIS:CG	1:A:299:ARG:HD2	2.51	0.46
5:I:26:PRO:HA	5:I:35:LEU:HD23	1.96	0.46
1:B:166:GLU:HA	1:B:166:GLU:OE2	2.14	0.46
1:B:201:VAL:HG11	1:B:215:PHE:CE2	2.51	0.46
5:J:157:PHE:HD1	5:J:197:THR:HG22	1.81	0.46
1:B:211:ARG:CZ	1:B:286:GLN:HE21	2.29	0.46
5:J:109:ILE:HG22	5:J:309:LEU:HD22	1.98	0.46
2:D:286:HIS:HD2	2:D:314:ASP:HA	1.81	0.46
3:F:207:MET:HE2	3:F:236:VAL:HG21	1.97	0.46
3:F:255:LYS:O	3:F:258:PRO:HD2	2.16	0.46
5:J:130:MET:HG3	5:J:302:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:207:MET:HE2	3:E:236:VAL:HG21	1.97	0.45
5:I:30:VAL:O	5:I:38:TYR:OH	2.27	0.45
1:B:248:HIS:CG	1:B:299:ARG:HD2	2.51	0.45
3:F:170:ARG:NH2	3:F:266:CYS:O	2.49	0.45
4:H:27:ILE:HD11	4:H:72:PHE:HB2	1.97	0.45
5:J:26:PRO:HB2	5:J:36:ILE:HD11	1.98	0.45
1:A:211:ARG:CZ	1:A:286:GLN:HE21	2.29	0.45
3:E:255:LYS:O	3:E:258:PRO:HD2	2.16	0.45
3:E:170:ARG:NH2	3:E:266:CYS:O	2.49	0.45
3:F:188:ARG:HB2	3:F:188:ARG:NH1	2.30	0.45
4:H:27:ILE:HD12	4:H:27:ILE:HA	1.74	0.45
4:G:206:ILE:HG21	4:G:228:VAL:HG11	1.97	0.45
5:I:97:LEU:HD21	5:I:101:VAL:CG2	2.46	0.45
2:C:97:HIS:ND1	2:C:126:TYR:OH	2.46	0.45
3:F:422:GLN:O	3:F:426:VAL:HG23	2.15	0.45
1:A:237:GLY:HA2	5:I:194:ARG:CZ	2.47	0.45
2:D:128:GLN:O	2:D:132:ASN:ND2	2.49	0.45
2:D:242:ASN:HB3	2:D:278:PHE:CE2	2.52	0.45
1:B:193:PRO:HG2	2:C:304:GLU:HB3	1.98	0.45
4:H:206:ILE:HG21	4:H:228:VAL:HG11	1.97	0.45
5:J:30:VAL:O	5:J:38:TYR:OH	2.27	0.45
4:G:20:MET:HE1	4:G:28:ARG:HH11	1.81	0.45
1:A:250:SER:HG	1:A:252:CYS:HG	1.64	0.45
5:I:328:LYS:HD3	5:I:328:LYS:N	2.31	0.45
5:I:215:LEU:HD23	5:I:215:LEU:HA	1.90	0.45
2:C:128:GLN:O	2:C:132:ASN:ND2	2.49	0.45
2:C:242:ASN:HB3	2:C:278:PHE:CE2	2.52	0.45
2:D:37:GLU:HA	2:D:37:GLU:OE2	2.17	0.45
1:B:75:LEU:HD22	1:B:156:ILE:HD11	1.99	0.45
2:D:188:HIS:HE1	2:D:215:THR:OG1	2.00	0.44
1:B:186:LYS:HE3	2:C:297:PHE:CD2	2.52	0.44
4:G:303:LEU:HA	2:C:110:HIS:HB2	2.00	0.44
2:C:43:ARG:HB2	2:C:137:ILE:HG21	1.98	0.44
4:H:154:GLU:O	4:H:154:GLU:HG2	2.18	0.44
5:J:309:LEU:O	5:J:311:SER:N	2.50	0.44
5:I:109:ILE:HG22	5:I:309:LEU:HD22	1.98	0.44
4:H:132:ARG:HA	4:H:132:ARG:HD2	1.87	0.44
1:B:332:THR:O	1:B:332:THR:OG1	2.35	0.44
1:A:75:LEU:HD22	1:A:156:ILE:HD11	1.99	0.44
2:D:45:ILE:HD13	2:D:64:GLU:OE1	2.17	0.44
2:D:281:GLU:CD	2:D:282:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:56:LEU:HA	4:G:56:LEU:HD23	1.67	0.44
2:C:37:GLU:OE2	2:C:37:GLU:HA	2.17	0.44
2:C:188:HIS:HE1	2:C:215:THR:OG1	2.00	0.44
3:F:499:LEU:HD13	4:H:239:PHE:CE2	2.53	0.44
4:G:103:ARG:HG2	2:C:112:LEU:HD13	1.98	0.44
4:G:211:GLY:HA3	4:H:181:ALA:HB1	2.00	0.44
5:I:89:SER:O	5:I:93:ILE:HG12	2.18	0.44
5:I:326:VAL:CG1	5:I:327:PRO:HD3	2.47	0.44
2:C:228:ARG:NH1	3:F:179:LEU:HD23	2.30	0.44
4:H:20:MET:HE1	4:H:28:ARG:HH11	1.81	0.44
4:G:237:ARG:HG3	4:G:305:LEU:HG	1.99	0.44
4:G:300:LEU:CD2	4:G:305:LEU:HD21	2.48	0.44
5:J:89:SER:O	5:J:93:ILE:HG12	2.18	0.44
5:J:328:LYS:HD3	5:J:328:LYS:N	2.31	0.44
2:C:45:ILE:HD13	2:C:64:GLU:OE1	2.17	0.44
4:H:240:PRO:HA	4:H:245:ASP:HB3	2.00	0.44
2:D:43:ARG:HB2	2:D:137:ILE:HG21	1.98	0.43
4:H:237:ARG:HG3	4:H:305:LEU:HG	1.99	0.43
1:A:136:ARG:NH1	1:A:260:PHE:O	2.51	0.43
4:G:154:GLU:O	4:G:154:GLU:HG2	2.18	0.43
2:C:286:HIS:HD2	2:C:314:ASP:HA	1.81	0.43
1:A:104:GLU:O	1:A:108:LYS:HG3	2.18	0.43
3:E:240:TYR:OH	3:E:251:ASP:OD2	2.22	0.43
2:C:81:MET:HE3	2:C:272:PHE:HB2	2.01	0.43
5:I:51:VAL:HG13	5:I:73:PRO:HA	2.00	0.43
5:J:325:GLN:HB3	5:J:328:LYS:HZ2	1.83	0.43
5:J:326:VAL:CG1	5:J:327:PRO:HD3	2.47	0.43
2:D:81:MET:HE3	2:D:272:PHE:HB2	2.01	0.43
2:D:193:GLU:OE1	3:E:364:ARG:NH2	2.51	0.43
4:G:25:ALA:O	4:G:29:THR:HG23	2.19	0.43
4:G:128:HIS:HB2	4:G:215:MET:HE1	2.00	0.43
4:G:243:GLN:HB3	4:H:185:TYR:CD1	2.54	0.43
4:H:25:ALA:O	4:H:29:THR:HG23	2.19	0.43
5:J:91:ARG:HB2	5:J:216:MET:HE2	2.00	0.43
4:G:27:ILE:HD12	4:G:27:ILE:HA	1.74	0.43
1:B:51:SER:O	1:B:53:ASP:N	2.43	0.43
2:C:281:GLU:CD	2:C:282:GLU:H	2.26	0.43
5:J:51:VAL:HG13	5:J:73:PRO:HA	2.00	0.43
5:I:309:LEU:O	5:I:311:SER:N	2.50	0.43
1:B:104:GLU:O	1:B:108:LYS:HG3	2.18	0.43
4:H:128:HIS:HB2	4:H:215:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:130:TYR:HB2	4:H:164:MET:HB2	2.01	0.43
1:A:154:ASP:OD2	1:A:154:ASP:N	2.51	0.43
1:A:170:LEU:HA	1:A:173:LYS:HG2	2.00	0.43
1:B:136:ARG:NH1	1:B:260:PHE:O	2.51	0.43
1:A:240:VAL:O	5:I:192:ARG:HA	2.19	0.42
2:C:340:MET:HE2	2:C:340:MET:HB2	1.86	0.42
4:H:47:ALA:O	4:H:51:SER:OG	2.31	0.42
2:D:11:LEU:HD21	2:D:45:ILE:HA	2.01	0.42
3:F:512:VAL:O	3:F:515:VAL:HG22	2.19	0.42
5:I:91:ARG:HB2	5:I:216:MET:HE2	2.00	0.42
1:B:157:SER:HB2	1:B:297:GLY:HA2	2.01	0.42
4:H:300:LEU:CD2	4:H:305:LEU:HD21	2.48	0.42
5:J:71:MET:HB3	5:J:72:LYS:H	1.48	0.42
4:G:13:GLN:HA	4:G:16:GLU:OE2	2.19	0.42
4:G:240:PRO:HA	4:G:245:ASP:HB3	2.00	0.42
5:I:86:THR:HG23	5:I:223:SER:HA	2.02	0.42
1:A:72:ASN:O	1:A:333:GLN:NE2	2.53	0.42
1:A:346:PRO:HG2	1:A:364:SER:HB2	2.02	0.42
4:G:231:GLU:OE1	4:G:231:GLU:N	2.53	0.42
2:C:11:LEU:HD21	2:C:45:ILE:HA	2.01	0.42
4:H:13:GLN:HA	4:H:16:GLU:OE2	2.19	0.42
5:J:86:THR:HG23	5:J:223:SER:HA	2.02	0.42
1:A:188:SER:O	1:A:243:ASP:HB2	2.19	0.42
2:D:225:VAL:HA	3:E:452:PHE:CZ	2.54	0.42
2:D:340:MET:HE2	2:D:340:MET:HB2	1.86	0.42
4:G:132:ARG:HA	4:G:132:ARG:HD2	1.87	0.42
1:A:157:SER:HB2	1:A:297:GLY:HA2	2.01	0.42
3:E:373:LEU:HD22	3:E:385:TYR:CD1	2.55	0.42
1:B:72:ASN:O	1:B:333:GLN:NE2	2.53	0.42
3:F:408:LEU:HD23	3:F:414:VAL:HA	2.02	0.42
4:G:130:TYR:HB2	4:G:164:MET:HB2	2.01	0.42
1:B:170:LEU:HA	1:B:173:LYS:HG2	2.00	0.42
1:B:188:SER:O	1:B:243:ASP:HB2	2.19	0.42
2:D:109:LEU:HD13	4:H:303:LEU:HD22	2.02	0.41
4:H:105:SER:OG	4:H:106:LEU:HD13	2.20	0.41
4:H:110:LYS:HE2	4:H:110:LYS:HB2	1.89	0.41
2:D:20:GLU:HA	2:D:20:GLU:OE1	2.21	0.41
3:F:173:TYR:CD2	3:F:187:SER:HB2	2.55	0.41
3:F:177:VAL:HG21	3:F:485:LEU:HB2	2.03	0.41
2:D:333:PRO:HA	2:D:336:ILE:HG12	2.02	0.41
3:E:512:VAL:O	3:E:515:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:OD2	1:B:154:ASP:N	2.51	0.41
2:C:274:LEU:O	2:C:344:TYR:OH	2.29	0.41
3:F:310:GLU:HG3	3:F:311:LYS:CD	2.50	0.41
3:F:373:LEU:HD22	3:F:385:TYR:CD1	2.54	0.41
4:H:79:ALA:O	4:H:82:GLU:HB2	2.21	0.41
1:A:63:GLN:HA	1:A:64:PRO:HD3	1.94	0.41
1:A:332:THR:O	1:A:332:THR:OG1	2.35	0.41
2:D:15:ILE:HD11	2:D:45:ILE:HG12	2.02	0.41
2:D:249:THR:HG22	3:E:389:PRO:HB2	2.02	0.41
3:E:310:GLU:HG3	3:E:311:LYS:CD	2.50	0.41
3:E:311:LYS:HG2	3:E:441:TYR:HB3	2.03	0.41
3:F:394:VAL:O	3:F:398:VAL:HG23	2.21	0.41
1:A:115:THR:O	1:A:115:THR:OG1	2.39	0.41
1:B:181:MET:HB3	1:B:287:ILE:HG23	2.03	0.41
1:B:237:GLY:HA2	5:J:194:ARG:NH1	2.36	0.41
2:C:15:ILE:HD11	2:C:45:ILE:HG12	2.02	0.41
2:C:20:GLU:OE1	2:C:20:GLU:HA	2.21	0.41
2:D:245:LEU:HD21	2:D:324:PHE:CE1	2.56	0.41
3:E:173:TYR:CD2	3:E:187:SER:HB2	2.55	0.41
5:I:2:GLU:OE1	5:I:122:ARG:NH2	2.48	0.41
2:D:221:ALA:HB1	3:E:487:LEU:HD12	2.02	0.41
2:C:245:LEU:HD21	2:C:324:PHE:CE1	2.56	0.41
3:F:515:VAL:O	3:F:518:VAL:HG23	2.20	0.41
1:A:199:ASP:O	1:A:201:VAL:HG23	2.21	0.41
2:D:51:TRP:CZ3	2:D:129:LEU:HD23	2.56	0.41
3:E:177:VAL:HG21	3:E:485:LEU:HB2	2.03	0.41
4:G:105:SER:OG	4:G:106:LEU:HD13	2.20	0.41
5:I:105:SER:OG	5:I:203:HIS:HB3	2.21	0.41
2:C:245:LEU:HD21	2:C:324:PHE:CZ	2.56	0.41
4:H:158:ASP:O	4:H:160:SER:N	2.52	0.41
4:H:227:TYR:HE1	4:H:283:LEU:HD12	1.86	0.41
1:A:181:MET:HB3	1:A:287:ILE:HG23	2.03	0.41
1:A:310:CYS:O	1:A:314:ILE:HG12	2.20	0.41
2:D:245:LEU:HD21	2:D:324:PHE:CZ	2.56	0.41
3:E:394:VAL:O	3:E:398:VAL:HG23	2.20	0.41
2:C:51:TRP:CZ3	2:C:129:LEU:HD23	2.56	0.41
3:F:170:ARG:HA	3:F:192:LEU:HD13	2.02	0.41
3:F:209:ARG:NE	5:J:122:ARG:O	2.51	0.41
3:F:311:LYS:HG2	3:F:441:TYR:HB3	2.03	0.41
1:A:51:SER:O	1:A:53:ASP:N	2.43	0.41
3:E:170:ARG:HA	3:E:192:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:CYS:O	1:B:314:ILE:HG12	2.20	0.41
3:F:403:LEU:HD13	3:F:420:THR:HG23	2.03	0.41
5:J:40:LEU:O	5:J:44:GLU:N	2.44	0.41
1:B:346:PRO:HG2	1:B:364:SER:HB2	2.02	0.40
3:F:421:ALA:HA	3:F:492:THR:CG2	2.49	0.40
5:J:215:LEU:HD23	5:J:215:LEU:HA	1.90	0.40
1:A:56:PHE:O	1:A:60:SER:OG	2.28	0.40
2:D:42:LEU:HD13	2:D:85:VAL:HG21	2.03	0.40
2:D:271:MET:HE1	2:D:339:LEU:HD13	2.04	0.40
3:E:408:LEU:HD23	3:E:414:VAL:HA	2.02	0.40
2:C:271:MET:HE1	2:C:339:LEU:HD13	2.04	0.40
2:C:286:HIS:CD2	2:C:314:ASP:HA	2.55	0.40
2:D:286:HIS:CD2	2:D:314:ASP:HA	2.56	0.40
3:E:515:VAL:O	3:E:518:VAL:HG23	2.20	0.40
4:G:79:ALA:O	4:G:82:GLU:HB2	2.21	0.40
1:B:270:ASP:OD2	1:B:274:ARG:NE	2.55	0.40
2:C:333:PRO:HA	2:C:336:ILE:HG12	2.02	0.40
4:H:17:ASP:OD1	4:H:20:MET:HE3	2.22	0.40
1:A:350:LEU:HA	1:A:368:ILE:HB	2.04	0.40
2:C:49:HIS:CE1	2:C:60:LEU:HD21	2.56	0.40
5:J:105:SER:OG	5:J:203:HIS:HB3	2.21	0.40
4:G:227:TYR:HE1	4:G:283:LEU:HD12	1.86	0.40
4:G:303:LEU:HD22	2:C:109:LEU:HB3	2.03	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 PDB entries followed by that with respect to all EM entries.

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	410/721 (57%)	388 (95%)	21 (5%)	1 (0%)	43 72
1	B	410/721 (57%)	389 (95%)	20 (5%)	1 (0%)	43 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	323/351 (92%)	309 (96%)	14 (4%)	0	100	100
2	D	323/351 (92%)	309 (96%)	14 (4%)	0	100	100
3	E	351/523 (67%)	348 (99%)	3 (1%)	0	100	100
3	F	351/523 (67%)	348 (99%)	3 (1%)	0	100	100
4	G	281/305 (92%)	272 (97%)	9 (3%)	0	100	100
4	H	281/305 (92%)	272 (97%)	9 (3%)	0	100	100
5	I	222/452 (49%)	210 (95%)	11 (5%)	1 (0%)	24	55
5	J	222/452 (49%)	210 (95%)	11 (5%)	1 (0%)	24	55
All	All	3174/4704 (68%)	3055 (96%)	115 (4%)	4 (0%)	49	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	310	CYS
5	J	310	CYS
1	A	52	PHE
1	B	52	PHE

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 PDB entries followed by that with respect to all EM entries.

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	355/626 (57%)	332 (94%)	23 (6%)	15	43
1	B	355/626 (57%)	332 (94%)	23 (6%)	15	43
2	C	279/298 (94%)	268 (96%)	11 (4%)	28	64
2	D	279/298 (94%)	268 (96%)	11 (4%)	28	64
3	E	309/444 (70%)	290 (94%)	19 (6%)	17	46
3	F	309/444 (70%)	290 (94%)	19 (6%)	17	46
4	G	241/260 (93%)	215 (89%)	26 (11%)	6	21
4	H	241/260 (93%)	215 (89%)	26 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	203/398 (51%)	186 (92%)	17 (8%)	10	32
5	J	203/398 (51%)	186 (92%)	17 (8%)	10	32
All	All	2774/4052 (68%)	2582 (93%)	192 (7%)	16	41

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	115	THR
1	A	119	VAL
1	A	124	THR
1	A	127	LEU
1	A	130	SER
1	A	146	SER
1	A	151	VAL
1	A	166	GLU
1	A	199	ASP
1	A	250	SER
1	A	273	VAL
1	A	328	THR
1	A	329	ASP
1	A	332	THR
1	A	348	VAL
1	A	364	SER
1	A	377	SER
1	A	394	THR
1	A	432	THR
1	A	435	VAL
1	A	447	SER
1	A	450	SER
2	D	13	GLU
2	D	37	GLU
2	D	47	THR
2	D	59	GLU
2	D	111	LYS
2	D	112	LEU
2	D	149	GLU
2	D	171	SER
2	D	214	THR
2	D	227	SER
2	D	284	SER

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Mol	Chain	Res	Type
3	E	167	VAL
3	E	169	THR
3	E	171	LYS
3	E	181	SER
3	E	189	GLN
3	E	191	SER
3	E	197	SER
3	E	198	ILE
3	E	201	SER
3	E	241	THR
3	E	272	SER
3	E	286	SER
3	E	313	VAL
3	E	343	SER
3	E	392	SER
3	E	416	SER
3	E	492	THR
3	E	510	SER
3	E	518	VAL
4	G	4	LYS
4	G	5	GLU
4	G	7	ILE
4	G	15	LYS
4	G	19	ASP
4	G	24	VAL
4	G	27	ILE
4	G	43	GLN
4	G	45	LEU
4	G	51	SER
4	G	54	GLU
4	G	55	THR
4	G	62	SER
4	G	73	LEU
4	G	76	ILE
4	G	83	TYR
4	G	87	SER
4	G	90	LYS
4	G	92	ILE
4	G	95	GLU
4	G	106	LEU
4	G	149	SER
4	G	152	VAL

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Mol	Chain	Res	Type
4	G	154	GLU
4	G	202	GLU
4	G	273	VAL
5	I	1	MET
5	I	75	ILE
5	I	76	VAL
5	I	77	CYS
5	I	84	MET
5	I	86	THR
5	I	97	LEU
5	I	99	THR
5	I	101	VAL
5	I	204	LEU
5	I	220	SER
5	I	222	THR
5	I	265	SER
5	I	302	VAL
5	I	307	GLU
5	I	316	LEU
5	I	328	LYS
1	B	53	ASP
1	B	115	THR
1	B	119	VAL
1	B	124	THR
1	B	127	LEU
1	B	130	SER
1	B	146	SER
1	B	151	VAL
1	B	166	GLU
1	B	199	ASP
1	B	250	SER
1	B	273	VAL
1	B	328	THR
1	B	329	ASP
1	B	332	THR
1	B	348	VAL
1	B	364	SER
1	B	377	SER
1	B	394	THR
1	B	432	THR
1	B	435	VAL
1	B	447	SER

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Mol	Chain	Res	Type
1	B	450	SER
2	C	13	GLU
2	C	37	GLU
2	C	47	THR
2	C	59	GLU
2	C	111	LYS
2	C	112	LEU
2	C	149	GLU
2	C	171	SER
2	C	214	THR
2	C	227	SER
2	C	284	SER
3	F	167	VAL
3	F	169	THR
3	F	171	LYS
3	F	181	SER
3	F	189	GLN
3	F	191	SER
3	F	197	SER
3	F	198	ILE
3	F	201	SER
3	F	241	THR
3	F	272	SER
3	F	286	SER
3	F	313	VAL
3	F	343	SER
3	F	392	SER
3	F	416	SER
3	F	492	THR
3	F	510	SER
3	F	518	VAL
4	H	4	LYS
4	H	5	GLU
4	H	7	ILE
4	H	15	LYS
4	H	19	ASP
4	H	24	VAL
4	H	27	ILE
4	H	43	GLN
4	H	45	LEU
4	H	51	SER
4	H	54	GLU

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Mol	Chain	Res	Type
4	H	55	THR
4	H	62	SER
4	H	73	LEU
4	H	76	ILE
4	H	83	TYR
4	H	87	SER
4	H	90	LYS
4	H	92	ILE
4	H	95	GLU
4	H	106	LEU
4	H	149	SER
4	H	152	VAL
4	H	154	GLU
4	H	202	GLU
4	H	273	VAL
5	J	1	MET
5	J	75	ILE
5	J	76	VAL
5	J	77	CYS
5	J	84	MET
5	J	86	THR
5	J	97	LEU
5	J	99	THR
5	J	101	VAL
5	J	204	LEU
5	J	220	SER
5	J	222	THR
5	J	265	SER
5	J	302	VAL
5	J	307	GLU
5	J	316	LEU
5	J	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	177	ASN
1	A	214	HIS
1	A	219	GLN
1	A	286	GLN
2	D	53	ASN

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Mol	Chain	Res	Type
2	D	72	GLN
2	D	130	GLN
2	D	154	GLN
2	D	162	ASN
2	D	188	HIS
2	D	260	HIS
2	D	261	HIS
2	D	286	HIS
2	D	309	HIS
3	E	185	GLN
3	E	194	GLN
3	E	213	GLN
3	E	223	ASN
3	E	265	GLN
3	E	281	ASN
3	E	347	GLN
3	E	371	HIS
3	E	448	GLN
3	E	464	GLN
4	G	208	ASN
4	G	214	GLN
4	G	222	GLN
4	G	243	GLN
5	I	196	HIS
5	I	323	ASN
1	B	72	ASN
1	B	177	ASN
1	B	214	HIS
1	B	219	GLN
1	B	286	GLN
2	C	53	ASN
2	C	72	GLN
2	C	130	GLN
2	C	154	GLN
2	C	162	ASN
2	C	188	HIS
2	C	260	HIS
2	C	261	HIS
2	C	286	HIS
2	C	309	HIS
3	F	185	GLN
3	F	194	GLN

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Mol	Chain	Res	Type
3	F	213	GLN
3	F	223	ASN
3	F	265	GLN
3	F	347	GLN
3	F	371	HIS
3	F	448	GLN
3	F	464	GLN
4	H	208	ASN
4	H	214	GLN
4	H	222	GLN
5	J	196	HIS
5	J	323	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-26098. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.