Full wwPDB X-ray Structure Validation Report (i)

Mar 15, 2026 – 02:11 PM UTC

PDB ID	:	6A3V / pdb_00006a3v
Title	:	Complex structure of human 4-1BB and 4-1BBL
Authors	:	Li, Y.; Zhang, C.; Chai, Y.; Qi, J.; Tien, P.; Gao, S.; Gao, G.F.
Deposited on	:	2018-06-17
Resolution	:	3.39 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 (i) 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 (i)) were used in the production of this report:

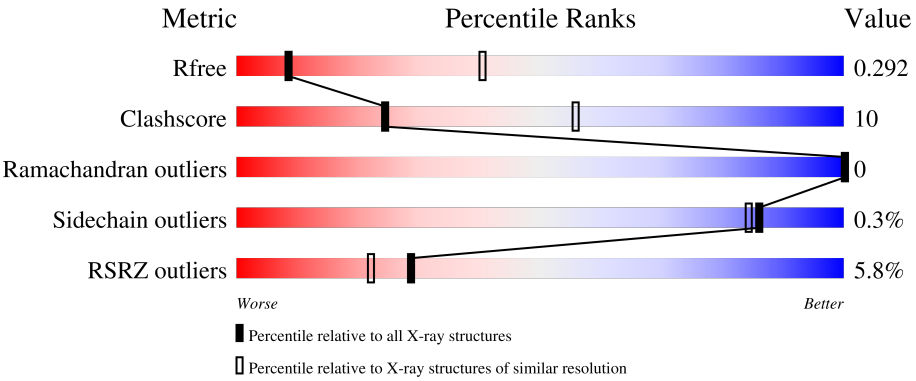
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 <=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	203	3% 54% 20% 27%
1	C	203	% 59% 15% 26%
1	E	203	3% 55% 18% 27%
1	G	203	% 59% 15% 26%
1	I	203	% 55% 17% 29%

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Mol	Chain	Length	Quality of chain
1	K	203	2% 58% 16% 26%
1	M	203	2% 53% 21% 27%
1	O	203	2% 56% 16% 28%
1	Q	203	2% 57% 15% 28%
1	S	203	2% 56% 17% 27%
1	U	203	% 54% 18% 28%
1	W	203	% 59% 14% 27%
2	B	163	13% 67% 17% 15%
2	D	163	6% 70% 12% 18%
2	F	163	6% 66% 17% 18%
2	H	163	8% 64% 16% 20%
2	J	163	4% 55% 18% 27%
2	L	163	9% 62% 20% 18%
2	N	163	10% 57% 25% 18%
2	P	163	9% 63% 21% 15%
2	R	163	6% 60% 13% 27%
2	T	163	6% 55% 23% 22%
2	V	163	5% 62% 13% 24%
2	X	163	9% 60% 21% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25073 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1120	718	198	203	1			
1	C	150	Total	C	N	O	S	0	0	0
			1124	720	199	204	1			
1	E	148	Total	C	N	O	S	0	0	0
			1112	712	197	202	1			
1	G	150	Total	C	N	O	S	0	0	0
			1132	723	203	205	1			
1	I	145	Total	C	N	O	S	0	0	0
			1092	701	194	196	1			
1	K	150	Total	C	N	O	S	0	0	0
			1125	719	200	205	1			
1	M	149	Total	C	N	O	S	0	0	0
			1120	718	198	203	1			
1	O	147	Total	C	N	O	S	0	0	0
			1106	710	196	199	1			
1	Q	147	Total	C	N	O	S	0	0	0
			1103	707	196	199	1			
1	S	148	Total	C	N	O	S	0	0	0
			1115	715	197	202	1			
1	U	147	Total	C	N	O	S	0	0	0
			1107	709	196	201	1			
1	W	149	Total	C	N	O	S	0	0	0
			1120	718	198	203	1			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	HIS	-	expression tag	UNP P41273
A	256	HIS	-	expression tag	UNP P41273
A	257	HIS	-	expression tag	UNP P41273
A	258	HIS	-	expression tag	UNP P41273
A	259	HIS	-	expression tag	UNP P41273

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Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P41273
C	255	HIS	-	expression tag	UNP P41273
C	256	HIS	-	expression tag	UNP P41273
C	257	HIS	-	expression tag	UNP P41273
C	258	HIS	-	expression tag	UNP P41273
C	259	HIS	-	expression tag	UNP P41273
C	260	HIS	-	expression tag	UNP P41273
E	255	HIS	-	expression tag	UNP P41273
E	256	HIS	-	expression tag	UNP P41273
E	257	HIS	-	expression tag	UNP P41273
E	258	HIS	-	expression tag	UNP P41273
E	259	HIS	-	expression tag	UNP P41273
E	260	HIS	-	expression tag	UNP P41273
G	255	HIS	-	expression tag	UNP P41273
G	256	HIS	-	expression tag	UNP P41273
G	257	HIS	-	expression tag	UNP P41273
G	258	HIS	-	expression tag	UNP P41273
G	259	HIS	-	expression tag	UNP P41273
G	260	HIS	-	expression tag	UNP P41273
I	255	HIS	-	expression tag	UNP P41273
I	256	HIS	-	expression tag	UNP P41273
I	257	HIS	-	expression tag	UNP P41273
I	258	HIS	-	expression tag	UNP P41273
I	259	HIS	-	expression tag	UNP P41273
I	260	HIS	-	expression tag	UNP P41273
K	255	HIS	-	expression tag	UNP P41273
K	256	HIS	-	expression tag	UNP P41273
K	257	HIS	-	expression tag	UNP P41273
K	258	HIS	-	expression tag	UNP P41273
K	259	HIS	-	expression tag	UNP P41273
K	260	HIS	-	expression tag	UNP P41273
M	255	HIS	-	expression tag	UNP P41273
M	256	HIS	-	expression tag	UNP P41273
M	257	HIS	-	expression tag	UNP P41273
M	258	HIS	-	expression tag	UNP P41273
M	259	HIS	-	expression tag	UNP P41273
M	260	HIS	-	expression tag	UNP P41273
O	255	HIS	-	expression tag	UNP P41273
O	256	HIS	-	expression tag	UNP P41273
O	257	HIS	-	expression tag	UNP P41273
O	258	HIS	-	expression tag	UNP P41273
O	259	HIS	-	expression tag	UNP P41273

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Chain	Residue	Modelled	Actual	Comment	Reference
O	260	HIS	-	expression tag	UNP P41273
Q	255	HIS	-	expression tag	UNP P41273
Q	256	HIS	-	expression tag	UNP P41273
Q	257	HIS	-	expression tag	UNP P41273
Q	258	HIS	-	expression tag	UNP P41273
Q	259	HIS	-	expression tag	UNP P41273
Q	260	HIS	-	expression tag	UNP P41273
S	255	HIS	-	expression tag	UNP P41273
S	256	HIS	-	expression tag	UNP P41273
S	257	HIS	-	expression tag	UNP P41273
S	258	HIS	-	expression tag	UNP P41273
S	259	HIS	-	expression tag	UNP P41273
S	260	HIS	-	expression tag	UNP P41273
U	255	HIS	-	expression tag	UNP P41273
U	256	HIS	-	expression tag	UNP P41273
U	257	HIS	-	expression tag	UNP P41273
U	258	HIS	-	expression tag	UNP P41273
U	259	HIS	-	expression tag	UNP P41273
U	260	HIS	-	expression tag	UNP P41273
W	255	HIS	-	expression tag	UNP P41273
W	256	HIS	-	expression tag	UNP P41273
W	257	HIS	-	expression tag	UNP P41273
W	258	HIS	-	expression tag	UNP P41273
W	259	HIS	-	expression tag	UNP P41273
W	260	HIS	-	expression tag	UNP P41273

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1015	600	190	203	22			
2	D	134	Total	C	N	O	S	0	0	0
			988	585	186	195	22			
2	F	134	Total	C	N	O	S	0	0	0
			989	585	186	196	22			
2	H	131	Total	C	N	O	S	0	0	0
			969	572	182	193	22			
2	J	119	Total	C	N	O	S	0	0	0
			882	524	163	175	20			
2	L	134	Total	C	N	O	S	0	0	0
			989	585	186	196	22			
2	N	133	Total	C	N	O	S	0	0	0
			982	580	185	195	22			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	138	Total	C	N	O	S	0	0	0
			1015	600	190	203	22			
2	R	119	Total	C	N	O	S	0	0	0
			871	517	157	175	22			
2	T	127	Total	C	N	O	S	0	0	0
			931	552	172	185	22			
2	V	124	Total	C	N	O	S	0	0	0
			921	544	174	183	20			
2	X	132	Total	C	N	O	S	0	0	0
			977	579	184	192	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	HIS	-	expression tag	UNP Q07011
B	182	HIS	-	expression tag	UNP Q07011
B	183	HIS	-	expression tag	UNP Q07011
B	184	HIS	-	expression tag	UNP Q07011
B	185	HIS	-	expression tag	UNP Q07011
B	186	HIS	-	expression tag	UNP Q07011
D	181	HIS	-	expression tag	UNP Q07011
D	182	HIS	-	expression tag	UNP Q07011
D	183	HIS	-	expression tag	UNP Q07011
D	184	HIS	-	expression tag	UNP Q07011
D	185	HIS	-	expression tag	UNP Q07011
D	186	HIS	-	expression tag	UNP Q07011
F	181	HIS	-	expression tag	UNP Q07011
F	182	HIS	-	expression tag	UNP Q07011
F	183	HIS	-	expression tag	UNP Q07011
F	184	HIS	-	expression tag	UNP Q07011
F	185	HIS	-	expression tag	UNP Q07011
F	186	HIS	-	expression tag	UNP Q07011
H	181	HIS	-	expression tag	UNP Q07011
H	182	HIS	-	expression tag	UNP Q07011
H	183	HIS	-	expression tag	UNP Q07011
H	184	HIS	-	expression tag	UNP Q07011
H	185	HIS	-	expression tag	UNP Q07011
H	186	HIS	-	expression tag	UNP Q07011
J	181	HIS	-	expression tag	UNP Q07011
J	182	HIS	-	expression tag	UNP Q07011
J	183	HIS	-	expression tag	UNP Q07011
J	184	HIS	-	expression tag	UNP Q07011
J	185	HIS	-	expression tag	UNP Q07011

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Chain	Residue	Modelled	Actual	Comment	Reference
J	186	HIS	-	expression tag	UNP Q07011
L	181	HIS	-	expression tag	UNP Q07011
L	182	HIS	-	expression tag	UNP Q07011
L	183	HIS	-	expression tag	UNP Q07011
L	184	HIS	-	expression tag	UNP Q07011
L	185	HIS	-	expression tag	UNP Q07011
L	186	HIS	-	expression tag	UNP Q07011
N	181	HIS	-	expression tag	UNP Q07011
N	182	HIS	-	expression tag	UNP Q07011
N	183	HIS	-	expression tag	UNP Q07011
N	184	HIS	-	expression tag	UNP Q07011
N	185	HIS	-	expression tag	UNP Q07011
N	186	HIS	-	expression tag	UNP Q07011
P	181	HIS	-	expression tag	UNP Q07011
P	182	HIS	-	expression tag	UNP Q07011
P	183	HIS	-	expression tag	UNP Q07011
P	184	HIS	-	expression tag	UNP Q07011
P	185	HIS	-	expression tag	UNP Q07011
P	186	HIS	-	expression tag	UNP Q07011
R	181	HIS	-	expression tag	UNP Q07011
R	182	HIS	-	expression tag	UNP Q07011
R	183	HIS	-	expression tag	UNP Q07011
R	184	HIS	-	expression tag	UNP Q07011
R	185	HIS	-	expression tag	UNP Q07011
R	186	HIS	-	expression tag	UNP Q07011
T	181	HIS	-	expression tag	UNP Q07011
T	182	HIS	-	expression tag	UNP Q07011
T	183	HIS	-	expression tag	UNP Q07011
T	184	HIS	-	expression tag	UNP Q07011
T	185	HIS	-	expression tag	UNP Q07011
T	186	HIS	-	expression tag	UNP Q07011
V	181	HIS	-	expression tag	UNP Q07011
V	182	HIS	-	expression tag	UNP Q07011
V	183	HIS	-	expression tag	UNP Q07011
V	184	HIS	-	expression tag	UNP Q07011
V	185	HIS	-	expression tag	UNP Q07011
V	186	HIS	-	expression tag	UNP Q07011
X	181	HIS	-	expression tag	UNP Q07011
X	182	HIS	-	expression tag	UNP Q07011
X	183	HIS	-	expression tag	UNP Q07011
X	184	HIS	-	expression tag	UNP Q07011
X	185	HIS	-	expression tag	UNP Q07011

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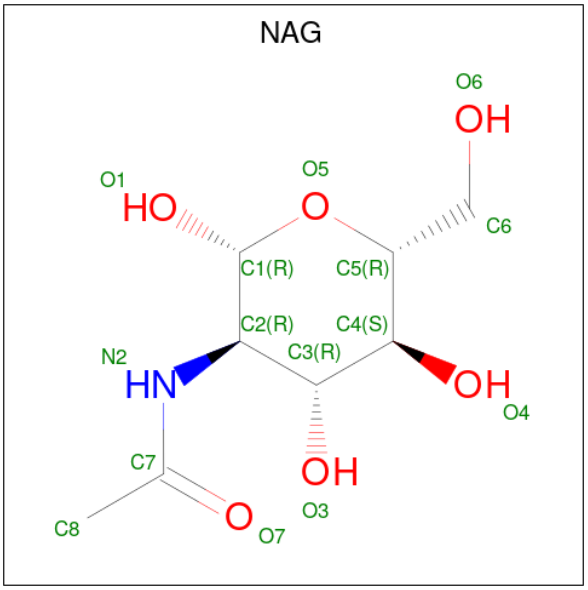
Chain	Residue	Modelled	Actual	Comment	Reference
X	186	HIS	-	expression tag	UNP Q07011

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	N	1	Total	C	N	O	0	0
			14	8	1	5		
3	P	1	Total	C	N	O	0	0
			14	8	1	5		
3	R	1	Total	C	N	O	0	0
			14	8	1	5		
3	T	1	Total	C	N	O	0	0
			14	8	1	5		

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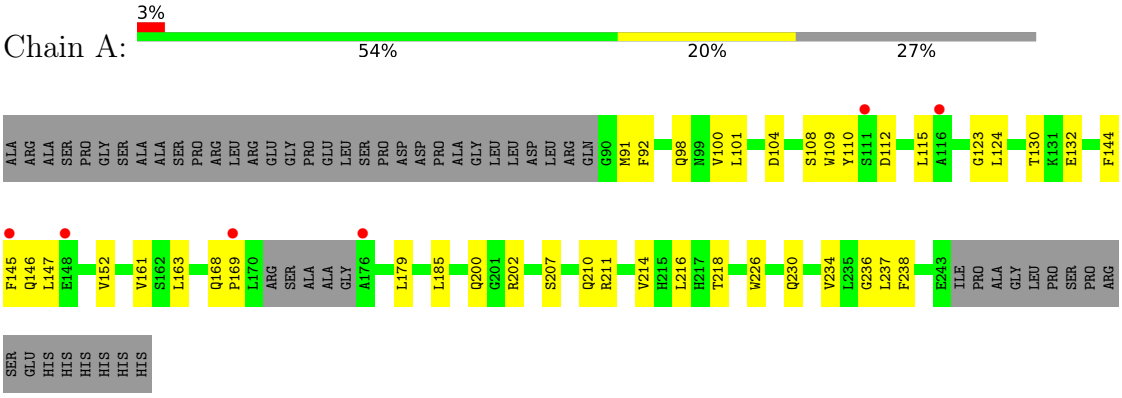
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total	C	N	O	0	0
			14	8	1	5		
3	X	1	Total	C	N	O	0	0
			14	8	1	5		

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.

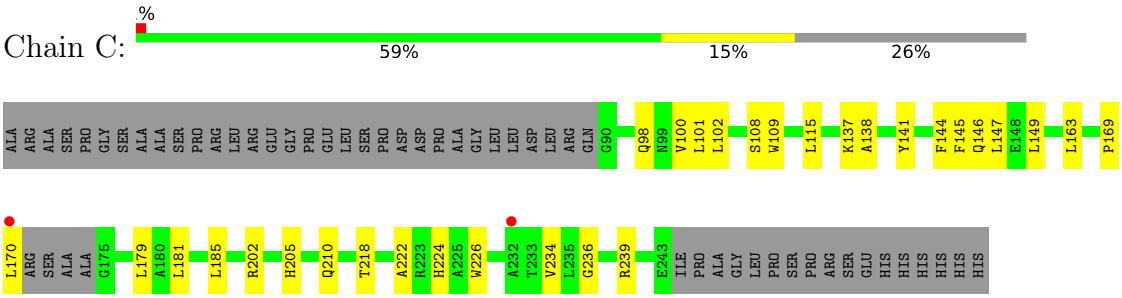
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain A:



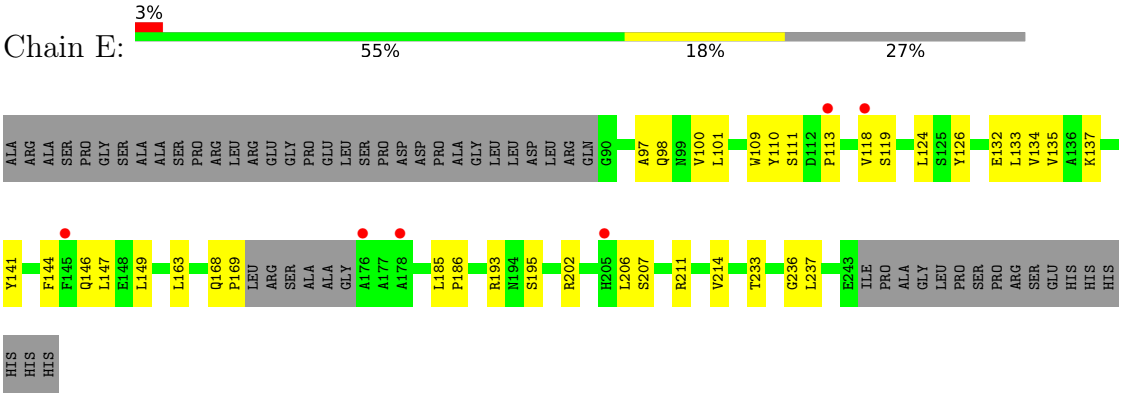
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain C:



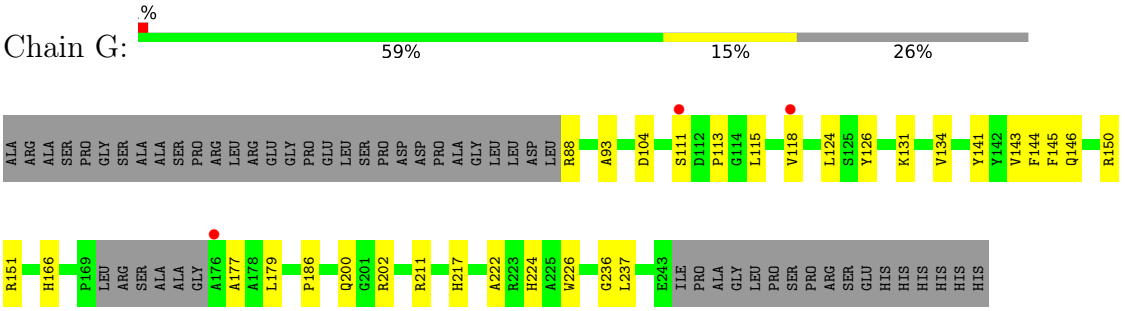
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain E:



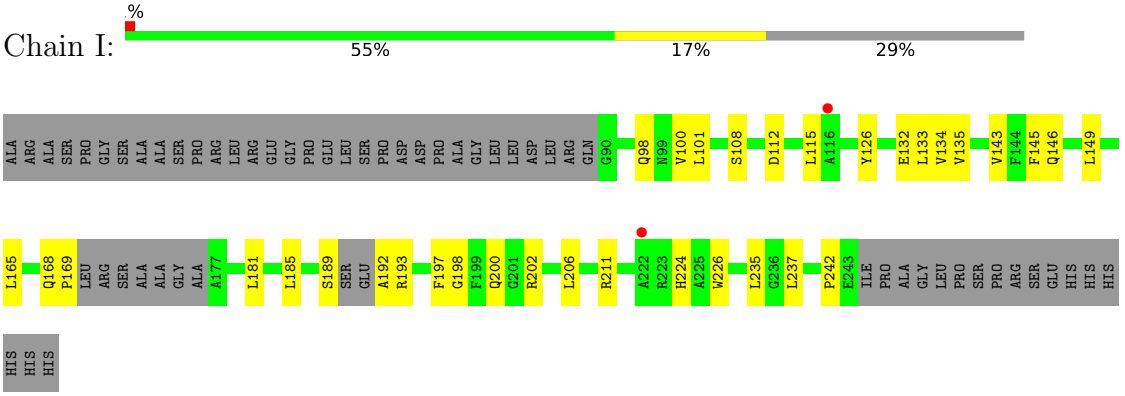
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain G:



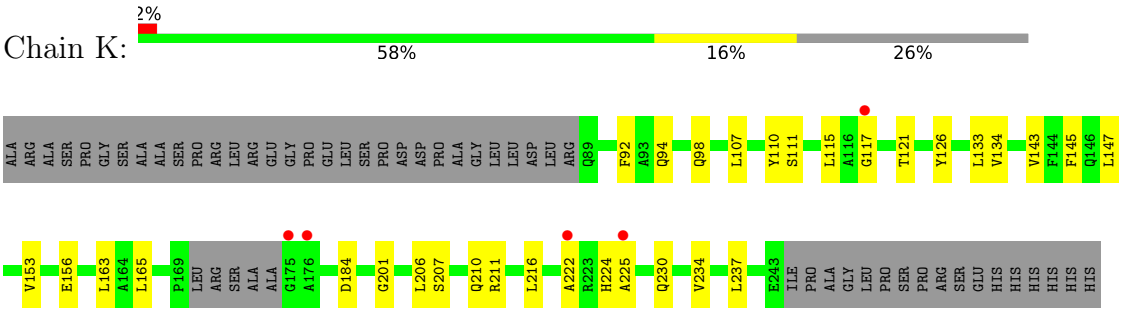
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain I:



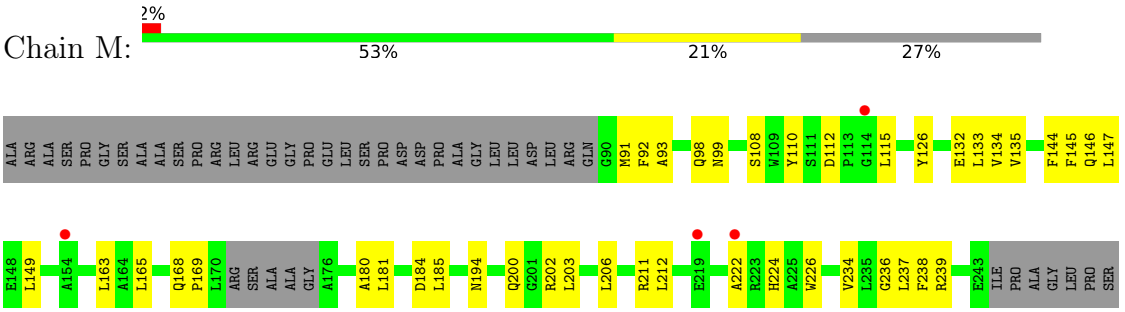
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain K:



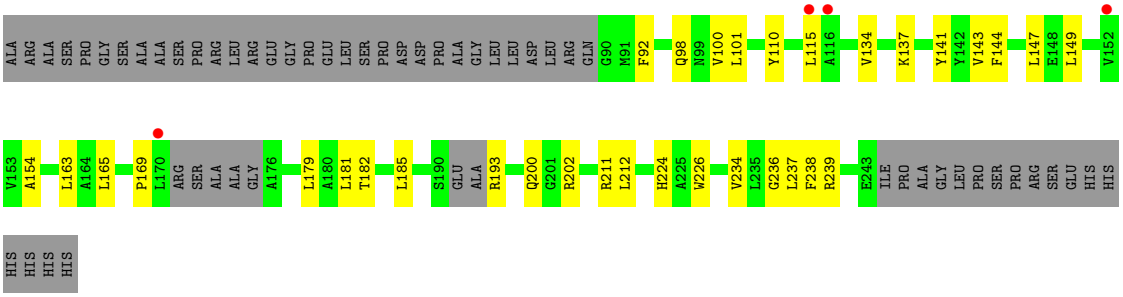
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain M:



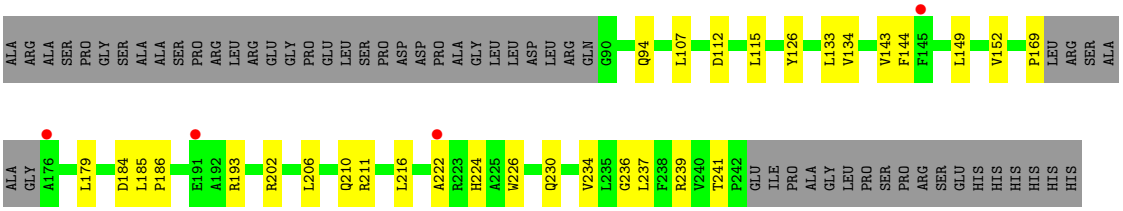
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain O:



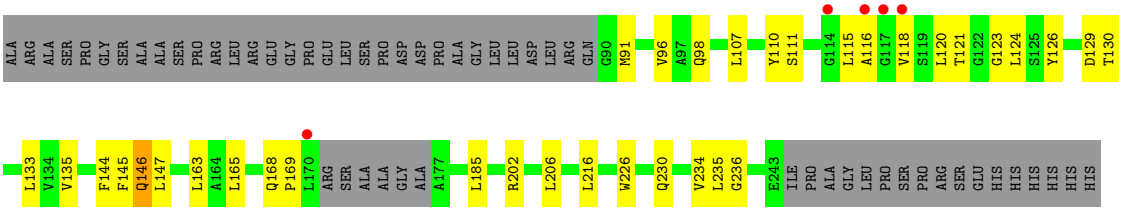
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain Q:



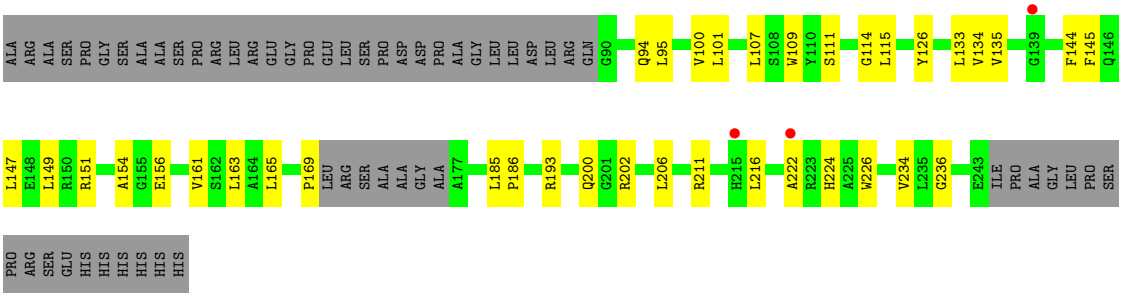
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain S:



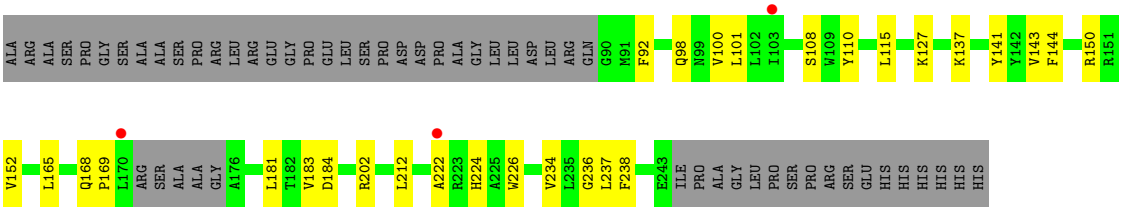
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain U:



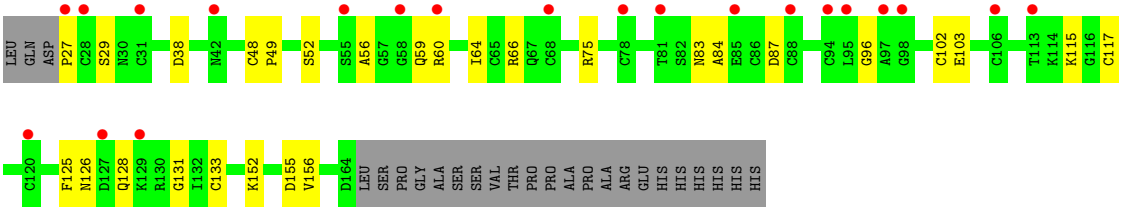
• Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain W:



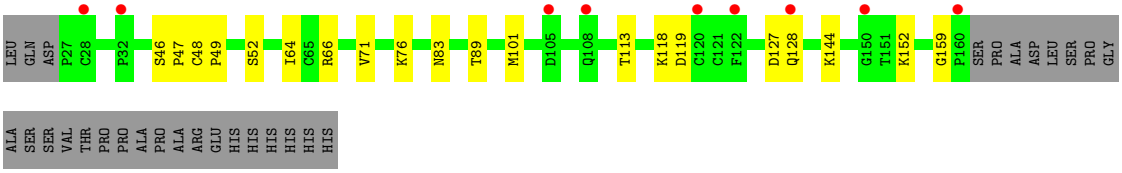
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain B:



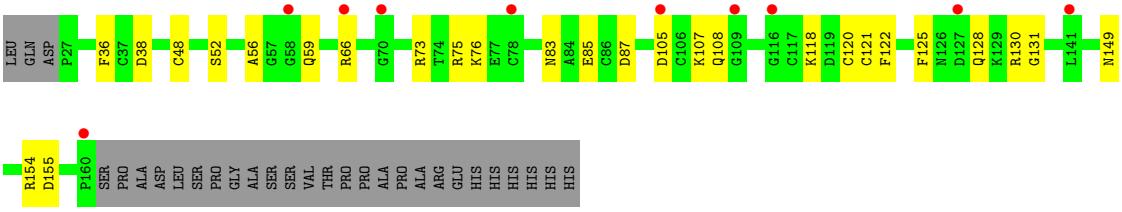
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain D:



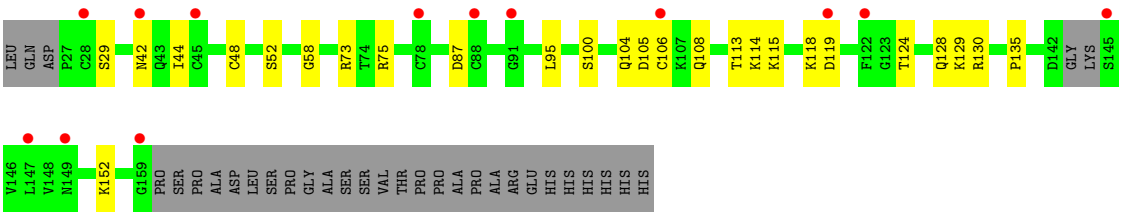
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain F:



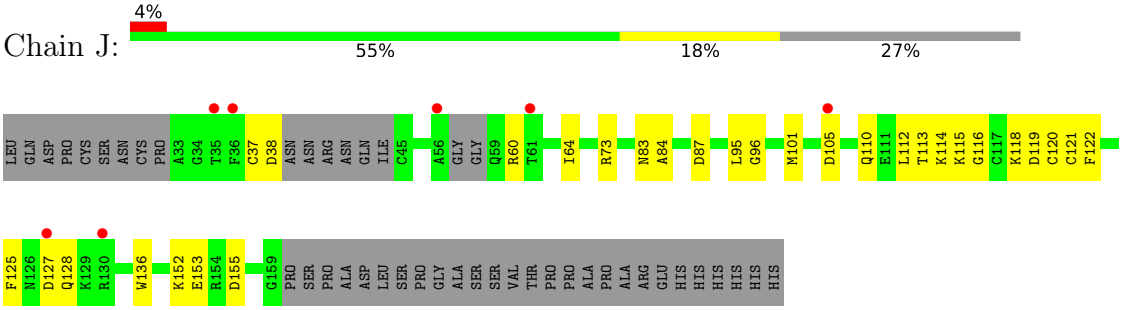
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain H:



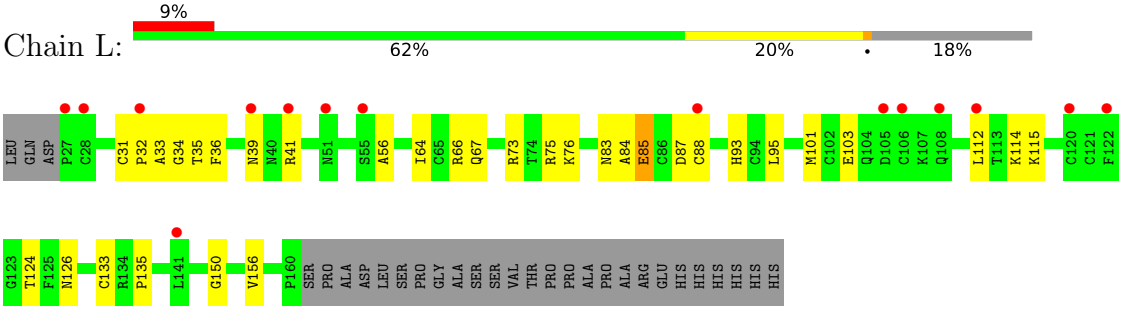
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain J:



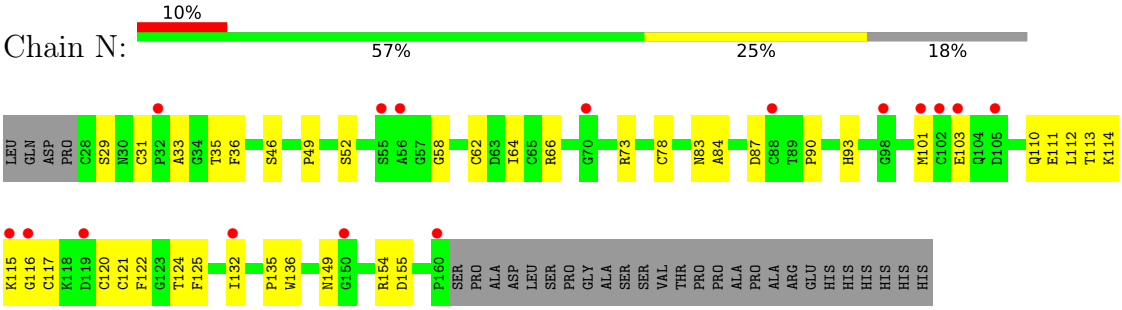
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain L:



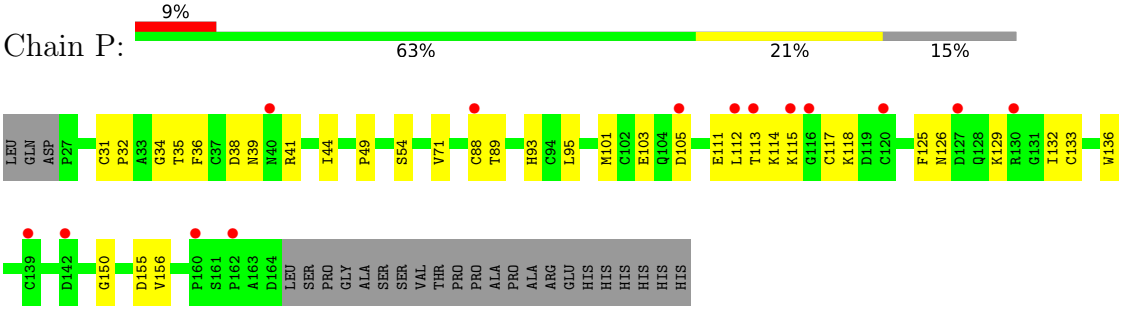
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain N:



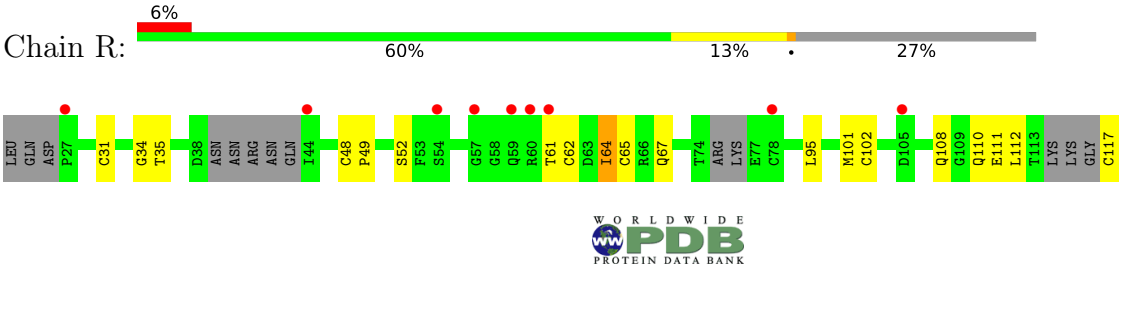
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain P:



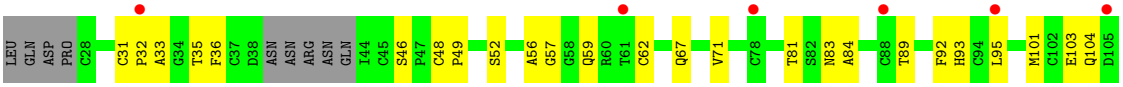
• Molecule 2: Tumor necrosis factor receptor superfamily member 9

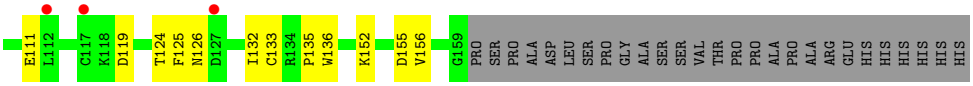
Chain R:



• Molecule 2: Tumor necrosis factor receptor superfamily member 9

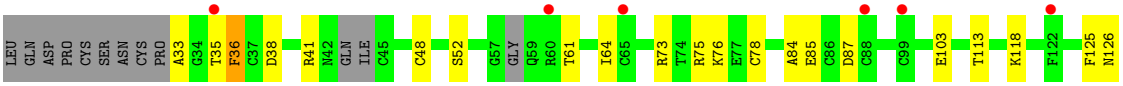
Chain T:

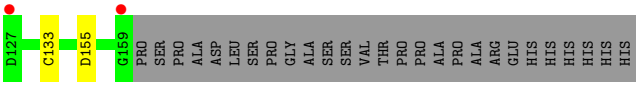




• Molecule 2: Tumor necrosis factor receptor superfamily member 9

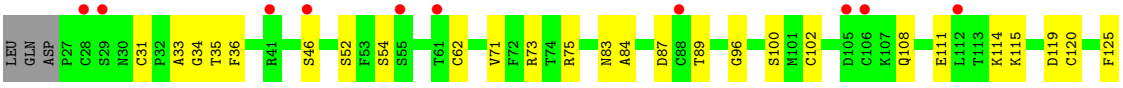
Chain V:

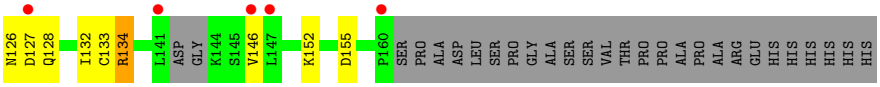




• Molecule 2: Tumor necrosis factor receptor superfamily member 9

Chain X:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	126.09Å 137.19Å 140.32Å 90.00° 111.80° 90.00°	Depositor
Resolution (Å)	44.67 – 3.39 44.67 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.67-3.39) 98.7 (44.67-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.264 , 0.293 0.263 , 0.292	Depositor DCC
R_{free} test set	3101 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	25073	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG

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	0.11	0/1143	0.34	0/1553
1	C	0.14	0/1147	0.40	0/1558
1	E	0.10	0/1135	0.34	0/1542
1	G	0.11	0/1155	0.36	0/1568
1	I	0.10	0/1114	0.33	0/1512
1	K	0.10	0/1148	0.34	0/1559
1	M	0.11	0/1143	0.33	0/1553
1	O	0.10	0/1128	0.32	0/1531
1	Q	0.10	0/1126	0.32	0/1530
1	S	0.22	0/1138	0.34	0/1546
1	U	0.10	0/1130	0.33	0/1535
1	W	0.11	0/1143	0.34	0/1553
2	B	0.23	0/1032	0.48	0/1387
2	D	0.14	0/1004	0.46	0/1348
2	F	0.13	0/1005	0.43	0/1349
2	H	0.14	0/983	0.51	0/1318
2	J	0.13	0/893	0.42	0/1193
2	L	0.14	0/1005	0.48	0/1349
2	N	0.17	0/997	0.52	0/1338
2	P	0.18	0/1032	0.51	0/1387
2	R	0.30	0/882	0.54	1/1182 (0.1%)
2	T	0.14	0/944	0.44	0/1264
2	V	0.16	0/932	0.50	2/1245 (0.2%)
2	X	0.18	0/992	0.46	0/1330
All	All	0.15	0/25351	0.41	3/34230 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	64	ILE	CB-CA-C	-7.09	102.12	111.13
2	V	36	PHE	CA-C-N	5.30	128.12	120.38
2	V	36	PHE	C-N-CA	5.30	128.12	120.38

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	1120	0	1130	33	0
1	C	1124	0	1133	24	0
1	E	1112	0	1119	26	0
1	G	1132	0	1140	20	0
1	I	1092	0	1102	22	0
1	K	1125	0	1130	21	0
1	M	1120	0	1130	31	0
1	O	1106	0	1118	23	0
1	Q	1103	0	1113	24	0
1	S	1115	0	1125	27	0
1	U	1107	0	1114	29	0
1	W	1120	0	1130	20	0
2	B	1015	0	936	18	0
2	D	988	0	915	12	0
2	F	989	0	915	16	0
2	H	969	0	891	16	0
2	J	882	0	818	22	0
2	L	989	0	915	26	0
2	N	982	0	907	29	0
2	P	1015	0	936	23	0
2	R	871	0	787	18	0
2	T	931	0	860	25	0
2	V	921	0	852	15	0
2	X	977	0	907	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	D	14	0	13	0	0
3	F	14	0	13	0	0
3	H	14	0	13	0	0
3	J	14	0	13	0	0
3	L	14	0	13	0	0
3	N	14	0	13	0	0
3	P	14	0	13	0	0
3	R	14	0	13	0	0
3	T	14	0	13	0	0
3	V	14	0	13	0	0
3	X	14	0	13	1	0
All	All	25073	0	24279	489	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 10.

All (489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PRO:HD2	1:C:210:GLN:HE21	1.49	0.78
1:C:115:LEU:HD12	2:D:64:ILE:HG12	1.70	0.74
2:T:31:CYS:HB2	2:T:35:THR:HG21	1.70	0.73
2:R:64:ILE:HG22	2:R:65:CYS:N	2.01	0.73
1:K:115:LEU:HD23	2:L:64:ILE:HG12	1.70	0.72
1:M:194:ASN:ND2	2:N:101:MET:SD	2.63	0.72
1:U:193:ARG:NH1	1:W:184:ASP:OD1	2.22	0.72
2:L:75:ARG:HB3	2:L:85:GLU:HB3	1.72	0.71
2:V:75:ARG:HD3	2:V:85:GLU:HG2	1.72	0.70
1:M:115:LEU:HD12	2:N:64:ILE:HG12	1.72	0.70
1:A:168:GLN:HB2	1:A:169:PRO:HD3	1.73	0.69
2:H:75:ARG:NE	2:H:87:ASP:OD2	2.20	0.69
1:M:112:ASP:HB3	1:M:115:LEU:HD23	1.74	0.69
1:A:132:GLU:OE1	1:A:168:GLN:HG3	1.93	0.69
1:S:230:GLN:HE22	2:T:67:GLN:H	1.41	0.69
1:I:115:LEU:HD12	2:J:64:ILE:HG12	1.73	0.68
1:M:234:VAL:HG21	1:O:202:ARG:HH21	1.57	0.68
2:L:75:ARG:NE	2:L:87:ASP:OD2	2.23	0.68
1:G:202:ARG:HH21	1:K:234:VAL:HG21	1.58	0.68
1:A:168:GLN:HB2	1:A:211:ARG:HB2	1.74	0.68
1:M:149:LEU:HD22	1:M:185:LEU:HD21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:GLN:NE2	1:K:201:GLY:O	2.26	0.67
1:A:115:LEU:HD12	2:B:64:ILE:HG12	1.77	0.67
1:A:202:ARG:HH21	1:C:234:VAL:HG21	1.59	0.67
1:C:205:HIS:NE2	1:E:119:SER:OG	2.28	0.66
2:J:95:LEU:HD11	2:J:116:GLY:H	1.61	0.66
1:M:126:TYR:HA	1:M:133:LEU:HA	1.78	0.65
2:F:149:ASN:O	2:F:154:ARG:NH2	2.28	0.65
2:T:124:THR:HA	2:T:135:PRO:HA	1.78	0.65
2:R:64:ILE:CG2	2:R:65:CYS:N	2.60	0.64
2:X:108:GLN:NE2	2:X:127:ASP:OD1	2.31	0.64
2:R:64:ILE:HG22	2:R:65:CYS:O	1.99	0.63
2:N:66:ARG:HG3	2:N:83:ASN:HD21	1.64	0.63
2:L:114:LYS:H	2:L:114:LYS:HD2	1.64	0.62
1:U:134:VAL:HG22	1:U:211:ARG:HG3	1.79	0.62
1:M:147:LEU:HD22	1:M:163:LEU:HG	1.80	0.62
2:H:73:ARG:N	2:H:87:ASP:O	2.32	0.62
2:T:32:PRO:HA	2:T:57:GLY:HA2	1.80	0.62
1:U:149:LEU:HD22	1:U:185:LEU:HD21	1.80	0.62
2:J:113:THR:OG1	2:J:118:LYS:N	2.29	0.62
2:N:112:LEU:HA	2:N:117:CYS:HA	1.82	0.62
2:X:126:ASN:HB2	2:X:133:CYS:HA	1.81	0.62
2:F:75:ARG:NE	2:F:87:ASP:OD2	2.26	0.61
2:X:34:GLY:O	2:X:54:SER:OG	2.16	0.61
1:Q:149:LEU:HD22	1:Q:185:LEU:HD21	1.82	0.61
1:E:132:GLU:OE2	1:E:168:GLN:HG3	2.01	0.61
1:G:134:VAL:HG22	1:G:211:ARG:HG3	1.82	0.61
1:A:144:PHE:CZ	1:A:236:GLY:HA3	2.36	0.61
1:W:168:GLN:HB2	1:W:169:PRO:HD3	1.83	0.61
1:M:165:LEU:HD11	1:M:212:LEU:HD23	1.83	0.60
1:K:156:GLU:OE1	1:K:224:HIS:NE2	2.35	0.60
1:S:146:GLN:HE22	1:U:202:ARG:HB3	1.67	0.60
2:D:66:ARG:HG3	2:D:83:ASN:HD21	1.67	0.60
2:N:31:CYS:HB3	2:N:35:THR:HG21	1.82	0.60
2:X:146:VAL:HG21	3:X:301:NAG:H81	1.82	0.60
1:A:124:LEU:HD21	1:A:237:LEU:HD22	1.85	0.59
1:E:118:VAL:HG23	1:E:119:SER:H	1.66	0.59
2:T:119:ASP:OD2	2:T:152:LYS:HD3	2.02	0.59
2:F:66:ARG:HG3	2:F:83:ASN:HD21	1.66	0.59
1:I:189:SER:HB2	1:I:192:ALA:HB2	1.83	0.59
2:H:42:ASN:HB2	2:H:44:ILE:HG23	1.83	0.59
1:K:107:LEU:HD21	1:K:216:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:36:PHE:HB3	2:X:62:CYS:SG	2.41	0.59
1:A:145:PHE:HE2	1:A:163:LEU:HB3	1.67	0.58
2:L:31:CYS:HB3	2:L:35:THR:HB	1.84	0.58
2:L:33:ALA:O	2:L:35:THR:HG23	2.03	0.58
1:E:186:PRO:HG2	1:E:193:ARG:HB2	1.85	0.58
2:F:118:LYS:HG3	2:F:120:CYS:H	1.68	0.58
2:N:111:GLU:OE2	2:N:132:ILE:HG23	2.02	0.58
1:Q:115:LEU:HD22	2:R:49:PRO:HG2	1.86	0.58
1:S:115:LEU:HD21	2:T:49:PRO:HG2	1.85	0.58
1:C:147:LEU:HD22	1:C:163:LEU:HG	1.86	0.58
1:C:145:PHE:HB3	1:C:181:LEU:HD12	1.86	0.58
2:P:32:PRO:O	2:P:35:THR:OG1	2.14	0.58
1:W:144:PHE:CZ	1:W:236:GLY:HA3	2.38	0.58
2:F:73:ARG:N	2:F:87:ASP:O	2.27	0.57
2:P:105:ASP:OD2	2:P:129:LYS:HB3	2.04	0.57
1:O:144:PHE:CZ	1:O:236:GLY:HA3	2.39	0.57
1:S:234:VAL:HG21	1:U:202:ARG:HH21	1.70	0.57
2:X:119:ASP:OD2	2:X:152:LYS:HD3	2.05	0.57
1:E:147:LEU:HD22	1:E:163:LEU:HG	1.87	0.57
2:R:31:CYS:HB3	2:R:35:THR:HG21	1.87	0.57
1:O:110:TYR:HB3	1:O:115:LEU:HD23	1.86	0.56
2:L:73:ARG:N	2:L:87:ASP:O	2.34	0.56
1:O:143:VAL:HG22	1:O:237:LEU:HG	1.87	0.56
1:Q:222:ALA:C	1:Q:224:HIS:H	2.13	0.56
2:T:33:ALA:HB1	2:T:81:THR:HG22	1.88	0.56
1:A:112:ASP:HB3	1:A:115:LEU:HD23	1.88	0.56
1:S:118:VAL:HB	1:S:120:LEU:HG	1.87	0.56
1:E:169:PRO:HG3	1:E:211:ARG:HH21	1.70	0.56
2:L:83:ASN:OD1	2:L:84:ALA:N	2.39	0.56
1:S:96:VAL:HG21	1:S:116:ALA:HB3	1.88	0.56
1:O:234:VAL:HG21	1:Q:202:ARG:HH21	1.71	0.55
2:L:76:LYS:HB3	2:L:85:GLU:HB2	1.89	0.55
2:J:37:CYS:SG	2:J:38:ASP:N	2.79	0.55
1:A:234:VAL:HG21	1:E:202:ARG:HH21	1.71	0.55
1:E:144:PHE:CZ	1:E:236:GLY:HA3	2.41	0.55
1:W:143:VAL:HG22	1:W:237:LEU:HG	1.89	0.55
1:M:203:LEU:O	1:Q:94:GLN:NE2	2.37	0.55
1:M:144:PHE:CZ	1:M:236:GLY:HA3	2.42	0.55
1:Q:134:VAL:HG22	1:Q:211:ARG:HG3	1.89	0.55
2:J:96:GLY:HA2	2:J:115:LYS:HD2	1.88	0.55
1:K:206:LEU:HD22	1:K:210:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:VAL:O	2:D:89:THR:OG1	2.25	0.54
1:E:134:VAL:HG22	1:E:211:ARG:HG3	1.89	0.54
2:B:155:ASP:OD1	2:B:156:VAL:N	2.41	0.54
1:G:146:GLN:HE22	1:I:202:ARG:HB3	1.71	0.54
1:S:126:TYR:HA	1:S:133:LEU:HA	1.90	0.54
2:X:31:CYS:HB3	2:X:35:THR:HG21	1.90	0.54
2:B:126:ASN:HB2	2:B:133:CYS:HA	1.89	0.54
1:G:151:ARG:NH2	1:G:186:PRO:O	2.39	0.54
1:E:97:ALA:HB3	1:E:233:THR:HB	1.89	0.54
1:Q:206:LEU:HD22	1:Q:210:GLN:HG2	1.88	0.54
1:S:144:PHE:CZ	1:S:236:GLY:HA3	2.42	0.54
1:A:91:MET:HE1	1:A:123:GLY:HA3	1.90	0.54
1:W:110:TYR:HD2	1:W:115:LEU:HD13	1.73	0.54
2:J:60:ARG:NH1	1:K:207:SER:OG	2.42	0.53
2:N:113:THR:N	2:N:116:GLY:O	2.30	0.53
2:J:105:ASP:N	2:J:105:ASP:OD1	2.41	0.53
1:E:124:LEU:HD21	1:E:237:LEU:HD22	1.91	0.53
1:A:147:LEU:HD13	1:A:163:LEU:HD11	1.89	0.53
1:M:112:ASP:OD2	2:N:49:PRO:HB3	2.08	0.53
2:T:33:ALA:O	2:T:35:THR:HG23	2.09	0.53
2:R:112:LEU:HA	2:R:117:CYS:SG	2.49	0.53
2:V:126:ASN:HB2	2:V:133:CYS:HA	1.90	0.53
1:G:222:ALA:C	1:G:224:HIS:H	2.17	0.52
2:N:125:PHE:HB3	2:N:136:TRP:CD1	2.44	0.52
2:R:128:GLN:OE1	1:U:211:ARG:NH1	2.42	0.52
1:C:144:PHE:CZ	1:C:236:GLY:HA3	2.44	0.52
1:S:147:LEU:HD13	1:S:163:LEU:HD11	1.90	0.52
1:C:222:ALA:C	1:C:224:HIS:H	2.18	0.52
1:Q:144:PHE:CZ	1:Q:236:GLY:HA3	2.44	0.52
1:M:145:PHE:HB3	1:M:181:LEU:HD12	1.92	0.52
2:N:31:CYS:HB3	2:N:35:THR:CG2	2.39	0.52
2:N:93:HIS:HE1	2:N:103:GLU:HB2	1.74	0.52
2:X:35:THR:HA	2:X:46:SER:O	2.10	0.52
2:L:124:THR:HG22	2:L:135:PRO:HA	1.91	0.52
1:U:169:PRO:HD3	1:U:211:ARG:HE	1.75	0.52
1:A:147:LEU:HD22	1:A:163:LEU:HG	1.92	0.52
2:L:39:ASN:C	2:L:41:ARG:H	2.18	0.52
1:O:193:ARG:HD2	1:Q:184:ASP:HB2	1.92	0.52
2:R:110:GLN:HA	2:R:120:CYS:H	1.75	0.52
2:V:76:LYS:H	2:V:85:GLU:HB3	1.75	0.52
1:U:222:ALA:C	1:U:224:HIS:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:165:LEU:HD11	1:W:212:LEU:HD23	1.92	0.52
2:X:75:ARG:NH2	2:X:87:ASP:OD2	2.38	0.52
2:F:76:LYS:HB3	2:F:85:GLU:HB2	1.92	0.51
1:U:145:PHE:HZ	1:U:165:LEU:HB2	1.75	0.51
2:N:35:THR:HA	2:N:46:SER:O	2.10	0.51
2:L:34:GLY:C	2:L:35:THR:HG1	2.17	0.51
1:Q:126:TYR:HA	1:Q:133:LEU:HA	1.93	0.51
2:D:113:THR:OG1	2:D:118:LYS:N	2.41	0.51
1:K:147:LEU:HD13	1:K:163:LEU:HD11	1.92	0.51
1:O:115:LEU:HD13	2:P:49:PRO:HG2	1.92	0.51
2:B:38:ASP:OD1	2:B:38:ASP:N	2.44	0.51
1:W:222:ALA:C	1:W:224:HIS:H	2.20	0.50
2:H:105:ASP:OD2	2:H:130:ARG:HG2	2.11	0.50
1:U:111:SER:HB3	1:U:126:TYR:CD2	2.47	0.50
2:V:78:CYS:HB2	2:V:84:ALA:HB2	1.92	0.50
2:L:93:HIS:HE1	2:L:103:GLU:HB2	1.77	0.50
1:M:135:VAL:HG21	1:M:206:LEU:HD13	1.92	0.50
1:U:144:PHE:CZ	1:U:236:GLY:HA3	2.46	0.50
1:A:132:GLU:OE1	1:A:211:ARG:HD3	2.12	0.50
2:H:114:LYS:O	2:H:115:LYS:HB2	2.12	0.50
2:R:34:GLY:HA2	2:R:48:CYS:SG	2.51	0.50
2:T:93:HIS:ND1	2:T:103:GLU:O	2.41	0.50
1:K:230:GLN:OE1	2:L:67:GLN:N	2.41	0.50
1:U:115:LEU:HD12	2:V:64:ILE:HG13	1.94	0.50
2:J:112:LEU:HD22	2:J:114:LYS:HD3	1.94	0.50
1:Q:143:VAL:HG22	1:Q:237:LEU:HG	1.93	0.50
2:T:71:VAL:O	2:T:89:THR:OG1	2.30	0.50
1:U:154:ALA:HB3	2:V:103:GLU:HG2	1.93	0.50
1:W:137:LYS:O	1:W:141:TYR:OH	2.28	0.50
2:D:119:ASP:OD2	2:D:152:LYS:HD3	2.11	0.50
1:M:147:LEU:HD13	1:M:163:LEU:HD11	1.93	0.50
2:P:31:CYS:HB3	2:P:35:THR:HB	1.93	0.50
1:S:146:GLN:OE1	1:U:200:GLN:NE2	2.45	0.50
2:T:35:THR:HA	2:T:46:SER:O	2.12	0.50
2:X:52:SER:HB2	2:X:62:CYS:HB3	1.94	0.50
1:C:202:ARG:HD2	1:E:146:GLN:OE1	2.12	0.50
2:P:126:ASN:HB2	2:P:133:CYS:HA	1.93	0.50
1:O:179:LEU:HD11	1:O:200:GLN:HG2	1.93	0.49
2:N:33:ALA:O	2:N:35:THR:HG23	2.12	0.49
2:L:126:ASN:HB2	2:L:133:CYS:HA	1.93	0.49
1:G:146:GLN:NE2	1:I:202:ARG:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:114:LYS:O	2:N:115:LYS:HB2	2.12	0.49
1:O:154:ALA:HB3	2:P:103:GLU:HG2	1.95	0.49
1:S:129:ASP:OD2	1:S:130:THR:HG23	2.13	0.49
1:C:170:LEU:C	1:C:170:LEU:HD12	2.38	0.49
1:Q:169:PRO:HD3	1:Q:211:ARG:HE	1.77	0.49
2:X:33:ALA:O	2:X:35:THR:HG23	2.13	0.49
2:T:36:PHE:HB3	2:T:62:CYS:SG	2.53	0.49
1:U:126:TYR:HA	1:U:133:LEU:HA	1.93	0.49
2:T:155:ASP:OD1	2:T:156:VAL:N	2.45	0.49
1:M:146:GLN:OE1	1:O:202:ARG:HB3	2.12	0.49
2:X:111:GLU:OE2	2:X:132:ILE:HG23	2.13	0.49
2:H:108:GLN:HG2	2:H:128:GLN:H	1.77	0.49
1:M:224:HIS:C	1:M:226:TRP:H	2.20	0.49
2:R:95:LEU:HD22	2:R:101:MET:HE3	1.95	0.49
2:F:36:PHE:CE2	2:F:38:ASP:HB3	2.49	0.48
1:E:147:LEU:HD13	1:E:163:LEU:HD11	1.94	0.48
1:I:149:LEU:HD22	1:I:185:LEU:HD21	1.94	0.48
2:P:113:THR:OG1	2:P:118:LYS:N	2.43	0.48
1:Q:107:LEU:HD21	1:Q:216:LEU:HD13	1.95	0.48
2:X:71:VAL:O	2:X:89:THR:OG1	2.32	0.48
1:C:149:LEU:HD22	1:C:185:LEU:HD21	1.95	0.48
2:F:128:GLN:HB3	2:F:131:GLY:HA3	1.94	0.48
1:E:149:LEU:HD22	1:E:185:LEU:HD21	1.95	0.48
2:J:127:ASP:OD1	2:J:127:ASP:N	2.45	0.48
2:N:29:SER:CB	2:N:58:GLY:HA3	2.43	0.48
2:B:75:ARG:HE	2:B:87:ASP:CG	2.22	0.48
1:K:134:VAL:HG22	1:K:211:ARG:HG3	1.96	0.48
2:P:125:PHE:CE2	2:P:155:ASP:HB2	2.48	0.48
1:A:185:LEU:HD13	1:A:226:TRP:CG	2.49	0.48
2:J:83:ASN:OD1	2:J:84:ALA:N	2.46	0.48
2:X:114:LYS:O	2:X:115:LYS:HB2	2.13	0.48
1:C:138:ALA:O	1:C:239:ARG:NH2	2.47	0.48
2:J:119:ASP:OD2	2:J:152:LYS:HD3	2.14	0.48
2:J:121:CYS:SG	2:J:122:PHE:N	2.87	0.48
2:J:125:PHE:CE2	2:J:155:ASP:HB2	2.48	0.48
2:L:31:CYS:HB3	2:L:35:THR:CG2	2.44	0.48
1:A:161:VAL:HG13	1:A:218:THR:HB	1.96	0.47
1:G:145:PHE:N	1:G:200:GLN:O	2.41	0.47
1:I:100:VAL:HG13	1:I:101:LEU:H	1.79	0.47
1:M:184:ASP:HB2	1:Q:193:ARG:NH1	2.29	0.47
1:O:134:VAL:HG22	1:O:211:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:LEU:HG	1:I:200:GLN:HB3	1.95	0.47
2:L:95:LEU:HD22	2:L:101:MET:HE3	1.96	0.47
2:R:111:GLU:OE2	2:R:132:ILE:HG23	2.14	0.47
1:U:145:PHE:CZ	1:U:165:LEU:HB2	2.49	0.47
1:C:115:LEU:HD22	2:D:49:PRO:HG2	1.97	0.47
2:J:125:PHE:HB3	2:J:136:TRP:HE1	1.79	0.47
1:O:149:LEU:HD22	1:O:185:LEU:HD21	1.95	0.47
1:Q:186:PRO:HG3	1:Q:193:ARG:HB2	1.96	0.47
2:R:49:PRO:O	2:R:52:SER:OG	2.31	0.47
1:I:134:VAL:HG22	1:I:211:ARG:HG3	1.96	0.47
2:J:101:MET:HE3	2:J:101:MET:HB2	1.81	0.47
2:D:46:SER:HB2	2:D:47:PRO:HD2	1.97	0.47
2:J:110:GLN:HG2	2:J:119:ASP:HA	1.96	0.47
2:P:39:ASN:C	2:P:41:ARG:H	2.22	0.47
1:U:151:ARG:NH2	1:U:186:PRO:O	2.44	0.47
1:K:153:VAL:HB	1:K:225:ALA:HB2	1.97	0.47
2:N:149:ASN:O	2:N:154:ARG:NH2	2.46	0.47
2:P:95:LEU:HG	2:P:115:LYS:HA	1.95	0.47
2:V:36:PHE:CD1	2:V:61:THR:HA	2.49	0.47
2:V:113:THR:OG1	2:V:118:LYS:N	2.47	0.47
2:V:125:PHE:CE2	2:V:155:ASP:HB2	2.49	0.47
2:H:48:CYS:HB3	2:H:52:SER:OG	2.15	0.47
1:G:111:SER:HB2	1:G:126:TYR:CD2	2.50	0.47
1:Q:112:ASP:HB3	1:Q:115:LEU:HD23	1.97	0.47
1:I:112:ASP:HB3	1:I:115:LEU:HD23	1.97	0.47
2:J:110:GLN:HA	2:J:120:CYS:H	1.80	0.47
1:K:98:GLN:HG3	1:K:110:TYR:CZ	2.49	0.47
1:G:144:PHE:CZ	1:G:236:GLY:HA3	2.49	0.46
2:X:96:GLY:HA2	2:X:115:LYS:HE3	1.97	0.46
1:E:109:TRP:HZ2	1:E:214:VAL:HB	1.80	0.46
2:N:29:SER:HB3	2:N:58:GLY:HA3	1.96	0.46
1:S:168:GLN:HB2	1:S:169:PRO:HD3	1.97	0.46
2:X:35:THR:O	2:X:36:PHE:HD2	1.98	0.46
2:L:95:LEU:HD21	2:L:115:LYS:HD3	1.97	0.46
2:P:34:GLY:N	2:P:54:SER:OG	2.49	0.46
1:E:100:VAL:HG13	1:E:101:LEU:H	1.80	0.46
1:S:185:LEU:HD13	1:S:226:TRP:CG	2.50	0.46
1:U:135:VAL:HG21	1:U:206:LEU:HD13	1.97	0.46
1:W:181:LEU:HD21	1:W:183:VAL:HG23	1.97	0.46
2:H:29:SER:HA	2:H:58:GLY:HA3	1.98	0.46
1:M:145:PHE:CZ	1:M:165:LEU:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:202:ARG:HH21	1:W:234:VAL:HG21	1.80	0.46
1:A:202:ARG:HB3	1:C:146:GLN:OE1	2.15	0.46
1:S:145:PHE:HZ	1:S:165:LEU:HB2	1.81	0.46
2:V:73:ARG:O	2:V:87:ASP:N	2.46	0.46
2:X:31:CYS:HB3	2:X:35:THR:CB	2.46	0.46
1:M:168:GLN:HB2	1:M:169:PRO:HD3	1.98	0.46
1:E:126:TYR:HA	1:E:133:LEU:HA	1.97	0.46
1:G:93:ALA:HB2	1:G:124:LEU:HD23	1.98	0.46
1:K:126:TYR:HA	1:K:133:LEU:HA	1.98	0.46
2:V:38:ASP:OD2	2:V:41:ARG:CZ	2.64	0.46
1:W:92:PHE:HA	1:W:238:PHE:HA	1.98	0.46
1:C:224:HIS:C	1:C:226:TRP:H	2.23	0.46
2:L:93:HIS:CE1	2:L:103:GLU:HB2	2.50	0.46
1:M:92:PHE:HA	1:M:238:PHE:HA	1.96	0.46
2:P:111:GLU:OE2	2:P:132:ILE:HG23	2.15	0.46
1:O:169:PRO:HD3	1:O:211:ARG:HE	1.81	0.45
2:P:35:THR:O	2:P:36:PHE:CD2	2.69	0.45
2:R:108:GLN:H	2:R:108:GLN:HG3	1.51	0.45
1:I:224:HIS:C	1:I:226:TRP:H	2.25	0.45
1:K:94:GLN:NE2	1:K:117:GLY:O	2.45	0.45
2:N:31:CYS:HB3	2:N:35:THR:CB	2.47	0.45
1:G:224:HIS:C	1:G:226:TRP:H	2.24	0.45
2:H:124:THR:HA	2:H:135:PRO:HA	1.98	0.45
1:I:145:PHE:CZ	1:I:165:LEU:HB2	2.52	0.45
1:A:98:GLN:HG3	1:A:110:TYR:CZ	2.51	0.45
2:N:73:ARG:O	2:N:87:ASP:N	2.49	0.45
2:N:73:ARG:HH11	2:N:90:PRO:HD3	1.82	0.45
1:U:95:LEU:HB3	1:U:109:TRP:HB3	1.98	0.45
2:B:125:PHE:CE2	2:B:155:ASP:HB2	2.51	0.45
1:E:137:LYS:HD3	1:E:137:LYS:HA	1.81	0.45
1:M:185:LEU:HD13	1:M:226:TRP:CG	2.51	0.45
1:O:224:HIS:C	1:O:226:TRP:H	2.23	0.45
1:S:230:GLN:NE2	2:T:67:GLN:H	2.10	0.45
1:C:147:LEU:HD13	1:C:163:LEU:HD11	1.97	0.45
1:E:111:SER:HB2	1:E:126:TYR:CD2	2.52	0.45
1:I:145:PHE:HE1	1:I:235:LEU:HD13	1.82	0.45
2:N:124:THR:HA	2:N:135:PRO:HA	1.99	0.45
2:R:48:CYS:HB3	2:R:52:SER:OG	2.17	0.45
1:E:135:VAL:HG21	1:E:206:LEU:HD13	1.98	0.45
2:J:73:ARG:O	2:J:87:ASP:N	2.50	0.45
1:S:145:PHE:HE1	1:S:235:LEU:HD13	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:OD1	2:B:84:ALA:N	2.50	0.45
1:C:98:GLN:NE2	1:C:109:TRP:O	2.45	0.45
2:F:125:PHE:CE2	2:F:155:ASP:HB2	2.52	0.45
2:T:56:ALA:HB3	2:T:59:GLN:HG3	1.98	0.45
1:U:224:HIS:C	1:U:226:TRP:H	2.25	0.45
1:W:150:ARG:NH2	2:X:100:SER:O	2.49	0.45
2:X:83:ASN:OD1	2:X:84:ALA:N	2.50	0.45
1:A:202:ARG:HD2	1:C:146:GLN:HE22	1.79	0.44
2:B:48:CYS:HB3	2:B:52:SER:OG	2.17	0.44
1:C:98:GLN:HB2	1:C:108:SER:HB2	1.99	0.44
2:B:128:GLN:HB3	2:B:131:GLY:H	1.81	0.44
1:C:102:LEU:HG	1:C:218:THR:HG21	1.98	0.44
2:J:114:LYS:O	2:J:115:LYS:HB2	2.17	0.44
1:A:145:PHE:N	1:A:200:GLN:O	2.49	0.44
1:A:152:VAL:O	2:B:102:CYS:N	2.50	0.44
1:K:222:ALA:C	1:K:224:HIS:H	2.25	0.44
2:N:93:HIS:CE1	2:N:103:GLU:HB2	2.51	0.44
2:T:124:THR:HG22	2:T:135:PRO:HG3	1.99	0.44
2:T:126:ASN:HB2	2:T:133:CYS:HA	1.98	0.44
2:B:103:GLU:OE2	2:B:117:CYS:HB2	2.18	0.44
2:N:78:CYS:HB2	2:N:84:ALA:HB2	2.00	0.44
2:X:31:CYS:HB3	2:X:35:THR:CG2	2.47	0.44
1:G:141:TYR:CD2	1:G:237:LEU:HD21	2.53	0.44
1:G:143:VAL:HG22	1:G:237:LEU:HD12	1.99	0.44
1:O:100:VAL:HG13	1:O:101:LEU:H	1.83	0.44
1:A:92:PHE:HA	1:A:238:PHE:HA	2.00	0.44
2:F:105:ASP:OD2	2:F:130:ARG:NE	2.51	0.44
2:L:66:ARG:HG3	2:L:83:ASN:HD21	1.83	0.44
2:T:95:LEU:HD22	2:T:101:MET:HE3	2.00	0.44
1:W:152:VAL:O	2:X:102:CYS:N	2.51	0.44
2:F:121:CYS:SG	2:F:122:PHE:N	2.91	0.44
1:S:98:GLN:HG3	1:S:110:TYR:CZ	2.52	0.44
2:V:33:ALA:O	2:V:35:THR:HG23	2.18	0.44
1:K:145:PHE:CZ	1:K:165:LEU:HB2	2.53	0.44
1:M:222:ALA:C	1:M:224:HIS:H	2.26	0.44
2:T:31:CYS:HB2	2:T:35:THR:CG2	2.44	0.44
2:H:128:GLN:HB3	2:H:129:LYS:H	1.56	0.43
2:L:31:CYS:HB3	2:L:35:THR:CB	2.48	0.43
2:V:35:THR:OG1	2:V:36:PHE:N	2.50	0.43
1:A:130:THR:HB	1:A:132:GLU:OE2	2.18	0.43
2:F:107:LYS:H	2:F:107:LYS:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:98:GLN:HG3	1:O:110:TYR:CZ	2.53	0.43
1:A:104:ASP:HA	1:A:216:LEU:O	2.18	0.43
2:N:125:PHE:CE2	2:N:155:ASP:HB2	2.54	0.43
1:U:94:GLN:HG3	1:U:234:VAL:HG13	2.00	0.43
2:D:144:LYS:HD3	2:D:159:GLY:HA2	1.99	0.43
2:F:56:ALA:HB3	2:F:59:GLN:HG3	2.01	0.43
1:K:111:SER:HB3	1:K:126:TYR:CD2	2.53	0.43
1:K:147:LEU:HD22	1:K:163:LEU:HG	1.99	0.43
1:M:93:ALA:O	1:M:237:LEU:N	2.49	0.43
1:O:147:LEU:HD13	1:O:163:LEU:HD11	2.00	0.43
1:U:114:GLY:O	2:V:61:THR:OG1	2.28	0.43
1:M:180:ALA:O	1:M:200:GLN:NE2	2.51	0.43
2:P:125:PHE:HB3	2:P:136:TRP:CD1	2.53	0.43
1:W:98:GLN:HB3	1:W:108:SER:HB2	2.01	0.43
1:A:207:SER:H	1:A:210:GLN:NE2	2.17	0.43
1:O:185:LEU:HD13	1:O:226:TRP:CG	2.54	0.43
2:R:52:SER:HB2	2:R:62:CYS:HB3	2.01	0.43
2:F:48:CYS:HB3	2:F:52:SER:OG	2.18	0.43
2:N:52:SER:HB2	2:N:62:CYS:HB3	2.00	0.43
1:Q:179:LEU:HD12	1:Q:179:LEU:HA	1.87	0.43
1:S:107:LEU:HD21	1:S:216:LEU:HD13	2.01	0.43
2:T:48:CYS:HB3	2:T:52:SER:OG	2.19	0.43
2:N:35:THR:O	2:N:36:PHE:CD2	2.72	0.43
1:O:165:LEU:HD21	1:O:212:LEU:HD23	2.01	0.43
2:P:71:VAL:O	2:P:89:THR:N	2.47	0.43
1:W:224:HIS:C	1:W:226:TRP:H	2.27	0.43
2:H:95:LEU:HG	2:H:115:LYS:HA	2.00	0.42
1:I:135:VAL:HG21	1:I:206:LEU:HD13	2.00	0.42
1:O:181:LEU:HD23	1:O:182:THR:N	2.34	0.42
1:W:98:GLN:HA	1:W:110:TYR:HE1	1.84	0.42
1:C:145:PHE:CE2	1:C:179:LEU:HB3	2.54	0.42
1:E:193:ARG:NH2	1:E:195:SER:O	2.52	0.42
1:K:143:VAL:HG22	1:K:237:LEU:HD12	2.01	0.42
1:A:98:GLN:HB3	1:A:108:SER:HB2	2.01	0.42
1:G:131:LYS:HE2	1:G:131:LYS:HB2	1.88	0.42
2:N:121:CYS:SG	2:N:122:PHE:N	2.92	0.42
2:P:101:MET:HE3	2:P:101:MET:HB2	1.92	0.42
1:S:145:PHE:CZ	1:S:165:LEU:HB2	2.54	0.42
1:E:98:GLN:HG3	1:E:110:TYR:CZ	2.55	0.42
1:E:113:PRO:HA	1:E:118:VAL:HG21	2.01	0.42
2:X:125:PHE:CE2	2:X:155:ASP:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:134:ARG:H	2:X:134:ARG:HG2	1.64	0.42
1:I:98:GLN:HB3	1:I:108:SER:HB2	2.01	0.42
2:P:112:LEU:HA	2:P:117:CYS:SG	2.60	0.42
2:D:101:MET:HE3	2:D:101:MET:HB2	1.89	0.42
2:H:104:GLN:C	2:H:106:CYS:H	2.26	0.42
1:K:92:PHE:O	1:K:121:THR:OG1	2.32	0.42
2:T:92:PHE:HA	2:T:104:GLN:HA	2.01	0.42
2:P:38:ASP:OD2	2:P:41:ARG:HD2	2.19	0.42
2:F:107:LYS:HD3	2:F:107:LYS:N	2.35	0.42
2:F:107:LYS:HG2	2:F:108:GLN:HB2	2.01	0.42
2:L:95:LEU:HD21	2:L:115:LYS:HA	2.01	0.42
2:P:44:ILE:HD12	2:P:44:ILE:HA	1.92	0.42
1:A:230:GLN:HE22	2:B:66:ARG:HE	1.68	0.42
1:C:145:PHE:HE2	1:C:179:LEU:HB3	1.85	0.42
1:G:166:HIS:HD2	1:G:177:ALA:HA	1.85	0.42
2:J:125:PHE:HB3	2:J:136:TRP:NE1	2.34	0.42
2:B:60:ARG:NH1	1:E:207:SER:OG	2.53	0.42
2:D:48:CYS:HB3	2:D:52:SER:OG	2.20	0.42
2:H:119:ASP:OD2	2:H:152:LYS:HD3	2.19	0.42
2:L:32:PRO:O	2:L:56:ALA:HA	2.19	0.42
1:M:184:ASP:HB2	1:Q:193:ARG:HH11	1.84	0.42
2:V:48:CYS:HB3	2:V:52:SER:OG	2.20	0.42
2:L:150:GLY:H	2:L:156:VAL:HG22	1.85	0.41
2:T:35:THR:O	2:T:36:PHE:CD2	2.73	0.41
1:A:100:VAL:HG13	1:A:101:LEU:H	1.84	0.41
1:A:115:LEU:HD22	2:B:49:PRO:HG2	2.02	0.41
1:G:104:ASP:OD2	1:G:217:HIS:ND1	2.53	0.41
1:M:98:GLN:HG3	1:M:110:TYR:CZ	2.54	0.41
1:M:202:ARG:HH21	1:Q:234:VAL:HG21	1.84	0.41
2:N:110:GLN:HB3	2:N:117:CYS:SG	2.60	0.41
2:P:93:HIS:NE2	2:P:103:GLU:HB2	2.35	0.41
1:S:91:MET:HA	1:S:121:THR:HG21	2.01	0.41
1:S:111:SER:HB3	1:S:126:TYR:CD2	2.55	0.41
1:S:124:LEU:HD11	1:S:135:VAL:HG22	2.01	0.41
1:A:146:GLN:NE2	1:E:202:ARG:HB3	2.35	0.41
1:M:99:ASN:OD1	1:M:108:SER:N	2.50	0.41
1:A:109:TRP:HZ2	1:A:214:VAL:HB	1.85	0.41
1:A:145:PHE:CD1	1:A:179:LEU:HD23	2.55	0.41
2:J:127:ASP:O	2:J:128:GLN:HB2	2.20	0.41
1:S:91:MET:HE1	1:S:123:GLY:HA3	2.03	0.41
2:N:31:CYS:HB3	2:N:35:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:150:GLY:H	2:P:156:VAL:HG22	1.86	0.41
2:T:111:GLU:OE2	2:T:132:ILE:HG23	2.19	0.41
2:B:27:PRO:C	2:B:29:SER:H	2.28	0.41
2:D:127:ASP:O	2:D:128:GLN:HB2	2.20	0.41
2:P:114:LYS:O	2:P:115:LYS:HB2	2.20	0.41
2:B:152:LYS:H	2:B:152:LYS:HD2	1.86	0.41
1:G:150:ARG:NH2	2:H:100:SER:O	2.54	0.41
2:H:113:THR:OG1	2:H:118:LYS:N	2.53	0.41
2:J:127:ASP:HB3	2:J:153:GLU:O	2.21	0.41
1:S:135:VAL:HG21	1:S:206:LEU:HD13	2.02	0.41
1:S:163:LEU:HD23	1:S:163:LEU:HA	1.91	0.41
1:U:107:LEU:HD21	1:U:216:LEU:HD12	2.01	0.41
1:W:110:TYR:CD2	1:W:115:LEU:HD13	2.54	0.41
2:X:127:ASP:O	2:X:128:GLN:HB2	2.21	0.41
1:A:168:GLN:CB	1:A:211:ARG:HB2	2.48	0.41
2:B:56:ALA:O	2:B:59:GLN:HG3	2.21	0.41
1:I:193:ARG:HD2	1:K:184:ASP:CG	2.45	0.41
1:Q:152:VAL:O	2:R:102:CYS:N	2.54	0.41
1:U:151:ARG:NH1	1:U:156:GLU:O	2.53	0.41
2:X:31:CYS:HB3	2:X:35:THR:HB	2.02	0.41
1:C:100:VAL:HG13	1:C:101:LEU:H	1.85	0.41
2:D:76:LYS:HB2	2:D:76:LYS:HE3	1.86	0.41
1:G:88:ARG:HA	1:I:242:PRO:HG3	2.02	0.41
1:G:113:PRO:HA	1:G:118:VAL:HG23	2.02	0.41
1:I:126:TYR:HA	1:I:133:LEU:HA	2.03	0.41
2:L:35:THR:OG1	2:L:36:PHE:N	2.52	0.41
1:M:132:GLU:OE2	1:M:168:GLN:HG3	2.21	0.41
1:M:134:VAL:HG22	1:M:211:ARG:HG3	2.03	0.41
2:P:36:PHE:O	2:P:36:PHE:CD1	2.74	0.41
2:T:125:PHE:HB3	2:T:136:TRP:CD1	2.56	0.41
1:U:149:LEU:HD21	1:U:161:VAL:HG21	2.03	0.41
2:H:108:GLN:HG2	2:H:128:GLN:N	2.36	0.41
1:I:143:VAL:HG22	1:I:237:LEU:HG	2.03	0.41
2:L:112:LEU:HD23	2:L:112:LEU:H	1.84	0.41
2:B:96:GLY:HA2	2:B:115:LYS:HD2	2.01	0.40
1:I:197:PHE:CG	1:I:198:GLY:N	2.89	0.40
1:Q:115:LEU:O	2:R:61:THR:OG1	2.35	0.40
1:Q:224:HIS:C	1:Q:226:TRP:H	2.29	0.40
1:Q:239:ARG:NE	1:Q:241:THR:O	2.46	0.40
1:U:145:PHE:HD1	1:U:145:PHE:HA	1.80	0.40
1:S:145:PHE:HD1	1:S:145:PHE:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:234:VAL:HG21	1:W:202:ARG:HH21	1.86	0.40
1:W:100:VAL:HG13	1:W:101:LEU:H	1.86	0.40
2:X:73:ARG:N	2:X:87:ASP:O	2.46	0.40
1:I:169:PRO:HD3	1:I:211:ARG:HB2	2.02	0.40
1:O:92:PHE:HA	1:O:238:PHE:HA	2.02	0.40
2:T:83:ASN:OD1	2:T:84:ALA:N	2.45	0.40
1:W:127:LYS:HE3	1:W:127:LYS:HB2	1.91	0.40
1:C:137:LYS:O	1:C:141:TYR:OH	2.39	0.40
1:G:115:LEU:HB2	1:G:118:VAL:HG22	2.04	0.40
1:M:91:MET:HB2	1:M:239:ARG:HB2	2.03	0.40
1:Q:230:GLN:NE2	2:R:67:GLN:O	2.54	0.40
1:U:147:LEU:HD13	1:U:163:LEU:HD11	2.03	0.40
1:E:141:TYR:CD2	1:E:237:LEU:HD21	2.57	0.40
1:I:132:GLU:OE2	1:I:168:GLN:HG3	2.21	0.40
1:O:137:LYS:O	1:O:141:TYR:OH	2.35	0.40
1:O:141:TYR:CD1	1:O:239:ARG:HA	2.57	0.40
1:U:100:VAL:HG13	1:U:101:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/203 (71%)	135 (93%)	10 (7%)	0	100	100
1	C	146/203 (72%)	138 (94%)	8 (6%)	0	100	100
1	E	144/203 (71%)	136 (94%)	8 (6%)	0	100	100
1	G	146/203 (72%)	138 (94%)	8 (6%)	0	100	100
1	I	139/203 (68%)	132 (95%)	7 (5%)	0	100	100
1	K	146/203 (72%)	139 (95%)	7 (5%)	0	100	100
1	M	145/203 (71%)	135 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	141/203 (70%)	133 (94%)	8 (6%)	0	100	100
1	Q	143/203 (70%)	137 (96%)	6 (4%)	0	100	100
1	S	144/203 (71%)	138 (96%)	6 (4%)	0	100	100
1	U	143/203 (70%)	134 (94%)	9 (6%)	0	100	100
1	W	145/203 (71%)	139 (96%)	6 (4%)	0	100	100
2	B	136/163 (83%)	123 (90%)	13 (10%)	0	100	100
2	D	132/163 (81%)	123 (93%)	9 (7%)	0	100	100
2	F	132/163 (81%)	121 (92%)	11 (8%)	0	100	100
2	H	127/163 (78%)	113 (89%)	14 (11%)	0	100	100
2	J	113/163 (69%)	100 (88%)	13 (12%)	0	100	100
2	L	132/163 (81%)	113 (86%)	19 (14%)	0	100	100
2	N	131/163 (80%)	117 (89%)	14 (11%)	0	100	100
2	P	136/163 (83%)	123 (90%)	13 (10%)	0	100	100
2	R	109/163 (67%)	91 (84%)	18 (16%)	0	100	100
2	T	123/163 (76%)	112 (91%)	11 (9%)	0	100	100
2	V	118/163 (72%)	102 (86%)	16 (14%)	0	100	100
2	X	128/163 (78%)	108 (84%)	20 (16%)	0	100	100
All	All	3244/4392 (74%)	2980 (92%)	264 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/155 (74%)	114 (100%)	0	100	100
1	C	114/155 (74%)	114 (100%)	0	100	100
1	E	113/155 (73%)	113 (100%)	0	100	100
1	G	115/155 (74%)	114 (99%)	1 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	111/155 (72%)	111 (100%)	0	100	100
1	K	114/155 (74%)	114 (100%)	0	100	100
1	M	114/155 (74%)	114 (100%)	0	100	100
1	O	113/155 (73%)	113 (100%)	0	100	100
1	Q	112/155 (72%)	112 (100%)	0	100	100
1	S	114/155 (74%)	113 (99%)	1 (1%)	70	76
1	U	113/155 (73%)	113 (100%)	0	100	100
1	W	114/155 (74%)	114 (100%)	0	100	100
2	B	119/140 (85%)	119 (100%)	0	100	100
2	D	116/140 (83%)	116 (100%)	0	100	100
2	F	116/140 (83%)	116 (100%)	0	100	100
2	H	114/140 (81%)	114 (100%)	0	100	100
2	J	103/140 (74%)	103 (100%)	0	100	100
2	L	116/140 (83%)	114 (98%)	2 (2%)	53	67
2	N	115/140 (82%)	114 (99%)	1 (1%)	70	76
2	P	119/140 (85%)	118 (99%)	1 (1%)	73	77
2	R	104/140 (74%)	104 (100%)	0	100	100
2	T	109/140 (78%)	109 (100%)	0	100	100
2	V	107/140 (76%)	107 (100%)	0	100	100
2	X	115/140 (82%)	113 (98%)	2 (2%)	53	67
All	All	2714/3540 (77%)	2706 (100%)	8 (0%)	86	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	179	LEU
2	L	85	GLU
2	L	88	CYS
2	N	120	CYS
2	P	88	CYS
1	S	146	GLN
2	X	120	CYS
2	X	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
2	B	51	ASN
2	B	59	GLN
1	C	146	GLN
1	E	205	HIS
1	E	217	HIS
2	H	104	GLN
1	I	194	ASN
2	J	110	GLN
2	L	93	HIS
1	M	205	HIS
1	M	217	HIS
2	N	67	GLN
2	N	110	GLN
2	N	138	ASN
2	P	40	ASN
1	S	98	GLN
2	T	126	ASN
2	X	39	ASN
2	X	51	ASN

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

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	301	2	14,14,15	0.33	0	17,19,21	0.48	0
3	NAG	P	301	2	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	H	301	2	14,14,15	0.32	0	17,19,21	0.53	0
3	NAG	X	301	2	14,14,15	0.32	0	17,19,21	0.54	0
3	NAG	V	301	2	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	B	301	2	14,14,15	0.33	0	17,19,21	0.53	0
3	NAG	R	301	2	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	J	301	2	14,14,15	0.29	0	17,19,21	0.50	0
3	NAG	L	301	2	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	T	301	2	14,14,15	0.26	0	17,19,21	0.57	0
3	NAG	N	301	2	14,14,15	0.46	0	17,19,21	0.53	0
3	NAG	F	301	2	14,14,15	0.31	0	17,19,21	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	301	2	-	0/6/23/26	0/1/1/1
3	NAG	P	301	2	-	2/6/23/26	0/1/1/1
3	NAG	H	301	2	-	2/6/23/26	0/1/1/1
3	NAG	X	301	2	-	0/6/23/26	0/1/1/1
3	NAG	V	301	2	-	2/6/23/26	0/1/1/1
3	NAG	B	301	2	-	2/6/23/26	0/1/1/1
3	NAG	R	301	2	-	2/6/23/26	0/1/1/1
3	NAG	J	301	2	-	4/6/23/26	0/1/1/1
3	NAG	L	301	2	-	1/6/23/26	0/1/1/1
3	NAG	T	301	2	-	4/6/23/26	0/1/1/1
3	NAG	N	301	2	-	3/6/23/26	0/1/1/1
3	NAG	F	301	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	301	NAG	O5-C5-C6-O6
3	F	301	NAG	C4-C5-C6-O6
3	J	301	NAG	C4-C5-C6-O6
3	J	301	NAG	C8-C7-N2-C2
3	J	301	NAG	O7-C7-N2-C2
3	N	301	NAG	C8-C7-N2-C2
3	N	301	NAG	O7-C7-N2-C2
3	F	301	NAG	O5-C5-C6-O6
3	L	301	NAG	O5-C5-C6-O6
3	T	301	NAG	O5-C5-C6-O6
3	P	301	NAG	C4-C5-C6-O6
3	T	301	NAG	C4-C5-C6-O6
3	R	301	NAG	O5-C5-C6-O6
3	V	301	NAG	O5-C5-C6-O6
3	R	301	NAG	C4-C5-C6-O6
3	P	301	NAG	O5-C5-C6-O6
3	H	301	NAG	C4-C5-C6-O6
3	T	301	NAG	C1-C2-N2-C7
3	B	301	NAG	C4-C5-C6-O6
3	V	301	NAG	C4-C5-C6-O6
3	N	301	NAG	C4-C5-C6-O6
3	H	301	NAG	O5-C5-C6-O6
3	B	301	NAG	O5-C5-C6-O6
3	T	301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	301	NAG	1	0

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, 95^{th} 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	149/203 (73%)	0.40	6 (4%) 42 30	16, 41, 89, 111	0
1	C	150/203 (73%)	0.28	2 (1%) 75 61	14, 39, 83, 121	0
1	E	148/203 (72%)	0.42	6 (4%) 41 29	17, 47, 92, 114	0
1	G	150/203 (73%)	0.33	3 (2%) 65 49	15, 41, 95, 130	0
1	I	145/203 (71%)	0.32	2 (1%) 73 59	17, 41, 85, 112	0
1	K	150/203 (73%)	0.36	5 (3%) 49 36	18, 48, 85, 119	0
1	M	149/203 (73%)	0.33	4 (2%) 56 42	18, 50, 88, 128	0
1	O	147/203 (72%)	0.41	4 (2%) 56 42	21, 48, 81, 103	0
1	Q	147/203 (72%)	0.42	4 (2%) 56 42	17, 51, 88, 143	0
1	S	148/203 (72%)	0.44	5 (3%) 48 35	21, 46, 92, 107	0
1	U	147/203 (72%)	0.30	3 (2%) 65 49	21, 50, 91, 109	0
1	W	149/203 (73%)	0.40	3 (2%) 65 49	23, 50, 101, 138	0
2	B	138/163 (84%)	0.98	21 (15%) 5 7	20, 68, 112, 141	0
2	D	134/163 (82%)	0.70	9 (6%) 24 19	21, 57, 105, 135	0
2	F	134/163 (82%)	0.80	10 (7%) 20 17	30, 70, 106, 129	0
2	H	131/163 (80%)	0.84	13 (9%) 13 12	27, 68, 107, 147	0
2	J	119/163 (73%)	0.57	7 (5%) 28 22	25, 58, 97, 122	0
2	L	134/163 (82%)	0.87	15 (11%) 10 11	34, 74, 120, 148	0
2	N	133/163 (81%)	0.89	16 (12%) 9 9	23, 67, 125, 157	0
2	P	138/163 (84%)	0.89	14 (10%) 12 12	31, 73, 112, 135	0
2	R	119/163 (73%)	0.94	9 (7%) 20 17	37, 76, 118, 150	0
2	T	127/163 (77%)	0.71	9 (7%) 22 18	23, 66, 103, 148	0
2	V	124/163 (76%)	0.70	8 (6%) 25 20	24, 66, 117, 132	0
2	X	132/163 (80%)	0.92	15 (11%) 10 10	36, 70, 102, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3342/4392 (76%)	0.58	193 (5%)	29	22	14, 56, 105, 157	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	105	ASP	5.4
2	H	42	ASN	4.4
2	P	105	ASP	4.3
1	O	152	VAL	4.3
2	R	78	CYS	4.3
1	W	170	LEU	4.0
2	F	105	ASP	3.9
2	H	78	CYS	3.8
2	T	32	PRO	3.7
1	E	176	ALA	3.6
1	G	176	ALA	3.6
2	F	160	PRO	3.5
2	B	88	CYS	3.5
2	R	59	GLN	3.5
2	L	141	LEU	3.5
1	Q	145	PHE	3.5
2	B	81	THR	3.5
2	N	56	ALA	3.5
2	R	105	ASP	3.4
2	V	127	ASP	3.4
2	L	106	CYS	3.4
2	X	88	CYS	3.3
2	N	103	GLU	3.3
2	H	28	CYS	3.3
2	B	27	PRO	3.3
2	X	127	ASP	3.2
2	H	159	GLY	3.2
2	T	105	ASP	3.1
2	X	141	LEU	3.1
2	F	109	GLY	3.1
2	T	95	LEU	3.1
2	P	120	CYS	3.1
2	N	98	GLY	3.1
2	J	35	THR	3.0
2	X	112	LEU	3.0
2	L	105	ASP	3.0
2	L	88	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	222	ALA	3.0
2	V	159	GLY	3.0
2	D	128	GLN	3.0
2	D	120	CYS	2.9
2	X	28	CYS	2.9
2	F	127	ASP	2.9
2	H	106	CYS	2.9
1	A	111	SER	2.9
2	L	112	LEU	2.9
2	B	28	CYS	2.9
2	T	88	CYS	2.9
1	U	222	ALA	2.8
1	I	222	ALA	2.8
1	K	222	ALA	2.8
2	L	27	PRO	2.8
2	B	58	GLY	2.8
2	H	147	LEU	2.8
2	V	99	CYS	2.8
1	G	111	SER	2.8
1	S	114	GLY	2.8
2	V	65	CYS	2.8
2	V	60	ARG	2.8
2	X	55	SER	2.8
2	D	105	ASP	2.8
1	U	139	GLY	2.8
2	L	108	GLN	2.8
2	H	149	ASN	2.7
2	D	160	PRO	2.7
2	L	41	ARG	2.7
2	R	27	PRO	2.7
2	T	78	CYS	2.7
2	N	116	GLY	2.7
2	D	150	GLY	2.7
2	J	105	ASP	2.7
2	B	42	ASN	2.7
1	O	116	ALA	2.6
1	M	219	GLU	2.6
2	P	113	THR	2.6
2	X	61	THR	2.6
2	X	106	CYS	2.6
2	N	160	PRO	2.6
2	R	57	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	97	ALA	2.6
2	D	28	CYS	2.6
2	N	55	SER	2.6
2	P	112	LEU	2.6
2	P	88	CYS	2.5
2	D	108	GLN	2.5
1	C	170	LEU	2.5
1	S	118	VAL	2.5
2	H	119	ASP	2.5
2	T	127	ASP	2.5
2	X	147	LEU	2.5
2	X	105	ASP	2.5
1	S	116	ALA	2.5
2	B	85	GLU	2.5
1	S	117	GLY	2.5
1	A	148	GLU	2.5
2	B	127	ASP	2.5
2	L	122	PHE	2.5
1	S	170	LEU	2.5
2	P	130	ARG	2.5
2	H	45	CYS	2.4
2	J	61	THR	2.4
2	F	58	GLY	2.4
1	K	176	ALA	2.4
2	B	120	CYS	2.4
2	D	122	PHE	2.4
2	V	88	CYS	2.4
1	O	115	LEU	2.4
1	E	178	ALA	2.4
2	X	41	ARG	2.4
2	P	139	CYS	2.4
1	E	113	PRO	2.4
2	F	116	GLY	2.4
2	P	116	GLY	2.4
1	Q	222	ALA	2.4
2	H	88	CYS	2.4
2	F	70	GLY	2.3
2	J	130	ARG	2.3
2	P	127	ASP	2.3
2	L	32	PRO	2.3
1	Q	176	ALA	2.3
2	B	55	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	40	ASN	2.3
1	W	103	ILE	2.3
2	P	160	PRO	2.3
2	T	61	THR	2.3
2	B	106	CYS	2.3
2	F	78	CYS	2.3
2	P	115	LYS	2.3
1	A	116	ALA	2.2
2	V	35	THR	2.2
2	N	115	LYS	2.2
2	N	102	CYS	2.2
2	X	146	VAL	2.2
1	A	176	ALA	2.2
1	M	154	ALA	2.2
2	X	160	PRO	2.2
1	E	205	HIS	2.2
2	B	113	THR	2.2
1	A	169	PRO	2.2
2	N	32	PRO	2.2
2	N	101	MET	2.2
2	R	44	ILE	2.2
2	L	51	ASN	2.2
2	F	141	LEU	2.2
1	K	225	ALA	2.2
2	N	88	CYS	2.2
2	J	36	PHE	2.2
2	R	61	THR	2.2
1	K	117	GLY	2.2
2	J	127	ASP	2.2
2	T	117	CYS	2.2
1	O	170	LEU	2.1
2	X	46	SER	2.1
1	K	175	GLY	2.1
2	F	66	ARG	2.1
2	L	120	CYS	2.1
2	J	56	ALA	2.1
1	Q	191	GLU	2.1
2	H	91	GLY	2.1
2	N	70	GLY	2.1
2	R	54	SER	2.1
1	E	118	VAL	2.1
2	L	28	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	119	ASP	2.1
1	U	215	HIS	2.1
2	L	55	SER	2.1
2	B	68	CYS	2.1
2	B	78	CYS	2.1
1	C	232	ALA	2.1
1	M	114	GLY	2.1
2	X	29	SER	2.1
2	N	132	ILE	2.1
2	B	94	CYS	2.1
1	I	116	ALA	2.1
1	W	222	ALA	2.1
2	N	150	GLY	2.1
1	A	145	PHE	2.1
2	D	32	PRO	2.1
2	H	122	PHE	2.1
2	H	145	SER	2.0
2	P	142	ASP	2.0
2	B	31	CYS	2.0
1	E	145	PHE	2.0
2	B	98	GLY	2.0
2	V	122	PHE	2.0
2	B	129	LYS	2.0
1	G	118	VAL	2.0
2	B	60	ARG	2.0
2	T	112	LEU	2.0
2	L	39	ASN	2.0
2	P	162	PRO	2.0
2	R	60	ARG	2.0
2	B	95	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	N	301	14/15	0.53	0.20	69,77,90,90	0
3	NAG	F	301	14/15	0.59	0.17	73,103,109,114	0
3	NAG	P	301	14/15	0.66	0.17	78,91,100,106	0
3	NAG	H	301	14/15	0.69	0.16	68,91,100,100	0
3	NAG	R	301	14/15	0.69	0.18	98,115,120,120	0
3	NAG	X	301	14/15	0.69	0.17	99,116,127,130	0
3	NAG	L	301	14/15	0.72	0.13	69,86,90,91	0
3	NAG	D	301	14/15	0.73	0.13	55,71,75,76	0
3	NAG	B	301	14/15	0.73	0.14	43,56,70,76	0
3	NAG	V	301	14/15	0.74	0.15	77,93,100,100	0
3	NAG	J	301	14/15	0.77	0.14	83,93,100,101	0
3	NAG	T	301	14/15	0.84	0.13	70,78,87,89	0

6.5 Other polymers (i)

There are no such residues in this entry.