



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2022 – 09:20 am GMT

PDB ID : 7OX1  
Title : Fab 7D6: hIL-9 complex  
Authors : De Vos, T.; Savvides, S.N.  
Deposited on : 2021-06-22  
Resolution : 2.49 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
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) : 2.31.3

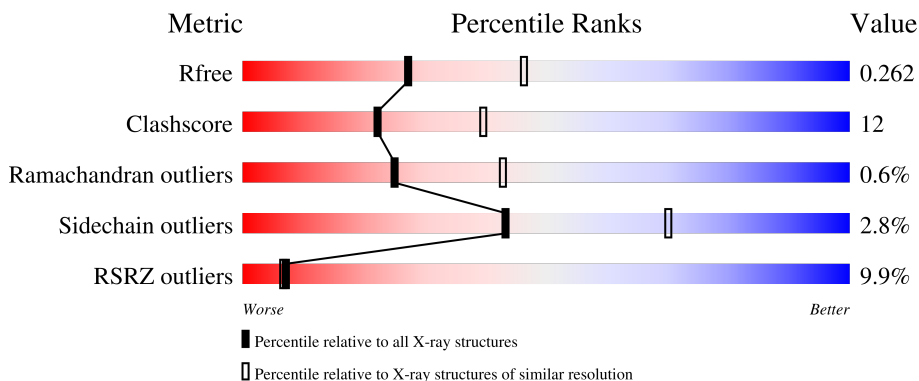
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	230	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9%      77%      18%      ••</p>
1	C	230	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      84%      13%      •</p>
1	E	230	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      76%      19%      ••</p>
1	H	230	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3%      80%      16%      ••</p>
2	B	215	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">10%      78%      15%      • 6%</p>

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Mol	Chain	Length	Quality of chain
2	D	215	<p>86% 12%</p>
2	F	215	<p>9% 72% 18% 9%</p>
2	L	215	<p>2% 84% 13%</p>
3	G	130	<p>21% 58% 25% 15%</p>
3	X	130	<p>26% 51% 28% 6% 14%</p>
3	Y	130	<p>20% 49% 28% 19%</p>
3	Z	130	<p>29% 61% 25% 5% 9%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32503 atoms, of which 15989 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 Heavy chain (Fab 7D6).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	222	3315	1064	1641	275	328	7	0	0	0
1	C	225	3340	1071	1652	278	332	7	0	0	0
1	E	222	3315	1064	1641	275	329	6	0	0	0
1	H	223	3322	1066	1644	276	330	6	0	0	0

- Molecule 2 is a protein called Light chain (Fab 7D6).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	203	2961	944	1451	255	307	4	0	1	0
2	D	211	3070	977	1507	264	318	4	0	0	0
2	F	195	2833	900	1387	248	294	4	0	2	0
2	L	210	3056	973	1500	263	316	4	0	0	0

- Molecule 3 is a protein called Interleukin-9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	G	111	1752	546	882	150	161	13	0	0	0
3	X	112	1793	557	909	155	160	12	0	0	0
3	Y	105	1669	522	844	142	150	11	0	0	0
3	Z	118	1852	575	931	162	169	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	15	GLY	-	expression tag	UNP P15248
G	16	SER	-	expression tag	UNP P15248
G	17	HIS	-	expression tag	UNP P15248
G	18	MET	-	expression tag	UNP P15248
X	15	GLY	-	expression tag	UNP P15248
X	16	SER	-	expression tag	UNP P15248
X	17	HIS	-	expression tag	UNP P15248
X	18	MET	-	expression tag	UNP P15248
Y	15	GLY	-	expression tag	UNP P15248
Y	16	SER	-	expression tag	UNP P15248
Y	17	HIS	-	expression tag	UNP P15248
Y	18	MET	-	expression tag	UNP P15248
Z	15	GLY	-	expression tag	UNP P15248
Z	16	SER	-	expression tag	UNP P15248
Z	17	HIS	-	expression tag	UNP P15248
Z	18	MET	-	expression tag	UNP P15248

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0
4	B	29	Total O 29 29	0	0
4	C	32	Total O 32 32	0	0
4	D	48	Total O 48 48	0	0
4	E	12	Total O 12 12	0	0
4	F	15	Total O 15 15	0	0
4	G	6	Total O 6 6	0	0
4	H	24	Total O 24 24	0	0
4	L	23	Total O 23 23	0	0
4	X	4	Total O 4 4	0	0
4	Y	4	Total O 4 4	0	0

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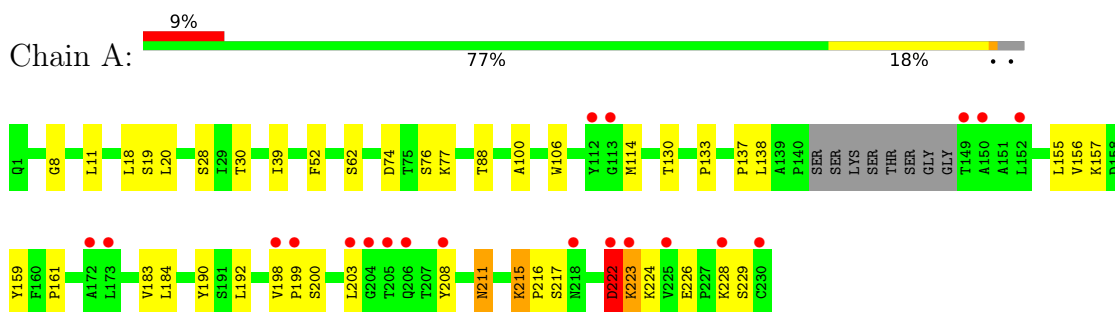
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	Z	1	Total	O	0	0
			1	1		

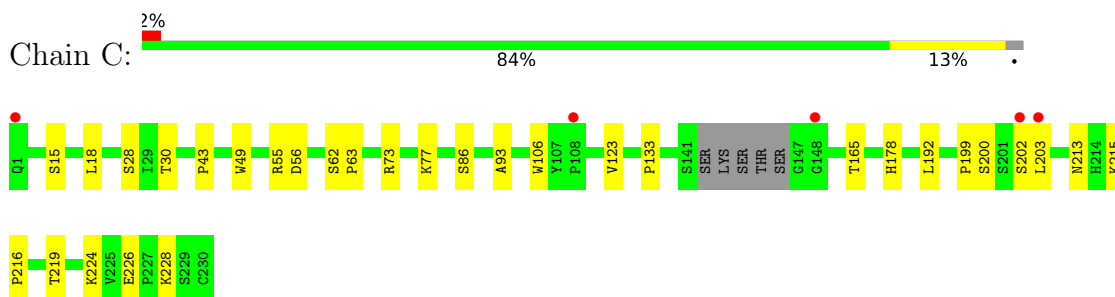
### 3 Residue-property plots [i](#)

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

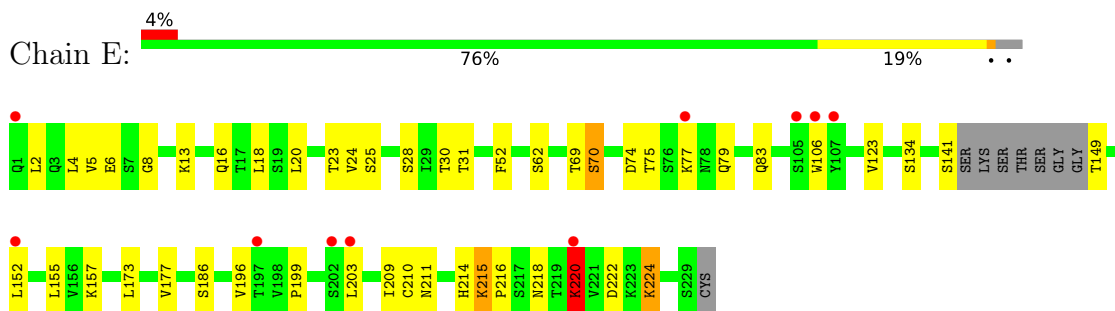
- Molecule 1: Heavy chain (Fab 7D6)



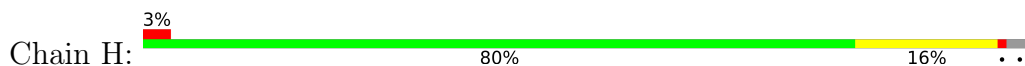
- Molecule 1: Heavy chain (Fab 7D6)

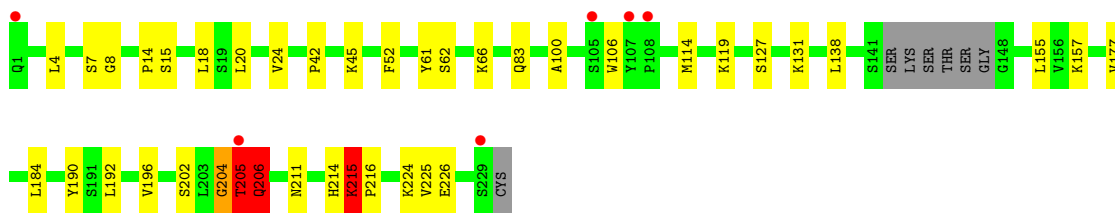


- Molecule 1: Heavy chain (Fab 7D6)

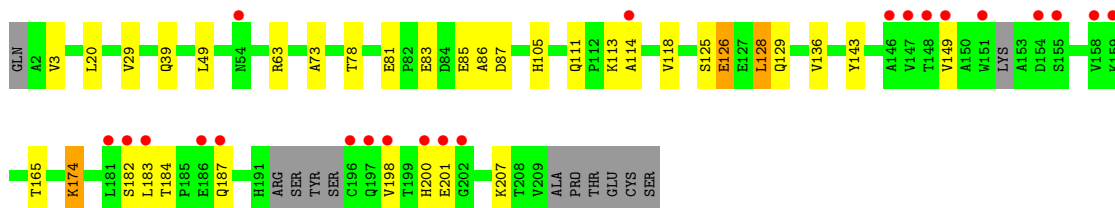
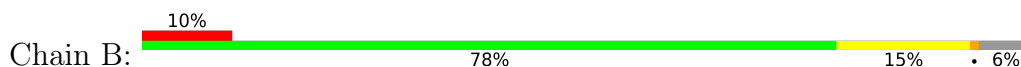


- Molecule 1: Heavy chain (Fab 7D6)

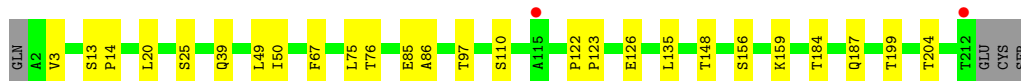
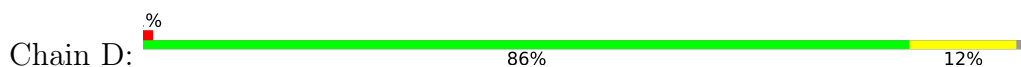




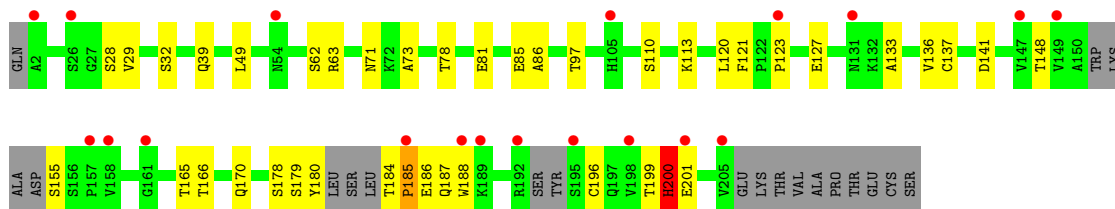
• Molecule 2: Light chain (Fab 7D6)



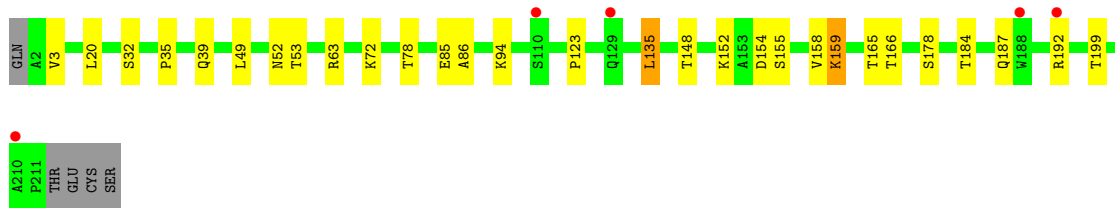
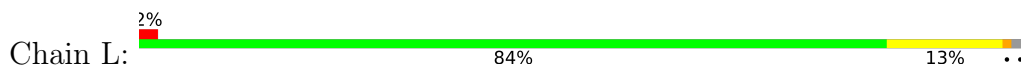
• Molecule 2: Light chain (Fab 7D6)



• Molecule 2: Light chain (Fab 7D6)



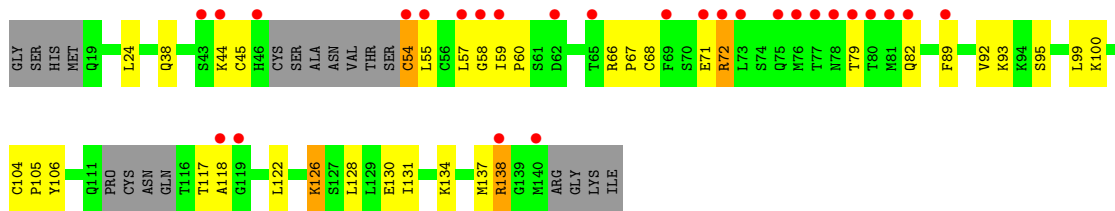
• Molecule 2: Light chain (Fab 7D6)



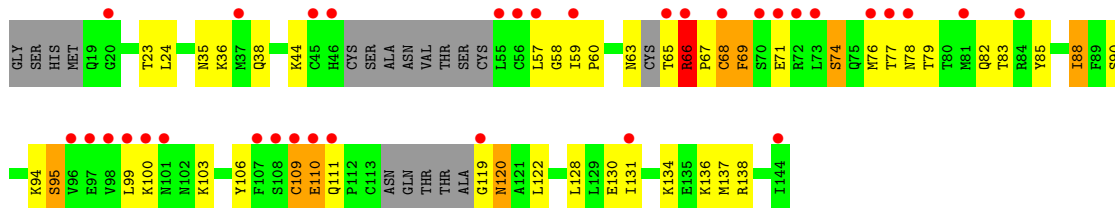
• Molecule 3: Interleukin-9



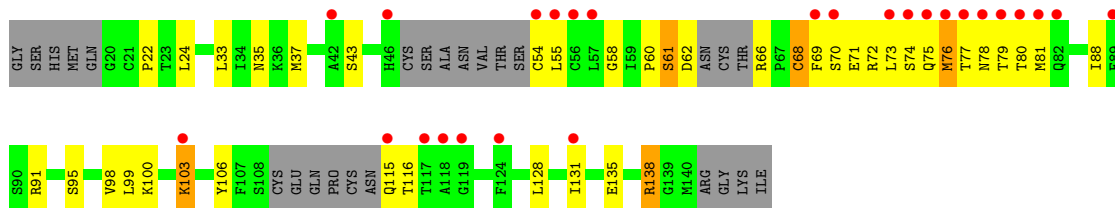




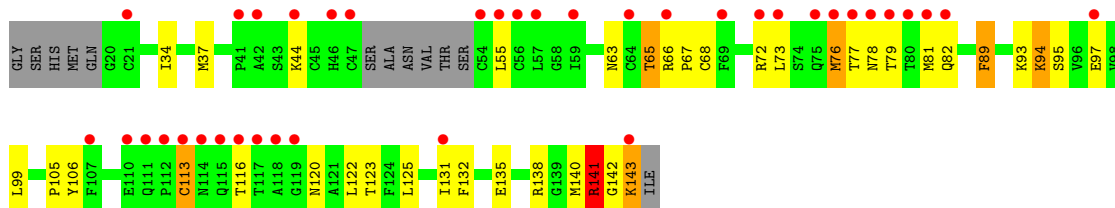
• Molecule 3: Interleukin-9



• Molecule 3: Interleukin-9



• Molecule 3: Interleukin-9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.35Å 102.75Å 164.37Å 90.00° 94.12° 90.00°	Depositor
Resolution (Å)	42.36 – 2.49 42.36 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.36-2.49) 97.7 (42.36-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.48Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.209 , 0.262 0.209 , 0.262	Depositor DCC
$R_{free}$ test set	4624 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtrriage
Anisotropy	0.198	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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

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	0.55	1/1720 (0.1%)	0.74	3/2348 (0.1%)
1	C	0.41	1/1734 (0.1%)	0.65	0/2366
1	E	0.59	5/1720 (0.3%)	0.80	7/2348 (0.3%)
1	H	0.53	3/1724 (0.2%)	0.80	5/2353 (0.2%)
2	B	0.46	1/1548 (0.1%)	0.68	3/2117 (0.1%)
2	D	0.39	0/1604	0.62	0/2196
2	F	0.53	2/1489 (0.1%)	0.73	3/2033 (0.1%)
2	L	0.45	1/1597 (0.1%)	0.89	5/2186 (0.2%)
3	G	0.59	2/882 (0.2%)	1.02	5/1182 (0.4%)
3	X	0.67	3/896 (0.3%)	0.78	4/1197 (0.3%)
3	Y	0.77	3/836 (0.4%)	0.86	4/1118 (0.4%)
3	Z	0.55	1/935 (0.1%)	0.79	3/1254 (0.2%)
All	All	0.53	23/16685 (0.1%)	0.77	42/22698 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	H	0	2
2	F	0	2
3	X	0	2
All	All	0	8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	138	ARG	CZ-NH1	16.18	1.54	1.33
1	A	222	ASP	CG-OD2	13.58	1.56	1.25
1	E	13	LYS	CD-CE	-10.61	1.24	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	113	LYS	CB-CG	-10.50	1.24	1.52
3	X	66	ARG	CG-CD	9.94	1.76	1.51
3	X	66	ARG	CB-CG	9.25	1.77	1.52
2	L	135	LEU	CG-CD2	8.22	1.82	1.51
3	G	138	ARG	CZ-NH2	-8.20	1.22	1.33
2	F	113	LYS	CD-CE	7.63	1.70	1.51
1	H	205	THR	CB-CG2	-7.03	1.29	1.52
1	E	220	LYS	CD-CE	-6.51	1.34	1.51
3	G	138	ARG	CD-NE	-6.32	1.35	1.46
3	Y	138	ARG	CZ-NH2	5.80	1.40	1.33
1	E	220	LYS	CB-CG	5.75	1.68	1.52
3	Z	89	PHE	CG-CD1	-5.73	1.30	1.38
2	B	174	LYS	CE-NZ	-5.64	1.34	1.49
1	H	204	GLY	C-O	5.48	1.32	1.23
1	E	220	LYS	CG-CD	5.43	1.71	1.52
1	E	220	LYS	CE-NZ	5.33	1.62	1.49
3	X	66	ARG	C-N	5.30	1.44	1.34
1	C	228	LYS	CB-CG	-5.14	1.38	1.52
3	Y	138	ARG	CB-CG	-5.13	1.38	1.52
1	H	215	LYS	CG-CD	5.06	1.69	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	135	LEU	CB-CG-CD1	24.84	153.22	111.00
3	G	138	ARG	NE-CZ-NH2	-15.37	112.61	120.30
3	G	57	LEU	CB-CG-CD1	15.07	136.62	111.00
2	L	135	LEU	CB-CG-CD2	-14.54	86.28	111.00
2	F	113	LYS	CA-CB-CG	13.32	142.71	113.40
1	H	205	THR	CA-CB-CG2	13.30	131.02	112.40
1	E	220	LYS	CD-CE-NZ	-13.22	81.29	111.70
1	A	222	ASP	CB-CG-OD2	11.68	128.81	118.30
3	G	138	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	222	ASP	CB-CG-OD1	-11.41	108.03	118.30
1	H	215	LYS	CA-CB-CG	11.23	138.11	113.40
3	Y	138	ARG	NE-CZ-NH2	10.67	125.64	120.30
2	F	200	HIS	CB-CA-C	-9.45	91.50	110.40
3	Z	141	ARG	NE-CZ-NH1	-9.40	115.60	120.30
3	X	66	ARG	CB-CG-CD	9.31	135.82	111.60
1	H	215	LYS	CB-CG-CD	8.96	134.89	111.60
1	H	215	LYS	CD-CE-NZ	-8.91	91.21	111.70
1	E	13	LYS	CB-CG-CD	8.43	133.53	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	126	LYS	CB-CG-CD	8.38	133.40	111.60
3	X	66	ARG	CG-CD-NE	7.91	128.40	111.80
2	L	135	LEU	CD1-CG-CD2	-7.75	87.25	110.50
3	Y	138	ARG	CB-CG-CD	-7.72	91.53	111.60
3	Y	138	ARG	NH1-CZ-NH2	-7.64	110.99	119.40
1	E	224	LYS	CA-CB-CG	7.48	129.86	113.40
1	E	203	LEU	CA-CB-CG	7.16	131.76	115.30
1	E	16	GLN	CA-CB-CG	7.10	129.02	113.40
2	L	159	LYS	CA-CB-CG	6.68	128.09	113.40
2	L	135	LEU	CA-CB-CG	-6.66	99.99	115.30
3	X	88	ILE	CG1-CB-CG2	6.36	125.39	111.40
1	H	215	LYS	CG-CD-CE	6.05	130.04	111.90
2	B	174	LYS	CA-CB-CG	5.77	126.09	113.40
2	B	174	LYS	CG-CD-CE	5.76	129.18	111.90
3	Y	138	ARG	N-CA-CB	-5.41	100.86	110.60
1	E	16	GLN	CB-CA-C	5.40	121.19	110.40
1	A	223	LYS	CA-CB-CG	-5.38	101.56	113.40
3	G	57	LEU	CB-CG-CD2	-5.34	101.92	111.00
3	Z	141	ARG	CB-CG-CD	-5.34	97.71	111.60
2	F	113	LYS	CB-CA-C	5.24	120.87	110.40
1	E	70	SER	N-CA-CB	-5.17	102.74	110.50
3	X	88	ILE	CB-CG1-CD1	5.10	128.17	113.90
2	B	126	GLU	N-CA-CB	-5.08	101.45	110.60
3	Z	89	PHE	CG-CD2-CE2	5.03	126.33	120.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ASP	Mainchain
1	E	220	LYS	Mainchain
2	F	186	GLU	Peptide
2	F	200	HIS	Sidechain
1	H	205	THR	Mainchain
1	H	206	GLN	Sidechain
3	X	109	CYS	Peptide
3	X	66	ARG	Sidechain

## 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	1674	1641	1640	43	1
1	C	1688	1652	1651	21	3
1	E	1674	1641	1640	39	1
1	H	1678	1644	1643	25	3
2	B	1510	1451	1447	44	0
2	D	1563	1507	1507	19	0
2	F	1446	1387	1373	39	0
2	L	1556	1500	1500	29	0
3	G	870	882	880	26	15
3	X	884	909	906	47	0
3	Y	825	844	844	44	15
3	Z	921	931	931	33	4
4	A	27	0	0	0	0
4	B	29	0	0	2	0
4	C	32	0	0	2	0
4	D	48	0	0	1	0
4	E	12	0	0	3	0
4	F	15	0	0	0	0
4	G	6	0	0	0	0
4	H	24	0	0	3	0
4	L	23	0	0	3	0
4	X	4	0	0	1	0
4	Y	4	0	0	3	0
4	Z	1	0	0	0	0
All	All	16514	15989	15962	378	21

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (378) 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)
3:X:66:ARG:CD	3:X:66:ARG:CG	1.76	1.63
3:X:66:ARG:CG	3:X:66:ARG:CB	1.77	1.55
2:L:135:LEU:CG	2:L:135:LEU:CD2	1.82	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:LEU:CD2	2:L:135:LEU:CD1	2.23	1.17
3:Y:68:CYS:SG	4:Y:201:HOH:O	2.04	1.15
2:L:135:LEU:CD2	2:L:135:LEU:CB	2.30	1.08
3:Y:72:ARG:NH1	3:Y:75:GLN:CD	2.08	1.07
2:L:135:LEU:CD2	2:L:135:LEU:HD13	1.89	1.01
1:A:211:ASN:HA	1:A:222:ASP:OD2	1.62	1.00
1:E:18:LEU:HD12	1:E:123:VAL:HG11	1.48	0.95
1:A:211:ASN:ND2	1:A:222:ASP:OD2	2.05	0.90
3:Y:72:ARG:NH1	3:Y:75:GLN:OE1	2.05	0.90
1:A:211:ASN:CA	1:A:222:ASP:OD2	2.20	0.89
3:Y:58:GLY:H	3:Y:72:ARG:HH21	1.20	0.89
3:Y:100:LYS:NZ	4:Y:201:HOH:O	2.02	0.88
3:Z:68:CYS:SG	3:Z:72:ARG:NH1	2.47	0.87
2:D:3:VAL:CG1	2:D:25:SER:OG	2.24	0.85
1:A:211:ASN:HD22	1:A:222:ASP:CG	1.80	0.84
1:C:49:TRP:CZ3	2:D:97:THR:HG23	2.12	0.84
2:F:120:LEU:HD22	2:F:196:CYS:HB2	1.60	0.84
2:D:3:VAL:HG13	2:D:25:SER:OG	1.78	0.83
2:L:135:LEU:HD13	2:L:135:LEU:HD21	1.59	0.82
1:H:119:LYS:NZ	4:H:301:HOH:O	2.12	0.82
2:L:123:PRO:HD3	2:L:135:LEU:CD1	2.10	0.82
1:C:63:PRO:HD3	2:D:97:THR:HG21	1.62	0.81
1:A:137:PRO:HG2	2:B:126:GLU:OE1	1.80	0.81
3:X:63:ASN:ND2	4:X:201:HOH:O	2.14	0.81
2:L:123:PRO:HD3	2:L:135:LEU:HD12	1.64	0.80
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.64	0.80
3:G:54:CYS:SG	3:G:55:LEU:N	2.55	0.79
2:L:178:SER:OG	4:L:301:HOH:O	2.01	0.79
3:Y:61:SER:OG	3:Y:62:ASP:N	2.13	0.78
2:F:39:GLN:HB2	2:F:49:LEU:HD11	1.66	0.78
1:A:211:ASN:CB	1:A:222:ASP:OD2	2.31	0.77
2:B:39:GLN:HB2	2:B:49:LEU:HD11	1.68	0.76
2:B:83:GLU:OE1	4:B:301:HOH:O	2.02	0.76
3:Z:68:CYS:SG	3:Z:72:ARG:CZ	2.74	0.76
3:X:106:TYR:HB3	3:X:131:ILE:HD11	1.68	0.75
2:D:126:GLU:OE1	4:D:301:HOH:O	2.05	0.74
1:H:215:LYS:NZ	4:H:302:HOH:O	2.19	0.74
3:Y:79:THR:HG22	3:Y:80:THR:H	1.53	0.74
1:A:28:SER:OG	1:A:30:THR:HG22	1.88	0.73
1:E:70:SER:OG	1:E:83:GLN:OE1	2.03	0.73
2:L:63:ARG:HB2	2:L:78:THR:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:67:PRO:O	3:X:69:PHE:N	2.21	0.72
1:C:49:TRP:HZ3	2:D:97:THR:HG23	1.54	0.72
2:L:135:LEU:CD2	2:L:135:LEU:HB2	2.19	0.72
3:X:77:THR:O	3:X:78:ASN:ND2	2.21	0.72
1:E:157:LYS:O	4:E:301:HOH:O	2.07	0.72
2:B:114:ALA:CB	2:B:174:LYS:HE2	2.21	0.71
3:Z:95:SER:O	3:Z:99:LEU:HD23	1.91	0.70
3:Y:72:ARG:HH11	3:Y:75:GLN:CD	1.89	0.70
2:L:165:THR:HG22	2:L:166:THR:O	1.92	0.70
3:Z:106:TYR:HB3	3:Z:131:ILE:HD11	1.74	0.69
3:Y:115:GLN:N	4:Y:202:HOH:O	2.25	0.68
2:D:199:THR:OG1	2:D:204:THR:HG22	1.93	0.68
3:X:95:SER:O	3:X:99:LEU:HD23	1.94	0.68
1:C:28:SER:OG	1:C:30:THR:HG22	1.94	0.68
3:Z:76:MET:SD	3:Z:82:GLN:NE2	2.67	0.67
1:A:183:VAL:HG12	2:B:165:THR:CG2	2.25	0.67
2:L:39:GLN:HB2	2:L:49:LEU:HD11	1.77	0.66
1:E:18:LEU:CD1	1:E:123:VAL:HG11	2.24	0.66
1:C:18:LEU:CD1	1:C:123:VAL:HG11	2.27	0.65
1:A:223:LYS:HG3	1:A:224:LYS:N	2.10	0.65
2:B:184:THR:HG23	2:B:187:GLN:H	1.60	0.65
2:L:123:PRO:CD	2:L:135:LEU:HD12	2.27	0.65
3:Y:37:MET:SD	3:Y:81:MET:SD	2.95	0.65
2:F:120:LEU:HD12	2:F:136:VAL:O	1.97	0.64
1:A:215:LYS:HG3	1:A:216:PRO:HD3	1.79	0.64
1:A:198:VAL:HG22	1:A:199:PRO:HD2	1.78	0.63
3:X:128:LEU:HA	3:X:131:ILE:HG22	1.80	0.63
2:B:114:ALA:HB2	2:B:174:LYS:HE2	1.79	0.63
1:A:137:PRO:CG	2:B:126:GLU:OE1	2.47	0.63
2:B:184:THR:HG22	2:B:187:GLN:HE21	1.63	0.63
3:X:79:THR:O	3:X:83:THR:HG23	1.99	0.62
1:A:100:ALA:HB2	1:A:114:MET:HG2	1.81	0.62
2:B:114:ALA:HB3	2:B:143:TYR:H	1.64	0.62
2:L:135:LEU:CD1	2:L:135:LEU:HD21	2.19	0.62
2:B:78:THR:HG22	2:F:63:ARG:N	2.15	0.62
3:X:68:CYS:HB2	3:X:109:CYS:HB2	1.82	0.62
3:Y:72:ARG:HD2	3:Y:72:ARG:O	1.98	0.62
3:Z:120:ASN:OD1	3:Z:123:THR:OG1	2.07	0.62
1:E:23:THR:HG22	1:E:79:GLN:HB3	1.82	0.62
3:Z:76:MET:CE	3:Z:76:MET:O	2.48	0.61
2:L:72:LYS:NZ	4:L:303:HOH:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:76:MET:O	3:Z:76:MET:HE3	2.01	0.61
2:B:63:ARG:HA	2:F:78:THR:HG21	1.83	0.61
1:E:8:GLY:HA3	1:E:20:LEU:HD23	1.83	0.60
3:Z:76:MET:SD	3:Z:76:MET:C	2.81	0.60
2:B:78:THR:CG2	2:F:62:SER:C	2.70	0.59
3:Y:72:ARG:HH11	3:Y:75:GLN:HB3	1.67	0.59
3:Z:65:THR:HB	3:Z:66:ARG:HH22	1.66	0.59
1:E:4:LEU:HD23	1:E:24:VAL:HG22	1.83	0.59
3:G:89:PHE:CE2	3:G:93:LYS:HD3	2.37	0.59
1:A:130:THR:HG21	1:A:217:SER:HA	1.84	0.59
1:A:183:VAL:HG12	2:B:165:THR:HG22	1.83	0.59
3:Z:89:PHE:C	3:Z:89:PHE:CD2	2.75	0.59
2:D:3:VAL:HG12	2:D:25:SER:OG	2.03	0.59
1:E:18:LEU:HD21	1:E:20:LEU:HG	1.85	0.59
1:E:28:SER:HB3	1:E:31:THR:HG22	1.85	0.58
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.86	0.58
3:G:92:VAL:O	3:G:95:SER:OG	2.21	0.58
3:X:71:GLU:HA	3:X:74:SER:HB2	1.85	0.57
1:H:131:LYS:NZ	4:H:304:HOH:O	2.36	0.57
3:Y:66:ARG:N	3:Y:66:ARG:HD2	2.20	0.57
1:A:198:VAL:HG21	1:A:208:TYR:CZ	2.39	0.57
3:X:65:THR:HG23	3:X:66:ARG:N	2.20	0.56
3:X:134:LYS:HD2	3:X:134:LYS:N	2.19	0.56
3:Z:89:PHE:HE2	3:Z:93:LYS:HE2	1.69	0.56
1:H:4:LEU:HD23	1:H:24:VAL:HG22	1.86	0.56
3:G:117:THR:HG22	3:G:118:ALA:H	1.70	0.56
2:B:63:ARG:HA	2:F:78:THR:CG2	2.36	0.56
3:X:106:TYR:HB3	3:X:131:ILE:CD1	2.37	0.55
2:L:52:ASN:ND2	4:L:304:HOH:O	2.38	0.55
1:A:198:VAL:CG2	1:A:199:PRO:HD2	2.37	0.55
2:D:39:GLN:HB2	2:D:49:LEU:HD11	1.89	0.55
2:B:114:ALA:HB1	2:B:174:LYS:HE2	1.89	0.55
1:E:18:LEU:HD23	1:E:18:LEU:C	2.27	0.55
2:F:123:PRO:HB3	2:F:127:GLU:OE2	2.05	0.55
1:E:134:SER:N	4:E:301:HOH:O	2.28	0.55
3:Y:72:ARG:NH1	3:Y:75:GLN:NE2	2.54	0.55
2:F:141:ASP:OD1	2:F:170:GLN:NE2	2.40	0.54
2:F:136:VAL:HG12	2:F:180:TYR:CE1	2.42	0.54
3:G:128:LEU:O	3:G:131:ILE:HG22	2.06	0.54
1:H:155:LEU:HG	1:H:157:LYS:HG3	1.88	0.54
2:B:78:THR:HG23	2:F:62:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:GLU:O	2:D:86:ALA:HB2	2.07	0.54
3:X:71:GLU:HA	3:X:74:SER:CB	2.38	0.54
3:X:103:LYS:HE3	3:X:103:LYS:HA	1.89	0.54
1:A:133:PRO:HB2	1:A:156:VAL:HG13	1.90	0.53
2:L:32:SER:OG	3:X:35:ASN:HB3	2.07	0.53
3:X:57:LEU:HG	3:X:58:GLY:H	1.73	0.53
1:A:198:VAL:HG21	1:A:208:TYR:OH	2.08	0.53
1:E:6:GLU:N	1:E:6:GLU:OE2	2.41	0.53
3:X:57:LEU:CG	3:X:58:GLY:H	2.21	0.53
3:G:82:GLN:HG2	3:G:89:PHE:CD2	2.44	0.53
3:Z:79:THR:CG2	3:Z:81:MET:HG3	2.38	0.53
3:Y:77:THR:HG23	3:Y:77:THR:O	2.07	0.53
3:G:105:PRO:CB	3:G:138:ARG:NH2	2.72	0.53
3:Y:58:GLY:N	3:Y:72:ARG:HH21	1.98	0.53
3:Y:71:GLU:N	3:Y:71:GLU:OE2	2.42	0.52
1:E:5:VAL:CG2	1:E:23:THR:OG1	2.57	0.52
3:Y:79:THR:HG22	3:Y:80:THR:N	2.22	0.52
1:A:183:VAL:HG12	2:B:165:THR:HG23	1.89	0.52
1:E:220:LYS:NZ	1:E:222:ASP:CG	2.62	0.52
2:F:85:GLU:O	2:F:86:ALA:HB2	2.10	0.52
2:B:125:SER:O	2:B:128:LEU:HD12	2.09	0.52
1:E:155:LEU:HG	1:E:157:LYS:HG3	1.91	0.52
3:G:59:ILE:N	3:G:60:PRO:HD3	2.24	0.52
2:B:87:ASP:OD1	2:B:105[B]:HIS:ND1	2.43	0.52
2:B:85:GLU:O	2:B:86:ALA:HB2	2.08	0.52
1:A:11:LEU:HD13	1:A:161:PRO:HG3	1.92	0.52
2:B:114:ALA:HB3	2:B:143:TYR:N	2.24	0.52
1:H:14:PRO:O	1:H:15:SER:CB	2.58	0.51
1:A:215:LYS:N	1:A:216:PRO:CD	2.74	0.51
3:Y:128:LEU:HA	3:Y:131:ILE:HG22	1.92	0.51
1:A:106:TRP:CE2	3:G:24:LEU:HB3	2.45	0.51
3:G:105:PRO:HB3	3:G:138:ARG:NH2	2.26	0.51
3:Y:77:THR:O	3:Y:77:THR:CG2	2.58	0.51
3:X:66:ARG:CD	3:X:66:ARG:HG2	2.19	0.51
2:B:83:GLU:OE2	2:B:83:GLU:N	2.38	0.51
2:D:123:PRO:HD3	2:D:135:LEU:HD13	1.93	0.51
3:G:67:PRO:O	3:G:72:ARG:NE	2.44	0.51
3:G:122:LEU:O	3:G:126:LYS:HG3	2.11	0.51
1:A:159:TYR:OH	1:A:192:LEU:HD23	2.12	0.50
3:Z:120:ASN:ND2	3:Z:122:LEU:HB3	2.25	0.50
1:C:18:LEU:HD11	1:C:123:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:LYS:NZ	1:E:222:ASP:OD2	2.44	0.50
2:L:123:PRO:HD3	2:L:135:LEU:HD11	1.93	0.50
3:X:71:GLU:HA	3:X:74:SER:H	1.76	0.50
1:A:211:ASN:CG	1:A:222:ASP:OD2	2.50	0.50
1:E:149:THR:HG22	1:E:199:PRO:HA	1.92	0.50
3:G:67:PRO:HG3	3:G:131:ILE:HD12	1.94	0.50
3:G:59:ILE:N	3:G:60:PRO:CD	2.75	0.50
3:X:74:SER:C	3:X:76:MET:H	2.15	0.50
2:B:29:VAL:HG11	2:B:73:ALA:HB2	1.94	0.49
3:G:59:ILE:HD11	3:G:72:ARG:HB3	1.93	0.49
3:X:38:GLN:HG2	3:X:122:LEU:HD21	1.94	0.49
1:H:202:SER:C	1:H:205:THR:H	2.15	0.49
1:A:200:SER:HA	1:A:203:LEU:CD2	2.42	0.49
1:C:133:PRO:HD2	1:C:219:THR:HG21	1.94	0.49
1:E:69:THR:HG22	1:E:70:SER:N	2.28	0.49
2:L:135:LEU:HB2	2:L:135:LEU:HD22	1.94	0.49
1:A:106:TRP:NE1	3:G:24:LEU:HB3	2.28	0.49
2:D:184:THR:OG1	2:D:187:GLN:HG3	2.13	0.49
3:X:128:LEU:HA	3:X:131:ILE:CG2	2.40	0.49
1:E:218:ASN:O	1:E:218:ASN:ND2	2.44	0.49
3:X:85:TYR:HB3	3:X:88:ILE:HG12	1.95	0.49
3:X:134:LYS:HE3	3:X:134:LYS:HA	1.95	0.49
1:H:214:HIS:CD2	1:H:216:PRO:HD2	2.48	0.49
3:X:66:ARG:CB	3:X:66:ARG:HG2	2.20	0.48
3:G:89:PHE:HA	3:G:92:VAL:HG12	1.93	0.48
3:Z:89:PHE:CD2	3:Z:89:PHE:O	2.66	0.48
1:H:215:LYS:N	1:H:216:PRO:CD	2.77	0.48
3:X:66:ARG:CD	3:X:66:ARG:HG3	2.19	0.48
1:E:157:LYS:N	4:E:301:HOH:O	2.46	0.48
1:E:5:VAL:O	1:E:5:VAL:HG23	2.13	0.48
1:C:199:PRO:O	1:C:202:SER:OG	2.31	0.48
2:D:20:LEU:HD12	2:D:20:LEU:N	2.28	0.48
2:F:97:THR:HG23	3:Y:91:ARG:NH2	2.28	0.48
1:C:224:LYS:HD3	1:C:226:GLU:OE2	2.14	0.48
1:E:2:LEU:HD12	1:E:25:SER:O	2.13	0.48
2:F:200:HIS:O	2:F:201:GLU:C	2.52	0.48
1:H:18:LEU:HD11	1:H:20:LEU:HD12	1.96	0.48
3:Y:135:GLU:O	3:Y:138:ARG:HB2	2.14	0.47
1:H:14:PRO:O	1:H:15:SER:OG	2.27	0.47
2:L:3:VAL:O	2:L:3:VAL:HG13	2.14	0.47
1:A:138:LEU:HD21	2:B:136:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HE3	1:A:226:GLU:HB3	1.95	0.47
2:B:3:VAL:HG12	4:B:319:HOH:O	2.13	0.47
3:Y:66:ARG:HG3	3:Y:106:TYR:HA	1.96	0.47
3:Z:76:MET:SD	3:Z:82:GLN:CD	2.93	0.47
2:F:155:SER:O	2:F:155:SER:OG	2.30	0.47
1:H:177:VAL:HG22	1:H:196:VAL:HB	1.96	0.47
2:L:94:LYS:HE2	3:X:88:ILE:HD11	1.97	0.47
3:Y:69:PHE:CD2	3:Y:131:ILE:HD13	2.50	0.47
3:Z:37:MET:SD	3:Z:81:MET:HG2	2.55	0.47
2:L:85:GLU:O	2:L:86:ALA:HB2	2.14	0.47
3:Y:73:LEU:O	3:Y:76:MET:HB3	2.15	0.47
1:C:18:LEU:HD12	1:C:123:VAL:HG11	1.97	0.47
2:L:20:LEU:N	2:L:20:LEU:HD12	2.30	0.47
3:Y:128:LEU:O	3:Y:131:ILE:CG2	2.64	0.46
2:B:78:THR:CG2	2:F:63:ARG:N	2.78	0.46
2:F:184:THR:OG1	2:F:187:GLN:HG3	2.15	0.46
3:X:57:LEU:O	3:X:59:ILE:HD12	2.14	0.46
1:H:42:PRO:HB2	1:H:45:LYS:HD2	1.96	0.46
2:L:154:ASP:O	2:L:155:SER:HB3	2.15	0.46
3:Y:54:CYS:SG	3:Y:55:LEU:N	2.85	0.46
1:E:106:TRP:CE2	3:Y:24:LEU:HB3	2.50	0.46
2:B:63:ARG:HB3	2:F:78:THR:HG22	1.96	0.46
2:B:136:VAL:O	2:B:136:VAL:HG23	2.15	0.46
2:F:165:THR:HG22	2:F:166:THR:O	2.16	0.46
2:B:201:GLU:OE1	2:B:201:GLU:HA	2.15	0.46
3:X:57:LEU:HG	3:X:58:GLY:N	2.31	0.46
3:X:66:ARG:CB	3:X:66:ARG:HG3	2.20	0.46
2:D:50:ILE:CD1	2:D:75:LEU:HD13	2.45	0.46
3:G:89:PHE:O	3:G:93:LYS:HG3	2.16	0.46
2:D:67:PHE:HE2	2:D:76:THR:HG1	1.63	0.46
3:Z:66:ARG:N	3:Z:67:PRO:CD	2.79	0.46
3:Z:106:TYR:HB3	3:Z:131:ILE:CD1	2.44	0.46
1:C:215:LYS:N	1:C:216:PRO:CD	2.79	0.45
3:G:60:PRO:HD2	3:G:117:THR:O	2.16	0.45
3:G:99:LEU:HD23	3:G:104:CYS:SG	2.56	0.45
3:X:128:LEU:O	3:X:131:ILE:CG2	2.65	0.45
2:B:149:VAL:O	2:B:149:VAL:HG13	2.15	0.45
3:G:67:PRO:HD2	3:G:106:TYR:O	2.16	0.45
3:Y:128:LEU:HA	3:Y:131:ILE:CG2	2.45	0.45
3:Y:95:SER:O	3:Y:98:VAL:HG12	2.16	0.45
2:F:136:VAL:HG12	2:F:180:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:110:GLU:O	3:X:111:GLN:HB2	2.16	0.45
2:B:149:VAL:O	2:B:149:VAL:CG1	2.63	0.45
2:D:14:PRO:HG3	2:D:110:SER:HB3	1.99	0.45
1:E:209:ILE:HG12	1:E:224:LYS:CB	2.47	0.45
2:F:165:THR:OG1	2:F:178:SER:N	2.45	0.45
3:Y:37:MET:CE	3:Y:81:MET:SD	3.04	0.45
2:D:122:PRO:HA	2:D:135:LEU:HD13	1.99	0.45
3:Z:116:THR:O	3:Z:116:THR:HG22	2.17	0.45
1:A:138:LEU:HD11	1:A:155:LEU:HB2	1.98	0.45
1:A:215:LYS:HG3	1:A:216:PRO:CD	2.46	0.45
2:B:78:THR:HG21	2:F:62:SER:O	2.16	0.45
1:C:192:LEU:HD12	1:C:192:LEU:C	2.37	0.45
2:F:165:THR:OG1	2:F:178:SER:O	2.24	0.45
3:X:128:LEU:O	3:X:131:ILE:HG22	2.17	0.45
2:B:118:VAL:HG12	2:B:207:LYS:HG3	1.98	0.45
3:X:130:GLU:O	3:X:134:LYS:HG2	2.16	0.45
1:A:184:LEU:HD13	1:A:190:TYR:CE2	2.52	0.44
2:B:125:SER:HA	2:B:128:LEU:HD11	1.99	0.44
1:A:28:SER:HG	1:A:30:THR:HG22	1.79	0.44
1:H:52:PHE:CD1	1:H:52:PHE:C	2.90	0.44
1:E:214:HIS:CE1	1:E:216:PRO:HB2	2.52	0.44
3:Y:88:ILE:HD12	3:Y:88:ILE:N	2.32	0.44
1:C:165:THR:OG1	1:C:213:ASN:HB2	2.18	0.44
3:X:23:THR:HG21	3:X:136:LYS:HA	2.00	0.44
1:E:18:LEU:HD11	1:E:123:VAL:HG21	1.99	0.44
1:H:184:LEU:HD13	1:H:190:TYR:CZ	2.53	0.44
1:H:225:VAL:O	1:H:225:VAL:HG23	2.17	0.44
1:H:61:TYR:HB2	1:H:66:LYS:HG3	1.99	0.43
1:H:138:LEU:HD21	1:H:155:LEU:HB2	2.00	0.43
3:Y:138:ARG:HA	3:Y:138:ARG:HD3	1.64	0.43
1:H:192:LEU:HD12	1:H:192:LEU:C	2.38	0.43
3:Y:70:SER:HB3	3:Y:71:GLU:OE2	2.18	0.43
2:B:63:ARG:CA	2:F:78:THR:CG2	2.96	0.43
2:F:137:CYS:HB3	2:F:179:SER:HB3	2.00	0.43
2:B:20:LEU:N	2:B:20:LEU:HD12	2.34	0.43
1:H:18:LEU:O	1:H:83:GLN:HA	2.19	0.43
1:A:155:LEU:HG	1:A:157:LYS:HG3	2.00	0.43
3:X:57:LEU:HD12	3:X:58:GLY:H	1.84	0.43
3:Z:79:THR:HG22	3:Z:81:MET:HG3	1.99	0.43
2:D:13:SER:HB3	2:D:14:PRO:HD2	1.99	0.43
2:F:148:THR:HB	2:F:199:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:94:LYS:HA	3:X:94:LYS:HD2	1.81	0.43
2:B:182:SER:O	2:B:183:LEU:HG	2.19	0.43
1:E:5:VAL:HG23	1:E:23:THR:OG1	2.19	0.43
1:E:155:LEU:HD21	1:E:157:LYS:HD2	2.01	0.43
2:F:121:PHE:HB2	2:F:136:VAL:HG23	2.00	0.43
2:B:81:GLU:OE2	2:F:81:GLU:OE2	2.37	0.42
1:E:74:ASP:OD2	1:E:77:LYS:HG3	2.19	0.42
1:E:152:LEU:O	1:E:152:LEU:HD12	2.19	0.42
3:G:58:GLY:CA	3:G:60:PRO:HD3	2.49	0.42
1:A:88:THR:HG21	1:C:15:SER:HA	2.00	0.42
3:X:138:ARG:O	3:X:138:ARG:HD3	2.19	0.42
1:A:39:ILE:N	1:A:39:ILE:HD12	2.35	0.42
1:A:100:ALA:HB2	1:A:114:MET:CG	2.47	0.42
1:H:100:ALA:HB2	1:H:114:MET:HG2	2.02	0.42
1:E:215:LYS:N	1:E:216:PRO:CD	2.83	0.42
1:A:18:LEU:HD12	1:A:19:SER:N	2.35	0.42
1:A:88:THR:HG22	1:C:86:SER:HB3	2.02	0.42
2:F:28:SER:HB3	2:F:71:ASN:HB3	2.02	0.42
1:A:52:PHE:CD1	1:A:52:PHE:C	2.92	0.42
2:F:32:SER:OG	3:Y:35:ASN:HB3	2.19	0.42
2:L:152:LYS:HA	2:L:158:VAL:HG23	2.02	0.42
3:Y:22:PRO:O	3:Y:99:LEU:HD21	2.20	0.42
2:F:184:THR:HB	2:F:185:PRO:HD2	2.01	0.42
3:Z:81:MET:SD	3:Z:125:LEU:HD11	2.60	0.42
2:B:78:THR:CG2	2:F:62:SER:O	2.68	0.42
2:B:128:LEU:HD12	2:B:129:GLN:N	2.35	0.42
1:C:56:ASP:OD2	4:C:301:HOH:O	2.21	0.42
1:E:30:THR:HG21	1:E:75:THR:HG23	2.02	0.42
1:E:152:LEU:HD12	1:E:152:LEU:C	2.41	0.42
2:L:148:THR:OG1	2:L:199:THR:HB	2.20	0.42
3:X:60:PRO:HG2	3:X:69:PHE:CE2	2.55	0.42
3:X:128:LEU:CA	3:X:131:ILE:HG22	2.47	0.42
3:Z:105:PRO:HD2	3:Z:135:GLU:OE1	2.19	0.42
3:G:130:GLU:O	3:G:134:LYS:HG3	2.20	0.42
2:L:184:THR:HG23	2:L:187:GLN:H	1.85	0.42
3:X:134:LYS:NZ	3:X:137:MET:CE	2.83	0.42
1:E:177:VAL:HG22	1:E:196:VAL:HB	2.02	0.41
3:G:79:THR:OG1	3:G:82:GLN:HB2	2.19	0.41
3:Y:72:ARG:HH11	3:Y:75:GLN:CB	2.31	0.41
3:Z:77:THR:O	3:Z:78:ASN:C	2.58	0.41
2:B:118:VAL:HG21	2:B:198:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:ALA:HB2	2:F:185:PRO:HA	2.02	0.41
3:Y:68:CYS:SG	3:Y:71:GLU:CD	2.98	0.41
2:F:123:PRO:CA	2:F:127:GLU:OE2	2.68	0.41
2:F:123:PRO:CB	2:F:127:GLU:OE2	2.68	0.41
1:H:106:TRP:CE2	3:X:24:LEU:HB3	2.56	0.41
3:Y:60:PRO:HG2	3:Y:69:PHE:CZ	2.55	0.41
3:Z:55:LEU:HD23	3:Z:55:LEU:N	2.35	0.41
3:Z:94:LYS:O	3:Z:94:LYS:HD2	2.20	0.41
3:G:68:CYS:O	3:G:72:ARG:HD2	2.21	0.41
1:H:205:THR:O	1:H:206:GLN:HB2	2.21	0.41
2:L:63:ARG:HB2	2:L:78:THR:CG2	2.46	0.41
3:Z:63:ASN:ND2	3:Z:131:ILE:HD12	2.36	0.41
1:A:228:LYS:HG2	1:A:229:SER:H	1.86	0.41
2:D:148:THR:OG1	2:D:199:THR:HB	2.20	0.41
3:X:57:LEU:CD1	3:X:58:GLY:H	2.34	0.41
3:Z:93:LYS:O	3:Z:97:GLU:HG2	2.21	0.41
1:C:43:PRO:HD3	1:C:93:ALA:HA	2.02	0.41
1:C:200:SER:HA	1:C:203:LEU:CD2	2.51	0.41
2:F:29:VAL:HG11	2:F:73:ALA:HB2	2.02	0.41
3:Y:116:THR:O	3:Y:116:THR:OG1	2.36	0.41
2:F:185:PRO:O	2:F:188:TRP:HB3	2.21	0.41
3:X:57:LEU:CG	3:X:58:GLY:N	2.83	0.41
3:Y:33:LEU:HD23	3:Y:33:LEU:HA	1.91	0.41
3:Y:95:SER:HA	3:Y:98:VAL:HG12	2.02	0.41
3:Z:34:ILE:HG23	3:Z:122:LEU:HD11	2.03	0.41
1:A:74:ASP:OD2	1:A:77:LYS:HE2	2.21	0.41
1:C:30:THR:O	1:C:55:ARG:HG3	2.21	0.41
1:E:52:PHE:CD1	1:E:52:PHE:C	2.94	0.41
3:Z:44:LYS:O	3:Z:44:LYS:HG3	2.20	0.41
3:Z:140:MET:O	3:Z:143:LYS:HG3	2.21	0.41
1:E:69:THR:CG2	1:E:70:SER:N	2.83	0.40
1:H:224:LYS:HZ3	1:H:226:GLU:HB3	1.86	0.40
3:Y:58:GLY:H	3:Y:72:ARG:NH2	2.02	0.40
3:Z:73:LEU:HD11	3:Z:89:PHE:CZ	2.57	0.40
2:B:200:HIS:O	2:B:201:GLU:HB3	2.21	0.40
1:C:106:TRP:HB3	4:C:324:HOH:O	2.21	0.40
1:E:173:LEU:HD21	1:E:196:VAL:HG21	2.02	0.40
1:E:220:LYS:NZ	1:E:222:ASP:OD1	2.53	0.40
3:G:38:GLN:HG2	3:G:122:LEU:HD21	2.03	0.40
1:E:209:ILE:HA	1:E:224:LYS:HA	2.04	0.40
3:X:119:GLY:O	3:X:120:ASN:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:O	1:C:73:ARG:NH1	2.52	0.40
2:F:123:PRO:HA	2:F:127:GLU:OE2	2.21	0.40
3:Y:95:SER:O	3:Y:98:VAL:CG1	2.70	0.40
2:B:78:THR:HG22	2:F:63:ARG:CA	2.51	0.40
2:L:35:PRO:HD2	2:L:53:THR:OG1	2.21	0.40
3:Z:65:THR:HB	3:Z:66:ARG:NH2	2.32	0.40

All (21) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:138:ARG:NH1	3:Y:138:ARG:NH2[1_545]	1.01	1.19
3:G:138:ARG:HH11	3:Y:138:ARG:NH2[1_545]	0.53	1.07
3:G:138:ARG:HH11	3:Y:138:ARG:HH22[1_545]	1.00	0.60
1:C:77:LYS:HE3	1:H:206:GLN:H[2_645]	1.12	0.48
3:G:138:ARG:CZ	3:Y:138:ARG:NH2[1_545]	1.72	0.48
3:G:138:ARG:NH1	3:Y:138:ARG:HH22[1_545]	1.18	0.42
3:G:138:ARG:NH1	3:Y:138:ARG:HH21[1_545]	1.20	0.40
3:G:138:ARG:HH11	3:Y:138:ARG:CZ[1_545]	1.21	0.39
1:C:77:LYS:NZ	1:H:204:GLY:O[2_645]	1.83	0.37
1:A:222:ASP:HB2	1:E:220:LYS:HE3[2_646]	1.24	0.36
3:G:138:ARG:HH11	3:Y:138:ARG:HH21[1_545]	1.24	0.36
1:C:77:LYS:HZ2	1:H:204:GLY:O[2_645]	1.25	0.35
3:G:138:ARG:HD2	3:Y:138:ARG:HH22[1_545]	1.25	0.35
3:G:138:ARG:CZ	3:Y:138:ARG:HH22[1_545]	1.32	0.28
3:Y:103:LYS:NZ	3:Z:142:GLY:O[1_465]	2.01	0.19
3:G:138:ARG:NH1	3:Y:138:ARG:CZ[1_545]	2.02	0.18
3:Y:103:LYS:HZ2	3:Z:142:GLY:O[1_465]	1.48	0.12
3:G:137:MET:O	3:Z:141:ARG:NH2[1_455]	2.09	0.11
3:G:138:ARG:NE	3:Y:138:ARG:HH22[1_545]	1.54	0.06
3:G:138:ARG:NE	3:Y:138:ARG:NH2[1_545]	2.18	0.02
3:G:137:MET:O	3:Z:141:ARG:HH22[1_455]	1.60	0.00

## 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	218/230 (95%)	211 (97%)	7 (3%)	0	100	100
1	C	221/230 (96%)	212 (96%)	9 (4%)	0	100	100
1	E	218/230 (95%)	209 (96%)	9 (4%)	0	100	100
1	H	219/230 (95%)	207 (94%)	11 (5%)	1 (0%)	29	48
2	B	198/215 (92%)	190 (96%)	8 (4%)	0	100	100
2	D	209/215 (97%)	202 (97%)	7 (3%)	0	100	100
2	F	189/215 (88%)	179 (95%)	8 (4%)	2 (1%)	14	26
2	L	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
3	G	105/130 (81%)	96 (91%)	8 (8%)	1 (1%)	15	28
3	X	104/130 (80%)	87 (84%)	14 (14%)	3 (3%)	4	6
3	Y	97/130 (75%)	89 (92%)	5 (5%)	3 (3%)	4	5
3	Z	114/130 (88%)	104 (91%)	8 (7%)	2 (2%)	8	14
All	All	2100/2300 (91%)	1987 (95%)	101 (5%)	12 (1%)	25	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	206	GLN
3	X	68	CYS
3	X	110	GLU
3	Y	43	SER
3	Y	78	ASN
3	Y	103	LYS
3	Z	113	CYS
3	G	45	CYS
2	F	110	SER
2	F	185	PRO
3	Z	65	THR
3	X	120	ASN

### 5.3.2 Protein sidechains [i](#)

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	190/196 (97%)	186 (98%)	4 (2%)	53	78
1	C	191/196 (97%)	189 (99%)	2 (1%)	76	90
1	E	190/196 (97%)	183 (96%)	7 (4%)	34	60
1	H	190/196 (97%)	184 (97%)	6 (3%)	39	65
2	B	170/180 (94%)	167 (98%)	3 (2%)	59	81
2	D	176/180 (98%)	174 (99%)	2 (1%)	73	89
2	F	164/180 (91%)	163 (99%)	1 (1%)	86	95
2	L	175/180 (97%)	173 (99%)	2 (1%)	73	89
3	G	102/118 (86%)	96 (94%)	6 (6%)	19	37
3	X	103/118 (87%)	95 (92%)	8 (8%)	12	24
3	Y	96/118 (81%)	92 (96%)	4 (4%)	30	54
3	Z	108/118 (92%)	101 (94%)	7 (6%)	17	33
All	All	1855/1976 (94%)	1803 (97%)	52 (3%)	43	70

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	76	SER
1	A	211	ASN
1	A	215	LYS
2	B	111	GLN
2	B	113	LYS
2	B	128	LEU
1	C	62	SER
1	C	178	HIS
2	D	156	SER
2	D	159	LYS
1	E	62	SER
1	E	141	SER
1	E	186	SER
1	E	210	CYS
1	E	211	ASN
1	E	215	LYS
1	E	220	LYS
2	F	200	HIS

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Mol	Chain	Res	Type
3	G	44	LYS
3	G	54	CYS
3	G	66	ARG
3	G	71	GLU
3	G	72	ARG
3	G	100	LYS
1	H	7	SER
1	H	62	SER
1	H	127	SER
1	H	206	GLN
1	H	211	ASN
1	H	215	LYS
2	L	159	LYS
2	L	192	ARG
3	X	36	LYS
3	X	44	LYS
3	X	69	PHE
3	X	74	SER
3	X	82	GLN
3	X	90	SER
3	X	95	SER
3	X	100	LYS
3	Y	61	SER
3	Y	68	CYS
3	Y	74	SER
3	Y	76	MET
3	Z	76	MET
3	Z	94	LYS
3	Z	113	CYS
3	Z	132	PHE
3	Z	138	ARG
3	Z	141	ARG
3	Z	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	129	GLN
2	B	187	GLN
2	D	187	GLN
1	E	41	GLN
2	F	111	GLN

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Mol	Chain	Res	Type
2	F	129	GLN
2	F	187	GLN
2	L	52	ASN
3	Z	63	ASN
3	Z	82	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	222/230 (96%)	0.51	20 (9%) 9 9	35, 63, 113, 138	0
1	C	225/230 (97%)	0.17	5 (2%) 62 65	35, 50, 86, 111	0
1	E	222/230 (96%)	0.57	10 (4%) 33 36	43, 80, 105, 115	0
1	H	223/230 (96%)	0.20	6 (2%) 54 58	36, 56, 85, 128	0
2	B	203/215 (94%)	0.64	22 (10%) 5 5	32, 62, 120, 145	0
2	D	211/215 (98%)	0.09	2 (0%) 84 86	29, 48, 73, 92	0
2	F	195/215 (90%)	0.70	19 (9%) 7 7	34, 66, 127, 204	0
2	L	210/215 (97%)	0.29	5 (2%) 59 62	32, 58, 101, 117	0
3	G	111/130 (85%)	1.09	27 (24%) 0 0	43, 88, 131, 144	0
3	X	112/130 (86%)	1.48	34 (30%) 0 0	50, 93, 136, 153	0
3	Y	105/130 (80%)	1.37	26 (24%) 0 0	50, 96, 135, 157	0
3	Z	118/130 (90%)	1.49	38 (32%) 0 0	45, 96, 141, 161	0
All	All	2157/2300 (93%)	0.59	214 (9%) 7 7	29, 64, 124, 204	0

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	77	THR	8.0
2	F	198	VAL	7.4
3	Y	73	LEU	6.4
3	Z	47	CYS	6.4
3	Z	54	CYS	5.7
1	A	203	LEU	5.5
3	X	65	THR	5.4
3	G	57	LEU	5.4
3	X	119	GLY	5.3
3	X	77	THR	5.3
3	Y	57	LEU	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	131	ASN	5.2
3	G	55	LEU	5.2
3	Y	119	GLY	5.1
3	Z	115	GLN	5.1
3	X	55	LEU	5.0
3	Y	76	MET	5.0
3	Z	78	ASN	5.0
2	F	158	VAL	4.9
3	X	76	MET	4.9
3	X	110	GLU	4.9
2	B	198	VAL	4.9
3	Z	55	LEU	4.8
3	Y	55	LEU	4.7
1	E	203	LEU	4.6
3	Z	64	CYS	4.5
3	G	81	MET	4.5
1	A	149	THR	4.5
3	X	109	CYS	4.3
3	Y	77	THR	4.3
3	Y	118	ALA	4.3
3	Z	76	MET	4.2
2	F	157	PRO	4.2
3	G	118	ALA	4.2
2	F	161	GLY	4.1
1	H	205	THR	4.1
1	A	230	CYS	4.0
2	B	186	GLU	4.0
2	F	192	ARG	4.0
3	G	73	LEU	3.9
3	Z	81	MET	3.8
1	H	1	GLN	3.8
2	B	151	TRP	3.8
2	B	149	VAL	3.8
3	G	75	GLN	3.7
3	Y	75	GLN	3.7
1	H	229	SER	3.7
3	Z	119	GLY	3.7
3	Z	114	ASN	3.6
3	Y	46	HIS	3.6
2	F	185	PRO	3.6
3	Y	89	PHE	3.6
2	L	110	SER	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	X	56	CYS	3.6
2	F	205	VAL	3.6
3	Z	42	ALA	3.6
1	C	1	GLN	3.6
3	X	46	HIS	3.6
3	X	100	LYS	3.6
1	E	1	GLN	3.5
2	B	196	CYS	3.5
2	F	123	PRO	3.5
3	X	108	SER	3.5
3	G	54	CYS	3.5
2	F	195	SER	3.4
3	Y	78	ASN	3.4
3	X	107	PHE	3.4
3	Y	54	CYS	3.4
3	X	131	ILE	3.4
2	F	189	LYS	3.4
1	A	172	ALA	3.4
3	Y	74	SER	3.3
1	A	173	LEU	3.3
3	Z	116	THR	3.3
3	Y	131	ILE	3.3
2	L	210	ALA	3.3
3	X	84	ARG	3.3
3	Z	117	THR	3.3
3	Z	131	ILE	3.3
3	X	78	ASN	3.3
3	Y	82	GLN	3.3
3	Z	46	HIS	3.2
2	F	188	TRP	3.2
2	B	146	ALA	3.2
3	Z	79	THR	3.2
1	A	206	GLN	3.2
2	B	155	SER	3.2
3	Z	44	LYS	3.2
3	Y	80	THR	3.2
3	X	72	ARG	3.2
3	X	73	LEU	3.2
3	Z	75	GLN	3.1
1	A	205	THR	3.1
1	A	223	LYS	3.1
3	Y	81	MET	3.1

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Mol	Chain	Res	Type	RSRZ
3	Y	56	CYS	3.0
3	G	79	THR	3.0
3	G	119	GLY	3.0
3	G	77	THR	3.0
3	G	62	ASP	2.9
1	A	199	PRO	2.9
3	Z	118	ALA	2.9
3	Z	69	PHE	2.9
2	B	187	GLN	2.9
3	Z	80	THR	2.8
3	Z	112	PRO	2.8
2	B	148	THR	2.8
1	E	202	SER	2.8
3	Z	82	GLN	2.8
2	F	201	GLU	2.8
3	Y	69	PHE	2.8
2	F	26	SER	2.8
2	B	181	LEU	2.7
3	G	140	MET	2.7
2	F	105[A]	HIS	2.7
2	B	201	GLU	2.7
2	L	192	ARG	2.7
1	E	152	LEU	2.7
2	B	182	SER	2.7
3	X	70	SER	2.7
3	Z	110	GLU	2.7
3	G	43	SER	2.7
3	Y	79	THR	2.7
2	B	183	LEU	2.7
3	Z	66	ARG	2.6
3	X	57	LEU	2.6
3	X	111	GLN	2.6
3	Z	72	ARG	2.6
2	B	158	VAL	2.6
2	F	149	VAL	2.6
3	Y	115	GLN	2.6
3	Z	59	ILE	2.6
3	X	97	GLU	2.6
3	G	46	HIS	2.6
3	G	65	THR	2.6
3	Z	113	CYS	2.6
2	D	115	ALA	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	69	PHE	2.5
3	Z	56	CYS	2.5
3	X	81	MET	2.5
3	G	80	THR	2.5
3	X	68	CYS	2.5
3	Y	42	ALA	2.5
2	B	202	GLY	2.5
2	L	129	GLN	2.5
2	B	159	LYS	2.5
3	Z	143	LYS	2.5
3	G	78	ASN	2.5
3	Z	111	GLN	2.4
3	Y	70	SER	2.4
1	C	148	GLY	2.4
2	F	147	VAL	2.4
3	Z	107	PHE	2.4
3	X	96	VAL	2.4
1	A	218	ASN	2.4
3	Z	41	PRO	2.4
2	B	154	ASP	2.4
3	X	66	ARG	2.4
2	B	197	GLN	2.4
2	B	147	VAL	2.4
3	G	76	MET	2.4
3	Y	124	PHE	2.4
1	A	152	LEU	2.4
3	Z	57	LEU	2.4
3	G	72	ARG	2.3
1	C	203	LEU	2.3
3	G	58	GLY	2.3
1	A	208	TYR	2.3
3	X	71	GLU	2.3
3	X	99	LEU	2.3
3	X	59	ILE	2.3
1	A	150	ALA	2.3
1	C	202	SER	2.3
3	Y	103	LYS	2.3
3	G	71	GLU	2.3
1	A	225	VAL	2.2
2	F	2	ALA	2.2
3	G	59	ILE	2.2
1	E	106	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	228	LYS	2.2
3	G	44	LYS	2.2
1	E	107	TYR	2.2
3	X	45	CYS	2.2
1	A	222	ASP	2.2
1	E	197	THR	2.2
3	X	98	VAL	2.2
2	B	114	ALA	2.2
3	X	101	ASN	2.2
1	A	113	GLY	2.2
1	H	105	SER	2.2
1	H	108	PRO	2.2
2	L	188	TRP	2.2
3	G	138	ARG	2.2
2	B	54	ASN	2.2
1	E	77	LYS	2.2
1	E	220	LYS	2.2
2	F	54	ASN	2.1
3	G	89	PHE	2.1
3	X	20	GLY	2.1
2	D	212	THR	2.1
3	Y	117	THR	2.1
3	Z	97	GLU	2.1
3	G	82	GLN	2.1
1	H	107	TYR	2.1
2	B	200	HIS	2.1
3	Z	21	CYS	2.1
3	Z	73	LEU	2.1
3	X	37	MET	2.1
1	A	198	VAL	2.1
1	E	105	SER	2.0
1	A	112	TYR	2.0
1	A	204	GLY	2.0
3	X	144	ILE	2.0
1	C	108	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.