



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 04:30 PM EDT

PDB ID : 3PNW
Title : Crystal Structure of the tudor domain of human TDRD3 in complex with an anti-TDRD3 FAB
Authors : Loppnau, P.; Tempel, W.; Wernimont, A.K.; Lam, R.; Ravichandran, M.; Adams-Cioaba, M.A.; Persson, H.; Sidhu, S.S.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Cossar, D.; Structural Genomics Consortium (SGC)
Deposited on : unknown
Resolution : 2.05 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

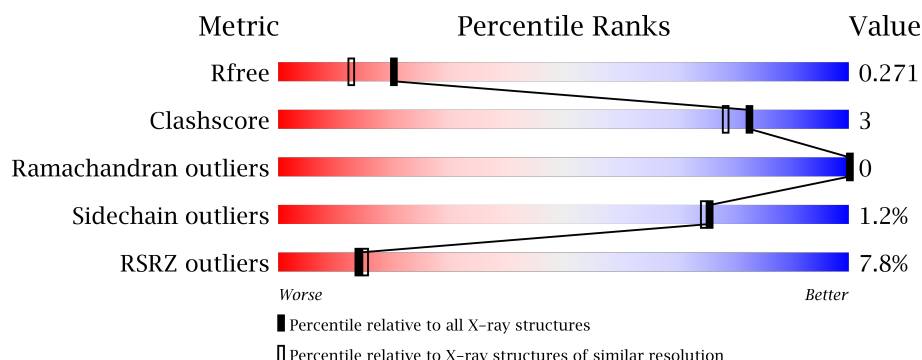
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	228	<div> <div>5%</div> <div>82%</div> <div>10%</div> <div>7%</div> </div>
1	D	228	<div> <div>13%</div> <div>87%</div> <div>7%</div> <div>7%</div> </div>
1	G	228	<div> <div>7%</div> <div>89%</div> <div>7%</div> <div>7%</div> </div>
1	J	228	<div> <div>8%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	M	228	<div> <div>5%</div> <div>80%</div> <div>14%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	228	
1	S	228	
1	V	228	
2	B	246	
2	E	246	
2	H	246	
2	K	246	
2	N	246	
2	Q	246	
2	T	246	
2	W	246	
3	C	77	
3	F	77	
3	I	77	
3	L	77	
3	O	77	
3	R	77	
3	U	77	
3	X	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	B	1872	-	-	-	X
4	UNX	B	1875	-	-	-	X
4	UNX	B	1889	-	-	-	X
4	UNX	B	1906	-	-	-	X
4	UNX	B	1946	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	E	1814	-	-	X	-
4	UNX	G	1820	-	-	X	-
4	UNX	G	1824	-	-	-	X
4	UNX	G	1885	-	-	-	X
4	UNX	H	1887	-	-	-	X
4	UNX	J	1821	-	-	-	X
4	UNX	J	1866	-	-	-	X
4	UNX	J	1867	-	-	-	X
4	UNX	M	1852	-	-	-	X
4	UNX	N	1822	-	-	-	X
4	UNX	P	1832	-	-	-	X
4	UNX	P	1886	-	-	-	X
4	UNX	Q	1835	-	-	-	X
4	UNX	T	1865	-	-	-	X
4	UNX	T	1890	-	-	-	X
4	UNX	V	1971	-	-	-	X
4	UNX	W	1857	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31176 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 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	4	0
			1639	1045	269	320	5			
1	D	213	Total	C	N	O	S	0	2	0
			1619	1028	267	319	5			
1	G	213	Total	C	N	O	S	0	4	0
			1639	1039	271	324	5			
1	J	213	Total	C	N	O	S	0	2	0
			1632	1033	269	325	5			
1	M	214	Total	C	N	O	S	0	4	0
			1648	1049	272	322	5			
1	P	213	Total	C	N	O	S	0	4	0
			1645	1042	271	327	5			
1	S	214	Total	C	N	O	S	0	3	0
			1633	1041	266	321	5			
1	V	212	Total	C	N	O	S	0	1	0
			1602	1021	259	317	5			

- Molecule 2 is a protein called FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1650	1040	275	328	7			
2	E	226	Total	C	N	O	S	0	2	0
			1676	1057	281	331	7			
2	H	218	Total	C	N	O	S	0	3	0
			1624	1029	267	319	9			
2	K	218	Total	C	N	O	S	0	0	0
			1610	1020	267	316	7			
2	N	226	Total	C	N	O	S	0	2	0
			1663	1048	278	330	7			
2	Q	218	Total	C	N	O	S	0	2	0
			1618	1026	268	317	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	225	Total	C	N	O	S	0	2	0
			1654	1047	273	327	7			
2	W	220	Total	C	N	O	S	0	1	0
			1624	1029	267	321	7			

- Molecule 3 is a protein called Tudor domain-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	60	Total	C	N	O	S	0	0	0
			482	316	71	92	3			
3	F	53	Total	C	N	O	S	0	1	0
			434	285	64	83	2			
3	I	55	Total	C	N	O	S	0	0	0
			436	286	64	84	2			
3	L	54	Total	C	N	O	S	0	0	0
			423	275	63	83	2			
3	O	61	Total	C	N	O	S	0	1	0
			482	315	70	95	2			
3	R	61	Total	C	N	O	S	0	1	0
			488	321	70	93	4			
3	U	54	Total	C	N	O	S	0	0	0
			433	284	66	81	2			
3	X	53	Total	C	N	O	S	0	1	0
			404	266	61	75	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
F	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
I	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
L	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
O	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
R	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
U	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2
X	539	GLY	-	EXPRESSION TAG	UNP Q9H7E2

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	11	Total	X	0	0
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	9	Total X 9 9	0	0
4	J	7	Total X 7 7	0	0
4	Q	8	Total X 8 8	0	0
4	D	5	Total X 5 5	0	0
4	K	6	Total X 6 6	0	0
4	E	11	Total X 11 11	0	0
4	H	16	Total X 16 16	0	0
4	B	12	Total X 12 12	0	0
4	I	1	Total X 1 1	0	0
4	C	2	Total X 2 2	0	0
4	V	7	Total X 7 7	0	0
4	W	10	Total X 10 10	0	0
4	A	7	Total X 7 7	0	0
4	T	12	Total X 12 12	0	0
4	N	12	Total X 12 12	0	0
4	R	1	Total X 1 1	0	0
4	S	2	Total X 2 2	0	0
4	F	1	Total X 1 1	0	0
4	M	3	Total X 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	69	Total O 69 69	0	0
5	B	111	Total O 111 111	0	0
5	C	13	Total O 13 13	0	0
5	D	51	Total O 51 51	0	0
5	E	107	Total O 107 107	0	0
5	F	2	Total O 2 2	0	0
5	G	52	Total O 52 52	0	0
5	H	82	Total O 82 82	0	0
5	I	8	Total O 8 8	0	0
5	J	60	Total O 60 60	0	0
5	K	89	Total O 89 89	0	0
5	L	2	Total O 2 2	0	0
5	M	55	Total O 55 55	0	0
5	N	104	Total O 104 104	0	0
5	O	7	Total O 7 7	0	0
5	P	60	Total O 60 60	0	0
5	Q	106	Total O 106 106	0	0
5	R	14	Total O 14 14	0	0
5	S	45	Total O 45 45	0	0
5	T	108	Total O 108 108	0	0
5	U	6	Total O 6 6	0	0
5	V	42	Total O 42 42	0	0

Continued on next page...

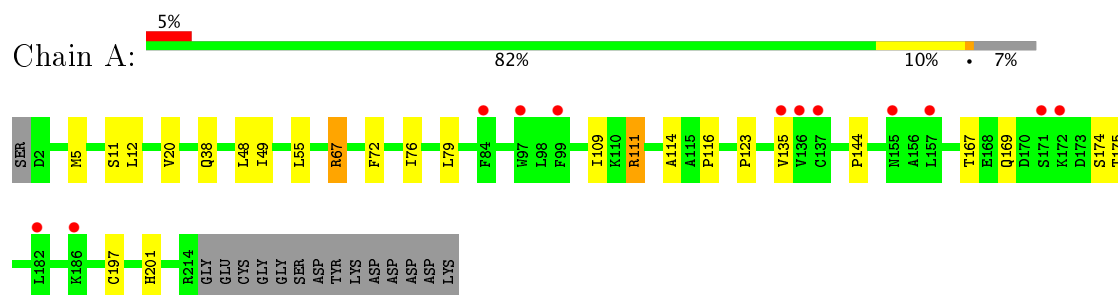
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	W	81	Total	O	0	0
			81	81		
5	X	1	Total	O	0	0
			1	1		

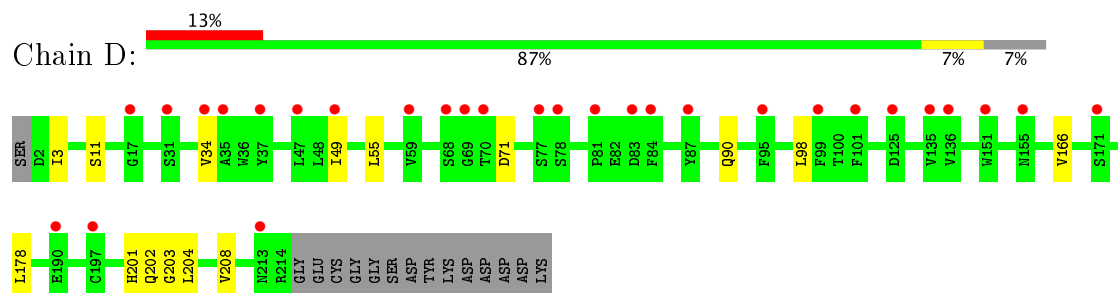
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

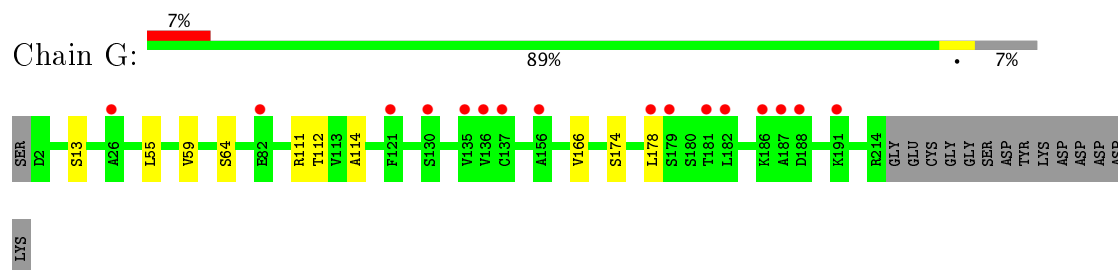
- Molecule 1: FAB light chain



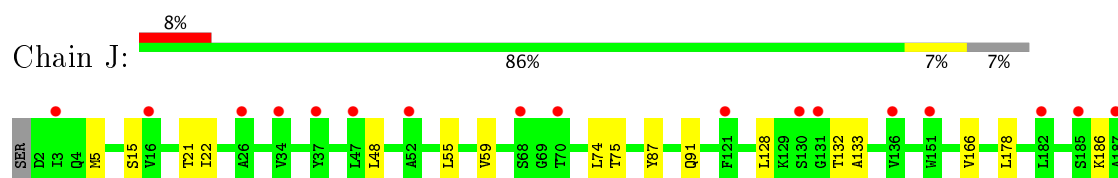
- Molecule 1: FAB light chain

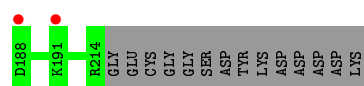


- Molecule 1: FAB light chain

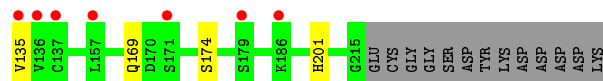
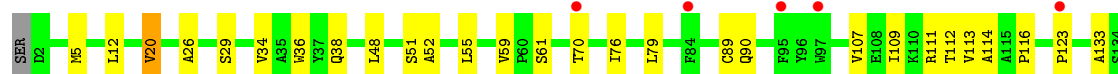
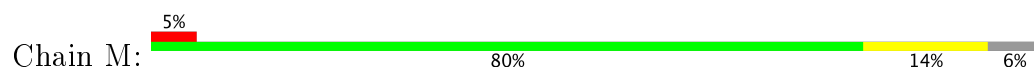


- Molecule 1: FAB light chain

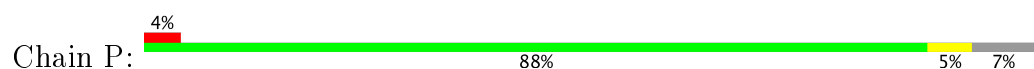




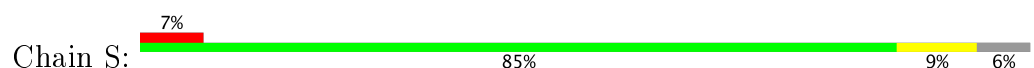
- Molecule 1: FAB light chain



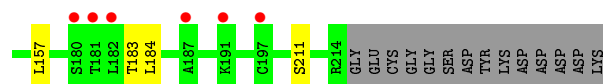
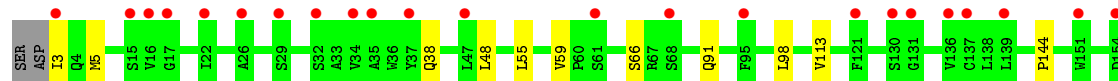
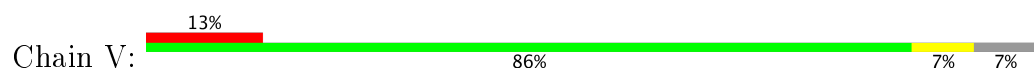
- Molecule 1: FAB light chain



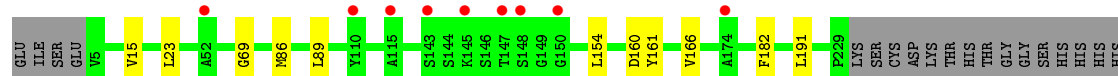
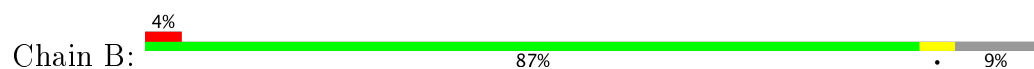
- Molecule 1: FAB light chain



- Molecule 1: FAB light chain

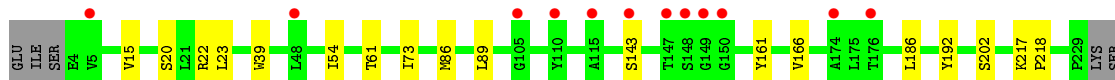
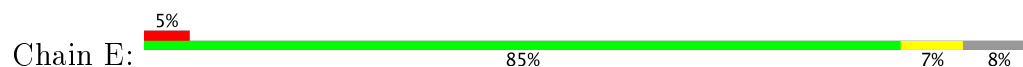


- Molecule 2: FAB heavy chain

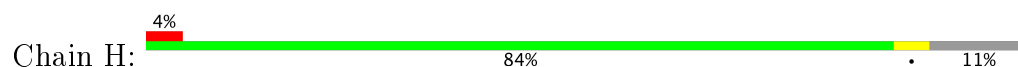


HIS
HIS

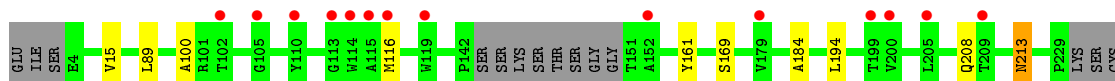
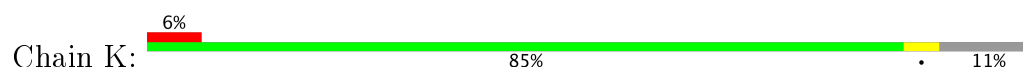
● Molecule 2: FAB heavy chain

CYS
ASP
LYS
THR
HIS
THR
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS

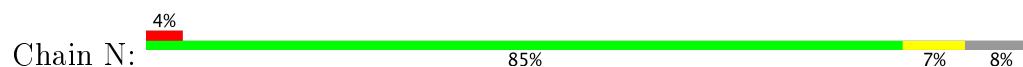
● Molecule 2: FAB heavy chain

HIS
HIS
HIS

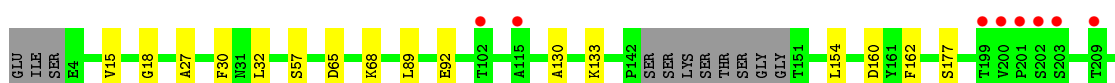
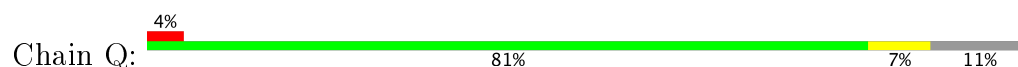
● Molecule 2: FAB heavy chain

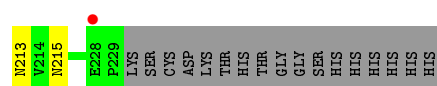
ASP
LYS
THR
HIS
THR
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS

● Molecule 2: FAB heavy chain

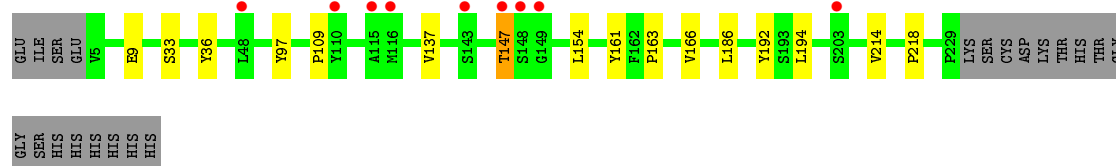
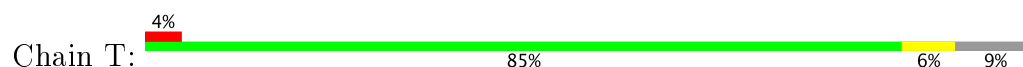
THR
HIS
THR
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS

● Molecule 2: FAB heavy chain

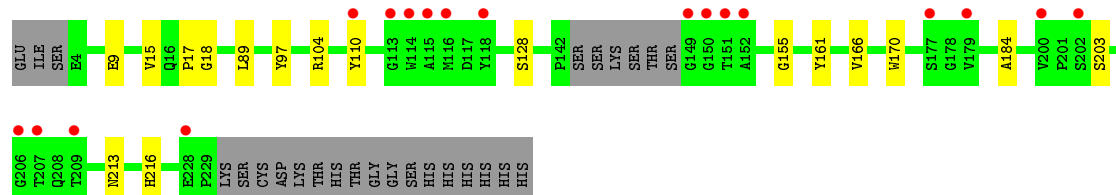
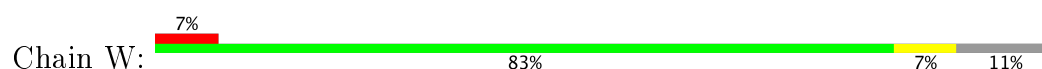




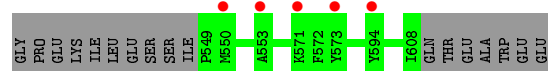
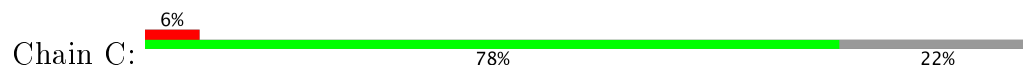
• Molecule 2: FAB heavy chain



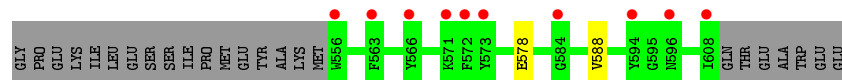
• Molecule 2: FAB heavy chain



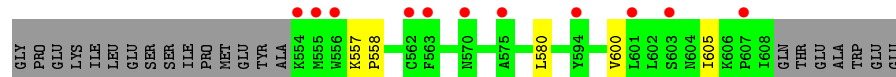
• Molecule 3: Tudor domain-containing protein 3



• Molecule 3: Tudor domain-containing protein 3

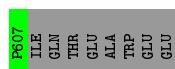


• Molecule 3: Tudor domain-containing protein 3



• Molecule 3: Tudor domain-containing protein 3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.71Å 93.73Å 159.93Å 80.96° 82.82° 90.06°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.05) 92.6 (30.00-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.264 0.231 , 0.271	Depositor DCC
R_{free} test set	2162 reflections (0.82%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31176	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.12 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.1425e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

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	0.63	0/1690	0.61	0/2305
1	D	0.63	0/1667	0.61	0/2274
1	G	0.63	0/1693	0.60	0/2307
1	J	0.59	0/1679	0.60	0/2288
1	M	0.63	0/1702	0.61	0/2320
1	P	0.62	0/1698	0.61	0/2315
1	S	0.61	0/1684	0.57	0/2297
1	V	0.62	0/1646	0.60	0/2246
2	B	0.73	0/1692	0.69	0/2312
2	E	0.72	0/1724	0.66	0/2352
2	H	0.74	0/1674	0.70	0/2286
2	K	0.67	0/1651	0.66	0/2256
2	N	0.75	0/1711	0.68	0/2338
2	Q	0.75	0/1665	0.70	0/2275
2	T	0.71	0/1702	0.66	0/2326
2	W	0.76	0/1668	0.66	0/2278
3	C	0.62	0/497	0.56	0/675
3	F	0.56	0/450	0.50	0/612
3	I	0.61	0/449	0.55	0/612
3	L	0.52	0/435	0.49	0/594
3	O	0.59	0/500	0.51	0/683
3	R	0.61	0/506	0.54	0/689
3	U	0.55	0/446	0.51	0/607
3	X	0.61	0/419	0.53	0/573
All	All	0.67	0/30648	0.63	0/41820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1639	0	1543	17	0
1	D	1619	0	1509	6	0
1	G	1639	0	1559	7	0
1	J	1632	0	1551	11	0
1	M	1648	0	1574	20	0
1	P	1645	0	1559	7	0
1	S	1633	0	1534	13	0
1	V	1602	0	1499	8	0
2	B	1650	0	1573	6	0
2	E	1676	0	1617	12	0
2	H	1624	0	1554	6	0
2	K	1610	0	1537	5	0
2	N	1663	0	1587	9	0
2	Q	1618	0	1552	9	0
2	T	1654	0	1578	9	0
2	W	1624	0	1550	8	0
3	C	482	0	442	0	0
3	F	434	0	400	1	0
3	I	436	0	389	4	0
3	L	423	0	376	0	0
3	O	482	0	417	3	0
3	R	488	0	438	3	0
3	U	433	0	394	4	0
3	X	404	0	352	9	0
4	A	7	0	0	0	0
4	B	12	0	0	0	0
4	C	2	0	0	0	0
4	D	5	0	0	0	0
4	E	11	0	0	2	0
4	F	1	0	0	0	0
4	G	9	0	0	2	0
4	H	16	0	0	0	0
4	I	1	0	0	0	0
4	J	7	0	0	0	0
4	K	6	0	0	0	0
4	M	3	0	0	0	0
4	N	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	11	0	0	0	0
4	Q	8	0	0	0	0
4	R	1	0	0	0	0
4	S	2	0	0	0	0
4	T	12	0	0	0	0
4	V	7	0	0	0	0
4	W	10	0	0	0	0
5	A	69	0	0	0	0
5	B	111	0	0	1	0
5	C	13	0	0	0	0
5	D	51	0	0	0	0
5	E	107	0	0	1	0
5	F	2	0	0	0	0
5	G	52	0	0	0	0
5	H	82	0	0	0	0
5	I	8	0	0	0	0
5	J	60	0	0	0	0
5	K	89	0	0	0	0
5	L	2	0	0	0	0
5	M	55	0	0	0	0
5	N	104	0	0	1	0
5	O	7	0	0	0	0
5	P	60	0	0	0	0
5	Q	106	0	0	0	0
5	R	14	0	0	0	0
5	S	45	0	0	0	0
5	T	108	0	0	0	0
5	U	6	0	0	0	0
5	V	42	0	0	0	0
5	W	81	0	0	0	0
5	X	1	0	0	0	0
All	All	31176	0	28084	168	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 3.

All (168) 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:E:143:SER:OG	4:E:1814:UNX:UNK	1.42	0.99
1:G:64:SER:OG	4:G:1820:UNX:UNK	1.48	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:29:SER:CB	1:S:70:THR:HG22	2.23	0.69
2:E:143:SER:HG	4:E:1814:UNX:UNK	1.35	0.68
1:M:12[B]:LEU:HD23	1:M:107:VAL:HG13	1.74	0.67
1:D:204:LEU:HD13	1:D:208:VAL:HG23	1.76	0.66
1:A:76:ILE:HG21	1:A:79:LEU:HD12	1.80	0.63
1:J:166:VAL:HG22	1:J:178:LEU:HD12	1.81	0.63
1:J:22:ILE:HD12	1:J:74:LEU:HD23	1.81	0.62
3:I:600:VAL:CG2	3:I:605:ILE:HD11	2.31	0.61
1:M:123:PRO:HD3	1:M:135:VAL:HG22	1.83	0.60
2:Q:15:VAL:HG11	2:Q:89:LEU:HD13	1.83	0.60
2:N:161:TYR:CE1	2:N:166:VAL:HG13	2.36	0.59
1:G:111:ARG:HD2	1:G:174:SER:HB2	1.84	0.59
1:S:166:VAL:HG22	1:S:178:LEU:HD12	1.85	0.59
3:X:587:ALA:HB2	3:X:602:LEU:HD21	1.83	0.59
1:G:111:ARG:HH12	1:G:114:ALA:HB2	1.69	0.58
1:M:20:VAL:HG13	1:M:76[A]:ILE:HB	1.86	0.58
3:U:574:ARG:HG2	3:U:592:ILE:HD12	1.85	0.58
2:K:169:SER:HB3	2:K:213:ASN:HB2	1.85	0.58
1:V:38:GLN:HB2	1:V:48:LEU:HD11	1.85	0.57
1:D:49:ILE:HD13	1:D:55:LEU:HA	1.86	0.57
3:U:587:ALA:HB2	3:U:602:LEU:HD21	1.86	0.56
2:E:22:ARG:NH1	5:E:790:HOH:O	2.37	0.56
1:M:20:VAL:HG13	1:M:76[B]:ILE:HB	1.87	0.56
2:T:137:VAL:HG21	2:T:214:VAL:HG21	1.88	0.56
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.88	0.55
1:D:201[B]:HIS:CD2	1:D:203:GLY:H	2.24	0.55
1:J:128:LEU:HD22	1:J:186:LYS:HG3	1.87	0.55
1:D:166:VAL:HG22	1:D:178:LEU:HD12	1.89	0.55
2:T:186:LEU:HD13	2:T:192:TYR:CZ	2.42	0.55
1:M:111:ARG:HH12	1:M:114:ALA:HB2	1.72	0.54
2:H:208:GLN:HG2	2:H:210:TYR:CZ	2.43	0.54
1:M:20:VAL:HG11	1:M:79:LEU:HD13	1.89	0.54
1:M:29:SER:CB	1:M:70:THR:HG22	2.38	0.54
1:D:34:VAL:HA	1:D:90:GLN:O	2.08	0.53
1:M:111:ARG:HD2	1:M:174:SER:HB2	1.91	0.53
1:A:111:ARG:HH12	1:A:114:ALA:HB2	1.73	0.53
2:W:15:VAL:HG11	2:W:89:LEU:HD13	1.91	0.52
1:A:109:ILE:HG22	1:A:169:GLN:OE1	2.09	0.52
2:T:166:VAL:CG2	2:T:194:LEU:HD21	2.39	0.52
3:I:600:VAL:HG23	3:I:605:ILE:HD11	1.92	0.51
1:M:112:THR:HG22	1:M:113:VAL:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:3:ILE:HD12	1:V:98:LEU:HD12	1.93	0.51
1:A:111:ARG:NH1	1:A:175:THR:HG22	2.25	0.51
2:H:25:CYS:SG	2:H:99[B]:CYS:HB3	2.50	0.51
1:J:5:MET:HE3	1:J:91:GLN:HB2	1.92	0.51
1:M:20:VAL:CG1	1:M:79:LEU:HD13	2.40	0.51
3:X:577:VAL:HG11	3:X:580:LEU:HD11	1.92	0.51
2:H:25:CYS:SG	2:H:99[B]:CYS:CB	2.99	0.50
2:B:161:TYR:CE2	2:B:166:VAL:HG13	2.46	0.50
1:A:111:ARG:HD2	1:A:174:SER:HB2	1.92	0.50
1:J:5:MET:CE	1:J:91:GLN:HB2	2.41	0.50
3:I:557:LYS:HA	3:I:580:LEU:HD11	1.94	0.49
1:A:49:ILE:HD13	1:A:55:LEU:HA	1.94	0.49
2:E:54:ILE:HD12	2:E:61:THR:HG22	1.95	0.49
1:P:111:ARG:HD2	1:P:174:SER:HB2	1.94	0.48
3:O:561:GLU:OE1	3:O:592:ILE:HD11	2.13	0.48
2:E:161:TYR:CE1	2:E:166:VAL:HG13	2.49	0.48
1:P:31:SER:O	1:P:67:ARG:NH1	2.46	0.48
3:F:578:GLU:HB3	3:F:588:VAL:HG12	1.96	0.48
2:T:9:GLU:OE1	2:T:97:TYR:O	2.32	0.48
3:O:556:TRP:O	3:O:580:LEU:HD11	2.14	0.48
3:X:564:ALA:HB3	3:X:591:PHE:CE1	2.49	0.48
3:X:577:VAL:HA	3:X:589:VAL:HG12	1.96	0.48
2:B:69:GLY:O	5:B:1101:HOH:O	2.20	0.47
3:R:557:LYS:HA	3:R:580:LEU:HD11	1.96	0.47
2:W:17:PRO:HD3	2:W:128:SER:C	2.34	0.47
1:D:3:ILE:HD12	1:D:98:LEU:HD12	1.95	0.47
2:E:39:TRP:HD1	2:E:73:ILE:HD12	1.79	0.47
1:A:123:PRO:HD3	1:A:135:VAL:HG22	1.96	0.47
1:M:38:GLN:HB2	1:M:48:LEU:HD11	1.97	0.47
1:A:109:ILE:HG22	1:A:169:GLN:CD	2.35	0.47
1:M:36:TRP:CZ3	1:M:89:CYS:HB3	2.49	0.47
1:G:166:VAL:HG22	1:G:178:LEU:HD12	1.96	0.47
2:K:15:VAL:HG11	2:K:89:LEU:HD13	1.96	0.46
3:X:600:VAL:HG21	3:X:605:ILE:CG2	2.45	0.46
1:S:201[B]:HIS:CD2	1:S:203:GLY:H	2.34	0.46
3:X:563:PHE:O	3:X:605:ILE:HA	2.15	0.46
1:S:48:LEU:HD11	1:S:87:TYR:CE2	2.50	0.46
1:S:127:GLN:NE2	1:S:132:THR:HG22	2.31	0.46
1:V:113:VAL:HG22	1:V:144:PRO:HD3	1.98	0.46
1:A:111:ARG:HH12	1:A:114:ALA:CB	2.29	0.46
3:U:564:ALA:HB3	3:U:591:PHE:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:5:MET:CE	1:V:91:GLN:HB2	2.46	0.46
1:J:48:LEU:HD11	1:J:87:TYR:HE2	1.81	0.45
2:Q:65:ASP:HA	2:Q:68:LYS:HE3	1.97	0.45
2:N:212:CYS:SG	2:N:225:LYS:HB3	2.56	0.45
2:Q:57:SER:HB3	3:R:581:HIS:NE2	2.31	0.45
3:X:580:LEU:N	3:X:580:LEU:HD12	2.32	0.45
2:N:68:LYS:NZ	5:N:842:HOH:O	2.48	0.45
2:T:109:PRO:HB3	3:U:567:TRP:CE2	2.51	0.45
1:A:67:ARG:HB3	1:A:72:PHE:CD2	2.51	0.45
2:H:15:VAL:HG11	2:H:89:LEU:HD13	1.98	0.45
2:E:20:SER:HA	2:E:86:MET:O	2.17	0.45
2:B:23:LEU:HD21	2:B:86:MET:HE1	1.98	0.45
2:B:15:VAL:HG11	2:B:89:LEU:HD13	1.98	0.45
1:J:55:LEU:HD11	1:J:59:VAL:HG12	1.99	0.45
2:E:54:ILE:HD12	2:E:61:THR:CG2	2.47	0.44
1:S:5:MET:HE1	1:S:91:GLN:HB2	1.98	0.44
1:J:48:LEU:HA	1:J:59:VAL:HG21	1.99	0.44
2:N:144[B]:SER:OG	2:N:152:ALA:HB2	2.17	0.44
2:N:172:SER:O	2:Q:92:GLU:HB3	2.17	0.44
1:A:12:LEU:CD2	1:A:20:VAL:HG13	2.47	0.44
1:V:55:LEU:HD11	1:V:59:VAL:CG1	2.47	0.44
1:A:116:PRO:HD3	1:A:201[B]:HIS:CD2	2.52	0.44
1:M:109:ILE:HG22	1:M:169:GLN:OE1	2.17	0.44
1:G:64:SER:HG	4:G:1820:UNX:UNK	1.59	0.44
3:I:558:PRO:HD3	3:I:580:LEU:HD12	1.99	0.44
2:E:186:LEU:HD13	2:E:192:TYR:CZ	2.53	0.44
2:N:186:LEU:HD13	2:N:192:TYR:CZ	2.53	0.44
2:Q:57:SER:HB3	3:R:581:HIS:CD2	2.53	0.44
1:A:111:ARG:HH11	1:A:175:THR:HG22	1.83	0.43
3:X:587:ALA:HB2	3:X:602:LEU:CD2	2.48	0.43
2:E:217:LYS:N	2:E:218:PRO:CD	2.82	0.43
1:P:111:ARG:HH12	1:P:114:ALA:CB	2.30	0.43
2:T:147:THR:HG21	1:V:157:LEU:HD11	1.99	0.43
1:V:55:LEU:HD11	1:V:59:VAL:HG12	2.00	0.43
2:Q:18:GLY:HA3	2:W:18:GLY:HA3	2.00	0.43
2:N:27:ALA:HB2	2:N:32:LEU:HD13	2.00	0.43
1:P:111:ARG:NH1	1:P:175:THR:HG22	2.33	0.43
2:K:161:TYR:OH	2:K:184:ALA:HB2	2.19	0.43
1:M:116:PRO:HD3	1:M:201[B]:HIS:CD2	2.54	0.43
1:S:60:PRO:HB2	1:S:62:ARG:HG2	1.99	0.43
1:P:49:ILE:HD13	1:P:55:LEU:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:166:VAL:HG12	2:W:216:HIS:CD2	2.54	0.43
2:Q:130:ALA:HB3	2:Q:162:PHE:CE2	2.54	0.42
2:W:9:GLU:OE1	2:W:97:TYR:O	2.38	0.42
2:K:194:LEU:C	2:K:194:LEU:HD12	2.40	0.42
1:A:167:THR:HG23	2:B:182:PHE:CE1	2.55	0.42
1:M:34:VAL:HA	1:M:90:GLN:O	2.20	0.42
1:J:21:THR:HG22	1:J:75:THR:HG23	2.02	0.42
2:N:57:SER:HB3	3:O:581:HIS:NE2	2.35	0.42
2:Q:133:LYS:NZ	2:Q:160:ASP:O	2.43	0.42
1:G:111:ARG:NH1	1:G:112:THR:O	2.53	0.41
1:J:48:LEU:HD11	1:J:87:TYR:CE2	2.56	0.41
1:P:51:SER:O	1:P:52:ALA:HB3	2.20	0.41
2:T:161:TYR:CE1	2:T:166:VAL:HG13	2.55	0.41
2:E:15:VAL:HG11	2:E:89:LEU:HD13	2.02	0.41
2:N:43:ALA:HB3	2:N:46:LYS:HG3	2.02	0.41
1:P:111:ARG:HH11	1:P:175:THR:HG22	1.85	0.41
2:H:101:ARG:CZ	2:H:103:VAL:HG11	2.50	0.41
1:S:97[A]:TRP:CH2	2:T:36:TYR:CE2	3.09	0.41
2:H:102:THR:HG21	2:H:114:TRP:HA	2.02	0.41
2:W:104:ARG:HG3	2:W:110:TYR:HB3	2.02	0.41
2:W:155:GLY:HA2	2:W:170:TRP:CZ2	2.55	0.41
1:A:12:LEU:HD21	1:A:20:VAL:HG13	2.03	0.41
2:B:160:ASP:HB3	2:B:191:LEU:HD13	2.03	0.41
1:G:55:LEU:HD11	1:G:59:VAL:HG12	2.02	0.41
1:M:5:MET:SD	1:M:26:ALA:HB2	2.61	0.41
3:X:581:HIS:ND1	3:X:583:SER:HB3	2.36	0.41
1:M:123:PRO:HG3	1:M:133:ALA:HB1	2.04	0.40
2:Q:27:ALA:HB1	2:Q:30:PHE:CE1	2.56	0.40
1:S:5:MET:HE1	1:S:91:GLN:CB	2.51	0.40
1:V:183:THR:O	1:V:184:LEU:HD23	2.21	0.40
2:E:23:LEU:HD21	2:E:86:MET:HE1	2.03	0.40
1:S:164:GLU:HA	1:S:179:SER:O	2.20	0.40
2:K:100:ALA:HB1	2:K:116:MET:HB3	2.03	0.40
1:M:55:LEU:HD11	1:M:59:VAL:HG12	2.03	0.40
2:T:163:PRO:HD2	2:T:218:PRO:HB2	2.03	0.40
1:A:144:PRO:O	1:A:201[B]:HIS:HE1	2.05	0.40
1:J:132:THR:HG22	1:J:133:ALA:N	2.37	0.40
1:M:51:SER:O	1:M:52:ALA:HB3	2.22	0.40
1:S:34:VAL:HA	1:S:90:GLN:O	2.22	0.40
2:W:161:TYR:OH	2:W:184:ALA:HB2	2.21	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	215/228 (94%)	209 (97%)	6 (3%)	0	100	100
1	D	213/228 (93%)	204 (96%)	9 (4%)	0	100	100
1	G	215/228 (94%)	204 (95%)	11 (5%)	0	100	100
1	J	213/228 (93%)	204 (96%)	9 (4%)	0	100	100
1	M	216/228 (95%)	208 (96%)	8 (4%)	0	100	100
1	P	215/228 (94%)	205 (95%)	10 (5%)	0	100	100
1	S	215/228 (94%)	203 (94%)	12 (6%)	0	100	100
1	V	211/228 (92%)	201 (95%)	10 (5%)	0	100	100
2	B	223/246 (91%)	220 (99%)	3 (1%)	0	100	100
2	E	226/246 (92%)	222 (98%)	4 (2%)	0	100	100
2	H	217/246 (88%)	212 (98%)	5 (2%)	0	100	100
2	K	214/246 (87%)	209 (98%)	5 (2%)	0	100	100
2	N	226/246 (92%)	223 (99%)	3 (1%)	0	100	100
2	Q	216/246 (88%)	213 (99%)	3 (1%)	0	100	100
2	T	225/246 (92%)	222 (99%)	3 (1%)	0	100	100
2	W	217/246 (88%)	212 (98%)	5 (2%)	0	100	100
3	C	58/77 (75%)	58 (100%)	0	0	100	100
3	F	52/77 (68%)	52 (100%)	0	0	100	100
3	I	53/77 (69%)	53 (100%)	0	0	100	100
3	L	52/77 (68%)	52 (100%)	0	0	100	100
3	O	60/77 (78%)	59 (98%)	1 (2%)	0	100	100
3	R	60/77 (78%)	60 (100%)	0	0	100	100
3	U	52/77 (68%)	52 (100%)	0	0	100	100
3	X	52/77 (68%)	50 (96%)	2 (4%)	0	100	100
All	All	3916/4408 (89%)	3807 (97%)	109 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	175/200 (88%)	170 (97%)	5 (3%)	48	40
1	D	173/200 (86%)	170 (98%)	3 (2%)	66	63
1	G	182/200 (91%)	181 (100%)	1 (0%)	91	91
1	J	182/200 (91%)	181 (100%)	1 (0%)	91	91
1	M	181/200 (90%)	179 (99%)	2 (1%)	78	77
1	P	182/200 (91%)	178 (98%)	4 (2%)	57	51
1	S	174/200 (87%)	173 (99%)	1 (1%)	89	89
1	V	171/200 (86%)	169 (99%)	2 (1%)	75	74
2	B	180/205 (88%)	179 (99%)	1 (1%)	89	89
2	E	184/205 (90%)	183 (100%)	1 (0%)	91	91
2	H	178/205 (87%)	176 (99%)	2 (1%)	78	77
2	K	174/205 (85%)	172 (99%)	2 (1%)	78	77
2	N	181/205 (88%)	179 (99%)	2 (1%)	78	77
2	Q	176/205 (86%)	171 (97%)	5 (3%)	49	42
2	T	178/205 (87%)	175 (98%)	3 (2%)	66	63
2	W	175/205 (85%)	173 (99%)	2 (1%)	78	77
3	C	49/67 (73%)	49 (100%)	0	100	100
3	F	45/67 (67%)	45 (100%)	0	100	100
3	I	43/67 (64%)	43 (100%)	0	100	100
3	L	42/67 (63%)	42 (100%)	0	100	100
3	O	46/67 (69%)	46 (100%)	0	100	100
3	R	48/67 (72%)	48 (100%)	0	100	100
3	U	43/67 (64%)	43 (100%)	0	100	100
3	X	37/67 (55%)	36 (97%)	1 (3%)	50	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3199/3776 (85%)	3161 (99%)	38 (1%)	75	74

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	11	SER
1	A	67	ARG
1	A	111	ARG
1	A	197	CYS
2	B	154	LEU
1	D	11	SER
1	D	71	ASP
1	D	202	GLN
2	E	202	SER
1	G	13	SER
2	H	208	GLN
2	H	213	ASN
1	J	15	SER
2	K	208	GLN
2	K	213	ASN
1	M	20	VAL
1	M	61	SER
2	N	154	LEU
2	N	194	LEU
1	P	111	ARG
1	P	132	THR
1	P	150	GLN
1	P	155	ASN
2	Q	32	LEU
2	Q	154	LEU
2	Q	177	SER
2	Q	213	ASN
2	Q	215	ASN
1	S	11	SER
2	T	33	SER
2	T	147	THR
2	T	154	LEU
1	V	66	SER
1	V	211	SER
2	W	203	SER
2	W	213	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	563	PHE

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

Mol	Chain	Res	Type
2	B	215	ASN
2	E	85	GLN
2	E	87	ASN
2	K	180	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 143 ligands modelled in this entry, 143 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	213/228 (93%)	0.42	12 (5%) 25 28	34, 57, 74, 78	0
1	D	213/228 (93%)	0.78	29 (13%) 3 3	44, 63, 88, 98	0
1	G	213/228 (93%)	0.54	16 (7%) 15 16	40, 57, 79, 90	0
1	J	213/228 (93%)	0.66	19 (8%) 10 11	41, 62, 85, 93	0
1	M	214/228 (93%)	0.59	12 (5%) 25 28	41, 61, 76, 88	0
1	P	213/228 (93%)	0.41	10 (4%) 32 35	36, 54, 78, 90	0
1	S	214/228 (93%)	0.61	16 (7%) 15 16	42, 61, 84, 93	0
1	V	212/228 (92%)	0.77	29 (13%) 3 3	41, 61, 82, 90	0
2	B	225/246 (91%)	0.13	9 (4%) 39 43	31, 42, 58, 68	0
2	E	226/246 (91%)	0.23	12 (5%) 27 29	32, 46, 73, 86	0
2	H	218/246 (88%)	0.26	9 (4%) 38 42	32, 44, 65, 78	0
2	K	218/246 (88%)	0.23	14 (6%) 20 22	31, 45, 70, 84	0
2	N	226/246 (91%)	0.15	9 (3%) 39 43	32, 43, 61, 75	0
2	Q	218/246 (88%)	0.17	9 (4%) 38 42	29, 43, 60, 71	0
2	T	225/246 (91%)	0.12	9 (4%) 39 43	32, 44, 67, 80	0
2	W	220/246 (89%)	0.27	18 (8%) 12 13	32, 46, 71, 85	0
3	C	60/77 (77%)	0.20	5 (8%) 12 12	40, 57, 82, 86	0
3	F	53/77 (68%)	0.99	10 (18%) 1 1	57, 81, 102, 110	0
3	I	55/77 (71%)	1.04	11 (20%) 1 1	49, 70, 98, 103	0
3	L	54/77 (70%)	0.79	8 (14%) 3 2	50, 81, 119, 126	0
3	O	61/77 (79%)	0.97	11 (18%) 2 1	50, 74, 103, 111	0
3	R	61/77 (79%)	0.14	3 (4%) 30 33	40, 58, 85, 95	0
3	U	54/77 (70%)	0.65	5 (9%) 9 10	45, 72, 98, 105	0
3	X	53/77 (68%)	1.78	21 (39%) 0 0	60, 91, 120, 130	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3932/4408 (89%)	0.44	306 (7%) 14 15	29, 53, 84, 130	0

All (306) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	608	ILE	5.7
2	E	147	THR	5.6
3	I	594	TYR	5.6
1	G	187	ALA	5.5
3	X	575	ALA	5.3
3	X	603	SER	5.3
3	I	575	ALA	5.3
3	I	554	LYS	4.9
2	T	147	THR	4.8
2	H	200	VAL	4.8
2	K	200	VAL	4.6
3	X	591	PHE	4.6
3	L	594	TYR	4.4
2	N	110	TYR	4.3
1	S	70	THR	4.2
3	X	556	TRP	4.2
3	X	560	ASP	4.2
3	I	556	TRP	4.2
2	E	110	TYR	4.2
1	V	3	ILE	4.2
3	X	572	PHE	4.1
3	L	563	PHE	4.1
3	O	600	VAL	4.1
3	O	563	PHE	4.1
1	A	171	SER	4.0
1	G	136	VAL	4.0
1	V	17	GLY	4.0
3	L	584	GLY	4.0
3	O	573	TYR	3.9
3	X	593	ASP	3.9
2	T	149	GLY	3.9
1	V	136	VAL	3.9
2	E	143	SER	3.8
3	I	563	PHE	3.8
2	K	115	ALA	3.8
2	T	110	TYR	3.8
3	X	563	PHE	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	22	ILE	3.7
3	U	584	GLY	3.7
1	D	213	ASN	3.7
2	H	228	GLU	3.7
3	X	594	TYR	3.7
1	V	182	LEU	3.6
1	D	81	PRO	3.6
1	V	187	ALA	3.6
1	J	70	THR	3.6
1	M	70	THR	3.6
2	T	143	SER	3.6
3	O	548	ILE	3.6
1	V	191	LYS	3.5
3	X	567	TRP	3.5
3	U	594	TYR	3.5
2	Q	115	ALA	3.5
1	J	182	LEU	3.5
2	W	200	VAL	3.5
1	S	213	ASN	3.4
1	D	69	GLY	3.4
2	Q	200	VAL	3.4
1	G	26	ALA	3.4
2	E	148	SER	3.4
3	X	569	ASP	3.4
2	W	115	ALA	3.4
1	M	135	VAL	3.3
2	N	143	SER	3.3
2	W	228	GLU	3.3
2	K	209	THR	3.3
3	U	608	ILE	3.3
1	V	130	SER	3.3
2	T	115	ALA	3.3
3	X	570	ASN	3.3
3	R	594	TYR	3.3
1	A	135	VAL	3.3
3	X	577	VAL	3.3
3	F	556	TRP	3.3
2	H	115	ALA	3.2
1	J	191	LYS	3.2
2	H	4	GLU	3.2
1	J	37	TYR	3.2
1	P	121	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	187	ALA	3.2
2	E	115	ALA	3.2
2	W	110	TYR	3.2
2	W	149	GLY	3.2
2	W	152	ALA	3.2
1	J	3	ILE	3.2
1	M	186	LYS	3.2
2	Q	228	GLU	3.1
1	D	171	SER	3.1
3	O	594	TYR	3.1
3	I	555	MET	3.1
1	D	49	ILE	3.1
2	Q	203	SER	3.1
3	X	583	SER	3.1
1	J	187	ALA	3.0
2	T	203	SER	3.0
3	X	555	MET	3.0
3	X	601	LEU	3.0
1	J	34	VAL	3.0
1	V	61	SER	3.0
1	D	68	SER	3.0
3	R	548	ILE	3.0
2	B	143	SER	3.0
2	W	177	SER	3.0
1	P	136	VAL	2.9
3	C	573	TYR	2.9
2	K	110	TYR	2.9
3	L	572	PHE	2.9
1	J	136	VAL	2.9
1	A	186	LYS	2.9
1	J	185	SER	2.9
1	S	135	VAL	2.9
3	F	584	GLY	2.9
3	F	566	TYR	2.9
1	V	131	GLY	2.8
2	K	113	GLY	2.8
2	E	149	GLY	2.8
2	W	116	MET	2.8
1	G	182	LEU	2.8
1	D	37	TYR	2.8
1	S	2	ASP	2.8
1	S	155	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	X	565	LEU	2.8
2	B	147	THR	2.8
2	H	114	TRP	2.7
1	J	26	ALA	2.7
1	D	70	THR	2.7
2	N	209	THR	2.7
2	Q	209	THR	2.7
3	O	592	ILE	2.7
3	F	563	PHE	2.7
2	T	148	SER	2.7
2	W	206	GLY	2.7
1	S	81	PRO	2.7
2	B	110	TYR	2.7
1	D	59	VAL	2.7
1	A	155	ASN	2.7
3	I	603	SER	2.7
3	O	574	ARG	2.7
2	Q	102	THR	2.7
1	V	37	TYR	2.6
3	U	556	TRP	2.6
1	P	156	ALA	2.6
3	O	572	PHE	2.6
1	V	47	LEU	2.6
1	J	52	ALA	2.6
1	S	190	GLU	2.6
2	K	116	MET	2.6
1	P	188	ASP	2.6
1	D	87	TYR	2.6
3	X	604	ASN	2.6
1	D	135	VAL	2.6
1	S	37	TYR	2.6
2	W	151	THR	2.6
3	C	571	LYS	2.6
1	G	135	VAL	2.6
1	D	31	SER	2.6
3	L	556	TRP	2.6
1	M	137	CYS	2.5
2	Q	202[A]	SER	2.5
1	D	136	VAL	2.5
2	W	150	GLY	2.5
1	J	130	SER	2.5
1	D	35	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	5	VAL	2.5
3	O	549	PRO	2.5
1	V	32	SER	2.5
1	V	151	TRP	2.5
2	Q	199	THR	2.5
1	V	137	CYS	2.5
3	F	573	TYR	2.5
3	C	553	ALA	2.5
3	X	578	GLU	2.5
1	A	84	PHE	2.5
2	H	209	THR	2.4
2	B	150	GLY	2.4
1	G	121	PHE	2.4
2	K	102	THR	2.4
1	A	136	VAL	2.4
2	B	174	ALA	2.4
1	G	178	LEU	2.4
2	E	150	GLY	2.4
1	D	190	GLU	2.4
1	G	191	LYS	2.4
1	G	188	ASP	2.4
2	N	174	ALA	2.4
2	Q	201	PRO	2.4
1	D	99	PHE	2.4
1	S	99	PHE	2.4
3	X	558	PRO	2.4
1	V	180	SER	2.4
1	M	95	PHE	2.4
1	D	83	ASP	2.4
1	D	34	VAL	2.4
1	P	186	LYS	2.4
1	S	171	SER	2.4
3	F	594	TYR	2.4
1	J	121	PHE	2.3
1	V	95	PHE	2.3
1	V	34	VAL	2.3
2	K	152	ALA	2.3
3	O	584	GLY	2.3
1	M	157	LEU	2.3
2	W	114	TRP	2.3
1	M	136	VAL	2.3
1	J	188	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	174	ALA	2.3
2	T	116	MET	2.3
1	S	21	THR	2.3
2	N	147	THR	2.3
1	D	47	LEU	2.3
1	V	121	PHE	2.3
1	S	136	VAL	2.3
1	V	16	VAL	2.3
1	P	137	CYS	2.3
2	H	116	MET	2.3
1	D	78	SER	2.3
1	J	68	SER	2.3
3	U	563	PHE	2.3
1	V	26	ALA	2.3
3	X	557	LYS	2.3
1	V	68	SER	2.3
2	B	148	SER	2.3
3	L	603	SER	2.3
3	O	559	GLY	2.3
1	G	186	LYS	2.3
1	D	125	ASP	2.3
1	S	47	LEU	2.2
1	V	35	ALA	2.2
1	D	151	TRP	2.2
1	V	15	SER	2.2
1	P	182	LEU	2.2
1	P	135	VAL	2.2
1	V	29	SER	2.2
3	L	583	SER	2.2
1	A	97[A]	TRP	2.2
2	E	176	THR	2.2
1	A	157	LEU	2.2
1	D	77	SER	2.2
1	J	16	VAL	2.2
2	W	113	GLY	2.2
1	D	155	ASN	2.2
2	N	149	GLY	2.2
1	D	84	PHE	2.2
1	G	156	ALA	2.2
2	K	199	THR	2.2
1	M	171	SER	2.2
1	V	154	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	114	TRP	2.2
2	W	202	SER	2.2
1	V	139	LEU	2.2
3	L	601	LEU	2.2
2	W	118	TYR	2.2
1	D	17	GLY	2.2
2	B	52	ALA	2.2
2	K	119	TRP	2.1
1	A	137	CYS	2.1
1	D	101	PHE	2.1
3	C	594	TYR	2.1
1	G	130	SER	2.1
3	F	571	LYS	2.1
1	J	151	TRP	2.1
1	P	153	VAL	2.1
1	D	95	PHE	2.1
1	A	172	LYS	2.1
1	S	186	LYS	2.1
2	T	48	LEU	2.1
1	S	69	GLY	2.1
1	A	99	PHE	2.1
2	K	205	LEU	2.1
1	M	84	PHE	2.1
3	I	607	PRO	2.1
1	G	181	THR	2.1
1	V	181	THR	2.1
1	M	97[A]	TRP	2.1
2	H	203	SER	2.1
1	M	123	PRO	2.1
2	W	179	VAL	2.1
3	I	570	ASN	2.1
2	W	209	THR	2.1
3	F	572	PHE	2.1
2	N	145	LYS	2.1
1	D	197	CYS	2.1
1	G	137	CYS	2.1
1	G	179	SER	2.0
1	S	77	SER	2.0
3	I	562	CYS	2.1
3	F	596[A]	ASN	2.0
2	N	157	LEU	2.0
3	C	550	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	N	150	GLY	2.0
2	E	48	LEU	2.0
3	I	601	LEU	2.0
2	B	115	ALA	2.0
2	K	179	VAL	2.0
2	E	105	GLY	2.0
2	K	105	GLY	2.0
1	M	179	SER	2.0
2	H	177	SER	2.0
1	G	82	GLU	2.0
1	A	182	LEU	2.0
1	J	47	LEU	2.0
1	V	197	CYS	2.0
2	W	207	THR	2.0
3	R	575	ALA	2.0
1	J	131	GLY	2.0
2	B	145	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	N	1822	1/1	0.94	0.35	13.36	30,30,30,30	0
4	UNX	B	1906	1/1	0.94	0.18	8.78	30,30,30,30	0
4	UNX	B	1946	1/1	0.87	0.27	7.85	30,30,30,30	0
4	UNX	B	1872	1/1	0.98	0.35	7.51	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	W	1857	1/1	0.94	0.20	7.27	30,30,30,30	0
4	UNX	J	1866	1/1	0.83	0.26	6.97	30,30,30,30	0
4	UNX	J	1821	1/1	0.91	0.30	6.67	30,30,30,30	0
4	UNX	B	1889	1/1	0.71	0.34	5.86	30,30,30,30	0
4	UNX	J	1867	1/1	0.96	0.39	5.16	30,30,30,30	0
4	UNX	P	1886	1/1	0.78	0.19	5.06	30,30,30,30	0
4	UNX	B	1875	1/1	0.73	0.18	4.02	30,30,30,30	0
4	UNX	Q	1835	1/1	0.94	0.26	3.30	30,30,30,30	0
4	UNX	G	1885	1/1	0.95	0.32	3.29	30,30,30,30	0
4	UNX	T	1890	1/1	0.88	0.18	3.06	30,30,30,30	0
4	UNX	P	1832	1/1	0.97	0.18	3.03	30,30,30,30	0
4	UNX	M	1852	1/1	0.96	0.18	2.86	30,30,30,30	0
4	UNX	H	1887	1/1	0.96	0.12	2.40	30,30,30,30	0
4	UNX	V	1971	1/1	0.94	0.30	2.09	30,30,30,30	0
4	UNX	G	1824	1/1	0.78	0.14	2.05	30,30,30,30	0
4	UNX	T	1865	1/1	0.96	0.16	2.00	30,30,30,30	0
4	UNX	V	1879	1/1	0.91	0.19	1.91	30,30,30,30	0
4	UNX	H	1850	1/1	0.97	0.25	1.76	30,30,30,30	0
4	UNX	E	1815	1/1	0.96	0.39	1.56	30,30,30,30	0
4	UNX	H	1963	1/1	0.90	0.23	1.42	30,30,30,30	0
4	UNX	G	1829	1/1	0.96	0.20	1.31	30,30,30,30	0
4	UNX	B	1871	1/1	0.88	0.17	1.30	30,30,30,30	0
4	UNX	Q	1926	1/1	0.95	0.15	1.30	30,30,30,30	0
4	UNX	E	1893	1/1	0.88	0.15	1.27	30,30,30,30	0
4	UNX	J	1816	1/1	0.96	0.25	1.24	30,30,30,30	0
4	UNX	E	1942	1/1	0.95	0.17	1.16	30,30,30,30	0
4	UNX	T	1830	1/1	0.92	0.23	1.11	30,30,30,30	0
4	UNX	D	1939	1/1	0.90	0.18	1.02	30,30,30,30	0
4	UNX	A	1843	1/1	0.98	0.14	1.01	30,30,30,30	0
4	UNX	P	1828	1/1	0.96	0.15	1.00	30,30,30,30	0
4	UNX	A	1956	1/1	0.94	0.13	0.99	30,30,30,30	0
4	UNX	B	1949	1/1	0.87	0.12	0.97	30,30,30,30	0
4	UNX	H	1870	1/1	0.86	0.15	0.76	30,30,30,30	0
4	UNX	J	1936	1/1	0.82	0.13	0.73	30,30,30,30	0
4	UNX	G	1916	1/1	0.88	0.21	0.56	30,30,30,30	0
4	UNX	N	1899	1/1	0.92	0.15	0.53	30,30,30,30	0
4	UNX	T	1910	1/1	0.91	0.17	0.49	30,30,30,30	0
4	UNX	K	1849	1/1	0.97	0.12	0.42	30,30,30,30	0
4	UNX	N	1877	1/1	0.96	0.20	0.27	30,30,30,30	0
4	UNX	W	1883	1/1	0.88	0.23	0.13	30,30,30,30	0
4	UNX	W	1874	1/1	0.87	0.11	0.04	30,30,30,30	0
4	UNX	J	1908	1/1	0.75	0.11	-0.22	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	E	1965	1/1	0.95	0.23	-0.37	30,30,30,30	0
4	UNX	Q	1861	1/1	0.92	0.13	-0.40	30,30,30,30	0
4	UNX	W	1862	1/1	0.96	0.10	-0.44	30,30,30,30	0
4	UNX	H	1839	1/1	0.93	0.12	-0.51	30,30,30,30	0
4	UNX	N	1894	1/1	0.86	0.12	-0.54	30,30,30,30	0
4	UNX	T	1921	1/1	0.96	0.12	-0.65	30,30,30,30	0
4	UNX	H	1920	1/1	0.90	0.11	-0.67	30,30,30,30	0
4	UNX	B	1844	1/1	0.96	0.14	-0.69	30,30,30,30	0
4	UNX	R	1896	1/1	0.86	0.10	-0.83	30,30,30,30	0
4	UNX	I	1819	1/1	0.88	0.12	-0.87	30,30,30,30	0
4	UNX	H	1948	1/1	0.91	0.11	-0.89	30,30,30,30	0
4	UNX	T	1848	1/1	0.85	0.12	-0.90	30,30,30,30	0
4	UNX	C	1873	1/1	0.95	0.09	-0.93	30,30,30,30	0
4	UNX	W	1845	1/1	0.93	0.09	-1.16	30,30,30,30	0
4	UNX	K	1882	1/1	0.94	0.09	-1.21	30,30,30,30	0
4	UNX	J	1868	1/1	0.94	0.10	-1.23	30,30,30,30	0
4	UNX	Q	1842	1/1	0.97	0.08	-1.33	30,30,30,30	0
4	UNX	B	1947	1/1	0.94	0.11	-1.35	30,30,30,30	0
4	UNX	A	1860	1/1	0.96	0.08	-1.36	30,30,30,30	0
4	UNX	M	1966	1/1	0.93	0.10	-1.42	30,30,30,30	0
4	UNX	P	1903	1/1	0.94	0.11	-1.58	30,30,30,30	0
4	UNX	A	1859	1/1	0.97	0.11	-1.63	30,30,30,30	0
4	UNX	V	1841	1/1	0.98	0.07	-1.68	30,30,30,30	0
4	UNX	V	1964	1/1	0.95	0.09	-1.85	30,30,30,30	0
4	UNX	G	1820	1/1	0.95	0.09	-1.93	30,30,30,30	0
4	UNX	P	1851	1/1	0.98	0.07	-2.06	30,30,30,30	0
4	UNX	W	1913	1/1	0.88	0.07	-2.24	30,30,30,30	0
4	UNX	K	1888	1/1	0.89	0.10	-2.28	30,30,30,30	0
4	UNX	D	1925	1/1	0.95	0.07	-2.35	30,30,30,30	0
4	UNX	N	1876	1/1	0.98	0.08	-2.46	30,30,30,30	0
4	UNX	H	1941	1/1	0.94	0.09	-2.57	30,30,30,30	0
4	UNX	D	1834	1/1	0.96	0.07	-2.91	30,30,30,30	0
4	UNX	P	1934	1/1	0.93	0.08	-3.53	30,30,30,30	0
4	UNX	E	1904	1/1	0.92	0.07	-3.62	30,30,30,30	0
4	UNX	W	1951	1/1	0.84	0.24	-	30,30,30,30	0
4	UNX	H	1954	1/1	0.86	0.27	-	30,30,30,30	0
4	UNX	N	1969	1/1	0.83	0.10	-	30,30,30,30	0
4	UNX	B	1927	1/1	0.95	0.14	-	30,30,30,30	0
4	UNX	S	1864	1/1	0.90	0.19	-	30,30,30,30	0
4	UNX	P	1827	1/1	0.92	0.11	-	30,30,30,30	0
4	UNX	W	1884	1/1	0.91	0.08	-	30,30,30,30	0
4	UNX	H	1900	1/1	0.95	0.07	-	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	H	1944	1/1	0.78	0.21	-	30,30,30,30	0
4	UNX	D	1881	1/1	0.95	0.08	-	30,30,30,30	0
4	UNX	N	1937	1/1	0.93	0.16	-	30,30,30,30	0
4	UNX	K	1891	1/1	0.89	0.08	-	30,30,30,30	0
4	UNX	T	1924	1/1	0.96	0.22	-	30,30,30,30	0
4	UNX	M	1952	1/1	0.92	0.16	-	30,30,30,30	0
4	UNX	T	1898	1/1	0.85	0.11	-	30,30,30,30	0
4	UNX	H	1953	1/1	0.98	0.16	-	30,30,30,30	0
4	UNX	T	1846	1/1	0.97	0.04	-	30,30,30,30	0
4	UNX	G	1918	1/1	0.90	0.16	-	30,30,30,30	0
4	UNX	H	1919	1/1	0.87	0.11	-	30,30,30,30	0
4	UNX	E	1897	1/1	0.97	0.08	-	30,30,30,30	0
4	UNX	B	1914	1/1	0.83	0.21	-	30,30,30,30	0
4	UNX	W	1854	1/1	0.95	0.08	-	30,30,30,30	0
4	UNX	T	1928	1/1	0.88	0.24	-	30,30,30,30	0
4	UNX	V	1932	1/1	0.98	0.09	-	30,30,30,30	0
4	UNX	A	1972	1/1	0.88	0.19	-	30,30,30,30	0
4	UNX	T	1940	1/1	0.96	0.22	-	30,30,30,30	0
4	UNX	Q	1901	1/1	0.84	0.14	-	30,30,30,30	0
4	UNX	V	1856	1/1	0.95	0.19	-	30,30,30,30	0
4	UNX	P	1826	1/1	0.91	0.07	-	30,30,30,30	0
4	UNX	A	1950	1/1	0.95	0.11	-	30,30,30,30	0
4	UNX	N	1968	1/1	0.92	0.12	-	30,30,30,30	0
4	UNX	Q	1961	1/1	0.90	0.10	-	30,30,30,30	0
4	UNX	C	1855	1/1	0.81	0.12	-	30,30,30,30	0
4	UNX	S	1915	1/1	0.81	0.14	-	30,30,30,30	0
4	UNX	H	1858	1/1	0.97	0.12	-	30,30,30,30	0
4	UNX	H	1935	1/1	0.86	0.17	-	30,30,30,30	0
4	UNX	E	1814	1/1	0.89	0.31	-	30,30,30,30	0
4	UNX	K	1836	1/1	0.94	0.12	-	30,30,30,30	0
4	UNX	Q	1917	1/1	0.88	0.09	-	30,30,30,30	0
4	UNX	V	1823	1/1	0.80	0.12	-	30,30,30,30	0
4	UNX	P	1817	1/1	0.93	0.06	-	30,30,30,30	0
4	UNX	N	1958	1/1	0.90	0.13	-	30,30,30,30	0
4	UNX	G	1880	1/1	0.93	0.18	-	30,30,30,30	0
4	UNX	N	1938	1/1	0.87	0.19	-	30,30,30,30	0
4	UNX	E	1905	1/1	0.85	0.16	-	30,30,30,30	0
4	UNX	P	1929	1/1	0.95	0.09	-	30,30,30,30	0
4	UNX	H	1962	1/1	0.80	0.21	-	30,30,30,30	0
4	UNX	E	1957	1/1	0.95	0.11	-	30,30,30,30	0
4	UNX	N	1967	1/1	0.94	0.12	-	30,30,30,30	0
4	UNX	B	1902	1/1	0.94	0.08	-	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	UNX	G	1931	1/1	0.94	0.11	-	30,30,30,30	0
4	UNX	K	1863	1/1	0.98	0.05	-	30,30,30,30	0
4	UNX	A	1943	1/1	0.94	0.11	-	30,30,30,30	0
4	UNX	E	1923	1/1	0.97	0.11	-	30,30,30,30	0
4	UNX	F	1847	1/1	0.97	0.07	-	30,30,30,30	0
4	UNX	G	1818	1/1	0.88	0.10	-	30,30,30,30	0
4	UNX	W	1907	1/1	0.90	0.24	-	30,30,30,30	0
4	UNX	E	1945	1/1	0.95	0.14	-	30,30,30,30	0
4	UNX	P	1909	1/1	0.81	0.15	-	30,30,30,30	0
4	UNX	Q	1895	1/1	0.86	0.30	-	30,30,30,30	0
4	UNX	D	1955	1/1	0.81	0.18	-	30,30,30,30	0
4	UNX	T	1959	1/1	0.95	0.17	-	30,30,30,30	0
4	UNX	N	1878	1/1	0.85	0.13	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.