



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:26 AM UTC

PDB ID : 4R96 / pdb_00004r96
Title : Structure of a Llama Glama Fab 48A2 against human cMet
Authors : Klarenbeek, A.; El Mazouari, K.; Desmyter, A.; Blanchetot, C.; Hultberg, A.; Roovers, R.C.; Cambillau, C.; Spinelli, S.; Del-Favero, J.; Verrips, T.; de Haard, H.; Achour, I.
Deposited on : 2014-09-03
Resolution : 3.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

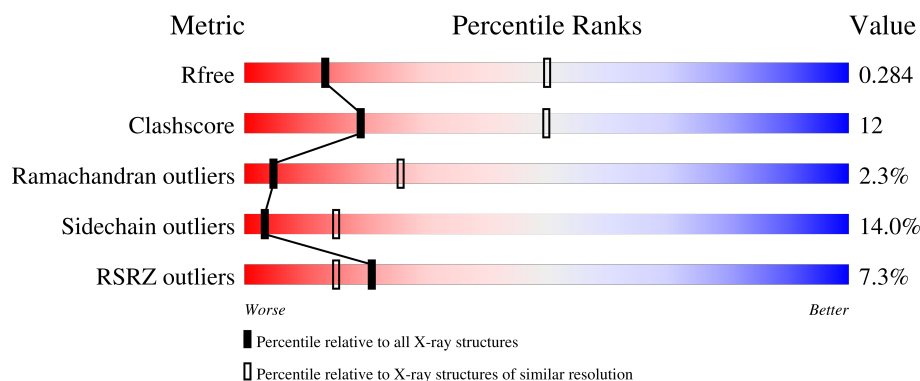
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	221	6% 76% 20% ..
1	C	221	8% 74% 22% ..
1	E	221	11% 75% 21% .
1	L	221	4% 81% 15% .
2	B	219	6% 62% 24% 9% ..

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Mol	Chain	Length	Quality of chain
2	D	219	8% 58% 26% 10%
2	F	219	10% 68% 20% 7%
2	H	219	5% 60% 31% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13536 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 Llama glama Fab 48A2 against human cMet L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1703	1068	288	342	5			
1	C	219	Total	C	N	O	S	0	0	0
			1703	1068	288	342	5			
1	E	221	Total	C	N	O	S	0	0	0
			1714	1074	290	344	6			
1	L	221	Total	C	N	O	S	0	0	0
			1718	1076	290	346	6			

- Molecule 2 is a protein called Llama glama Fab 48A2 against human cMet H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1606	1015	263	322	6			
2	D	213	Total	C	N	O	S	0	0	0
			1612	1018	266	322	6			
2	F	213	Total	C	N	O	S	0	0	0
			1612	1018	266	322	6			
2	H	217	Total	C	N	O	S	0	0	0
			1634	1030	270	328	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	C	16	Total	O	0	0
			16	16		
3	E	28	Total	O	0	0
			28	28		
3	L	29	Total	O	0	0
			29	29		

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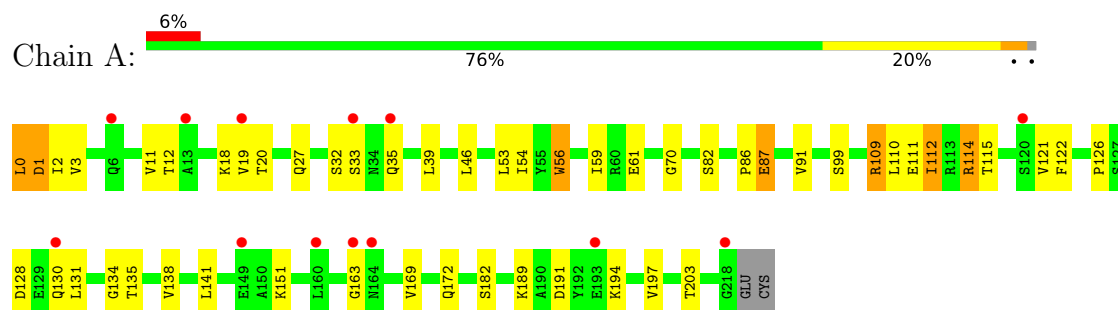
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	40	Total 40	O 40	0	0
3	D	25	Total 25	O 25	0	0
3	F	35	Total 35	O 35	0	0
3	H	22	Total 22	O 22	0	0

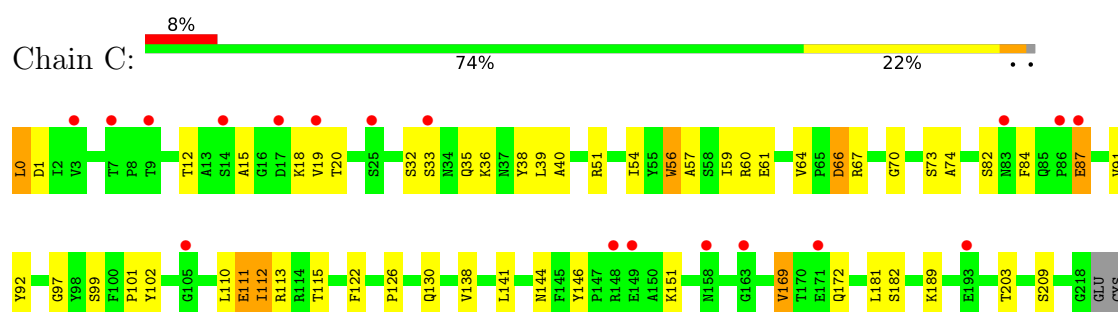
3 Residue-property plots [i](#)

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.

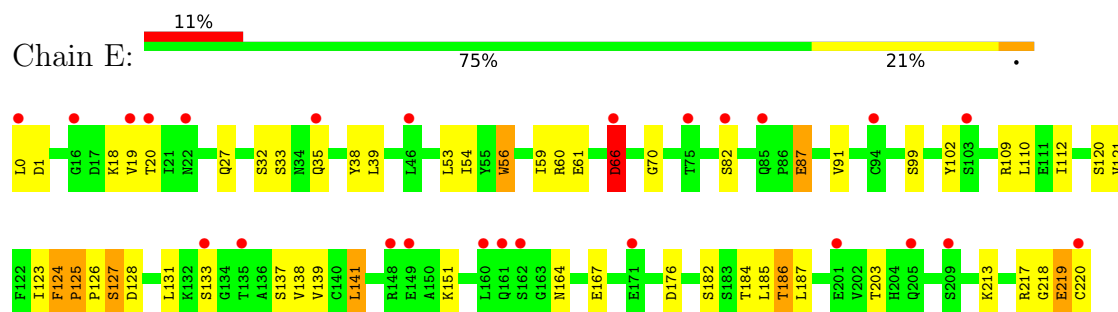
- Molecule 1: Llama glama Fab 48A2 against human cMet L chain



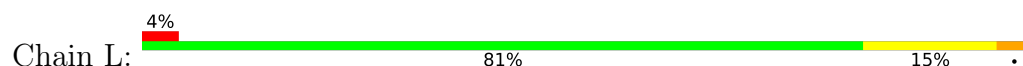
- Molecule 1: Llama glama Fab 48A2 against human cMet L chain

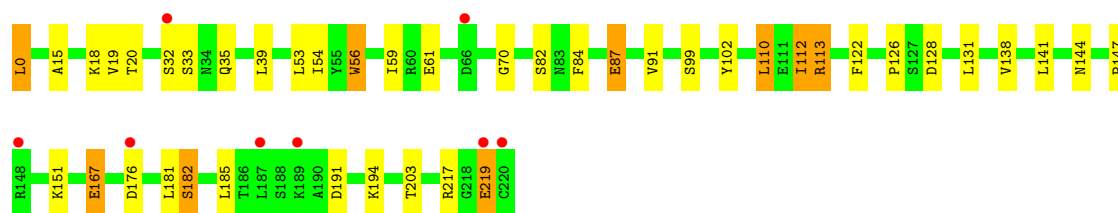


- Molecule 1: Llama glama Fab 48A2 against human cMet L chain

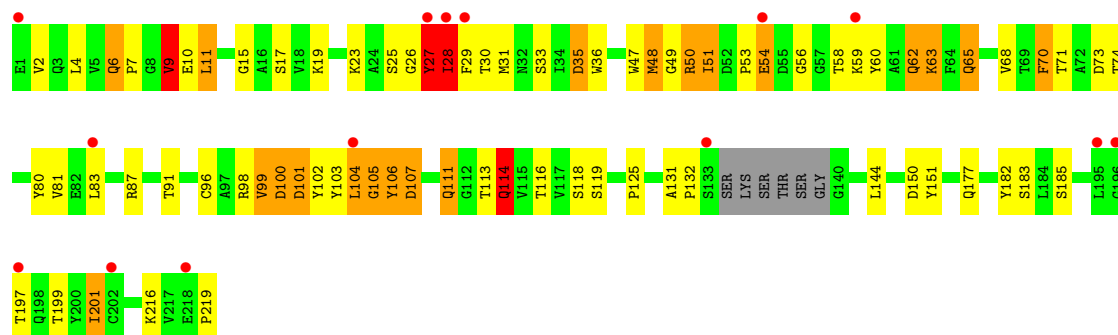


- Molecule 1: Llama glama Fab 48A2 against human cMet L chain

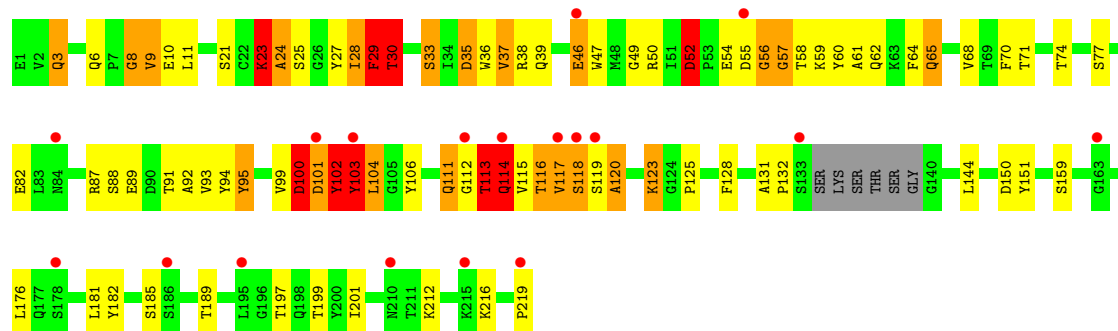




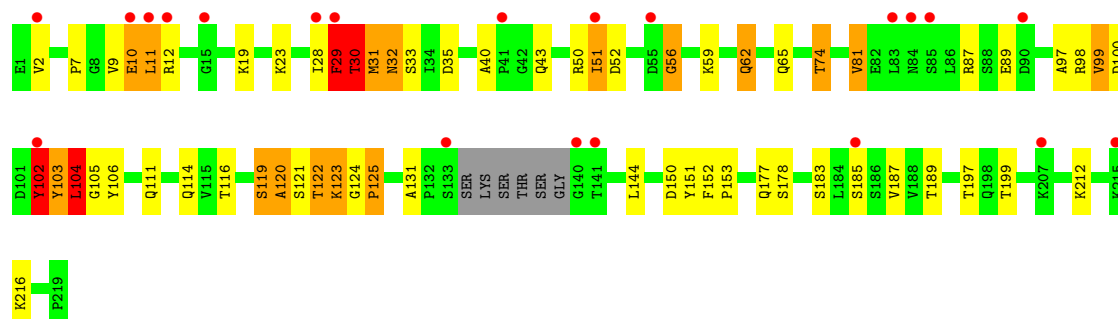
• Molecule 2: Llama glama Fab 48A2 against human cMet H chain



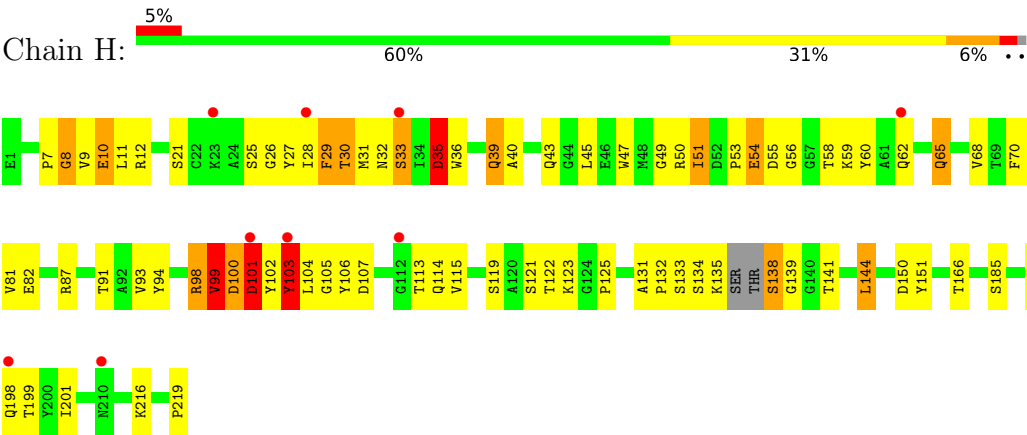
• Molecule 2: Llama glama Fab 48A2 against human cMet H chain



• Molecule 2: Llama glama Fab 48A2 against human cMet H chain



● Molecule 2: Llama glama Fab 48A2 against human cMet H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.02Å 121.54Å 185.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.39 – 3.31 43.39 – 3.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.39-3.31) 97.5 (43.39-3.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.217 , 0.261 0.241 , 0.284	Depositor DCC
R_{free} test set	3580 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.891	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13536	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.78	0/1741	1.18	5/2365 (0.2%)
1	C	0.77	0/1741	1.19	8/2365 (0.3%)
1	E	0.85	3/1752 (0.2%)	1.24	10/2380 (0.4%)
1	L	0.75	0/1756	1.20	4/2385 (0.2%)
2	B	0.87	2/1645 (0.1%)	1.39	14/2247 (0.6%)
2	D	0.85	1/1651 (0.1%)	1.40	26/2254 (1.2%)
2	F	0.82	1/1651 (0.1%)	1.36	14/2254 (0.6%)
2	H	0.81	1/1673 (0.1%)	1.34	14/2283 (0.6%)
All	All	0.81	8/13610 (0.1%)	1.29	95/18533 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	111	GLN	CA-C	10.44	1.58	1.52
2	H	103	TYR	C-N	6.56	1.42	1.33
1	E	125	PRO	N-CD	5.88	1.55	1.47
1	E	124	PHE	C-N	5.87	1.40	1.33
2	F	120	ALA	CA-C	-5.53	1.45	1.53
2	B	114	GLN	C-O	-5.40	1.17	1.23
2	B	28	ILE	CG1-CD1	5.21	1.72	1.51
1	E	125	PRO	C-N	5.05	1.40	1.33

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	30	THR	CA-C-N	9.92	139.55	121.70
2	F	30	THR	C-N-CA	9.92	139.55	121.70
2	D	23	LYS	CA-C-N	9.86	139.45	121.70
2	D	23	LYS	C-N-CA	9.86	139.45	121.70
2	B	25	SER	N-CA-C	-8.71	99.70	110.41
2	H	131	ALA	N-CA-C	8.60	120.91	110.07
2	B	105	GLY	CA-C-N	8.31	136.65	121.70
2	B	105	GLY	C-N-CA	8.31	136.65	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	25	SER	N-CA-C	8.19	123.54	111.34
2	H	103	TYR	CA-C-N	7.95	136.02	121.70
2	H	103	TYR	C-N-CA	7.95	136.02	121.70
1	E	66	ASP	CA-CB-CG	7.77	120.37	112.60
2	D	52	ASP	CA-CB-CG	7.44	120.04	112.60
2	B	29	PHE	N-CA-C	-7.28	100.90	110.43
2	D	111	GLN	N-CA-C	7.15	120.28	108.48
2	F	29	PHE	CA-CB-CG	7.11	120.91	113.80
1	C	0	LEU	CA-C-N	7.09	131.26	121.33
1	C	0	LEU	C-N-CA	7.09	131.26	121.33
2	F	7	PRO	N-CA-C	7.02	121.94	111.41
2	D	102	TYR	N-CA-C	-6.64	98.00	108.63
2	B	35	ASP	CA-CB-CG	6.64	119.24	112.60
1	E	125	PRO	CA-C-N	-6.49	113.08	119.76
1	E	125	PRO	C-N-CA	-6.49	113.08	119.76
2	H	134	SER	N-CA-C	-6.43	97.11	110.80
2	D	101	ASP	N-CA-C	-6.43	104.20	111.14
2	H	27	TYR	N-CA-C	6.41	116.46	108.19
2	B	29	PHE	CA-CB-CG	6.35	120.15	113.80
2	D	102	TYR	CA-C-N	6.27	133.52	121.54
2	D	102	TYR	C-N-CA	6.27	133.52	121.54
1	A	1	ASP	CA-CB-CG	6.22	118.83	112.60
2	H	103	TYR	CA-CB-CG	6.22	125.10	113.90
2	B	104	LEU	N-CA-C	6.20	119.62	109.76
2	F	29	PHE	CB-CA-C	6.20	117.43	109.80
2	D	29	PHE	CA-CB-CG	6.19	119.99	113.80
1	E	124	PHE	CA-C-N	-6.18	114.02	120.38
1	E	124	PHE	C-N-CA	-6.18	114.02	120.38
2	F	56	GLY	CA-C-N	6.11	126.91	120.43
2	F	56	GLY	C-N-CA	6.11	126.91	120.43
1	A	0	LEU	CA-C-N	6.11	133.21	121.54
1	A	0	LEU	C-N-CA	6.11	133.21	121.54
1	A	33	SER	N-CA-C	6.09	118.00	111.36
2	D	106	TYR	N-CA-C	6.04	118.04	108.67
2	B	100	ASP	CA-C-N	6.02	130.23	120.60
2	B	100	ASP	C-N-CA	6.02	130.23	120.60
2	F	120	ALA	N-CA-C	-5.97	102.62	110.33
2	F	131	ALA	N-CA-C	5.87	117.29	109.83
2	B	106	TYR	CA-C-N	5.85	128.12	120.28
2	B	106	TYR	C-N-CA	5.85	128.12	120.28
1	C	189	LYS	CA-C-N	5.84	128.43	120.54
1	C	189	LYS	C-N-CA	5.84	128.43	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	114	GLN	CA-C-N	5.83	132.47	121.97
2	D	114	GLN	C-N-CA	5.83	132.47	121.97
1	L	33	SER	N-CA-C	5.78	117.66	111.36
2	D	95	TYR	N-CA-C	5.78	118.66	109.24
1	E	33	SER	N-CA-C	5.78	117.66	111.36
2	H	101	ASP	CA-C-N	5.77	129.77	122.16
2	H	101	ASP	C-N-CA	5.77	129.77	122.16
1	C	33	SER	N-CA-C	5.76	117.64	111.36
2	H	100	ASP	N-CA-C	-5.76	100.29	109.96
2	D	117	VAL	CA-C-N	5.71	132.45	121.54
2	D	117	VAL	C-N-CA	5.71	132.45	121.54
2	B	131	ALA	N-CA-C	5.69	117.05	109.83
2	F	30	THR	CB-CA-C	5.68	121.72	110.42
2	D	92	ALA	N-CA-C	5.67	115.32	107.73
1	E	218	GLY	CA-C-N	5.66	132.35	121.54
1	E	218	GLY	C-N-CA	5.66	132.35	121.54
2	D	103	TYR	CA-CB-CG	5.61	124.00	113.90
1	A	121	VAL	N-CA-C	5.55	116.58	108.58
2	D	100	ASP	CA-C-N	5.53	127.96	120.44
2	D	100	ASP	C-N-CA	5.53	127.96	120.44
2	H	113	THR	CB-CA-C	5.52	118.68	110.62
2	B	70	PHE	CA-CB-CG	5.48	119.28	113.80
1	L	147	PRO	CA-C-N	5.47	127.61	120.28
1	L	147	PRO	C-N-CA	5.47	127.61	120.28
2	D	131	ALA	N-CA-C	5.47	116.77	109.83
1	C	66	ASP	CA-C-N	5.42	127.80	120.38
1	C	66	ASP	C-N-CA	5.42	127.80	120.38
2	D	28	ILE	N-CA-CB	5.35	120.06	111.23
2	D	114	GLN	N-CA-C	5.33	122.15	110.80
1	E	124	PHE	N-CA-C	5.32	121.80	108.40
2	F	103	TYR	N-CA-C	-5.26	99.94	108.41
2	H	26	GLY	N-CA-C	5.24	122.51	115.59
2	H	133	SER	CA-C-N	5.24	131.54	121.54
2	H	133	SER	C-N-CA	5.24	131.54	121.54
2	F	125	PRO	CA-N-CD	-5.15	104.78	112.00
1	E	176	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	101	ASP	N-CA-C	5.14	118.66	112.38
1	L	217	ARG	N-CA-C	5.14	121.74	110.80
2	D	3	GLN	N-CA-C	5.12	116.52	107.61
2	D	8	GLY	CA-C-N	5.10	130.87	121.70
2	D	8	GLY	C-N-CA	5.10	130.87	121.70
2	H	35	ASP	CA-CB-CG	5.09	117.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	ASP	CA-CB-CG	5.02	117.62	112.60
2	F	178	SER	CA-C-N	5.02	129.10	120.72
2	F	178	SER	C-N-CA	5.02	129.10	120.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1703	0	1645	33	0
1	C	1703	0	1645	34	0
1	E	1714	0	1652	32	0
1	L	1718	0	1656	19	0
2	B	1606	0	1548	53	0
2	D	1612	0	1559	66	0
2	F	1612	0	1559	46	0
2	H	1634	0	1576	46	0
3	A	39	0	0	1	0
3	B	40	0	0	0	0
3	C	16	0	0	0	0
3	D	25	0	0	1	0
3	E	28	0	0	2	0
3	F	35	0	0	0	0
3	H	22	0	0	0	0
3	L	29	0	0	1	0
All	All	13536	0	12840	305	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 12.

All (305) 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)
2:F:30:THR:CB	2:F:31:MET:HB2	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:123:LYS:NZ	2:F:150:ASP:O	1.78	1.16
2:B:50:ARG:HH11	2:B:50:ARG:HG2	1.14	1.12
2:F:30:THR:HB	2:F:31:MET:CB	1.84	1.06
2:F:100:ASP:HB3	2:F:102:TYR:CE2	1.93	1.02
2:D:103:TYR:HB2	2:D:104:LEU:HA	1.42	1.00
1:C:15:ALA:O	2:B:15:GLY:HA3	1.63	0.98
2:B:9:VAL:CG2	2:B:114:GLN:HB3	1.96	0.95
1:C:12:THR:HG22	1:C:111:GLU:OE1	1.67	0.94
2:F:125:PRO:HB3	2:F:151:TYR:HB3	1.46	0.94
2:H:51:ILE:HD12	2:H:58:THR:HG22	1.49	0.94
1:L:19:VAL:HG11	1:L:110:LEU:HD21	1.51	0.93
2:F:100:ASP:HB3	2:F:102:TYR:HE2	1.33	0.92
1:E:137:SER:HA	1:E:185:LEU:O	1.68	0.92
1:C:12:THR:CG2	1:C:111:GLU:OE1	2.19	0.91
1:A:19:VAL:HG11	1:A:110:LEU:HD21	1.49	0.91
2:F:123:LYS:NZ	2:F:150:ASP:C	2.31	0.87
1:E:123:ILE:HG13	1:E:124:PHE:H	1.37	0.87
2:B:9:VAL:HG23	2:B:114:GLN:HB3	1.55	0.87
2:B:30:THR:HG22	2:B:31:MET:H	1.38	0.87
1:E:123:ILE:HG13	1:E:124:PHE:N	1.90	0.86
2:F:30:THR:HB	2:F:31:MET:HB2	0.87	0.85
1:A:12:THR:HG22	1:A:111:GLU:HB3	1.58	0.84
2:F:10:GLU:OE2	2:F:12:ARG:HG2	1.78	0.84
2:F:33:SER:HB2	2:F:99:VAL:HG13	1.60	0.84
2:D:117:VAL:HG12	2:D:120:ALA:CB	2.12	0.80
2:F:11:LEU:HD11	2:F:152:PHE:HZ	1.47	0.79
2:B:70:PHE:HD1	2:B:81:VAL:HG22	1.47	0.79
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.65	0.79
1:A:130:GLN:NE2	1:A:135:THR:HG22	1.98	0.78
2:D:8:GLY:CA	2:D:113:THR:HG23	2.14	0.78
2:F:11:LEU:HD11	2:F:152:PHE:CZ	2.20	0.77
1:E:141:LEU:HD13	2:F:187:VAL:HG21	1.66	0.77
2:D:100:ASP:O	2:D:104:LEU:HB3	1.84	0.77
2:H:102:TYR:O	2:H:104:LEU:HA	1.87	0.74
2:D:33:SER:O	2:D:99:VAL:HG12	1.88	0.73
2:F:33:SER:HB2	2:F:99:VAL:CG1	2.19	0.73
2:B:70:PHE:CD1	2:B:81:VAL:HG22	2.24	0.72
1:E:126:PRO:HG2	3:E:306:HOH:O	1.89	0.72
2:H:60:TYR:HB2	2:H:65:GLN:HG3	1.72	0.71
2:H:93:VAL:HG22	2:H:114:GLN:HG2	1.72	0.71
2:H:123:LYS:HE3	2:H:150:ASP:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:TYR:CB	2:D:104:LEU:HA	2.20	0.70
2:B:6:GLN:O	2:B:111:GLN:OE1	2.10	0.70
2:D:29:PHE:CE2	2:D:77:SER:HA	2.27	0.70
2:D:91:THR:HG23	2:D:115:VAL:HA	1.72	0.69
2:B:50:ARG:HH11	2:B:50:ARG:CG	2.01	0.69
2:D:117:VAL:HG12	2:D:120:ALA:HB3	1.73	0.69
1:A:12:THR:HG22	1:A:111:GLU:CB	2.23	0.69
1:C:36:LYS:HB3	1:C:56:TRP:CZ3	2.28	0.69
1:C:112:ILE:HG22	1:C:172:GLN:HE22	1.58	0.68
2:D:8:GLY:HA2	2:D:113:THR:HG23	1.75	0.67
1:A:130:GLN:HE21	1:A:135:THR:HG22	1.58	0.67
2:F:2:VAL:HG11	2:F:98:ARG:HH21	1.59	0.67
1:E:127:SER:O	1:E:131:LEU:HD11	1.95	0.67
1:A:0:LEU:HB3	1:A:27:GLN:HE22	1.60	0.66
2:D:212:LYS:HB3	2:F:212:LYS:HE3	1.76	0.66
1:C:19:VAL:HG11	1:C:110:LEU:CD2	2.26	0.66
2:D:104:LEU:H	2:D:104:LEU:HD22	1.60	0.66
1:C:60:ARG:HD3	1:C:64:VAL:O	1.95	0.66
2:D:56:GLY:O	2:D:58:THR:HG23	1.96	0.65
1:A:134:GLY:HA2	1:A:189:LYS:HB2	1.79	0.65
2:D:117:VAL:HG12	2:D:120:ALA:HB2	1.78	0.65
1:L:176:ASP:HB3	3:L:306:HOH:O	1.96	0.64
2:F:32:ASN:HD21	2:F:100:ASP:CG	2.06	0.64
2:B:9:VAL:HG22	2:B:114:GLN:O	1.97	0.64
2:D:8:GLY:HA3	2:D:113:THR:CG2	2.28	0.63
2:D:103:TYR:HB2	2:D:104:LEU:CA	2.25	0.63
1:C:115:THR:HG21	2:B:119:SER:HB3	1.80	0.63
2:F:123:LYS:HZ2	2:F:150:ASP:C	2.06	0.63
1:A:128:ASP:HA	1:A:131:LEU:HD12	1.79	0.63
2:B:2:VAL:HG22	2:B:27:TYR:HB3	1.80	0.63
2:D:24:ALA:HB3	2:D:77:SER:O	1.98	0.63
2:B:50:ARG:HG2	2:B:50:ARG:NH1	1.94	0.62
1:A:86:PRO:HA	1:A:112:ILE:HD12	1.81	0.62
1:E:126:PRO:HD3	1:E:138:VAL:HG22	1.82	0.62
2:H:93:VAL:HG22	2:H:114:GLN:CG	2.29	0.61
2:B:51:ILE:HG12	2:B:58:THR:HG22	1.82	0.61
2:B:182:TYR:HE1	2:H:191:PRO:HB3	1.64	0.61
2:H:103:TYR:HB2	2:H:105:GLY:H	1.66	0.61
2:H:132:PRO:HG3	2:H:144:LEU:HB3	1.81	0.61
1:C:113:ARG:HA	1:C:146:TYR:OH	2.02	0.60
1:A:112:ILE:HG22	1:A:172:GLN:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLY:HA3	2:D:113:THR:HG23	1.84	0.60
2:B:60:TYR:HB2	2:B:65:GLN:HG3	1.82	0.59
2:F:11:LEU:HD12	2:F:116:THR:HB	1.84	0.59
2:D:9:VAL:HB	2:D:113:THR:OG1	2.01	0.59
2:F:122:THR:HG22	2:F:122:THR:O	2.02	0.59
1:E:127:SER:O	1:E:131:LEU:CD1	2.51	0.58
2:F:123:LYS:HG2	2:F:124:GLY:N	2.18	0.58
2:D:30:THR:O	2:D:54:GLU:HB2	2.03	0.58
2:F:9:VAL:HG12	2:F:114:GLN:O	2.04	0.58
2:H:199:THR:HG23	2:H:216:LYS:HE2	1.85	0.58
2:B:35:ASP:HB3	2:B:50:ARG:HA	1.86	0.58
1:E:164:ASN:O	1:E:186:THR:OG1	2.22	0.57
2:H:28:ILE:HG22	2:H:30:THR:HG22	1.86	0.57
2:D:46:GLU:OE1	2:D:64:PHE:HZ	1.88	0.57
2:H:29:PHE:O	2:H:30:THR:HB	2.05	0.57
2:H:10:GLU:OE1	2:H:12:ARG:NH2	2.37	0.57
1:L:167:GLU:HA	1:L:182:SER:O	2.04	0.56
2:B:26:GLY:HA3	2:B:27:TYR:C	2.31	0.56
1:A:126:PRO:HD3	1:A:138:VAL:HG22	1.88	0.56
2:D:37:VAL:HG22	2:D:47:TRP:HA	1.86	0.56
2:H:135:LYS:O	2:H:138:SER:N	2.38	0.56
1:A:11:VAL:O	1:A:111:GLU:HB2	2.06	0.56
1:C:12:THR:HG21	1:C:111:GLU:OE1	2.01	0.56
2:B:35:ASP:OD2	2:B:99:VAL:HG22	2.05	0.56
2:D:112:GLY:CA	2:D:113:THR:HG22	2.35	0.56
2:B:27:TYR:CG	2:B:28:ILE:N	2.74	0.56
2:D:23:LYS:HA	2:D:24:ALA:HB3	1.88	0.56
2:H:103:TYR:CB	2:H:105:GLY:H	2.19	0.55
2:D:46:GLU:OE1	2:D:64:PHE:CZ	2.59	0.55
2:H:99:VAL:HG23	2:H:106:TYR:CE1	2.41	0.55
1:C:56:TRP:CZ3	2:D:103:TYR:O	2.59	0.55
1:E:66:ASP:HB3	2:B:201:ILE:HD13	1.87	0.55
2:B:17:SER:OG	2:B:83:LEU:O	2.24	0.55
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.88	0.55
1:A:122:PHE:HB2	1:A:141:LEU:HB3	1.89	0.55
1:A:163:GLY:HA2	2:H:166:THR:HG21	1.89	0.55
2:B:35:ASP:OD1	2:B:106:TYR:OH	2.20	0.55
1:E:139:VAL:HG22	1:E:184:THR:HG23	1.89	0.55
2:F:40:ALA:HB3	2:F:43:GLN:HB2	1.89	0.55
2:D:114:GLN:HE21	2:D:115:VAL:N	2.05	0.55
1:C:122:PHE:HB2	1:C:141:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:TYR:OH	2:F:50:ARG:NH2	2.40	0.54
1:L:126:PRO:HD3	1:L:138:VAL:HG22	1.90	0.54
1:A:109:ARG:HH11	1:A:109:ARG:CG	2.20	0.54
2:B:11:LEU:HD11	2:B:118:SER:HB3	1.89	0.54
2:D:100:ASP:HB3	2:D:102:TYR:O	2.07	0.54
2:D:102:TYR:O	2:D:103:TYR:CD2	2.61	0.54
2:D:23:LYS:HA	2:D:24:ALA:CB	2.37	0.54
2:H:51:ILE:HD12	2:H:58:THR:CG2	2.32	0.54
2:H:132:PRO:HD2	2:H:219:PRO:HA	1.90	0.54
2:D:94:TYR:CE1	2:D:114:GLN:HG2	2.42	0.54
2:H:9:VAL:HG22	2:H:114:GLN:HB2	1.89	0.54
1:C:126:PRO:HD3	1:C:138:VAL:HG22	1.89	0.54
2:H:30:THR:HA	2:H:53:PRO:HB2	1.90	0.54
1:E:60:ARG:NH1	2:B:199:THR:HG21	2.23	0.53
2:F:121:SER:O	2:F:123:LYS:N	2.42	0.53
2:F:29:PHE:HD2	2:F:29:PHE:O	1.92	0.53
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.91	0.53
1:A:18:LYS:HG3	1:A:82:SER:HA	1.90	0.53
2:B:47:TRP:HZ2	2:B:50:ARG:HD3	1.73	0.53
2:H:30:THR:HG23	2:H:31:MET:HG2	1.91	0.53
2:H:8:GLY:O	2:H:9:VAL:HG23	2.09	0.52
1:L:122:PHE:HB2	1:L:141:LEU:HB3	1.90	0.52
1:C:54:ILE:HG21	1:C:70:GLY:HA3	1.92	0.52
1:E:18:LYS:HG3	1:E:82:SER:HA	1.91	0.52
2:B:30:THR:HG22	2:B:31:MET:N	2.18	0.52
2:B:60:TYR:HD2	2:B:65:GLN:HG3	1.73	0.52
2:B:35:ASP:OD2	2:B:50:ARG:HD2	2.10	0.52
1:C:18:LYS:HG3	1:C:82:SER:HA	1.91	0.51
2:D:117:VAL:O	2:D:118:SER:O	2.28	0.51
1:L:18:LYS:HG3	1:L:82:SER:HA	1.92	0.51
2:B:199:THR:HG23	2:B:216:LYS:HE2	1.91	0.51
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.75	0.51
1:L:167:GLU:HB2	1:L:181:LEU:HD21	1.93	0.51
2:D:103:TYR:CB	2:D:104:LEU:CA	2.87	0.51
2:D:199:THR:HG23	2:D:216:LYS:HE2	1.93	0.51
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.73	0.51
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.46	0.50
2:B:35:ASP:HB2	2:B:49:GLY:O	2.11	0.50
2:F:104:LEU:N	2:F:104:LEU:HD22	2.27	0.50
2:H:29:PHE:HE2	2:H:74:THR:HA	1.76	0.50
2:H:36:TRP:CE2	2:H:81:VAL:HG23	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:HG2	1:A:115:THR:N	2.26	0.50
1:C:151:LYS:HB3	1:C:203:THR:HB	1.94	0.50
2:F:125:PRO:HB3	2:F:151:TYR:CB	2.32	0.50
1:L:84:PHE:CE2	1:L:112:ILE:HG13	2.46	0.50
1:A:46:LEU:HD11	3:A:307:HOH:O	2.12	0.49
1:E:124:PHE:HB2	1:E:139:VAL:O	2.12	0.49
2:B:60:TYR:CD2	2:B:65:GLN:HG3	2.47	0.49
2:B:30:THR:HG21	2:B:54:GLU:N	2.27	0.49
1:A:2:ILE:HG12	1:A:27:GLN:HB2	1.93	0.49
2:B:36:TRP:CZ3	2:B:96:CYS:HB2	2.47	0.49
2:H:9:VAL:HG13	2:H:114:GLN:O	2.11	0.49
1:L:128:ASP:HA	1:L:131:LEU:HD12	1.94	0.49
2:D:33:SER:HA	2:D:52:ASP:HA	1.95	0.49
2:H:102:TYR:O	2:H:103:TYR:HB2	2.13	0.49
1:E:124:PHE:O	1:E:138:VAL:HG13	2.13	0.49
2:H:51:ILE:CD1	2:H:58:THR:HG22	2.34	0.49
1:L:151:LYS:HB3	1:L:203:THR:HB	1.94	0.49
1:C:112:ILE:HG22	1:C:172:GLN:NE2	2.25	0.49
1:E:38:TYR:CD2	2:F:104:LEU:HD23	2.48	0.49
1:E:151:LYS:HB3	1:E:203:THR:HB	1.95	0.48
1:C:19:VAL:HG11	1:C:110:LEU:HD23	1.95	0.48
2:B:177:GLN:NE2	2:B:183:SER:HB2	2.28	0.48
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.95	0.48
2:D:212:LYS:HB3	2:F:212:LYS:CE	2.42	0.48
2:H:70:PHE:CD1	2:H:81:VAL:HG22	2.48	0.48
2:B:35:ASP:OD2	2:B:99:VAL:CG2	2.61	0.48
2:D:117:VAL:CG1	2:D:120:ALA:HB2	2.44	0.48
1:A:151:LYS:HB3	1:A:203:THR:HB	1.94	0.48
2:F:122:THR:HG23	2:F:153:PRO:HD3	1.96	0.47
2:D:8:GLY:HA3	2:D:113:THR:HG21	1.96	0.47
2:F:11:LEU:CD1	2:F:152:PHE:CZ	2.95	0.47
2:H:33:SER:HA	2:H:53:PRO:HD3	1.96	0.47
1:A:56:TRP:HB2	1:A:59:ILE:HG12	1.96	0.47
2:H:32:ASN:HD22	2:H:98:ARG:NH2	2.12	0.47
1:C:1:ASP:OD1	1:C:101:PRO:HD2	2.15	0.47
2:B:7:PRO:O	2:B:113:THR:OG1	2.28	0.47
2:D:117:VAL:CG1	2:D:120:ALA:CB	2.88	0.47
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.80	0.46
1:C:92:TYR:CD2	1:C:110:LEU:HD13	2.51	0.46
2:B:36:TRP:O	2:B:48:MET:HB2	2.15	0.46
2:D:114:GLN:NE2	2:D:116:THR:HG22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLY:CA	2:D:113:THR:CG2	2.87	0.46
2:H:39:GLN:HG3	2:H:45:LEU:HG	1.96	0.46
1:A:12:THR:CG2	1:A:111:GLU:CB	2.93	0.46
1:E:213:LYS:HD3	3:E:310:HOH:O	2.16	0.46
2:B:33:SER:HA	2:B:53:PRO:HD3	1.98	0.46
2:D:100:ASP:O	2:D:104:LEU:CB	2.60	0.46
1:C:102:TYR:OH	2:D:50:ARG:NH2	2.49	0.46
2:D:6:GLN:CG	2:D:111:GLN:H	2.29	0.46
2:D:60:TYR:CE1	2:D:70:PHE:CD2	3.04	0.46
2:F:177:GLN:NE2	2:F:183:SER:HB2	2.31	0.46
2:H:9:VAL:CG2	2:H:114:GLN:HB2	2.46	0.46
1:C:130:GLN:HG3	2:D:128:PHE:CE2	2.51	0.45
2:D:60:TYR:HB2	2:D:65:GLN:HE21	1.81	0.45
1:C:19:VAL:HG11	1:C:110:LEU:HD21	1.98	0.45
2:H:9:VAL:HG22	2:H:114:GLN:H	1.81	0.45
2:F:119:SER:C	2:F:120:ALA:O	2.53	0.45
1:C:102:TYR:OH	2:D:104:LEU:HD23	2.17	0.45
2:D:29:PHE:O	2:D:29:PHE:CD2	2.70	0.45
2:H:35:ASP:OD1	2:H:35:ASP:N	2.49	0.45
2:B:91:THR:HG23	2:B:116:THR:HA	1.98	0.45
2:D:35:ASP:CB	2:D:49:GLY:O	2.65	0.45
2:H:28:ILE:HG22	2:H:30:THR:CG2	2.47	0.45
1:C:40:ALA:HA	1:C:54:ILE:O	2.17	0.45
1:C:38:TYR:N	1:C:38:TYR:CD1	2.85	0.44
1:L:19:VAL:HG11	1:L:110:LEU:CD2	2.34	0.44
2:D:61:ALA:HB3	2:D:64:PHE:HD1	1.82	0.44
2:F:97:ALA:HB1	2:F:106:TYR:HB3	1.99	0.44
1:A:54:ILE:HG21	1:A:70:GLY:HA3	1.99	0.44
1:A:130:GLN:HE21	1:A:135:THR:CG2	2.30	0.44
2:D:114:GLN:HE21	2:D:115:VAL:C	2.25	0.44
1:A:111:GLU:OE2	1:A:111:GLU:HA	2.17	0.44
1:C:209:SER:HB3	1:L:113:ARG:CD	2.47	0.44
1:E:123:ILE:O	1:E:124:PHE:CG	2.70	0.44
2:B:30:THR:HG21	2:B:54:GLU:CA	2.47	0.44
2:F:103:TYR:O	2:F:103:TYR:CD1	2.70	0.44
1:E:0:LEU:HD13	1:E:27:GLN:NE2	2.32	0.44
1:L:56:TRP:CZ2	2:H:102:TYR:HB3	2.52	0.44
1:E:56:TRP:HB2	1:E:59:ILE:HG12	1.99	0.44
1:L:54:ILE:HG21	1:L:70:GLY:HA3	2.00	0.44
2:F:29:PHE:HE2	2:F:74:THR:HA	1.83	0.44
1:E:87:GLU:H	1:E:87:GLU:HG2	1.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:ILE:HG21	1:E:70:GLY:HA3	2.00	0.44
2:F:50:ARG:HG2	2:F:51:ILE:N	2.32	0.44
1:A:169:VAL:HG23	2:H:198:GLN:HE22	1.83	0.43
2:F:199:THR:HG23	2:F:216:LYS:HE2	1.99	0.43
2:D:123:LYS:HE3	2:D:181:LEU:HD22	2.00	0.43
1:C:97:GLY:O	2:D:104:LEU:CD2	2.66	0.43
2:B:2:VAL:CG2	2:B:27:TYR:HB3	2.48	0.43
2:B:36:TRP:CH2	2:B:96:CYS:HB2	2.53	0.43
2:D:36:TRP:HD1	2:D:70:PHE:HE1	1.66	0.43
2:H:29:PHE:O	2:H:29:PHE:CD2	2.71	0.43
1:A:87:GLU:H	1:A:87:GLU:HG2	1.47	0.43
1:E:121:VAL:HG12	1:E:213:LYS:HG3	1.99	0.43
2:D:29:PHE:O	2:D:30:THR:HG23	2.19	0.43
2:F:19:LYS:HA	2:F:81:VAL:O	2.19	0.43
1:A:0:LEU:HB3	1:A:27:GLN:NE2	2.31	0.43
1:L:56:TRP:HB2	1:L:59:ILE:HG12	2.00	0.43
2:F:30:THR:CB	2:F:31:MET:CB	2.67	0.43
2:F:50:ARG:HG2	2:F:51:ILE:H	1.83	0.43
2:D:112:GLY:HA3	2:D:113:THR:HG22	1.99	0.43
1:C:56:TRP:HD1	1:C:59:ILE:HD12	1.84	0.42
2:B:30:THR:HG21	2:B:54:GLU:HA	2.00	0.42
2:F:121:SER:O	2:F:123:LYS:HB3	2.19	0.42
1:E:131:LEU:C	1:E:133:SER:N	2.77	0.42
2:B:63:LYS:HB2	2:B:63:LYS:HE3	1.73	0.42
2:H:71:THR:OG1	2:H:80:TYR:HB2	2.20	0.42
2:B:4:LEU:HD11	2:B:98:ARG:HB2	2.02	0.42
2:D:10:GLU:HG2	3:D:313:HOH:O	2.19	0.42
1:C:84:PHE:CE2	1:C:112:ILE:HG13	2.55	0.42
2:B:19:LYS:HD2	2:B:80:TYR:CD2	2.55	0.42
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.55	0.42
1:C:169:VAL:HG22	1:C:181:LEU:HD12	2.01	0.42
1:E:141:LEU:HD22	2:F:187:VAL:HG11	2.02	0.42
1:L:191:ASP:HA	1:L:194:LYS:HD2	2.02	0.42
2:D:176:LEU:HD13	2:D:182:TYR:CZ	2.55	0.42
1:L:102:TYR:HB2	2:H:47:TRP:CG	2.54	0.41
2:D:55:ASP:O	2:D:57:GLY:N	2.52	0.41
2:H:7:PRO:HD2	2:H:21:SER:O	2.20	0.41
1:L:0:LEU:N	1:L:0:LEU:CD2	2.83	0.41
1:E:185:LEU:HG	1:E:186:THR:N	2.34	0.41
2:D:33:SER:O	2:D:99:VAL:CG1	2.64	0.41
1:E:38:TYR:CE2	2:F:104:LEU:HD23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:PHE:HE2	1:E:141:LEU:HD23	1.85	0.41
2:D:36:TRP:HA	2:D:95:TYR:O	2.21	0.41
1:A:191:ASP:HA	1:A:194:LYS:HD2	2.03	0.41
1:C:102:TYR:HB2	2:D:47:TRP:CG	2.55	0.41
1:A:0:LEU:HD13	1:A:27:GLN:HE22	1.86	0.41
1:C:15:ALA:O	2:B:15:GLY:CA	2.51	0.41
2:D:132:PRO:HD2	2:D:219:PRO:HA	2.03	0.41
2:F:103:TYR:O	2:F:105:GLY:N	2.53	0.41
1:C:87:GLU:H	1:C:87:GLU:HG2	1.47	0.41
2:D:35:ASP:HB2	2:D:49:GLY:O	2.21	0.40
2:B:100:ASP:HB2	2:B:107:ASP:OD1	2.20	0.40
2:B:105:GLY:HA3	2:B:106:TYR:CD1	2.57	0.40
2:B:132:PRO:HD2	2:B:219:PRO:HA	2.03	0.40
1:E:19:VAL:HG11	1:E:110:LEU:HD11	2.03	0.40
1:E:128:ASP:HA	1:E:131:LEU:CD1	2.51	0.40
1:L:87:GLU:H	1:L:87:GLU:HG2	1.46	0.40
2:H:94:TYR:CD1	2:H:115:VAL:HG23	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/221 (98%)	201 (93%)	15 (7%)	1 (0%)	24	56
1	C	217/221 (98%)	205 (94%)	9 (4%)	3 (1%)	9	34
1	E	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	24	56
1	L	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	9	34
2	B	209/219 (95%)	190 (91%)	14 (7%)	5 (2%)	4	25
2	D	209/219 (95%)	177 (85%)	20 (10%)	12 (6%)	1	9
2	F	209/219 (95%)	186 (89%)	18 (9%)	5 (2%)	4	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	213/219 (97%)	185 (87%)	18 (8%)	10 (5%)	2	13
All	All	1712/1760 (97%)	1551 (91%)	121 (7%)	40 (2%)	5	26

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	E	219	GLU
1	L	219	GLU
2	D	24	ALA
2	D	56	GLY
2	D	103	TYR
2	D	114	GLN
2	D	118	SER
2	F	56	GLY
2	F	122	THR
2	H	30	THR
2	H	56	GLY
2	H	98	ARG
2	H	99	VAL
2	B	56	GLY
2	D	57	GLY
2	H	8	GLY
2	H	54	GLU
2	H	139	GLY
1	L	144	ASN
2	B	62	GLN
2	D	27	TYR
2	D	30	THR
2	D	120	ALA
2	D	150	ASP
1	C	144	ASN
2	B	27	TYR
2	F	102	TYR
2	H	103	TYR
1	C	74	ALA
1	L	15	ALA
2	B	9	VAL
2	B	150	ASP
2	F	104	LEU
2	H	91	THR
1	C	57	ALA

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Mol	Chain	Res	Type
2	D	28	ILE
2	D	113	THR
2	F	62	GLN
2	H	101	ASP

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	193/195 (99%)	177 (92%)	16 (8%)	10	35
1	C	193/195 (99%)	175 (91%)	18 (9%)	8	31
1	E	194/195 (100%)	169 (87%)	25 (13%)	4	18
1	L	195/195 (100%)	177 (91%)	18 (9%)	8	31
2	B	179/185 (97%)	147 (82%)	32 (18%)	2	8
2	D	180/185 (97%)	140 (78%)	40 (22%)	1	5
2	F	180/185 (97%)	152 (84%)	28 (16%)	2	12
2	H	182/185 (98%)	150 (82%)	32 (18%)	2	9
All	All	1496/1520 (98%)	1287 (86%)	209 (14%)	3	15

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	20	THR
1	A	32	SER
1	A	35	GLN
1	A	39	LEU
1	A	53	LEU
1	A	56	TRP
1	A	61	GLU
1	A	87	GLU
1	A	91	VAL
1	A	99	SER

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Mol	Chain	Res	Type
1	A	109	ARG
1	A	112	ILE
1	A	114	ARG
1	A	182	SER
1	A	197	VAL
1	C	0	LEU
1	C	20	THR
1	C	32	SER
1	C	35	GLN
1	C	39	LEU
1	C	51	ARG
1	C	56	TRP
1	C	61	GLU
1	C	66	ASP
1	C	67	ARG
1	C	73	SER
1	C	87	GLU
1	C	91	VAL
1	C	99	SER
1	C	111	GLU
1	C	112	ILE
1	C	169	VAL
1	C	182	SER
1	E	1	ASP
1	E	20	THR
1	E	32	SER
1	E	35	GLN
1	E	39	LEU
1	E	53	LEU
1	E	56	TRP
1	E	61	GLU
1	E	66	ASP
1	E	87	GLU
1	E	91	VAL
1	E	99	SER
1	E	109	ARG
1	E	112	ILE
1	E	120	SER
1	E	125	PRO
1	E	127	SER
1	E	141	LEU
1	E	167	GLU

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Mol	Chain	Res	Type
1	E	182	SER
1	E	186	THR
1	E	187	LEU
1	E	217	ARG
1	E	219	GLU
1	E	220	CYS
1	L	0	LEU
1	L	20	THR
1	L	32	SER
1	L	35	GLN
1	L	39	LEU
1	L	53	LEU
1	L	56	TRP
1	L	61	GLU
1	L	87	GLU
1	L	91	VAL
1	L	99	SER
1	L	110	LEU
1	L	112	ILE
1	L	113	ARG
1	L	167	GLU
1	L	182	SER
1	L	185	LEU
1	L	219	GLU
2	B	6	GLN
2	B	9	VAL
2	B	10	GLU
2	B	11	LEU
2	B	23	LYS
2	B	27	TYR
2	B	28	ILE
2	B	48	MET
2	B	50	ARG
2	B	51	ILE
2	B	54	GLU
2	B	59	LYS
2	B	62	GLN
2	B	63	LYS
2	B	65	GLN
2	B	68	VAL
2	B	71	THR
2	B	73	ASP

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Mol	Chain	Res	Type
2	B	74	THR
2	B	87	ARG
2	B	99	VAL
2	B	101	ASP
2	B	102	TYR
2	B	103	TYR
2	B	104	LEU
2	B	107	ASP
2	B	111	GLN
2	B	114	GLN
2	B	144	LEU
2	B	185	SER
2	B	197	THR
2	B	201	ILE
2	D	3	GLN
2	D	9	VAL
2	D	11	LEU
2	D	21	SER
2	D	23	LYS
2	D	29	PHE
2	D	30	THR
2	D	33	SER
2	D	35	ASP
2	D	37	VAL
2	D	38	ARG
2	D	39	GLN
2	D	46	GLU
2	D	52	ASP
2	D	59	LYS
2	D	62	GLN
2	D	65	GLN
2	D	68	VAL
2	D	71	THR
2	D	74	THR
2	D	82	GLU
2	D	87	ARG
2	D	88	SER
2	D	89	GLU
2	D	93	VAL
2	D	100	ASP
2	D	101	ASP
2	D	102	TYR

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Mol	Chain	Res	Type
2	D	104	LEU
2	D	113	THR
2	D	114	GLN
2	D	116	THR
2	D	119	SER
2	D	123	LYS
2	D	144	LEU
2	D	159	SER
2	D	185	SER
2	D	189	THR
2	D	197	THR
2	D	201	ILE
2	F	10	GLU
2	F	11	LEU
2	F	23	LYS
2	F	28	ILE
2	F	29	PHE
2	F	30	THR
2	F	31	MET
2	F	32	ASN
2	F	35	ASP
2	F	51	ILE
2	F	52	ASP
2	F	59	LYS
2	F	62	GLN
2	F	65	GLN
2	F	74	THR
2	F	81	VAL
2	F	87	ARG
2	F	89	GLU
2	F	99	VAL
2	F	102	TYR
2	F	104	LEU
2	F	111	GLN
2	F	119	SER
2	F	123	LYS
2	F	144	LEU
2	F	185	SER
2	F	189	THR
2	F	197	THR
2	H	10	GLU
2	H	11	LEU

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Mol	Chain	Res	Type
2	H	25	SER
2	H	29	PHE
2	H	33	SER
2	H	35	ASP
2	H	39	GLN
2	H	50	ARG
2	H	51	ILE
2	H	54	GLU
2	H	55	ASP
2	H	59	LYS
2	H	62	GLN
2	H	65	GLN
2	H	68	VAL
2	H	74	THR
2	H	82	GLU
2	H	87	ARG
2	H	99	VAL
2	H	100	ASP
2	H	101	ASP
2	H	107	ASP
2	H	119	SER
2	H	121	SER
2	H	122	THR
2	H	138	SER
2	H	141	THR
2	H	144	LEU
2	H	185	SER
2	H	189	THR
2	H	197	THR
2	H	201	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	35	GLN
1	A	83	ASN
1	A	195	HIS
1	A	205	GLN
1	A	216	ASN
1	C	83	ASN
1	C	143	ASN

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Mol	Chain	Res	Type
1	C	172	GLN
1	C	195	HIS
1	C	205	GLN
1	E	27	GLN
1	E	83	ASN
1	E	130	GLN
1	L	83	ASN
1	L	143	ASN
1	L	195	HIS
2	B	32	ASN
2	B	65	GLN
2	B	84	ASN
2	B	111	GLN
2	D	3	GLN
2	D	62	GLN
2	D	65	GLN
2	D	84	ASN
2	D	114	GLN
2	D	170	HIS
2	F	32	ASN
2	F	62	GLN
2	F	65	GLN
2	F	111	GLN
2	F	114	GLN
2	H	62	GLN
2	H	170	HIS
2	H	198	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	219/221 (99%)	0.87	13 (5%)	28	19	20, 46, 67, 82	3 (1%)
1	C	219/221 (99%)	0.93	18 (8%)	17	13	21, 42, 69, 85	3 (1%)
1	E	221/221 (100%)	1.01	25 (11%)	10	9	19, 46, 73, 125	3 (1%)
1	L	221/221 (100%)	0.66	8 (3%)	46	31	14, 38, 59, 120	3 (1%)
2	B	213/219 (97%)	0.81	14 (6%)	24	16	21, 44, 65, 79	0
2	D	213/219 (97%)	0.93	18 (8%)	16	13	21, 45, 68, 85	0
2	F	213/219 (97%)	1.02	21 (9%)	13	11	23, 48, 70, 84	0
2	H	217/219 (99%)	0.76	10 (4%)	37	25	17, 42, 66, 75	0
All	All	1736/1760 (98%)	0.87	127 (7%)	21	15	14, 44, 67, 125	12 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	10	GLU	5.9
1	L	220	CYS	4.5
1	E	220	CYS	4.1
2	B	28	ILE	4.0
1	L	148	ARG	4.0
1	C	86	PRO	3.9
2	B	83	LEU	3.8
1	C	33	SER	3.6
2	D	114	GLN	3.6
2	H	101	ASP	3.4
1	E	82	SER	3.3
2	F	28	ILE	3.3
1	E	149	GLU	3.3
2	B	133	SER	3.2
2	F	84	ASN	3.2
1	C	148	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	35	GLN	3.2
1	C	149	GLU	3.1
2	D	133	SER	3.1
2	D	46	GLU	3.1
1	A	218	GLY	3.1
1	E	66	ASP	3.0
1	E	135	THR	3.0
1	C	105	GLY	3.0
2	F	83	LEU	2.9
1	A	33	SER	2.9
2	F	133	SER	2.9
1	L	219	GLU	2.9
1	E	103	SER	2.9
1	A	163	GLY	2.8
2	D	117	VAL	2.8
2	D	55	ASP	2.8
2	F	51	ILE	2.8
1	C	17	ASP	2.7
1	E	148	ARG	2.7
1	E	0	LEU	2.7
2	B	195	LEU	2.7
2	H	198	GLN	2.7
2	F	215	LYS	2.7
2	D	119	SER	2.7
2	F	185	SER	2.7
1	C	87	GLU	2.6
1	E	20	THR	2.6
1	C	9	THR	2.6
2	H	33	SER	2.6
1	E	171	GLU	2.6
2	B	1	GLU	2.6
2	H	62	GLN	2.6
1	E	201	GLU	2.5
2	F	11	LEU	2.5
2	H	23	LYS	2.5
2	F	41	PRO	2.5
2	D	195	LEU	2.5
2	F	141	THR	2.5
1	C	14	SER	2.5
2	D	101	ASP	2.5
1	E	94	CYS	2.4
1	C	158	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	75	THR	2.4
2	B	197	THR	2.4
2	H	210	ASN	2.4
2	F	15	GLY	2.4
2	B	54	GLU	2.4
2	F	207	LYS	2.4
1	A	149	GLU	2.4
1	C	171	GLU	2.4
1	C	25	SER	2.4
1	E	35	GLN	2.3
2	F	12	ARG	2.3
2	F	140	GLY	2.3
1	E	16	GLY	2.3
2	D	186	SER	2.3
2	D	103	TYR	2.3
1	C	193	GLU	2.3
1	E	160	LEU	2.3
2	B	29	PHE	2.3
1	A	6	GLN	2.3
1	E	19	VAL	2.3
1	C	163	GLY	2.3
2	H	112	GLY	2.3
1	L	66	ASP	2.3
2	F	90	ASP	2.3
1	E	133	SER	2.2
1	A	19	VAL	2.2
2	F	2	VAL	2.2
1	L	189	LYS	2.2
2	F	102	TYR	2.2
1	E	209	SER	2.2
2	F	29	PHE	2.2
1	C	7	THR	2.2
2	D	84	ASN	2.2
1	A	160	LEU	2.2
2	B	104	LEU	2.2
1	A	13	ALA	2.2
2	B	202	CYS	2.2
1	L	176	ASP	2.2
1	A	130	GLN	2.2
2	D	178	SER	2.2
1	E	205	GLN	2.1
2	B	59	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	118	SER	2.1
1	A	164	ASN	2.1
1	C	3	VAL	2.1
1	E	46	LEU	2.1
2	B	196	GLY	2.1
2	F	85	SER	2.1
2	D	215	LYS	2.1
2	H	74	THR	2.1
1	E	85	GLN	2.1
2	D	112	GLY	2.1
1	A	120	SER	2.1
1	E	162	SER	2.1
1	C	83	ASN	2.1
1	E	22	ASN	2.1
2	D	210	ASN	2.1
1	C	19	VAL	2.1
2	H	103	TYR	2.1
2	D	219	PRO	2.1
2	B	27	TYR	2.1
2	D	163	GLY	2.1
2	B	218	GLU	2.1
2	F	55	ASP	2.0
1	L	32	SER	2.0
2	H	28	ILE	2.0
1	E	161	GLN	2.0
1	A	193	GLU	2.0
1	L	187	LEU	2.0

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

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.