



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:56 PM GMT

PDB ID : 3AXY
Title : Structure of Florigen Activation Complex Consisting of Rice Florigen Hd3a, 14-3-3 Protein GF14 and Rice FD Homolog OsFD1
Authors : Ohki, I.; Furuita, K.; Hayashi, K.; Taoka, K.; Tsuji, H.; Nakagawa, A.; Shimamoto, K.; Kojima, C.
Deposited on : 2011-04-19
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

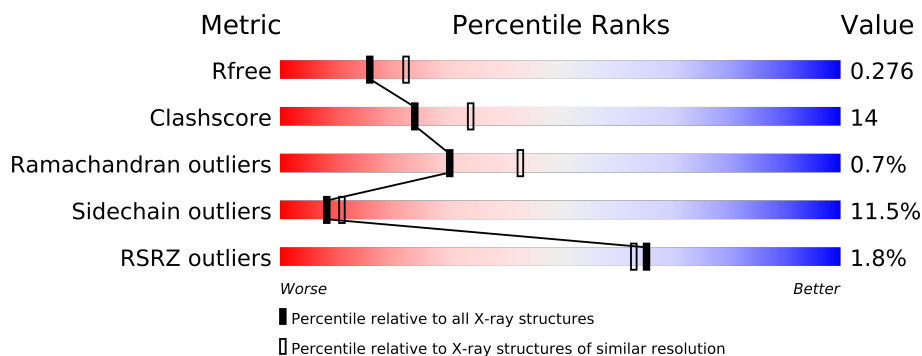
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	G	170	
1	H	170	
2	C	240	
2	D	240	
2	I	240	
2	J	240	
3	E	9	
3	F	9	
3	K	9	
3	L	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13751 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein HEADING DATE 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1312	831	229	246	6			
1	B	166	Total	C	N	O	S	0	0	0
			1312	831	229	246	6			
1	G	165	Total	C	N	O	S	0	0	0
			1306	828	228	244	6			
1	H	166	Total	C	N	O	S	0	0	0
			1312	831	229	246	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
A	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
A	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
A	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
A	5	MET	-	EXPRESSION TAG	UNP Q93WI9
A	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
A	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
A	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
B	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
B	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
B	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
B	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
B	5	MET	-	EXPRESSION TAG	UNP Q93WI9
B	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
B	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
B	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
G	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
G	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
G	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
G	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
G	5	MET	-	EXPRESSION TAG	UNP Q93WI9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
G	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
G	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
H	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
H	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
H	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
H	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
H	5	MET	-	EXPRESSION TAG	UNP Q93WI9
H	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
H	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
H	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9

- Molecule 2 is a protein called 14-3-3-like protein GF14-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	235	Total	C	N	O	S	0	0	0
			1875	1181	312	373	9			
2	D	235	Total	C	N	O	S	0	0	0
			1875	1181	312	373	9			
2	I	235	Total	C	N	O	S	0	0	0
			1875	1181	312	373	9			
2	J	234	Total	C	N	O	S	0	0	0
			1867	1176	311	372	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
C	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
C	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
C	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
C	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0
D	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
D	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
D	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
D	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
D	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0
I	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
I	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
I	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
I	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
I	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
J	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
J	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
J	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
J	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0

- Molecule 3 is a protein called Rice FD homolog OsFD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			
3	F	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			
3	K	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			
3	L	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	68	Total	O	0	0
			68	68		
4	C	118	Total	O	0	0
			118	118		
4	D	92	Total	O	0	0
			92	92		
4	E	9	Total	O	0	0
			9	9		
4	F	4	Total	O	0	0
			4	4		
4	G	120	Total	O	0	0
			120	120		
4	H	68	Total	O	0	0
			68	68		
4	I	104	Total	O	0	0
			104	104		
4	J	74	Total	O	0	0
			74	74		
4	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	4	Total	O	0	0
			4	4		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Protein HEADING DATE 3A

Chain A: 



- Molecule 1: Protein HEADING DATE 3A

Chain B: 



- Molecule 1: Protein HEADING DATE 3A

Chain G: 



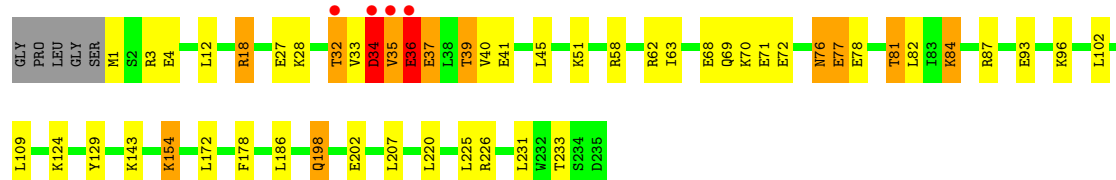
- Molecule 1: Protein HEADING DATE 3A

Chain H: 



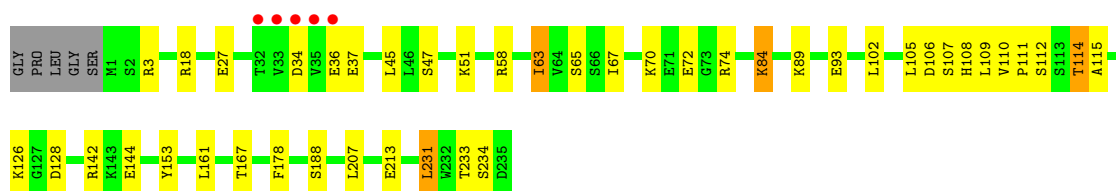
- Molecule 2: 14-3-3-like protein GF14-C

Chain C: 



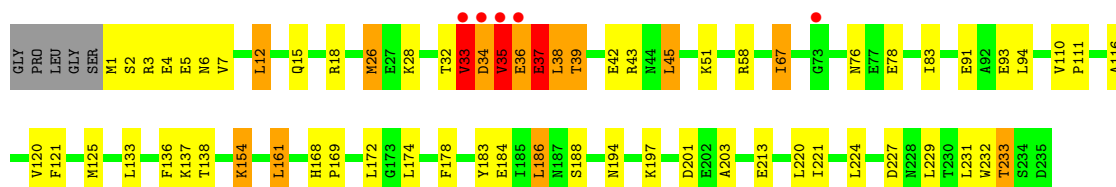
- Molecule 2: 14-3-3-like protein GF14-C

Chain D: 



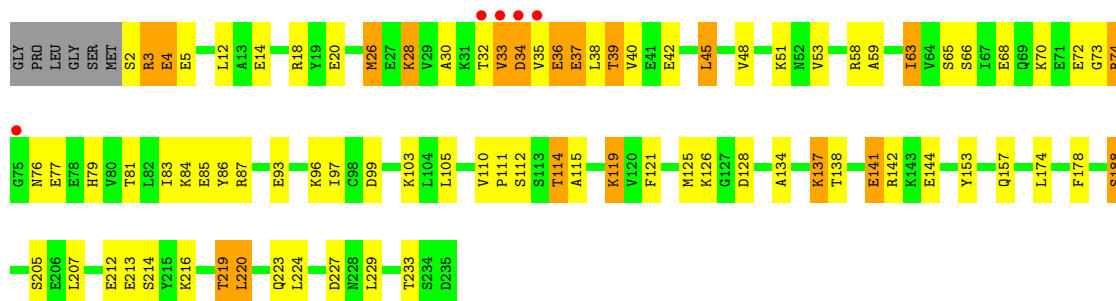
• Molecule 2: 14-3-3-like protein GF14-C

Chain I:



• Molecule 2: 14-3-3-like protein GF14-C

Chain J:



• Molecule 3: Rice FD homolog OsFD1

Chain E:



• Molecule 3: Rice FD homolog OsFD1

Chain F:



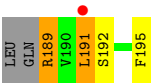
• Molecule 3: Rice FD homolog OsFD1

Chain K:



• Molecule 3: Rice FD homolog OsFD1

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.73Å 96.65Å 99.51Å 68.23° 87.90° 77.94°	Depositor
Resolution (Å)	50.00 – 2.40 37.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.40) 98.1 (37.86-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.227 , 0.276 0.227 , 0.276	Depositor DCC
R_{free} test set	7138 reflections (7.73%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 99449 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13751	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.9501e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1345	0.49	0/1831
1	B	0.33	0/1345	0.45	0/1831
1	G	0.37	0/1339	0.49	0/1824
1	H	0.34	0/1345	0.46	0/1831
2	C	0.38	0/1903	0.50	0/2563
2	D	0.35	0/1903	0.46	0/2563
2	I	0.37	0/1903	0.49	0/2563
2	J	0.34	0/1895	0.44	0/2553
3	E	0.43	0/50	0.92	1/64 (1.6%)
3	F	0.42	0/50	0.54	0/64
3	K	0.47	0/50	0.47	0/64
3	L	0.38	0/50	0.63	0/64
All	All	0.36	0/13178	0.48	1/17815 (0.0%)

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
2	C	0	3
2	I	0	3
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	191	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	129	TYR	Sidechain
2	C	36	GLU	Peptide
2	C	37	GLU	Peptide
2	I	33	VAL	Peptide
2	I	34	ASP	Peptide
2	I	37	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1312	0	0	11	0
1	B	1312	0	0	4	0
1	G	1306	0	0	11	0
1	H	1312	0	0	9	0
2	C	1875	0	0	22	0
2	D	1875	0	0	19	0
2	I	1875	0	1868	79	0
2	J	1867	0	1856	87	0
3	E	60	0	56	4	0
3	F	60	0	56	4	0
3	K	60	0	56	9	0
3	L	60	0	56	6	0
4	A	108	0	0	4	0
4	B	68	0	0	1	0
4	C	118	0	0	7	0
4	D	92	0	0	4	0
4	E	9	0	0	0	0
4	F	4	0	0	2	0
4	G	120	0	0	5	0
4	H	68	0	0	1	0
4	I	104	0	0	7	0
4	J	74	0	0	8	0
4	K	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	4	0	0	0	0
All	All	13751	0	3948	241	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (241) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:189:ARG:HG3	4:F:708:HOH:O	1.40	1.19
2:I:39:THR:HG23	2:I:42:GLU:HG3	1.31	1.10
2:J:39:THR:HG21	4:J:574:HOH:O	1.50	1.09
1:B:99:THR:CG2	1:B:100:ALA:N	2.21	1.02
2:I:26:MET:HE3	2:I:45:LEU:HB3	1.40	1.00
2:I:26:MET:CE	2:I:45:LEU:HB3	1.91	1.00
3:L:189:ARG:HG2	3:L:189:ARG:O	1.62	0.98
2:J:188:SER:HB3	4:J:598:HOH:O	1.61	0.98
2:J:33:VAL:HG13	2:J:36:GLU:H	1.28	0.95
2:J:110:VAL:CG1	2:J:111:PRO:HD3	1.97	0.93
2:J:110:VAL:HG12	2:J:111:PRO:HD3	1.50	0.93
2:I:39:THR:HG23	2:I:42:GLU:CG	2.00	0.92
1:H:99:THR:CG2	1:H:100:ALA:N	2.33	0.90
1:G:99:THR:CG2	1:G:100:ALA:N	2.37	0.88
2:I:26:MET:HE3	2:I:45:LEU:CB	2.03	0.88
2:J:212:GLU:O	2:J:216:LYS:HG3	1.75	0.87
1:A:99:THR:CG2	1:A:100:ALA:N	2.35	0.87
2:J:58:ARG:NH2	3:L:192:SEP:O1P	2.08	0.85
2:J:39:THR:HG22	2:J:42:GLU:OE1	1.77	0.84
2:J:121:PHE:CE1	2:J:125:MET:CE	2.62	0.83
2:J:87:ARG:HG2	2:J:87:ARG:HH11	1.44	0.82
2:J:121:PHE:HE1	2:J:125:MET:CE	1.94	0.81
2:J:20:GLU:HG2	4:J:240:HOH:O	1.80	0.80
3:K:189:ARG:HA	3:K:189:ARG:HH11	1.46	0.80
2:I:26:MET:CE	2:I:45:LEU:HD23	2.14	0.77
1:A:98:THR:CG2	2:C:226:ARG:NH1	2.47	0.77
2:I:26:MET:CE	2:I:45:LEU:CB	2.61	0.75
2:I:154:LYS:HE2	4:I:488:HOH:O	1.87	0.74
2:J:79:HIS:O	2:J:83:ILE:HG13	1.87	0.74
1:B:55:ARG:NH1	2:D:233:THR:O	2.21	0.74
2:C:18:ARG:NH1	2:D:93:GLU:OE2	2.20	0.74
2:J:219:THR:O	2:J:223:GLN:HG3	1.88	0.74
2:J:33:VAL:HG22	2:J:36:GLU:CB	2.18	0.73
2:J:121:PHE:HE1	2:J:125:MET:HE1	1.51	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:233:THR:O	2:J:233:THR:HG22	1.89	0.73
2:I:229:LEU:O	2:I:233:THR:HB	1.89	0.72
2:C:58:ARG:NH2	3:E:192:SEP:O1P	2.23	0.72
4:G:171:HOH:O	2:I:233:THR:HG21	1.89	0.71
2:I:220:LEU:HD12	2:I:221:ILE:HD13	1.72	0.71
2:J:30:ALA:HA	2:J:38:LEU:HD21	1.73	0.71
2:I:224:LEU:HD23	3:K:191:LEU:HD13	1.73	0.71
2:I:233:THR:HG23	4:I:417:HOH:O	1.91	0.71
2:I:26:MET:HE2	2:I:45:LEU:HB3	1.74	0.70
1:A:97:GLY:O	1:A:98:THR:CB	2.39	0.69
2:I:43:ARG:HD3	2:I:121:PHE:CZ	2.28	0.69
2:J:33:VAL:CG1	2:J:36:GLU:H	2.04	0.69
1:H:168:ARG:CZ	4:H:730:HOH:O	2.39	0.69
2:I:58:ARG:NH2	3:K:192:SEP:O1P	2.23	0.69
2:J:37:GLU:OE1	2:J:114:THR:HB	1.93	0.69
2:C:32:THR:CG2	2:C:33:VAL:N	2.56	0.68
2:J:33:VAL:HG22	2:J:36:GLU:HB2	1.75	0.68
2:D:233:THR:O	2:D:233:THR:CG2	2.42	0.67
2:C:35:VAL:O	2:C:35:VAL:CG1	2.43	0.67
2:J:2:SER:HB3	2:J:5:GLU:HB2	1.78	0.66
2:J:35:VAL:O	2:J:35:VAL:HG12	1.96	0.66
2:J:2:SER:N	4:J:600:HOH:O	2.29	0.66
2:J:105:LEU:O	2:J:110:VAL:HG12	1.96	0.65
2:I:36:GLU:O	2:I:37:GLU:C	2.35	0.65
3:E:189:ARG:HG2	3:E:189:ARG:O	1.96	0.65
2:J:33:VAL:HG13	2:J:36:GLU:N	2.06	0.65
2:I:227:ASP:HB3	4:I:258:HOH:O	1.97	0.65
1:A:105:GLN:NE2	4:A:173:HOH:O	2.30	0.65
2:I:35:VAL:HG13	2:I:35:VAL:O	1.96	0.65
2:I:26:MET:HE1	2:I:45:LEU:HD23	1.79	0.64
2:J:26:MET:CE	2:J:45:LEU:HB3	2.27	0.64
2:J:3:ARG:HH12	2:J:33:VAL:HG23	1.63	0.64
2:J:76:ASN:HB3	4:J:670:HOH:O	1.95	0.64
2:D:58:ARG:NH2	3:F:192:SEP:O1P	2.31	0.64
2:I:18:ARG:HH12	2:J:93:GLU:CD	2.02	0.63
2:J:233:THR:O	2:J:233:THR:CG2	2.47	0.63
2:I:39:THR:HG23	2:I:42:GLU:CD	2.19	0.62
2:I:2:SER:OG	2:I:5:GLU:HG3	1.99	0.62
2:I:33:VAL:O	2:I:33:VAL:HG12	1.98	0.62
2:C:34:ASP:O	4:C:752:HOH:O	2.16	0.62
2:J:39:THR:HG22	2:J:42:GLU:CD	2.19	0.61
1:G:6:ARG:CG	1:G:6:ARG:NH1	2.64	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:154:LYS:CE	4:I:488:HOH:O	2.44	0.60
2:J:3:ARG:NH1	2:J:33:VAL:HG23	2.16	0.60
2:J:33:VAL:HG22	2:J:36:GLU:HB3	1.84	0.59
2:I:93:GLU:CD	2:J:18:ARG:HH12	2.06	0.59
2:J:110:VAL:HG13	2:J:111:PRO:HD3	1.82	0.59
3:L:189:ARG:CG	3:L:189:ARG:O	2.43	0.59
2:C:36:GLU:CG	2:C:36:GLU:O	2.50	0.59
2:J:224:LEU:HD22	3:L:191:LEU:HD21	1.83	0.59
2:J:39:THR:OG1	2:J:40:VAL:N	2.35	0.59
2:J:114:THR:HG22	2:J:115:ALA:N	2.17	0.59
2:J:26:MET:HE3	2:J:45:LEU:CB	2.33	0.59
2:J:26:MET:CE	2:J:45:LEU:CB	2.80	0.58
2:C:93:GLU:OE2	2:D:18:ARG:NH1	2.35	0.58
2:C:68:GLU:OE1	2:C:87:ARG:NE	2.35	0.58
2:J:77:GLU:O	2:J:81:THR:OG1	2.10	0.58
2:J:110:VAL:CG1	2:J:111:PRO:CD	2.77	0.58
2:I:37:GLU:HG2	4:I:503:HOH:O	2.03	0.57
2:C:1:MET:N	4:C:565:HOH:O	2.37	0.57
2:J:36:GLU:O	2:J:37:GLU:HB2	2.04	0.57
2:I:26:MET:HE2	2:I:45:LEU:HD23	1.85	0.57
2:I:6:ASN:OD1	2:I:28:LYS:HE2	2.04	0.57
2:J:110:VAL:HG13	2:J:111:PRO:CD	2.35	0.57
2:D:231:LEU:O	2:D:234:SER:OG	2.23	0.57
1:G:93:THR:O	1:G:105:GLN:N	2.39	0.56
2:J:87:ARG:HG2	2:J:87:ARG:NH1	2.10	0.56
2:I:93:GLU:OE2	2:J:18:ARG:NH1	2.32	0.56
2:I:39:THR:CG2	2:I:42:GLU:HG3	2.22	0.55
2:J:26:MET:HE2	2:J:45:LEU:HB3	1.88	0.55
2:I:3:ARG:HD2	2:I:32:THR:OG1	2.07	0.55
2:I:32:THR:O	2:I:33:VAL:C	2.45	0.55
1:B:106:GLU:OE1	4:B:344:HOH:O	2.18	0.55
2:I:91:GLU:HA	2:I:94:LEU:HD12	1.88	0.54
1:A:49:MET:CG	4:A:194:HOH:O	2.55	0.54
2:I:67:ILE:HG22	2:I:83:ILE:HD13	1.89	0.54
2:I:184:GLU:OE1	3:K:190:VAL:HG11	2.07	0.54
2:C:28:LYS:CE	4:C:566:HOH:O	2.56	0.54
2:I:110:VAL:HB	2:I:111:PRO:HD3	1.89	0.53
2:J:39:THR:HG23	2:J:42:GLU:H	1.74	0.52
2:J:114:THR:O	2:J:119:LYS:HE2	2.09	0.52
2:J:72:GLU:OE1	4:J:747:HOH:O	2.19	0.52
2:C:33:VAL:CG2	2:C:36:GLU:O	2.57	0.52
3:F:189:ARG:N	4:F:708:HOH:O	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:15:ARG:NH2	4:G:222:HOH:O	2.41	0.52
2:I:18:ARG:NH1	2:J:93:GLU:CD	2.63	0.52
2:J:128:ASP:OD1	2:J:153:TYR:OH	2.25	0.52
3:E:191:LEU:C	3:E:191:LEU:HD23	2.30	0.51
2:C:124:LYS:NZ	3:E:195:PHE:OXT	2.43	0.51
2:I:18:ARG:NH1	2:J:93:GLU:OE2	2.42	0.51
2:I:233:THR:HG22	4:I:573:HOH:O	2.09	0.51
2:I:133:LEU:O	2:I:137:LYS:HG2	2.10	0.51
2:C:198:GLN:NE2	2:C:202:GLU:OE1	2.44	0.51
2:I:39:THR:CG2	2:I:42:GLU:CD	2.79	0.51
1:G:46:LYS:NZ	4:G:330:HOH:O	2.44	0.51
3:K:189:ARG:HA	3:K:189:ARG:NH1	2.22	0.50
2:D:167:THR:OG1	4:D:318:HOH:O	2.20	0.50
2:I:78:GLU:HA	2:I:78:GLU:OE1	2.11	0.50
2:D:106:ASP:OD1	2:D:126:LYS:NZ	2.45	0.50
2:I:233:THR:HG23	2:I:233:THR:O	2.11	0.50
2:I:220:LEU:HD11	4:I:400:HOH:O	2.11	0.50
2:D:114:THR:CG2	2:D:115:ALA:N	2.75	0.50
2:I:43:ARG:HD3	2:I:121:PHE:CE1	2.46	0.49
2:D:110:VAL:N	2:D:111:PRO:CD	2.75	0.49
1:A:37:LYS:NZ	4:A:438:HOH:O	2.45	0.49
2:J:26:MET:HE3	2:J:45:LEU:HB2	1.93	0.49
2:J:33:VAL:HG13	2:J:36:GLU:HB2	1.93	0.49
2:I:116:ALA:O	2:I:120:VAL:HG23	2.12	0.49
2:I:220:LEU:CD1	2:I:221:ILE:HD13	2.40	0.49
2:I:136:PHE:CE2	2:I:137:LYS:HD3	2.48	0.49
2:J:72:GLU:C	2:J:74:ARG:H	2.16	0.49
2:I:15:GLN:O	2:J:63:ILE:HD12	2.13	0.48
2:J:2:SER:OG	2:J:3:ARG:N	2.45	0.48
2:I:174:LEU:C	2:I:174:LEU:HD13	2.33	0.48
1:A:62:ASP:OD2	1:A:64:ARG:CD	2.62	0.48
2:D:36:GLU:CG	2:D:36:GLU:O	2.62	0.48
2:J:188:SER:CB	4:J:598:HOH:O	2.37	0.48
3:K:189:ARG:N	4:K:713:HOH:O	2.46	0.48
2:I:43:ARG:HD3	2:I:121:PHE:CE2	2.49	0.48
2:I:34:ASP:C	2:I:36:GLU:H	2.15	0.48
2:C:154:LYS:NZ	4:C:682:HOH:O	2.47	0.48
1:H:132:ARG:NH2	2:J:205:SER:HA	2.29	0.48
2:I:220:LEU:HD12	2:I:221:ILE:CD1	2.43	0.47
2:D:70:LYS:NZ	2:D:74:ARG:NH2	2.62	0.47
2:I:12:LEU:HD13	2:J:86:TYR:CD2	2.49	0.47
2:J:3:ARG:HH12	2:J:33:VAL:CG2	2.27	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:47:SER:OG	3:F:195:PHE:OXT	2.31	0.47
2:J:35:VAL:HA	2:J:112:SER:HB2	1.96	0.47
2:J:26:MET:CE	2:J:45:LEU:HD23	2.44	0.47
2:C:1:MET:N	4:C:626:HOH:O	2.48	0.47
2:I:220:LEU:C	2:I:220:LEU:HD13	2.36	0.47
2:D:107:SER:OG	2:D:108:HIS:ND1	2.48	0.46
2:J:28:LYS:O	2:J:32:THR:HG23	2.15	0.46
2:I:224:LEU:CD2	3:K:191:LEU:HD13	2.43	0.46
2:J:157:GLN:HA	2:J:174:LEU:HD21	1.98	0.46
2:I:26:MET:CE	2:I:45:LEU:CD2	2.88	0.46
1:H:96:PRO:O	1:H:99:THR:CB	2.63	0.46
2:C:78:GLU:CG	4:C:550:HOH:O	2.64	0.46
2:J:59:ALA:O	2:J:63:ILE:HG12	2.16	0.46
2:I:26:MET:HE2	2:I:45:LEU:CB	2.41	0.46
2:I:26:MET:HE3	2:I:45:LEU:HB2	1.94	0.46
2:J:26:MET:HE2	2:J:45:LEU:CB	2.45	0.46
2:C:62:ARG:NH2	4:C:304:HOH:O	2.48	0.46
1:H:6:ARG:NH2	1:H:8:ARG:NH1	2.65	0.45
2:I:161:LEU:O	2:I:161:LEU:HD22	2.16	0.45
2:I:76:ASN:HD22	2:I:76:ASN:N	2.15	0.45
1:A:6:ARG:NH2	1:H:132:ARG:NH1	2.64	0.45
2:J:227:ASP:OD2	3:L:189:ARG:NH2	2.50	0.44
2:C:76:ASN:OD1	2:C:76:ASN:N	2.50	0.44
2:I:183:TYR:CE1	2:I:232:TRP:CD1	3.06	0.44
1:G:143:ASN:ND2	4:G:221:HOH:O	2.51	0.44
2:J:53:VAL:HG12	2:J:97:ILE:HD13	1.99	0.44
2:I:38:LEU:HA	2:I:42:GLU:OE1	2.18	0.44
2:I:186:LEU:HD12	2:I:186:LEU:HA	1.81	0.44
2:D:84:LYS:NZ	4:D:671:HOH:O	2.51	0.44
2:J:26:MET:HE3	2:J:45:LEU:HB3	1.91	0.44
2:I:194:ASN:N	2:I:194:ASN:HD22	2.16	0.44
1:G:142:GLN:OE1	1:G:142:GLN:N	2.51	0.43
2:J:119:LYS:HE3	2:J:119:LYS:HB2	1.83	0.43
2:I:35:VAL:CG1	2:I:35:VAL:O	2.64	0.43
2:J:134:ALA:O	2:J:142:ARG:NH2	2.50	0.43
1:H:117:MET:N	1:H:168:ARG:NH1	2.67	0.43
2:I:36:GLU:HB2	2:I:37:GLU:H	1.62	0.43
2:D:128:ASP:OD1	2:D:153:TYR:OH	2.37	0.43
2:J:114:THR:CG2	2:J:115:ALA:N	2.81	0.43
3:L:195:PHE:CD1	3:L:195:PHE:C	2.91	0.43
2:I:172:LEU:HD21	2:I:203:ALA:HB2	2.01	0.43
2:J:33:VAL:HG12	2:J:34:ASP:N	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:121:PHE:CE1	2:J:125:MET:HE3	2.51	0.43
2:C:77:GLU:O	2:C:81:THR:CG2	2.67	0.43
1:G:40:SER:O	1:G:41:ASN:C	2.57	0.43
2:J:137:LYS:HA	2:J:137:LYS:HD2	1.51	0.42
2:I:26:MET:HE2	2:I:45:LEU:CG	2.48	0.42
2:I:35:VAL:C	2:I:36:GLU:HG3	2.39	0.42
2:I:1:MET:O	2:I:3:ARG:NH1	2.43	0.42
1:G:46:LYS:CE	4:G:330:HOH:O	2.67	0.42
2:J:220:LEU:O	2:J:220:LEU:HD22	2.18	0.42
2:I:3:ARG:NE	2:I:6:ASN:ND2	2.67	0.42
2:D:63:ILE:O	2:D:67:ILE:CD1	2.67	0.42
2:I:33:VAL:O	2:I:33:VAL:CG1	2.68	0.42
2:I:3:ARG:O	2:I:7:VAL:HG23	2.20	0.42
1:H:73:ASP:OD2	1:H:120:HIS:ND1	2.53	0.42
2:I:197:LYS:HE2	2:I:201:ASP:OD1	2.20	0.42
1:A:96:PRO:O	1:A:99:THR:CB	2.68	0.42
2:J:121:PHE:CE1	2:J:125:MET:HE2	2.52	0.42
2:C:72:GLU:OE2	2:C:84:LYS:NZ	2.53	0.42
2:D:233:THR:CG2	4:D:572:HOH:O	2.67	0.41
2:J:137:LYS:HG3	2:J:141:GLU:HB2	2.02	0.41
1:B:137:ALA:C	1:B:138:PRO:O	2.57	0.41
2:J:126:LYS:HE3	4:J:238:HOH:O	2.19	0.41
2:I:168:HIS:HA	2:I:169:PRO:HD3	1.95	0.41
1:G:74:PRO:O	1:G:85:ARG:NE	2.52	0.41
3:K:189:ARG:NH1	4:K:623:HOH:O	2.54	0.41
1:A:48:SER:N	1:A:169:GLU:OE2	2.54	0.41
2:I:91:GLU:HG2	2:I:136:PHE:CD2	2.56	0.41
1:A:143:ASN:ND2	4:A:463:HOH:O	2.54	0.41
2:J:14:GLU:OE2	2:J:48:VAL:HG11	2.21	0.41
2:J:68:GLU:OE1	2:J:87:ARG:NE	2.53	0.41
2:D:34:ASP:N	4:D:664:HOH:O	2.53	0.41
1:H:99:THR:CG2	1:H:103:PHE:CB	2.99	0.40
2:J:3:ARG:HG3	2:J:4:GLU:N	2.35	0.40
2:I:3:ARG:HE	2:I:6:ASN:ND2	2.20	0.40
2:J:99:ASP:OD2	2:J:103:LYS:HE2	2.22	0.40
1:G:167:GLN:O	1:G:168:ARG:C	2.60	0.40
2:C:39:THR:OG1	2:C:40:VAL:N	2.54	0.40
3:K:189:ARG:CZ	3:K:190:VAL:HG12	2.51	0.40
2:J:26:MET:HE2	2:J:45:LEU:HD23	2.02	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	164/170 (96%)	153 (93%)	11 (7%)	0	100	100
1	B	164/170 (96%)	159 (97%)	5 (3%)	0	100	100
1	G	163/170 (96%)	154 (94%)	7 (4%)	2 (1%)	19	26
1	H	164/170 (96%)	156 (95%)	8 (5%)	0	100	100
2	C	233/240 (97%)	224 (96%)	6 (3%)	3 (1%)	18	24
2	D	233/240 (97%)	221 (95%)	12 (5%)	0	100	100
2	I	233/240 (97%)	226 (97%)	3 (1%)	4 (2%)	14	17
2	J	232/240 (97%)	218 (94%)	12 (5%)	2 (1%)	25	35
3	E	4/9 (44%)	4 (100%)	0	0	100	100
3	F	4/9 (44%)	4 (100%)	0	0	100	100
3	K	4/9 (44%)	4 (100%)	0	0	100	100
3	L	4/9 (44%)	4 (100%)	0	0	100	100
All	All	1602/1676 (96%)	1527 (95%)	64 (4%)	11 (1%)	30	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	37	GLU
2	I	33	VAL
2	I	38	LEU
2	C	34	ASP
1	G	168	ARG
2	I	37	GLU
2	J	37	GLU
1	G	138	PRO
2	I	35	VAL
2	J	73	GLY
2	C	35	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	145/147 (99%)	132 (91%)	13 (9%)	14	20
1	B	145/147 (99%)	137 (94%)	8 (6%)	30	46
1	G	145/147 (99%)	137 (94%)	8 (6%)	30	46
1	H	145/147 (99%)	129 (89%)	16 (11%)	9	12
2	C	201/204 (98%)	166 (83%)	35 (17%)	3	3
2	D	201/204 (98%)	178 (89%)	23 (11%)	8	11
2	I	201/204 (98%)	182 (90%)	19 (10%)	12	18
2	J	200/204 (98%)	167 (84%)	33 (16%)	3	3
3	E	5/7 (71%)	4 (80%)	1 (20%)	2	2
3	F	5/7 (71%)	3 (60%)	2 (40%)	0	0
3	K	5/7 (71%)	4 (80%)	1 (20%)	2	2
3	L	5/7 (71%)	3 (60%)	2 (40%)	0	0
All	All	1403/1432 (98%)	1242 (88%)	161 (12%)	8	11

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	12	VAL
1	A	15	ARG
1	A	43	LEU
1	A	45	LEU
1	A	58	VAL
1	A	86	GLU
1	A	98	THR
1	A	99	THR
1	A	105	GLN
1	A	133	GLN
1	A	142	GLN
1	A	151	GLU
1	B	25	VAL
1	B	61	ASN

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Mol	Chain	Res	Type
1	B	78	SER
1	B	99	THR
1	B	116	THR
1	B	130	LEU
1	B	132	ARG
1	B	169	GLU
2	C	3	ARG
2	C	4	GLU
2	C	12	LEU
2	C	18	ARG
2	C	27	GLU
2	C	32	THR
2	C	34	ASP
2	C	36	GLU
2	C	39	THR
2	C	41	GLU
2	C	45	LEU
2	C	51	LYS
2	C	63	ILE
2	C	69	GLN
2	C	70	LYS
2	C	71	GLU
2	C	76	ASN
2	C	77	GLU
2	C	81	THR
2	C	82	LEU
2	C	84	LYS
2	C	96	LYS
2	C	102	LEU
2	C	109	LEU
2	C	143	LYS
2	C	154	LYS
2	C	172	LEU
2	C	178	PHE
2	C	186	LEU
2	C	198	GLN
2	C	207	LEU
2	C	220	LEU
2	C	225	LEU
2	C	231	LEU
2	C	233	THR
2	D	3	ARG

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Mol	Chain	Res	Type
2	D	27	GLU
2	D	37	GLU
2	D	45	LEU
2	D	51	LYS
2	D	63	ILE
2	D	65	SER
2	D	72	GLU
2	D	84	LYS
2	D	89	LYS
2	D	102	LEU
2	D	105	LEU
2	D	109	LEU
2	D	112	SER
2	D	114	THR
2	D	142	ARG
2	D	144	GLU
2	D	161	LEU
2	D	178	PHE
2	D	188	SER
2	D	207	LEU
2	D	213	GLU
2	D	231	LEU
3	E	191	LEU
3	F	189	ARG
3	F	190	VAL
1	G	6	ARG
1	G	7	ASP
1	G	8	ARG
1	G	69	LEU
1	G	78	SER
1	G	99	THR
1	G	132	ARG
1	G	151	GLU
1	H	6	ARG
1	H	7	ASP
1	H	21	LEU
1	H	25	VAL
1	H	44	GLU
1	H	46	LYS
1	H	61	ASN
1	H	62	ASP
1	H	99	THR

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Mol	Chain	Res	Type
1	H	106	GLU
1	H	114	ARG
1	H	116	THR
1	H	130	LEU
1	H	147	LYS
1	H	151	GLU
1	H	169	GLU
2	I	4	GLU
2	I	12	LEU
2	I	26	MET
2	I	35	VAL
2	I	36	GLU
2	I	39	THR
2	I	45	LEU
2	I	51	LYS
2	I	67	ILE
2	I	125	MET
2	I	138	THR
2	I	154	LYS
2	I	161	LEU
2	I	178	PHE
2	I	186	LEU
2	I	188	SER
2	I	213	GLU
2	I	231	LEU
2	I	233	THR
2	J	3	ARG
2	J	4	GLU
2	J	12	LEU
2	J	26	MET
2	J	28	LYS
2	J	33	VAL
2	J	34	ASP
2	J	36	GLU
2	J	39	THR
2	J	45	LEU
2	J	51	LYS
2	J	63	ILE
2	J	65	SER
2	J	66	SER
2	J	70	LYS
2	J	74	ARG

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Mol	Chain	Res	Type
2	J	84	LYS
2	J	85	GLU
2	J	96	LYS
2	J	114	THR
2	J	119	LYS
2	J	137	LYS
2	J	138	THR
2	J	141	GLU
2	J	144	GLU
2	J	178	PHE
2	J	188	SER
2	J	207	LEU
2	J	213	GLU
2	J	214	SER
2	J	219	THR
2	J	220	LEU
2	J	229	LEU
3	K	189	ARG
3	L	189	ARG
3	L	191	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	I	76	ASN
2	I	194	ASN
2	I	198	GLN
2	J	52	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SEP	E	192	3	9,9,10	5.91	2 (22%)	10,12,14	1.66	3 (30%)
3	SEP	F	192	3	9,9,10	5.80	3 (33%)	10,12,14	1.58	2 (20%)
3	SEP	K	192	3	9,9,10	5.88	2 (22%)	10,12,14	1.54	3 (30%)
3	SEP	L	192	3	9,9,10	5.88	3 (33%)	10,12,14	1.84	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	E	192	3	-	0/6/8/10	0/0/0/0
3	SEP	F	192	3	-	0/6/8/10	0/0/0/0
3	SEP	K	192	3	-	0/6/8/10	0/0/0/0
3	SEP	L	192	3	-	0/6/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	192	SEP	O-C	17.23	1.23	1.11
3	K	192	SEP	O-C	17.04	1.23	1.11
3	L	192	SEP	O-C	17.00	1.23	1.11
3	F	192	SEP	O-C	16.65	1.22	1.11
3	F	192	SEP	P-O1P	3.32	1.62	1.51
3	K	192	SEP	P-O1P	3.10	1.61	1.51
3	F	192	SEP	CA-C	2.88	1.53	1.48
3	L	192	SEP	P-O1P	2.86	1.60	1.51
3	E	192	SEP	P-O1P	2.76	1.60	1.51
3	L	192	SEP	CA-C	2.64	1.53	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	192	SEP	C-CA-N	-4.86	108.97	113.83
3	F	192	SEP	C-CA-N	-3.43	110.41	113.83
3	E	192	SEP	OG-CB-CA	2.99	112.93	108.69
3	E	192	SEP	P-OG-CB	-2.81	110.07	118.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	192	SEP	OG-CB-CA	2.57	112.33	108.69
3	K	192	SEP	O3P-P-OG	2.47	113.47	106.65
3	F	192	SEP	O3P-P-OG	2.42	113.33	106.65
3	K	192	SEP	P-OG-CB	-2.03	112.32	118.19
3	E	192	SEP	O3P-P-OG	2.01	112.19	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	166/170 (97%)	-0.37	4 (2%) 56 54	12, 25, 44, 60	0
1	B	166/170 (97%)	-0.18	3 (1%) 65 63	17, 32, 56, 68	0
1	G	165/170 (97%)	-0.29	1 (0%) 86 86	13, 23, 44, 60	0
1	H	166/170 (97%)	-0.41	1 (0%) 86 86	17, 32, 48, 69	0
2	C	235/240 (97%)	-0.32	4 (1%) 67 65	15, 27, 58, 76	0
2	D	235/240 (97%)	-0.22	5 (2%) 60 58	18, 33, 64, 80	0
2	I	235/240 (97%)	-0.20	5 (2%) 60 58	14, 27, 60, 75	0
2	J	234/240 (97%)	-0.13	5 (2%) 60 58	19, 35, 69, 77	0
3	E	7/9 (77%)	0.07	0 100 100	25, 28, 43, 53	0
3	F	7/9 (77%)	-0.08	0 100 100	25, 36, 44, 57	0
3	K	7/9 (77%)	-0.41	0 100 100	20, 29, 41, 52	0
3	L	7/9 (77%)	0.54	1 (14%) 3 3	28, 38, 49, 58	0
All	All	1630/1676 (97%)	-0.25	29 (1%) 65 63	12, 29, 57, 80	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	35	VAL	7.2
2	I	35	VAL	6.0
2	D	35	VAL	5.7
2	I	33	VAL	5.0
2	J	35	VAL	4.6
2	J	32	THR	4.5
2	D	34	ASP	4.5
2	I	34	ASP	4.2
1	A	130	LEU	3.7
2	J	34	ASP	3.7
2	J	33	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	170	ALA	3.5
2	D	36	GLU	3.0
2	D	33	VAL	3.0
1	A	170	ALA	2.9
1	H	170	ALA	2.8
2	C	34	ASP	2.8
1	A	132	ARG	2.6
2	C	32	THR	2.5
2	I	73	GLY	2.4
2	C	36	GLU	2.4
2	J	75	GLY	2.4
3	L	191	LEU	2.4
2	D	32	THR	2.3
2	I	36	GLU	2.2
1	A	136	TYR	2.1
1	B	130	LEU	2.1
1	G	136	TYR	2.1
1	B	136	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SEP	E	192	10/11	0.13	0.01	18,27,30,32	0
3	SEP	K	192	10/11	0.12	-0.42	10,21,23,26	0
3	SEP	L	192	10/11	0.10	-0.60	19,28,33,36	0
3	SEP	F	192	10/11	0.09	-0.83	16,27,29,31	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.