



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:03 pm BST

PDB ID : 1X27  
Title : Crystal Structure of Lck SH2-SH3 with SH2 binding site of p130Cas  
Authors : Nasertorabi, F.; Tars, K.; Becherer, K.; Kodandapani, R.; Liljas, L.; Vuori, K.; Ely, K.R.  
Deposited on : 2005-04-20  
Resolution : 2.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

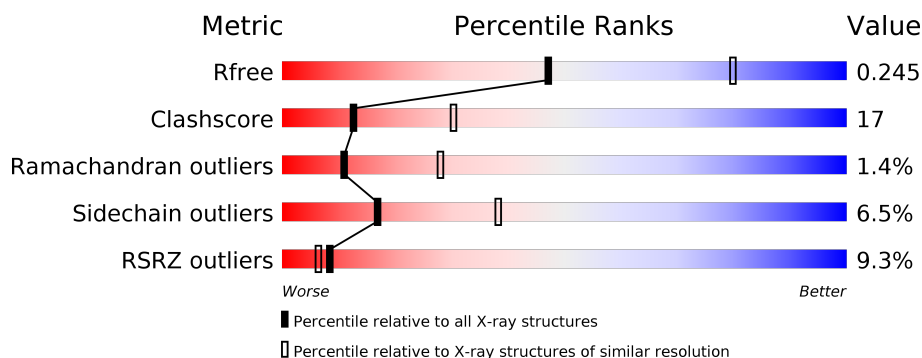
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	167	<div> <div>14%</div> <div> <div></div> <div>59%</div> <div>35%</div> <div>• •</div> </div> </div>
1	B	167	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>• •</div> </div> </div>
1	C	167	<div> <div>10%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>• •</div> </div> </div>
1	D	167	<div> <div>8%</div> <div> <div></div> <div>61%</div> <div>32%</div> <div>• •</div> </div> </div>
1	E	167	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>• •</div> </div> </div>
1	F	167	<div> <div>8%</div> <div> <div></div> <div>57%</div> <div>36%</div> <div>5% •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	9	<div><div><div></div><div></div><div></div></div><div>33% 11%44%44%</div></div>
2	J	9	<div><div><div></div><div></div><div></div></div><div>11% 33%33%33%</div></div>
2	K	9	<div><div><div></div><div></div><div></div></div><div>22% 22%33%44%</div></div>
2	L	9	<div><div><div></div><div></div><div></div></div><div>33% 33%33%33%</div></div>
2	M	9	<div><div><div></div><div></div><div></div></div><div>22% 33%22%44%</div></div>
2	N	9	<div><div><div></div><div></div><div></div></div><div>22% 22%44%33%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase LCK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1306	824	232	248	2			
1	B	164	Total	C	N	O	S	0	0	0
			1314	829	233	249	3			
1	C	164	Total	C	N	O	S	0	0	0
			1314	829	233	249	3			
1	D	163	Total	C	N	O	S	0	0	0
			1306	824	232	248	2			
1	E	163	Total	C	N	O	S	0	0	0
			1306	824	232	248	2			
1	F	163	Total	C	N	O	S	0	0	0
			1306	824	232	248	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLY	-	CLONING ARTIFACT	UNP P06239
A	61	SER	-	CLONING ARTIFACT	UNP P06239
A	62	HIS	-	CLONING ARTIFACT	UNP P06239
A	63	MET	-	CLONING ARTIFACT	UNP P06239
B	60	GLY	-	CLONING ARTIFACT	UNP P06239
B	61	SER	-	CLONING ARTIFACT	UNP P06239
B	62	HIS	-	CLONING ARTIFACT	UNP P06239
B	63	MET	-	CLONING ARTIFACT	UNP P06239
C	60	GLY	-	CLONING ARTIFACT	UNP P06239
C	61	SER	-	CLONING ARTIFACT	UNP P06239
C	62	HIS	-	CLONING ARTIFACT	UNP P06239
C	63	MET	-	CLONING ARTIFACT	UNP P06239
D	60	GLY	-	CLONING ARTIFACT	UNP P06239
D	61	SER	-	CLONING ARTIFACT	UNP P06239
D	62	HIS	-	CLONING ARTIFACT	UNP P06239
D	63	MET	-	CLONING ARTIFACT	UNP P06239
E	60	GLY	-	CLONING ARTIFACT	UNP P06239

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Chain	Residue	Modelled	Actual	Comment	Reference
E	61	SER	-	CLONING ARTIFACT	UNP P06239
E	62	HIS	-	CLONING ARTIFACT	UNP P06239
E	63	MET	-	CLONING ARTIFACT	UNP P06239
F	60	GLY	-	CLONING ARTIFACT	UNP P06239
F	61	SER	-	CLONING ARTIFACT	UNP P06239
F	62	HIS	-	CLONING ARTIFACT	UNP P06239
F	63	MET	-	CLONING ARTIFACT	UNP P06239

- Molecule 2 is a protein called CRK-associated substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	5	Total	C	N	O	P	0	0	0
			51	31	5	14	1			
2	J	6	Total	C	N	O	P	0	0	0
			61	37	8	15	1			
2	K	5	Total	C	N	O	P	0	0	0
			53	33	7	12	1			
2	L	6	Total	C	N	O	P	0	0	0
			61	37	8	15	1			
2	M	5	Total	C	N	O	P	0	0	0
			53	33	7	12	1			
2	N	6	Total	C	N	O	P	0	0	0
			61	37	8	15	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	762	PTR	TYR	MODIFIED RESIDUE	UNP Q63767
J	762	PTR	TYR	MODIFIED RESIDUE	UNP Q63767
K	762	PTR	TYR	MODIFIED RESIDUE	UNP Q63767
L	762	PTR	TYR	MODIFIED RESIDUE	UNP Q63767
M	762	PTR	TYR	MODIFIED RESIDUE	UNP Q63767
N	762	PTR	TYR	MODIFIED RESIDUE	UNP Q63767

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	A	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0

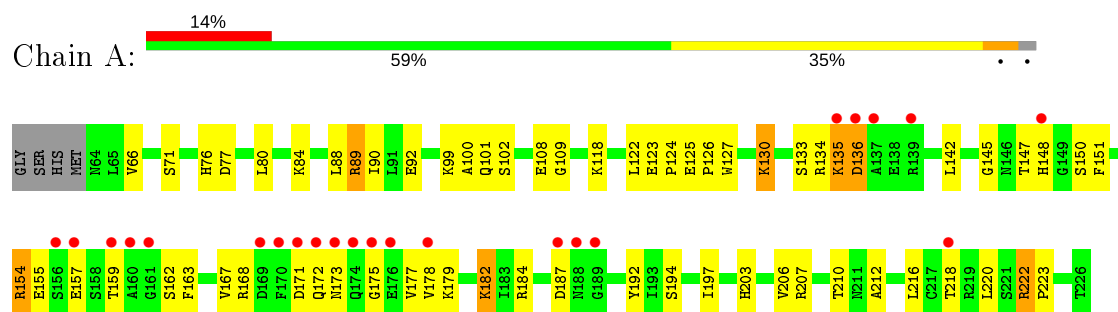
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	7	Total 7	O 7	0	0
4	C	8	Total 8	O 8	0	0
4	D	8	Total 8	O 8	0	0
4	E	12	Total 12	O 12	0	0
4	F	5	Total 5	O 5	0	0

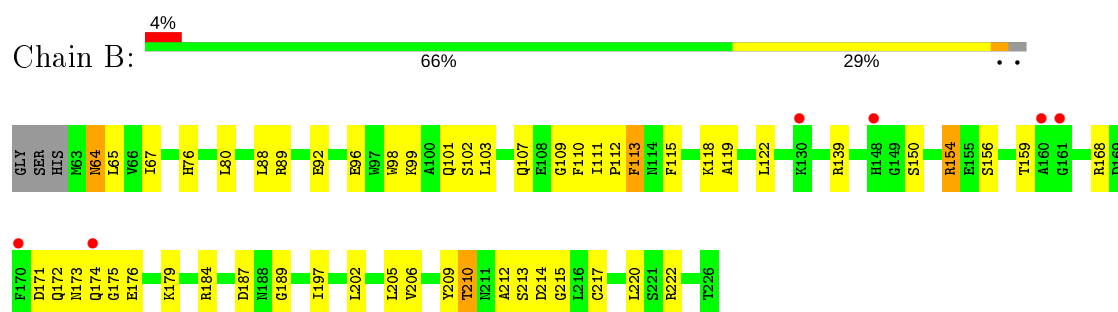
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

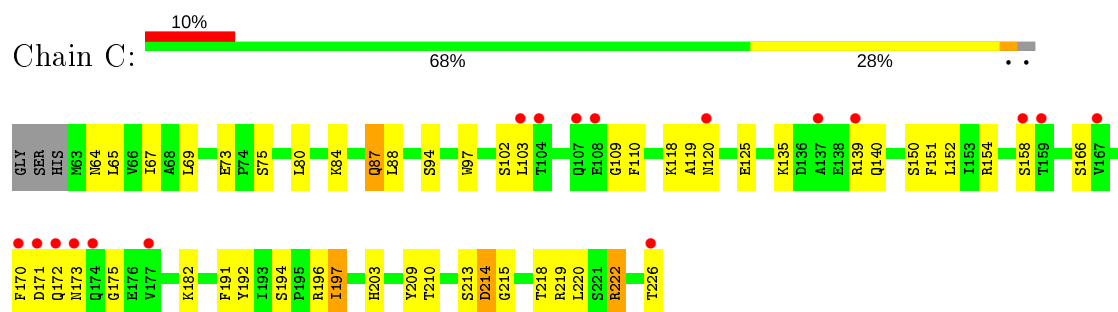
#### • Molecule 1: Proto-oncogene tyrosine-protein kinase LCK



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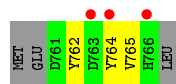
#### • Molecule 1: Proto-oncogene tyrosine-protein kinase LCK



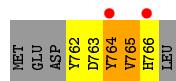
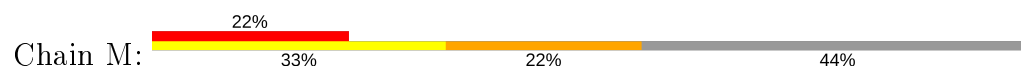




## ● Molecule 2: CRK-associated substrate



## ● Molecule 2: CRK-associated substrate



## ● Molecule 2: CRK-associated substrate



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.42Å 107.29Å 166.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 70.19 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 96.4 (70.19-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.247 , 0.317 0.240 , 0.245	Depositor DCC
$R_{free}$ test set	1866 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/1340	0.62	0/1811
1	B	0.49	0/1348	0.61	0/1821
1	C	0.47	0/1348	0.58	0/1821
1	D	0.46	0/1340	0.59	0/1811
1	E	0.50	0/1340	0.63	0/1811
1	F	0.47	0/1340	0.61	0/1811
2	I	0.50	0/34	0.59	0/44
2	J	0.49	0/45	0.52	0/59
2	K	0.43	0/38	0.47	0/51
2	L	0.47	0/45	0.60	0/59
2	M	0.44	0/38	0.43	0/51
2	N	0.44	0/45	0.55	0/59
All	All	0.47	0/8301	0.60	0/11209

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1306	0	1248	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1314	0	1257	38	0
1	C	1314	0	1257	45	0
1	D	1306	0	1248	43	0
1	E	1306	0	1248	46	0
1	F	1306	0	1248	54	0
2	I	51	0	32	3	0
2	J	61	0	39	3	0
2	K	53	0	38	4	0
2	L	61	0	39	3	0
2	M	53	0	38	9	0
2	N	61	0	39	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	7	0	0	0	0
4	B	7	0	0	1	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	12	0	0	0	0
4	F	5	0	0	0	0
All	All	8245	0	7731	266	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 17.

All (266) 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:89:ARG:HD2	1:A:101:GLN:HE21	1.34	0.92
1:F:123:GLU:HB2	1:F:124:PRO:HD3	1.60	0.84
1:C:215:GLY:HA3	2:K:765:VAL:HG23	1.60	0.84
1:B:210:THR:HG22	1:B:220:LEU:O	1.78	0.84
1:A:194:SER:HB2	2:I:765:VAL:HG11	1.60	0.83
1:E:210:THR:HG22	1:E:220:LEU:HB2	1.59	0.83
1:F:206:VAL:O	1:F:210:THR:HG23	1.78	0.83
1:B:215:GLY:HA2	2:J:765:VAL:HG13	1.62	0.81
1:E:171:ASP:HB3	1:E:174:GLN:HB2	1.64	0.79
1:B:65:LEU:HD11	1:B:103:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:NZ	1:A:203:HIS:HB3	2.00	0.77
1:C:80:LEU:HB2	1:C:109:GLY:HA3	1.64	0.77
1:E:67:ILE:HG13	1:E:119:ALA:HB2	1.66	0.77
1:F:213:SER:H	1:F:219:ARG:HE	1.31	0.76
1:B:76:HIS:HB3	1:D:147:THR:HG21	1.68	0.76
1:F:67:ILE:HG13	1:F:119:ALA:HB2	1.69	0.74
1:A:89:ARG:HD2	1:A:101:GLN:NE2	2.02	0.74
1:C:88:LEU:HD23	1:C:102:SER:HA	1.71	0.72
1:F:213:SER:HB3	1:F:219:ARG:HG3	1.70	0.72
1:D:64:ASN:HB3	1:D:120:ASN:HD21	1.55	0.71
1:A:222:ARG:HB3	1:F:110:PHE:CZ	2.25	0.71
1:E:123:GLU:HB2	1:E:124:PRO:HD3	1.72	0.70
1:E:193:ILE:CD1	1:E:205:LEU:HD11	2.22	0.70
1:C:67:ILE:HG13	1:C:119:ALA:HB2	1.74	0.69
1:C:194:SER:OG	1:C:196:ARG:HG3	1.92	0.69
1:C:154:ARG:NH1	1:C:166:SER:OG	2.26	0.69
1:C:182:LYS:HB3	1:C:182:LYS:NZ	2.08	0.68
1:D:215:GLY:O	2:L:765:VAL:HG23	1.94	0.68
1:D:154:ARG:HH11	1:D:154:ARG:HG2	1.60	0.67
1:C:210:THR:HG22	1:C:220:LEU:HB2	1.77	0.66
1:E:80:LEU:HB2	1:E:109:GLY:HA3	1.76	0.66
1:A:92:GLU:HB2	1:A:99:LYS:HB3	1.78	0.66
1:C:65:LEU:HD11	1:C:103:LEU:HD11	1.77	0.65
1:A:118:LYS:HE2	1:A:207:ARG:HH21	1.62	0.65
1:F:150:SER:HA	1:F:222:ARG:O	1.96	0.65
1:B:89:ARG:HD3	1:B:101:GLN:NE2	2.12	0.64
1:B:171:ASP:HB3	1:B:174:GLN:O	1.98	0.64
1:A:88:LEU:HD23	1:A:102:SER:HA	1.80	0.63
1:F:125:GLU:OE1	1:F:126:PRO:HD2	1.99	0.63
1:F:76:HIS:O	1:F:79:ASP:HB2	2.00	0.62
1:D:80:LEU:HB2	1:D:109:GLY:HA3	1.82	0.62
1:C:69:LEU:O	1:C:84:LYS:HD3	1.99	0.62
1:F:215:GLY:HA3	2:N:765:VAL:HG22	1.81	0.62
1:B:172:GLN:HE22	1:F:171:ASP:HB2	1.65	0.62
1:A:147:THR:HG23	1:F:77:ASP:HB2	1.83	0.61
1:C:150:SER:HA	1:C:222:ARG:O	2.01	0.61
1:A:150:SER:HA	1:A:222:ARG:O	2.00	0.61
1:A:101:GLN:HG3	1:A:108:GLU:HB3	1.81	0.60
1:A:130:LYS:HE3	1:A:155:GLU:OE1	2.02	0.60
1:C:210:THR:HG22	1:C:220:LEU:O	2.00	0.60
1:E:88:LEU:HD23	1:E:102:SER:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD21	1:A:178:VAL:HG23	1.84	0.60
1:F:197:ILE:HD13	1:F:209:TYR:OH	2.02	0.60
1:B:184:ARG:HH22	1:C:73:GLU:HB3	1.67	0.59
1:B:209:TYR:HA	1:B:212:ALA:O	2.02	0.59
1:C:191:PHE:O	1:C:192:TYR:HB3	2.02	0.59
1:F:215:GLY:HA3	2:N:765:VAL:HG13	1.83	0.59
1:F:171:ASP:OD2	1:F:174:GLN:HG2	2.03	0.58
1:E:143:ALA:HB1	1:E:144:PRO:HD2	1.85	0.58
1:A:159:THR:O	1:A:162:SER:HB2	2.04	0.57
1:F:173:ASN:HD22	1:F:173:ASN:N	2.01	0.56
1:A:76:HIS:HB3	1:F:147:THR:HG21	1.86	0.56
1:A:147:THR:HA	1:A:168:ARG:NH1	2.20	0.56
1:C:94:SER:HB3	1:C:97:TRP:O	2.06	0.56
1:A:216:LEU:C	1:A:218:THR:H	2.09	0.55
1:F:154:ARG:NH1	1:F:166:SER:OG	2.39	0.55
1:A:154:ARG:HH11	1:A:154:ARG:HG2	1.72	0.55
1:F:157:GLU:HB2	2:N:762:PTR:O3P	2.06	0.55
1:A:133:SER:OG	1:A:136:ASP:HB2	2.07	0.54
1:C:125:GLU:HA	1:C:125:GLU:OE1	2.08	0.54
1:F:136:ASP:O	1:F:140:GLN:HB2	2.07	0.54
4:B:227:HOH:O	2:N:766:HIS:HB3	2.08	0.54
1:F:159:THR:HB	1:F:162:SER:HB2	1.91	0.53
1:F:173:ASN:ND2	1:F:173:ASN:N	2.55	0.53
1:D:134:ARG:HD2	2:L:762:PTR:O2P	2.08	0.53
1:C:151:PHE:CD1	1:C:220:LEU:HB3	2.43	0.53
1:A:71:SER:N	1:E:187:ASP:OD2	2.42	0.53
1:F:174:GLN:HG3	1:F:177:VAL:CG1	2.38	0.53
1:C:152:LEU:HD12	1:C:152:LEU:C	2.29	0.52
1:A:84:LYS:HB2	1:E:187:ASP:OD2	2.09	0.52
1:B:89:ARG:HG3	1:B:101:GLN:HB3	1.91	0.52
1:E:112:PRO:HG2	1:E:115:PHE:HB2	1.90	0.52
1:C:170:PHE:CE2	1:C:175:GLY:HA2	2.44	0.52
1:E:150:SER:HA	1:E:222:ARG:O	2.09	0.52
1:A:135:LYS:HD2	1:A:135:LYS:H	1.75	0.51
1:D:205:LEU:HD23	1:D:205:LEU:C	2.31	0.51
1:C:182:LYS:HB3	1:C:182:LYS:HZ3	1.75	0.51
1:D:98:TRP:O	1:D:110:PHE:HA	2.11	0.51
1:B:168:ARG:HD3	1:B:176:GLU:HB3	1.92	0.51
1:D:150:SER:HA	1:D:222:ARG:O	2.10	0.51
1:B:80:LEU:HD13	1:B:107:GLN:HG2	1.93	0.51
1:C:135:LYS:HE2	1:C:139:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLU:HB3	1:D:124:PRO:HD3	1.92	0.51
1:E:212:ALA:HA	1:E:219:ARG:NE	2.25	0.51
1:C:110:PHE:CD2	1:E:222:ARG:HD3	2.46	0.50
1:C:215:GLY:HA2	2:K:766:HIS:H	1.75	0.50
1:B:96:GLU:OE2	1:C:196:ARG:HD2	2.10	0.50
1:F:92:GLU:HB2	1:F:99:LYS:HB3	1.93	0.50
1:A:118:LYS:HZ1	1:A:203:HIS:HB3	1.75	0.50
1:E:197:ILE:HD12	1:E:197:ILE:H	1.77	0.50
1:F:87:GLN:O	1:F:88:LEU:HD23	2.12	0.50
1:C:182:LYS:HB3	1:C:182:LYS:HZ2	1.76	0.50
1:A:135:LYS:H	1:A:135:LYS:CD	2.25	0.50
1:D:87:GLN:HG2	1:D:103:LEU:HD12	1.92	0.50
1:F:213:SER:HB3	1:F:219:ARG:HA	1.93	0.50
1:C:118:LYS:HD3	1:C:203:HIS:ND1	2.27	0.49
1:B:205:LEU:C	1:B:205:LEU:HD23	2.32	0.49
1:D:154:ARG:NH1	1:D:154:ARG:HG2	2.26	0.49
1:D:140:GLN:HE21	1:D:226:THR:HA	1.77	0.49
1:B:215:GLY:O	2:J:765:VAL:HA	2.11	0.49
1:F:123:GLU:CB	1:F:124:PRO:HD3	2.36	0.49
1:D:210:THR:HG22	1:D:220:LEU:O	2.12	0.49
1:A:80:LEU:HB2	1:A:109:GLY:CA	2.42	0.49
1:B:65:LEU:CD1	1:B:103:LEU:HD11	2.39	0.49
1:C:222:ARG:HG2	1:E:110:PHE:CD1	2.48	0.49
1:F:213:SER:CB	1:F:219:ARG:HG3	2.39	0.49
1:A:177:VAL:HG12	1:A:178:VAL:H	1.77	0.49
2:M:765:VAL:HG13	2:M:765:VAL:O	2.12	0.49
1:E:210:THR:HG22	1:E:220:LEU:CB	2.38	0.48
1:E:142:LEU:HD21	1:E:178:VAL:HG23	1.95	0.48
1:E:206:VAL:O	1:E:210:THR:HG23	2.13	0.48
1:A:127:TRP:HB3	1:A:223:PRO:HB3	1.96	0.48
1:B:80:LEU:HB2	1:B:109:GLY:HA3	1.95	0.48
1:E:193:ILE:HD12	1:E:205:LEU:HD11	1.95	0.48
1:B:179:LYS:HE2	1:B:217:CYS:SG	2.54	0.48
1:B:88:LEU:HD23	1:B:102:SER:HA	1.95	0.48
1:E:210:THR:CG2	1:E:220:LEU:HB2	2.37	0.48
1:C:171:ASP:O	1:C:175:GLY:N	2.47	0.47
1:B:98:TRP:O	1:B:110:PHE:HA	2.15	0.47
1:A:175:GLY:O	1:A:177:VAL:HG23	2.14	0.47
1:B:88:LEU:CD2	1:B:102:SER:HA	2.44	0.47
1:B:96:GLU:CD	1:C:196:ARG:HD2	2.35	0.47
1:A:134:ARG:NH2	2:I:761:ASP:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:HZ2	1:A:203:HIS:HB3	1.79	0.47
1:F:184:ARG:HG2	1:F:184:ARG:HH11	1.80	0.47
1:D:68:ALA:HA	1:D:116:VAL:HG12	1.96	0.47
1:F:127:TRP:HB3	1:F:223:PRO:HB3	1.97	0.47
1:F:182:LYS:HD3	1:F:183:ILE:N	2.30	0.47
1:A:80:LEU:HB2	1:A:109:GLY:HA3	1.97	0.47
1:C:171:ASP:C	1:C:173:ASN:H	2.18	0.47
1:D:87:GLN:CG	1:D:103:LEU:HD12	2.44	0.47
1:A:184:ARG:HD2	1:A:192:TYR:CE1	2.50	0.47
1:E:183:ILE:HG12	1:E:193:ILE:HD11	1.97	0.47
1:A:179:LYS:HE2	1:C:172:GLN:HE22	1.80	0.46
1:B:150:SER:HA	1:B:222:ARG:O	2.15	0.46
1:D:155:GLU:O	1:D:156:SER:C	2.53	0.46
1:E:210:THR:HG22	1:E:220:LEU:O	2.15	0.46
1:F:194:SER:C	1:F:196:ARG:H	2.18	0.46
1:B:156:SER:HB3	1:B:159:THR:O	2.15	0.46
1:B:202:LEU:O	1:B:206:VAL:HG23	2.15	0.46
1:E:94:SER:HB3	1:E:97:TRP:O	2.16	0.46
1:E:154:ARG:NH2	2:M:762:PTR:O2P	2.49	0.46
1:D:194:SER:C	1:D:196:ARG:H	2.19	0.46
1:F:67:ILE:HG12	1:F:87:GLN:HG2	1.97	0.46
1:F:147:THR:HB	1:F:148:HIS:H	1.37	0.46
1:D:157:GLU:CG	1:D:158:SER:N	2.78	0.46
1:F:186:LEU:HB3	1:F:189:GLY:O	2.15	0.46
1:A:151:PHE:HB3	1:A:167:VAL:HG23	1.97	0.46
1:D:157:GLU:HG2	2:L:762:PTR:O3P	2.16	0.46
1:A:123:GLU:HB2	1:A:124:PRO:HD3	1.98	0.45
1:C:182:LYS:HG2	2:K:762:PTR:CE2	2.46	0.45
1:D:154:ARG:NH1	1:D:166:SER:OG	2.49	0.45
1:A:135:LYS:HD2	1:A:135:LYS:N	2.31	0.45
1:D:65:LEU:CD2	1:D:87:GLN:HE21	2.29	0.45
1:A:206:VAL:O	1:A:210:THR:HG23	2.14	0.45
1:F:200:PRO:HG2	1:F:204:GLU:HG2	1.98	0.45
1:A:177:VAL:HG12	1:A:178:VAL:N	2.31	0.45
1:D:64:ASN:ND2	1:D:120:ASN:OD1	2.44	0.45
1:D:64:ASN:HB3	1:D:120:ASN:ND2	2.28	0.45
1:C:87:GLN:HG2	1:C:103:LEU:HD12	1.99	0.45
1:D:158:SER:OG	1:D:159:THR:N	2.49	0.45
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.82	0.45
1:D:172:GLN:HG2	1:D:173:ASN:N	2.32	0.45
1:A:163:PHE:O	1:A:182:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HD13	1:C:209:TYR:OH	2.17	0.45
1:E:169:ASP:OD2	1:E:217:CYS:HB2	2.18	0.45
1:B:64:ASN:OD1	1:B:64:ASN:N	2.50	0.44
1:F:152:LEU:HD12	1:F:152:LEU:C	2.37	0.44
1:B:89:ARG:CG	1:B:101:GLN:HB3	2.47	0.44
2:M:764:TYR:CD2	2:M:765:VAL:HG12	2.51	0.44
1:B:154:ARG:NH2	2:J:762:PTR:O3P	2.51	0.44
1:F:200:PRO:CG	1:F:204:GLU:HG2	2.48	0.44
1:F:147:THR:O	1:F:168:ARG:HD2	2.17	0.44
1:A:66:VAL:HG21	1:A:90:ILE:HD11	2.00	0.44
1:D:133:SER:HB3	1:D:136:ASP:OD1	2.18	0.44
1:D:179:LYS:HE3	1:D:217:CYS:SG	2.57	0.44
1:E:154:ARG:NH1	1:E:166:SER:OG	2.49	0.44
2:N:765:VAL:HG12	2:N:766:HIS:O	2.18	0.44
1:A:145:GLY:H	1:F:77:ASP:CG	2.21	0.44
1:C:151:PHE:HA	1:C:166:SER:O	2.17	0.44
1:E:197:ILE:N	1:E:197:ILE:HD12	2.33	0.44
2:M:764:TYR:HD2	2:M:765:VAL:HG12	1.82	0.44
1:A:118:LYS:CE	1:A:203:HIS:HB3	2.48	0.44
1:D:194:SER:C	1:D:196:ARG:N	2.71	0.44
1:D:168:ARG:NH1	1:D:176:GLU:OE2	2.48	0.44
1:B:184:ARG:NH2	1:C:73:GLU:HB3	2.31	0.43
1:D:112:PRO:HG2	1:D:115:PHE:HB2	1.98	0.43
1:E:134:ARG:NH1	2:M:762:PTR:O2P	2.48	0.43
1:C:110:PHE:CG	1:E:222:ARG:HD3	2.53	0.43
1:E:193:ILE:HD13	1:E:205:LEU:HD11	1.99	0.43
1:D:162:SER:HB3	1:D:182:LYS:NZ	2.33	0.43
1:B:67:ILE:HG12	1:B:119:ALA:HB2	2.00	0.43
1:C:218:THR:HG22	1:C:219:ARG:N	2.34	0.43
1:A:210:THR:HG22	1:A:220:LEU:HB2	2.01	0.43
1:F:66:VAL:HG21	1:F:90:ILE:HD11	2.01	0.43
1:E:194:SER:HB2	2:M:765:VAL:HB	2.00	0.43
2:N:762:PTR:N	2:N:762:PTR:HD1	2.33	0.43
1:E:123:GLU:CB	1:E:124:PRO:HD3	2.46	0.43
1:D:213:SER:O	1:D:215:GLY:N	2.52	0.43
1:E:205:LEU:C	1:E:205:LEU:HD23	2.39	0.43
1:F:210:THR:HG22	1:F:220:LEU:HB2	1.99	0.43
1:B:171:ASP:OD1	1:E:172:GLN:HG3	2.18	0.43
1:E:137:ALA:O	1:E:141:LEU:HB2	2.19	0.43
1:E:186:LEU:HA	1:E:186:LEU:HD12	1.90	0.43
1:E:180:HIS:HB2	2:M:762:PTR:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:GLU:H	1:E:99:LYS:HB3	1.83	0.42
1:F:213:SER:N	1:F:219:ARG:HE	2.08	0.42
1:E:186:LEU:HD13	1:E:192:TYR:CD2	2.54	0.42
1:B:213:SER:O	1:B:215:GLY:N	2.52	0.42
1:B:111:ILE:O	1:B:111:ILE:HG13	2.19	0.42
1:B:187:ASP:C	1:B:189:GLY:H	2.23	0.42
1:F:162:SER:HB3	1:F:182:LYS:HE3	2.00	0.42
1:F:215:GLY:CA	2:N:765:VAL:HG13	2.47	0.42
1:C:64:ASN:HB3	1:C:120:ASN:HD21	1.84	0.42
1:E:66:VAL:HB	1:E:116:VAL:HB	2.02	0.42
1:B:92:GLU:H	1:B:99:LYS:HB3	1.85	0.42
1:E:215:GLY:HA3	2:M:765:VAL:HG23	2.01	0.42
1:A:77:ASP:CG	1:F:145:GLY:H	2.22	0.42
1:A:157:GLU:HG2	2:I:762:PTR:O1P	2.19	0.42
1:A:171:ASP:OD2	1:A:173:ASN:HB3	2.19	0.42
1:D:88:LEU:HD23	1:D:111:ILE:HD13	2.02	0.42
1:F:184:ARG:HG2	1:F:184:ARG:NH1	2.34	0.42
1:F:196:ARG:HG2	1:F:197:ILE:HG13	2.02	0.42
1:D:134:ARG:HD3	1:D:157:GLU:OE2	2.20	0.41
1:F:209:TYR:HA	1:F:212:ALA:O	2.19	0.41
1:A:125:GLU:HA	1:A:126:PRO:HD3	1.87	0.41
1:F:93:GLN:HE21	1:F:93:GLN:HB3	1.63	0.41
2:M:763:ASP:HB3	2:M:766:HIS:NE2	2.35	0.41
1:F:217:CYS:O	1:F:218:THR:HG23	2.21	0.41
1:A:154:ARG:HG2	1:A:154:ARG:NH1	2.34	0.41
1:C:88:LEU:HD23	1:C:102:SER:CA	2.47	0.41
1:D:125:GLU:OE2	1:D:203:HIS:CE1	2.73	0.41
1:C:222:ARG:HB3	1:E:110:PHE:CZ	2.55	0.41
1:E:202:LEU:HA	1:E:202:LEU:HD23	1.81	0.41
1:B:122:LEU:CD1	1:B:202:LEU:HD12	2.51	0.41
1:C:182:LYS:CB	1:C:182:LYS:NZ	2.79	0.41
1:F:73:GLU:HA	1:F:74:PRO:HD3	1.93	0.41
1:A:100:ALA:O	1:A:108:GLU:HB2	2.21	0.41
1:D:162:SER:CB	1:D:182:LYS:HZ1	2.34	0.41
1:D:69:LEU:O	1:D:70:HIS:CD2	2.74	0.41
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.81	0.41
1:C:214:ASP:N	1:C:214:ASP:OD2	2.54	0.41
1:D:219:ARG:CG	1:D:219:ARG:HH11	2.34	0.41
1:C:215:GLY:CA	2:K:765:VAL:HG23	2.42	0.41
1:C:213:SER:O	1:C:215:GLY:N	2.54	0.41
1:D:125:GLU:OE2	1:D:203:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:VAL:O	1:D:210:THR:HG23	2.21	0.41
1:D:91:LEU:HD12	1:D:99:LYS:HG3	2.03	0.41
1:A:80:LEU:HD13	1:A:108:GLU:C	2.40	0.40
1:B:96:GLU:O	1:B:113:PHE:HB3	2.21	0.40
1:E:211:ASN:O	1:E:212:ALA:HB2	2.21	0.40
1:F:67:ILE:HG13	1:F:119:ALA:CB	2.44	0.40
1:B:112:PRO:HG2	1:B:115:PHE:HB2	2.03	0.40
1:D:70:HIS:HA	1:D:84:LYS:HG3	2.03	0.40
1:F:215:GLY:HA2	2:N:766:HIS:H	1.85	0.40
1:E:133:SER:OG	1:E:136:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	161/167 (96%)	144 (89%)	15 (9%)	2 (1%)	13	32
1	B	162/167 (97%)	153 (94%)	6 (4%)	3 (2%)	8	20
1	C	162/167 (97%)	144 (89%)	16 (10%)	2 (1%)	13	32
1	D	161/167 (96%)	141 (88%)	17 (11%)	3 (2%)	8	20
1	E	161/167 (96%)	148 (92%)	12 (8%)	1 (1%)	25	50
1	F	161/167 (96%)	148 (92%)	11 (7%)	2 (1%)	13	32
2	I	2/9 (22%)	2 (100%)	0	0	100	100
2	J	3/9 (33%)	0	3 (100%)	0	100	100
2	K	3/9 (33%)	3 (100%)	0	0	100	100
2	L	3/9 (33%)	2 (67%)	1 (33%)	0	100	100
2	M	3/9 (33%)	2 (67%)	0	1 (33%)	0	0
2	N	3/9 (33%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	985/1056 (93%)	890 (90%)	81 (8%)	14 (1%)	11	28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	ASP
1	E	130	LYS
1	F	130	LYS
1	F	187	ASP
2	M	765	VAL
1	B	175	GLY
1	C	214	ASP
1	D	130	LYS
1	D	175	GLY
1	B	173	ASN
1	D	156	SER
1	A	130	LYS
1	C	158	SER
1	A	212	ALA

### 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	141/144 (98%)	131 (93%)	10 (7%)	14	34
1	B	142/144 (99%)	135 (95%)	7 (5%)	25	52
1	C	142/144 (99%)	136 (96%)	6 (4%)	30	58
1	D	141/144 (98%)	132 (94%)	9 (6%)	17	39
1	E	141/144 (98%)	136 (96%)	5 (4%)	36	65
1	F	141/144 (98%)	126 (89%)	15 (11%)	6	15
2	I	4/8 (50%)	3 (75%)	1 (25%)	0	1
2	J	5/8 (62%)	4 (80%)	1 (20%)	1	3
2	K	4/8 (50%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	5/8 (62%)	4 (80%)	1 (20%)	1	3
2	M	4/8 (50%)	3 (75%)	1 (25%)	0	1
2	N	5/8 (62%)	4 (80%)	1 (20%)	1	3
All	All	875/912 (96%)	818 (94%)	57 (6%)	17	38

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ARG
1	A	135	LYS
1	A	136	ASP
1	A	148	HIS
1	A	154	ARG
1	A	172	GLN
1	A	182	LYS
1	A	187	ASP
1	A	197	ILE
1	A	222	ARG
1	B	64	ASN
1	B	113	PHE
1	B	118	LYS
1	B	139	ARG
1	B	154	ARG
1	B	197	ILE
1	B	210	THR
1	C	75	SER
1	C	87	GLN
1	C	140	GLN
1	C	197	ILE
1	C	222	ARG
1	C	226	THR
1	D	104	THR
1	D	154	ARG
1	D	155	GLU
1	D	172	GLN
1	D	186	LEU
1	D	197	ILE
1	D	217	CYS
1	D	219	ARG
1	D	222	ARG
1	E	88	LEU

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Mol	Chain	Res	Type
1	E	107	GLN
1	E	113	PHE
1	E	136	ASP
1	E	197	ILE
1	F	77	ASP
1	F	79	ASP
1	F	83	GLU
1	F	113	PHE
1	F	147	THR
1	F	154	ARG
1	F	167	VAL
1	F	172	GLN
1	F	173	ASN
1	F	176	GLU
1	F	182	LYS
1	F	197	ILE
1	F	214	ASP
1	F	218	THR
1	F	225	GLN
2	I	763	ASP
2	J	764	TYR
2	L	764	TYR
2	M	764	TYR
2	N	764	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	93	GLN
1	A	101	GLN
1	A	174	GLN
1	B	93	GLN
1	B	120	ASN
1	B	131	ASN
1	B	172	GLN
1	B	211	ASN
1	C	87	GLN
1	C	93	GLN
1	C	131	ASN
1	C	172	GLN
1	D	64	ASN

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Mol	Chain	Res	Type
1	D	70	HIS
1	D	87	GLN
1	D	93	GLN
1	D	107	GLN
1	D	120	ASN
1	D	140	GLN
1	D	203	HIS
1	D	211	ASN
1	E	70	HIS
1	E	87	GLN
1	E	174	GLN
1	E	203	HIS
1	E	211	ASN
1	F	70	HIS
1	F	93	GLN
1	F	101	GLN
1	F	140	GLN
1	F	148	HIS
1	F	172	GLN
1	F	173	ASN
1	F	174	GLN
1	F	203	HIS
2	K	766	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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
2	PTR	M	762	2	15,16,17	1.03	1 (6%)	19,22,24	0.66	0
2	PTR	N	762	2	15,16,17	1.16	1 (6%)	19,22,24	0.65	0
2	PTR	I	762	2	15,16,17	1.06	1 (6%)	19,22,24	0.64	0
2	PTR	L	762	2	15,16,17	0.91	1 (6%)	19,22,24	2.97	5 (26%)
2	PTR	J	762	2	15,16,17	1.12	1 (6%)	19,22,24	0.81	1 (5%)
2	PTR	K	762	2	15,16,17	0.99	1 (6%)	19,22,24	0.77	0

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
2	PTR	M	762	2	-	4/10/11/13	0/1/1/1
2	PTR	N	762	2	-	1/10/11/13	0/1/1/1
2	PTR	I	762	2	-	1/10/11/13	0/1/1/1
2	PTR	L	762	2	-	0/10/11/13	0/1/1/1
2	PTR	J	762	2	-	0/10/11/13	0/1/1/1
2	PTR	K	762	2	-	1/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	762	PTR	P-OH	2.60	1.63	1.59
2	M	762	PTR	P-OH	2.56	1.63	1.59
2	J	762	PTR	P-OH	2.50	1.63	1.59
2	I	762	PTR	P-OH	2.50	1.63	1.59
2	K	762	PTR	P-OH	2.37	1.62	1.59
2	L	762	PTR	P-OH	2.02	1.62	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	762	PTR	O3P-P-O1P	-7.32	82.01	110.68
2	L	762	PTR	O3P-P-OH	-6.93	83.58	105.24
2	L	762	PTR	O3P-P-O2P	-5.78	85.54	107.64
2	L	762	PTR	O2P-P-OH	3.64	116.62	105.24
2	L	762	PTR	OH-P-O1P	3.30	121.75	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	762	PTR	O3P-P-OH	2.06	111.68	105.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	762	PTR	C-CA-CB-CG
2	K	762	PTR	O-C-CA-CB
2	M	762	PTR	N-CA-CB-CG
2	M	762	PTR	CA-CB-CG-CD2
2	M	762	PTR	CA-CB-CG-CD1
2	I	762	PTR	C-CA-CB-CG
2	N	762	PTR	CZ-OH-P-O2P

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	762	PTR	3	0
2	N	762	PTR	2	0
2	I	762	PTR	1	0
2	L	762	PTR	2	0
2	J	762	PTR	1	0
2	K	762	PTR	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	163/167 (97%)	1.03	23 (14%) 2 1	34, 58, 87, 112	0
1	B	164/167 (98%)	0.66	6 (3%) 41 41	31, 52, 79, 92	0
1	C	164/167 (98%)	0.98	17 (10%) 6 4	37, 58, 84, 113	0
1	D	163/167 (97%)	0.83	14 (8%) 10 8	38, 58, 85, 106	0
1	E	163/167 (97%)	0.68	7 (4%) 35 33	33, 53, 79, 98	0
1	F	163/167 (97%)	0.79	14 (8%) 10 8	34, 56, 78, 85	0
2	I	4/9 (44%)	2.80	3 (75%) 0 0	99, 102, 108, 109	0
2	J	5/9 (55%)	1.69	1 (20%) 1 0	85, 86, 103, 110	0
2	K	4/9 (44%)	1.62	2 (50%) 0 0	90, 101, 104, 107	0
2	L	5/9 (55%)	1.78	3 (60%) 0 0	86, 91, 100, 103	0
2	M	4/9 (44%)	3.55	2 (50%) 0 0	96, 107, 110, 119	0
2	N	5/9 (55%)	2.13	2 (40%) 0 0	93, 94, 106, 111	0
All	All	1007/1056 (95%)	0.87	94 (9%) 8 6	31, 57, 88, 119	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	174	GLN	7.7
1	C	173	ASN	7.0
2	M	766	HIS	6.4
1	D	173	ASN	6.3
1	B	160	ALA	6.1
2	I	764	TYR	5.9
1	F	160	ALA	5.9
1	A	173	ASN	5.6
1	B	170	PHE	5.6
2	J	766	HIS	5.4
1	A	171	ASP	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	M	764	TYR	4.9
1	A	188	ASN	4.8
1	A	139	ARG	4.6
1	C	226	THR	4.5
1	C	104	THR	4.5
1	D	174	GLN	4.5
1	C	172	GLN	4.2
1	D	170	PHE	4.2
1	E	130	LYS	4.2
2	N	766	HIS	4.1
2	N	764	TYR	4.1
1	A	160	ALA	4.0
1	D	83	GLU	4.0
1	C	171	ASP	3.8
1	B	174	GLN	3.6
1	C	107	GLN	3.6
1	C	170	PHE	3.5
2	K	764	TYR	3.4
1	C	159	THR	3.4
1	F	139	ARG	3.4
1	A	172	GLN	3.3
1	F	131	ASN	3.3
1	A	175	GLY	3.2
2	L	766	HIS	3.2
1	A	187	ASP	3.2
1	A	156	SER	3.1
1	A	161	GLY	3.1
1	A	174	GLN	3.1
1	F	161	GLY	3.0
1	A	135	LYS	3.0
1	A	148	HIS	3.0
1	E	226	THR	3.0
1	A	189	GLY	2.9
1	E	83	GLU	2.9
1	E	214	ASP	2.9
1	D	87	GLN	2.8
1	D	217	CYS	2.8
1	D	103	LEU	2.8
1	F	130	LYS	2.8
1	A	178	VAL	2.8
1	E	139	ARG	2.8
1	D	159	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	188	ASN	2.7
1	F	136	ASP	2.7
1	E	135	LYS	2.7
1	D	104	THR	2.6
1	C	158	SER	2.6
1	C	103	LEU	2.6
1	F	226	THR	2.6
1	C	137	ALA	2.6
1	A	157	GLU	2.5
1	A	170	PHE	2.5
1	A	176	GLU	2.5
1	F	158	SER	2.5
1	F	128	PHE	2.5
1	A	137	ALA	2.5
1	F	159	THR	2.5
2	I	765	VAL	2.4
1	F	163	PHE	2.4
1	D	88	LEU	2.4
1	D	171	ASP	2.4
1	A	159	THR	2.4
1	D	94	SER	2.3
1	F	186	LEU	2.3
1	D	131	ASN	2.3
2	L	764	TYR	2.3
1	C	167	VAL	2.3
1	C	120	ASN	2.3
1	E	145	GLY	2.2
1	C	108	GLU	2.2
1	C	139	ARG	2.2
1	B	148	HIS	2.2
2	L	763	ASP	2.2
1	C	177	VAL	2.1
1	A	136	ASP	2.1
1	F	119	ALA	2.1
1	A	169	ASP	2.1
2	I	763	ASP	2.1
1	B	130	LYS	2.1
1	A	218	THR	2.0
1	B	161	GLY	2.0
2	K	766	HIS	2.0
1	D	172	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PTR	L	762	16/17	0.89	0.25	74,79,85,86	0
2	PTR	N	762	16/17	0.90	0.27	74,86,91,92	0
2	PTR	M	762	16/17	0.92	0.24	64,76,89,90	0
2	PTR	I	762	16/17	0.93	0.25	88,93,99,99	0
2	PTR	K	762	16/17	0.94	0.18	69,75,82,83	0
2	PTR	J	762	16/17	0.95	0.25	70,77,83,84	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	227	1/1	0.77	0.29	51,51,51,51	0
3	NA	D	10	1/1	0.81	0.39	50,50,50,50	0
3	NA	C	14	1/1	0.84	0.19	44,44,44,44	0
3	NA	E	227	1/1	0.93	0.17	43,43,43,43	0
3	NA	B	6	1/1	0.95	0.36	39,39,39,39	0
3	NA	F	21	1/1	0.97	0.21	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.