



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:43 AM UTC

PDB ID : 7OX1 / pdb_00007ox1
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

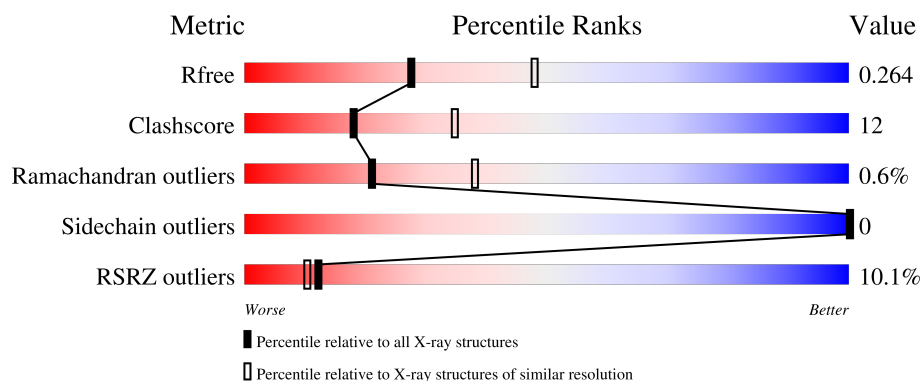
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 ≥ 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	5% 77% 19% .
1	C	230	2% 85% 13% .
1	E	230	7% 78% 17% .
1	H	230	3% 83% 13% ..
2	B	215	12% 78% 15% 6%

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Mol	Chain	Length	Quality of chain
2	D	215	% 88%10%•
2	F	215	15% 71%19%9%
2	L	215	83%14%•
3	G	130	17% 57%26%•15%
3	X	130	22% 54%28%••14%
3	Y	130	24% 49%29%•19%
3	Z	130	25% 62%27%•9%

2 Entry composition [i](#)

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

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

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

- Molecule 3 is a protein called Interleukin-9.

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

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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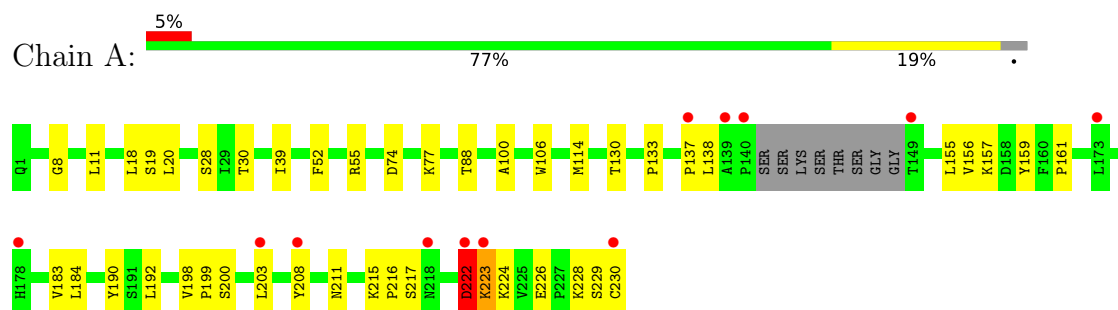
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	1	Total	O	0	0
			1	1		

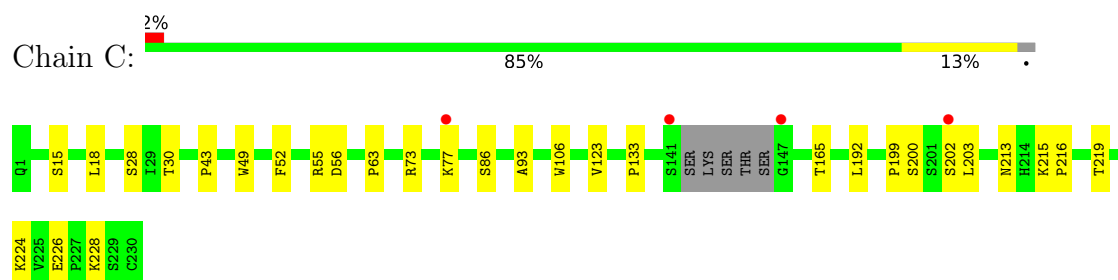
3 Residue-property plots [i](#)

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.

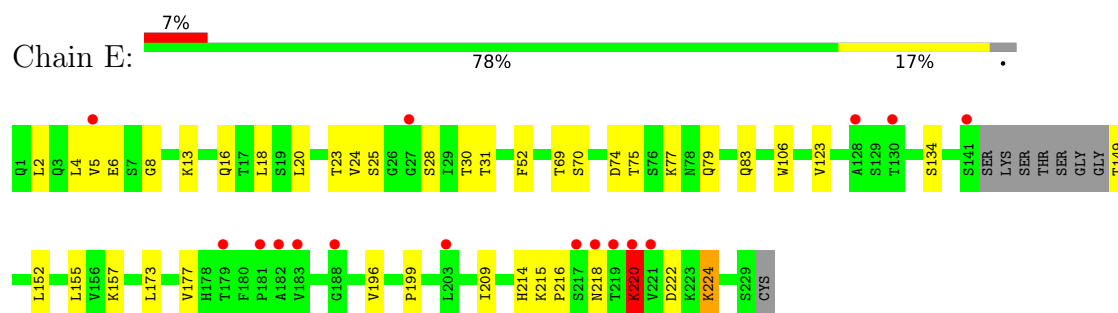
- Molecule 1: Heavy chain (Fab 7D6)



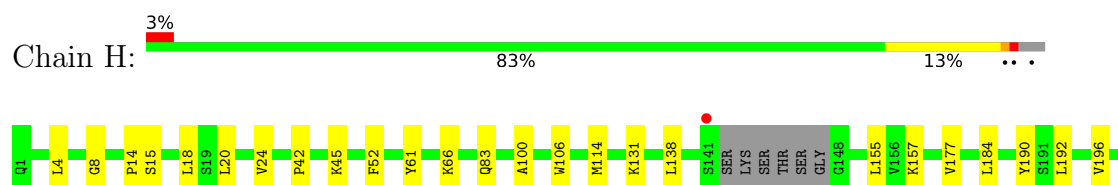
- Molecule 1: Heavy chain (Fab 7D6)

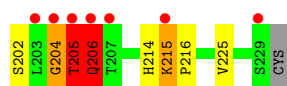


- Molecule 1: Heavy chain (Fab 7D6)

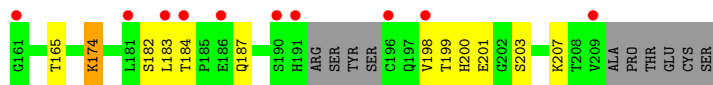
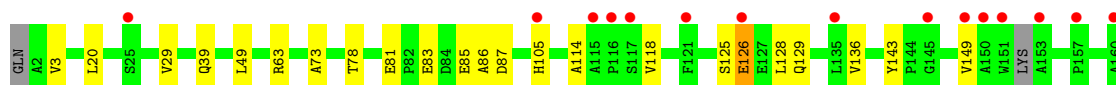
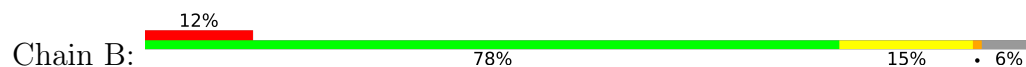


- Molecule 1: Heavy chain (Fab 7D6)

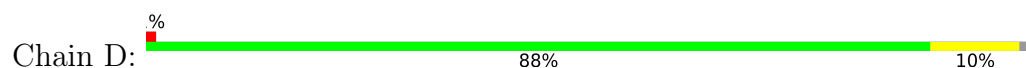




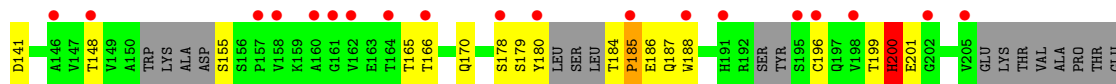
- Molecule 2: Light chain (Fab 7D6)



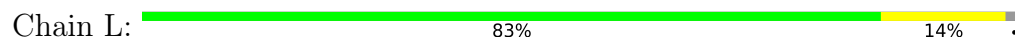
- Molecule 2: Light chain (Fab 7D6)



- Molecule 2: Light chain (Fab 7D6)

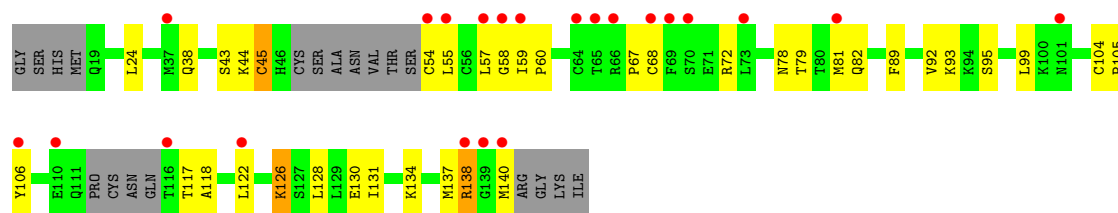


- Molecule 2: Light chain (Fab 7D6)

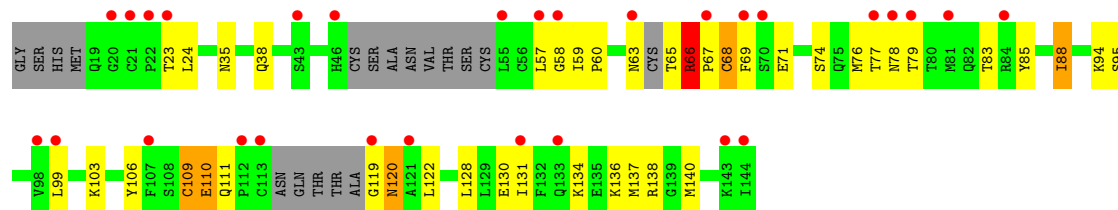


- Molecule 3: Interleukin-9

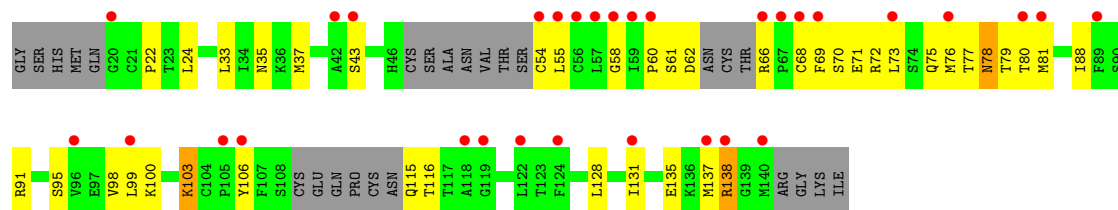




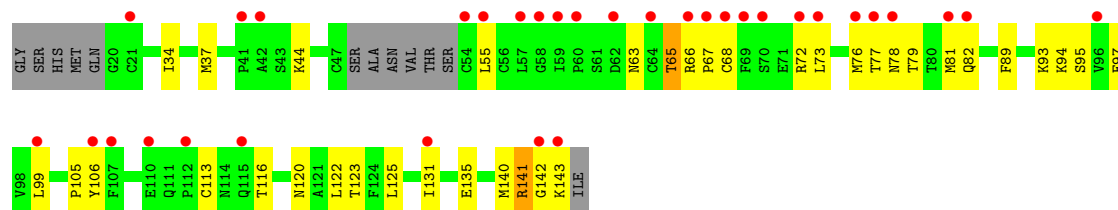
● Molecule 3: Interleukin-9



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.262 0.212 , 0.264	Depositor DCC
R_{free} test set	4625 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32503	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	1/1720 (0.1%)	0.66	2/2348 (0.1%)
1	C	0.36	0/1734	0.60	1/2366 (0.0%)
1	E	0.53	4/1720 (0.2%)	0.78	5/2348 (0.2%)
1	H	0.57	6/1724 (0.3%)	0.82	10/2353 (0.4%)
2	B	0.37	0/1548	0.68	3/2117 (0.1%)
2	D	0.32	0/1604	0.55	0/2196
2	F	0.46	2/1489 (0.1%)	0.74	3/2033 (0.1%)
2	L	0.43	2/1597 (0.1%)	0.72	4/2186 (0.2%)
3	G	0.60	3/882 (0.3%)	0.87	4/1182 (0.3%)
3	X	0.59	2/896 (0.2%)	0.80	3/1197 (0.3%)
3	Y	0.73	3/836 (0.4%)	0.85	4/1118 (0.4%)
3	Z	0.48	0/935	0.81	2/1254 (0.2%)
All	All	0.50	23/16685 (0.1%)	0.73	41/22698 (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)
1	A	222	ASP	CG-OD2	16.44	1.56	1.25
3	Y	138	ARG	CZ-NH1	15.24	1.54	1.32
2	F	113	LYS	CB-CG	-9.41	1.24	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	13	LYS	CD-CE	-9.24	1.24	1.52
2	L	135	LEU	CG-CD2	9.00	1.82	1.52
3	G	138	ARG	CZ-NH2	-8.51	1.22	1.33
1	H	204	GLY	C-N	8.46	1.45	1.33
3	X	66	ARG	CB-CG	8.36	1.77	1.52
3	X	66	ARG	CG-CD	8.12	1.76	1.52
3	G	138	ARG	CD-NE	-7.53	1.35	1.46
1	H	205	THR	CB-CG2	-7.09	1.29	1.52
1	H	204	GLY	C-O	6.96	1.32	1.24
1	H	205	THR	CA-CB	6.24	1.61	1.53
1	E	220	LYS	CG-CD	6.15	1.71	1.52
2	F	113	LYS	CD-CE	5.96	1.70	1.52
1	E	220	LYS	CD-CE	-5.82	1.34	1.52
1	H	206	GLN	CA-CB	5.77	1.63	1.53
1	H	215	LYS	CG-CD	5.74	1.69	1.52
3	Y	138	ARG	CZ-NH2	5.49	1.40	1.33
3	Y	138	ARG	CD-NE	5.25	1.53	1.46
1	E	220	LYS	CB-CG	5.21	1.68	1.52
2	L	34	TYR	C-O	-5.10	1.21	1.23
3	G	138	ARG	NE-CZ	-5.00	1.27	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	113	LYS	CA-CB-CG	14.30	142.71	114.10
2	L	135	LEU	CB-CG-CD1	14.17	153.22	110.70
1	H	205	THR	CA-CB-CG2	12.07	131.02	110.50
1	H	215	LYS	CA-CB-CG	12.00	138.11	114.10
2	L	135	LEU	CD1-CG-CD2	-10.70	87.25	110.80
3	X	66	ARG	CB-CG-CD	10.66	135.82	111.30
1	H	215	LYS	CB-CG-CD	10.26	134.89	111.30
2	F	200	HIS	CB-CA-C	-9.95	91.50	109.71
1	E	13	LYS	CB-CG-CD	9.66	133.53	111.30
3	G	126	LYS	CB-CG-CD	9.61	133.40	111.30
1	E	220	LYS	CD-CE-NZ	-9.57	81.29	111.90
3	G	57	LEU	CB-CG-CD1	8.64	136.62	110.70
3	Y	138	ARG	CB-CG-CD	-8.59	91.53	111.30
1	H	215	LYS	CG-CD-CE	8.15	130.04	111.30
2	L	135	LEU	CB-CG-CD2	-8.14	86.28	110.70
1	E	224	LYS	CA-CB-CG	7.88	129.86	114.10
2	B	174	LYS	CG-CD-CE	7.77	129.18	111.30
1	E	16	GLN	CA-CB-CG	7.46	129.02	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	66	ARG	CG-CD-NE	7.46	128.40	112.00
1	H	204	GLY	CA-C-N	-7.40	111.79	122.67
1	H	204	GLY	C-N-CA	-7.40	111.79	122.67
3	G	138	ARG	NE-CZ-NH2	-7.32	112.61	119.20
3	Y	138	ARG	NE-CZ-NH2	7.15	125.64	119.20
2	L	159	LYS	CA-CB-CG	7.00	128.09	114.10
1	H	205	THR	CA-C-O	-6.96	111.82	122.32
1	H	206	GLN	CB-CG-CD	6.89	124.32	112.60
3	X	88	ILE	CB-CG1-CD1	6.84	128.17	113.80
1	C	228	LYS	CG-CD-CE	6.54	126.33	111.30
1	H	215	LYS	CD-CE-NZ	-6.46	91.21	111.90
1	H	204	GLY	N-CA-C	-6.43	106.38	114.16
3	Y	138	ARG	NH1-CZ-NH2	-6.39	110.99	119.30
3	Y	138	ARG	N-CA-CB	-6.28	100.86	110.16
1	A	223	LYS	CA-CB-CG	-6.27	101.56	114.10
2	B	174	LYS	CA-CB-CG	6.00	126.09	114.10
3	Z	141	ARG	CB-CG-CD	-5.91	97.71	111.30
3	Z	141	ARG	NE-CZ-NH1	-5.90	115.60	121.50
2	B	126	GLU	N-CA-CB	-5.74	101.45	110.06
1	E	224	LYS	N-CA-CB	5.66	119.40	110.23
2	F	113	LYS	CB-CA-C	5.46	120.87	109.68
1	A	223	LYS	CB-CG-CD	5.38	123.68	111.30
3	G	126	LYS	CG-CD-CE	5.17	123.19	111.30

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

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	46	1
1	C	1688	1652	1651	22	3
1	E	1674	1641	1640	40	1
1	H	1678	1644	1643	23	3
2	B	1510	1451	1447	45	0
2	D	1563	1507	1507	18	0
2	F	1446	1387	1373	41	0
2	L	1556	1500	1500	31	0
3	G	870	882	880	32	15
3	X	884	909	906	49	0
3	Y	825	844	844	47	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	2	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	394	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 (394) 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
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
3:Y:72:ARG:NH1	3:Y:75:GLN:CD	2.08	1.11
2:L:135:LEU:CD2	2:L:135:LEU:CB	2.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Z:76:MET:HE3	3:Z:76:MET:O	1.70	0.91
1:A:211:ASN:ND2	1:A:222:ASP:OD2	2.05	0.90
1:A:211:ASN:CA	1:A:222:ASP:OD2	2.20	0.89
1:A:211:ASN:HD22	1:A:222:ASP:CG	1.80	0.89
3:Y:58:GLY:H	3:Y:72:ARG:HH21	1.20	0.89
3:Y:72:ARG:NH1	3:Y:75:GLN:OE1	2.05	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: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
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:72:ARG:HH11	3:Y:75:GLN:CD	1.89	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
1:E:70:SER:OG	1:E:83:GLN:OE1	2.03	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
3:Y:61:SER:OG	3:Y:62:ASP:N	2.13	0.74
1:A:28:SER:OG	1:A:30:THR:HG22	1.88	0.73
2:L:63:ARG:HB2	2:L:78:THR:HG22	1.70	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:78:THR:CG2	2:F:62:SER:C	2.70	0.64
3:Z:76:MET:SD	3:Z:76:MET:C	2.81	0.64
3:Z:89:PHE:C	3:Z:89:PHE:CD2	2.75	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
2:L:72:LYS:NZ	4:L:303:HOH:O	2.32	0.61
2:B:63:ARG:HA	2:F:78:THR:HG21	1.83	0.61
3:Y:100:LYS:NZ	4:Y:201:HOH:O	2.02	0.60
1:E:8:GLY:HA3	1:E:20:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:LEU:HD23	1:E:18:LEU:C	2.27	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
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
1:E:220:LYS:NZ	1:E:222:ASP:CG	2.62	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
2:F:165:THR:OG1	2:F:178:SER:O	2.24	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:211:ASN:CG	1:A:222:ASP:OD2	2.50	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
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
3:X:74:SER:C	3:X:76:MET:H	2.15	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
1:H:202:SER:C	1:H:205:THR:H	2.15	0.54
3:Z:76:MET:O	3:Z:76:MET:CE	2.48	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
1:H:14:PRO:O	1:H:15:SER:OG	2.27	0.52
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
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
3:Z:76:MET:SD	3:Z:82:GLN:CD	2.93	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
2:F:85:GLU:O	2:F:86:ALA:HB2	2.10	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
2:F:200:HIS:O	2:F:201:GLU:C	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:29:VAL:HG11	2:B:73:ALA:HB2	1.94	0.49
1:C:192:LEU:HD12	1:C:192:LEU:C	2.37	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:A:211:ASN:ND2	1:A:222:ASP:CG	2.61	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
3:X:134:LYS:NZ	3:X:137:MET:HE1	2.27	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:52:PHE:CD1	1:H:52:PHE:C	2.90	0.49
1:H:192:LEU:HD12	1:H:192:LEU:C	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:52:PHE:CD1	1:A:52:PHE:C	2.92	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
1:E:152:LEU:C	1:E:152:LEU:HD12	2.41	0.46
2:F:184:THR:OG1	2:F:187:GLN:HG3	2.15	0.46
3:G:81:MET:HE2	3:G:89:PHE:CE1	2.50	0.46
3:X:57:LEU:O	3:X:59:ILE:HD12	2.14	0.46
3:Z:77:THR:O	3:Z:78:ASN:C	2.58	0.46
1:H:42:PRO:HB2	1:H:45:LYS:HD2	1.96	0.46
1:E:106:TRP:CE2	3:Y:24:LEU:HB3	2.50	0.46
3:Y:68:CYS:SG	3:Y:71:GLU:CD	2.98	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:L:184:THR:OG1	2:L:186:GLU:OE2	2.26	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
3:Y:54:CYS:SG	3:Y:55:LEU:N	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:52:PHE:CD1	1:E:52:PHE:C	2.94	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
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
2:L:154:ASP:O	2:L:155:SER:HB3	2.15	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
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:110:GLU:O	3:X:111:GLN:HB2	2.16	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:A:229:SER:O	1:A:230:CYS:C	2.60	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
3:X:140:MET:HE3	3:Y:137:MET:SD	2.58	0.44
3:G:58:GLY:C	3:G:60:PRO:HD3	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD12	1:E:152:LEU:O	2.19	0.42
3:G:58:GLY:CA	3:G:60:PRO:HD3	2.49	0.42
3:Y:77:THR:O	3:Y:78:ASN:C	2.61	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
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
1:C:52:PHE:CD1	1:C:52:PHE:C	2.98	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
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
1:E:220:LYS:C	1:E:220:LYS:HD2	2.44	0.42
3:G:130:GLU:O	3:G:134:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:62:ASP:OD2	3:Y:62:ASP:C	2.62	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
2:B:118:VAL:HG21	2:B:198:VAL:CG1	2.50	0.41
2:F:133:ALA:HB2	2:F:185:PRO:HA	2.02	0.41
2:B:199:THR:HG23	2:B:203:SER:C	2.46	0.41
2:F:123:PRO:CA	2:F:127:GLU:OE2	2.68	0.41
3:G:44:LYS:O	3:G:45:CYS:C	2.63	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:G:43:SER:C	3:G:45:CYS:N	2.78	0.41
3:G:78:ASN:C	3:G:79:THR:HG23	2.45	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
2:L:166:THR:O	2:L:167:PRO:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:7:GLU:O	2:F:104:THR:OG1	2.34	0.40
2:F:184:THR:O	2:F:185:PRO:C	2.64	0.40
3:X:119:GLY:O	3:X:120:ASN:CB	2.69	0.40
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
1:A:55:ARG:HD3	3:G:140:MET:HE3	2.04	0.40
2:B:78:THR:HG22	2:F:63:ARG:CA	2.51	0.40
1:E:215:LYS:C	1:E:215:LYS:HD2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	43
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%)	11	22
2	L	208/215 (97%)	201 (97%)	7 (3%)	0	100	100
3	G	105/130 (81%)	96 (91%)	8 (8%)	1 (1%)	12	24
3	X	104/130 (80%)	87 (84%)	14 (14%)	3 (3%)	3	5
3	Y	97/130 (75%)	89 (92%)	5 (5%)	3 (3%)	3	5
3	Z	114/130 (88%)	104 (91%)	8 (7%)	2 (2%)	6	12
All	All	2100/2300 (91%)	1987 (95%)	101 (5%)	12 (1%)	21	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	206	GLN
3	X	68	CYS
3	X	110	GLU

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Mol	Chain	Res	Type
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 ⓘ

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%)	190 (100%)	0	100	100
1	C	191/196 (97%)	191 (100%)	0	100	100
1	E	190/196 (97%)	190 (100%)	0	100	100
1	H	190/196 (97%)	190 (100%)	0	100	100
2	B	170/180 (94%)	170 (100%)	0	100	100
2	D	176/180 (98%)	176 (100%)	0	100	100
2	F	164/180 (91%)	164 (100%)	0	100	100
2	L	175/180 (97%)	175 (100%)	0	100	100
3	G	102/118 (86%)	102 (100%)	0	100	100
3	X	103/118 (87%)	103 (100%)	0	100	100
3	Y	96/118 (81%)	96 (100%)	0	100	100
3	Z	108/118 (92%)	108 (100%)	0	100	100
All	All	1855/1976 (94%)	1855 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	129	GLN
2	B	187	GLN
2	B	191	HIS
2	B	200	HIS
1	C	206	GLN
2	D	187	GLN
2	D	191	HIS
1	E	41	GLN
2	F	54	ASN
2	F	111	GLN
2	F	129	GLN
3	G	19	GLN
1	H	1	GLN
1	H	16	GLN
1	H	206	GLN
2	L	52	ASN
2	L	191	HIS
3	X	78	ASN
3	X	102	ASN
3	Y	38	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/230 (96%)	0.49	12 (5%) 31 27	38, 68, 127, 153	0
1	C	225/230 (97%)	0.00	4 (1%) 67 64	38, 55, 97, 120	0
1	E	222/230 (96%)	0.92	16 (7%) 21 19	46, 87, 116, 132	0
1	H	223/230 (96%)	0.20	8 (3%) 46 41	38, 62, 94, 133	0
2	B	203/215 (94%)	0.58	25 (12%) 8 7	36, 66, 131, 158	1 (0%)
2	D	211/215 (98%)	-0.10	3 (1%) 73 70	32, 53, 82, 103	0
2	F	195/215 (90%)	0.86	33 (16%) 4 3	36, 72, 141, 225	1 (0%)
2	L	210/215 (97%)	0.19	1 (0%) 87 85	36, 63, 111, 133	0
3	G	111/130 (85%)	1.19	22 (19%) 3 2	45, 99, 140, 159	0
3	X	112/130 (86%)	1.43	29 (25%) 1 1	54, 104, 153, 167	0
3	Y	105/130 (80%)	1.46	31 (29%) 1 1	55, 106, 144, 175	0
3	Z	118/130 (90%)	1.41	33 (27%) 1 1	45, 106, 156, 177	0
All	All	2157/2300 (93%)	0.59	217 (10%) 12 10	32, 71, 136, 225	2 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	105[A]	HIS	6.7
2	F	105[A]	HIS	6.5
2	F	195	SER	5.3
2	F	158	VAL	5.2
2	B	151	TRP	4.2
3	X	57	LEU	4.2
1	E	220	LYS	4.0
2	F	160	ALA	4.0
3	X	55	LEU	3.9
2	B	196	CYS	3.9
2	B	209	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
3	Y	55	LEU	3.8
1	A	222	ASP	3.7
3	X	58	GLY	3.6
3	X	69	PHE	3.6
3	Z	67	PRO	3.6
3	X	113	CYS	3.4
1	A	223	LYS	3.4
3	Z	78	ASN	3.4
3	G	55	LEU	3.4
3	Z	77	THR	3.4
2	F	120	LEU	3.4
3	Y	67	PRO	3.4
3	Y	89	PHE	3.3
2	F	162	VAL	3.3
3	Z	76	MET	3.2
1	A	218	ASN	3.2
2	F	188	TRP	3.2
3	Y	81	MET	3.2
2	F	161	GLY	3.2
2	F	205	VAL	3.2
2	F	198	VAL	3.2
1	E	203	LEU	3.1
1	H	204	GLY	3.1
3	Z	58	GLY	3.1
3	G	138	ARG	3.1
3	Z	112	PRO	3.1
3	Y	106	TYR	3.0
2	F	196	CYS	3.0
3	Z	57	LEU	3.0
3	G	57	LEU	3.0
3	X	112	PRO	3.0
1	A	203	LEU	3.0
3	Z	142	GLY	3.0
1	A	140	PRO	2.9
2	F	123	PRO	2.9
3	Z	131	ILE	2.9
1	E	188	GLY	2.9
3	X	70	SER	2.9
1	E	183	VAL	2.9
3	G	139	GLY	2.9
1	E	179	THR	2.8
3	G	140	MET	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	64	CYS	2.8
3	X	20	GLY	2.8
3	X	119	GLY	2.8
3	X	131	ILE	2.8
2	B	115	ALA	2.8
3	G	81	MET	2.8
3	X	67	PRO	2.8
2	F	134	THR	2.8
3	Z	69	PHE	2.8
3	G	65	THR	2.7
3	X	63	ASN	2.7
2	F	2	ALA	2.7
3	Y	60	PRO	2.7
3	Z	107	PHE	2.7
1	E	182	ALA	2.7
2	B	126	GLU	2.7
3	Z	68	CYS	2.6
3	Z	81	MET	2.6
1	A	139	ALA	2.6
3	X	23	THR	2.6
3	Z	42	ALA	2.6
3	Z	143	LYS	2.6
1	A	173	LEU	2.6
2	B	186	GLU	2.6
1	E	27	GLY	2.6
2	B	198	VAL	2.6
3	Y	43	SER	2.6
2	F	130	ALA	2.6
2	B	191	HIS	2.6
2	F	180	TYR	2.6
3	G	122	LEU	2.6
3	Z	99	LEU	2.6
1	E	128	ALA	2.6
1	E	130	THR	2.6
2	B	153	ALA	2.6
3	Z	73	LEU	2.5
1	E	221	VAL	2.5
3	X	43	SER	2.5
2	F	135	LEU	2.5
3	X	99	LEU	2.5
3	X	107	PHE	2.5
3	Y	57	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	Z	55	LEU	2.5
2	B	117	SER	2.5
3	X	21	CYS	2.5
3	Y	58	GLY	2.5
2	F	146	ALA	2.5
3	Z	66	ARG	2.5
2	F	26	SER	2.5
3	X	22	PRO	2.5
3	Y	119	GLY	2.5
2	B	121	PHE	2.5
1	H	207	THR	2.5
2	F	166	THR	2.5
3	G	116	THR	2.5
3	G	59	ILE	2.4
3	G	73	LEU	2.4
3	Y	73	LEU	2.4
3	Y	69	PHE	2.4
2	D	2	ALA	2.4
1	H	229	SER	2.4
2	B	145	GLY	2.4
1	A	178	HIS	2.4
3	Z	72	ARG	2.4
2	F	54	ASN	2.4
3	Z	96	VAL	2.4
1	E	219	THR	2.4
1	H	141	SER	2.4
2	F	128	LEU	2.4
3	X	78	ASN	2.4
2	F	157	PRO	2.4
3	Z	82	GLN	2.4
3	X	46	HIS	2.4
3	Y	68	CYS	2.4
3	X	98	VAL	2.4
3	Y	118	ALA	2.4
3	X	144	ILE	2.3
1	A	230	CYS	2.3
3	G	54	CYS	2.3
3	Z	41	PRO	2.3
3	Z	54	CYS	2.3
3	Z	64	CYS	2.3
3	Y	42	ALA	2.3
2	D	212	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	141	SER	2.3
2	L	182	SER	2.3
3	G	37	MET	2.3
3	X	81	MET	2.3
3	Y	140	MET	2.3
2	F	94	LYS	2.3
2	F	121	PHE	2.3
3	Y	138	ARG	2.3
2	F	202	GLY	2.3
3	Z	62	ASP	2.3
3	Y	105	PRO	2.3
1	A	208	TYR	2.3
2	B	150	ALA	2.2
3	G	70	SER	2.2
3	Y	76	MET	2.2
3	Z	70	SER	2.2
2	B	116	PRO	2.2
2	F	185	PRO	2.2
3	G	101	ASN	2.2
3	G	68	CYS	2.2
3	Z	21	CYS	2.2
1	H	205	THR	2.2
3	Y	99	LEU	2.2
1	H	215	LYS	2.2
2	F	191	HIS	2.2
3	X	143	LYS	2.2
1	E	181	PRO	2.2
1	E	5	VAL	2.2
2	B	149	VAL	2.2
3	Y	137	MET	2.2
2	B	135	LEU	2.2
3	G	106	TYR	2.2
3	Y	56	CYS	2.2
3	Y	122	LEU	2.2
3	Y	59	ILE	2.2
3	Y	131	ILE	2.2
3	Z	59	ILE	2.2
1	E	141	SER	2.2
2	B	190	SER	2.2
3	G	110	GLU	2.2
1	E	218	ASN	2.1
2	B	183	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	X	77	THR	2.1
3	Z	110	GLU	2.1
3	Y	96	VAL	2.1
2	B	160	ALA	2.1
3	X	121	ALA	2.1
1	C	147	GLY	2.1
1	H	203	LEU	2.1
2	F	148	THR	2.1
3	G	58	GLY	2.1
3	Y	66	ARG	2.1
3	Y	54	CYS	2.1
1	A	137	PRO	2.1
3	Z	115	GLN	2.1
2	D	154	ASP	2.1
2	F	178	SER	2.1
3	Z	60	PRO	2.1
3	X	133	GLN	2.1
3	Y	124	PHE	2.1
2	B	181	LEU	2.1
3	G	66	ARG	2.1
3	X	84	ARG	2.1
3	Y	80	THR	2.1
2	B	25	SER	2.1
2	B	157	PRO	2.1
2	B	161	GLY	2.0
1	C	77	LYS	2.0
2	F	164	THR	2.0
3	X	79	THR	2.0
3	Z	106	TYR	2.0
1	H	206	GLN	2.0
3	G	69	PHE	2.0
2	F	127	GLU	2.0
2	F	131	ASN	2.0
3	Y	20	GLY	2.0
1	A	149	THR	2.0
2	B	184	THR	2.0
1	C	202	SER	2.0
1	E	217	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.