



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 01:56 PM BST

PDB ID : 6A3V
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

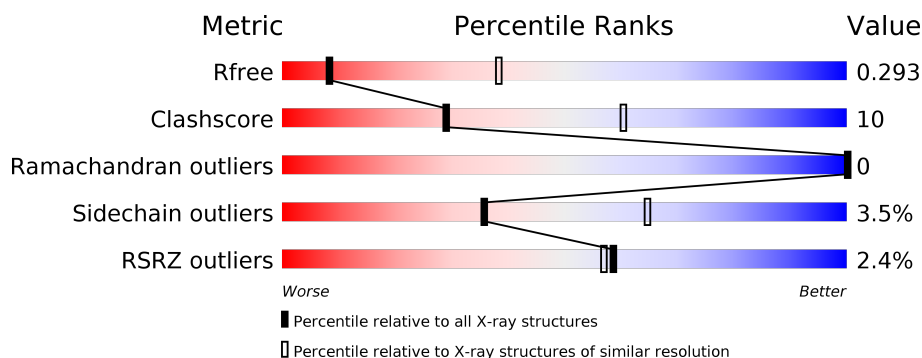
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	<div> <div>55%</div> <div>17%</div> <div>•</div> <div>27%</div> </div>
1	C	203	<div> <div>59%</div> <div>14%</div> <div>•</div> <div>26%</div> </div>
1	E	203	<div> <div>53%</div> <div>20%</div> <div>•</div> <div>27%</div> </div>
1	G	203	<div> <div>59%</div> <div>13%</div> <div>•</div> <div>26%</div> </div>
1	I	203	<div> <div>55%</div> <div>16%</div> <div>•</div> <div>29%</div> </div>
1	K	203	<div> <div>59%</div> <div>13%</div> <div>•</div> <div>26%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	203	
1	O	203	
1	Q	203	
1	S	203	
1	U	203	
1	W	203	
2	B	163	
2	D	163	
2	F	163	
2	H	163	
2	J	163	
2	L	163	
2	N	163	
2	P	163	
2	R	163	
2	T	163	
2	V	163	
2	X	163	

2 Entry composition

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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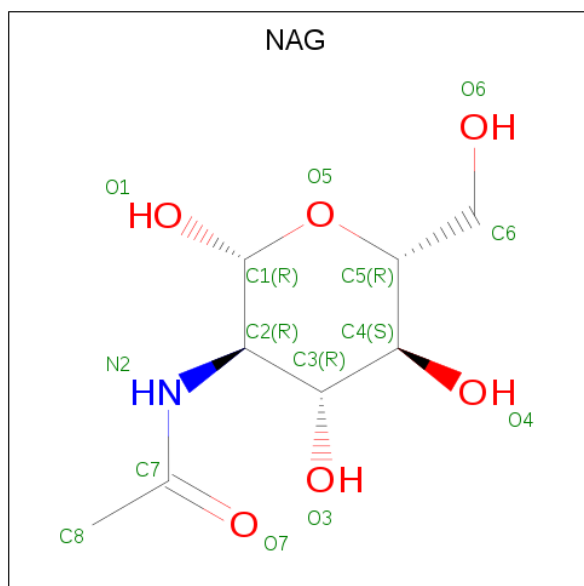
Chain	Residue	Modelled	Actual	Comment	Reference
J	186	HIS	-	expression tag	UNP Q07011
L	181	HIS	-	expression tag	UNP Q07011
L	182	HIS	-	expression tag	UNP Q07011
L	183	HIS	-	expression tag	UNP Q07011
L	184	HIS	-	expression tag	UNP Q07011
L	185	HIS	-	expression tag	UNP Q07011
L	186	HIS	-	expression tag	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 (three-letter code: 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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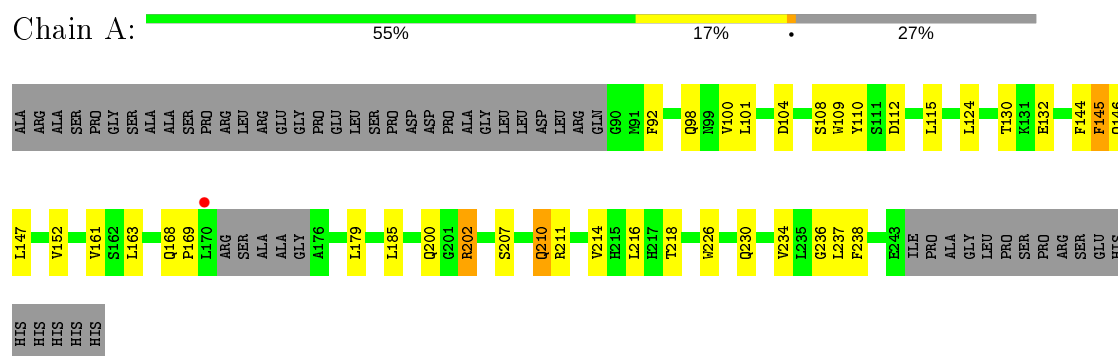
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	V	1	Total	C	N	O	0	0
			14	8	1	5		
3	X	1	Total	C	N	O	0	0
			14	8	1	5		

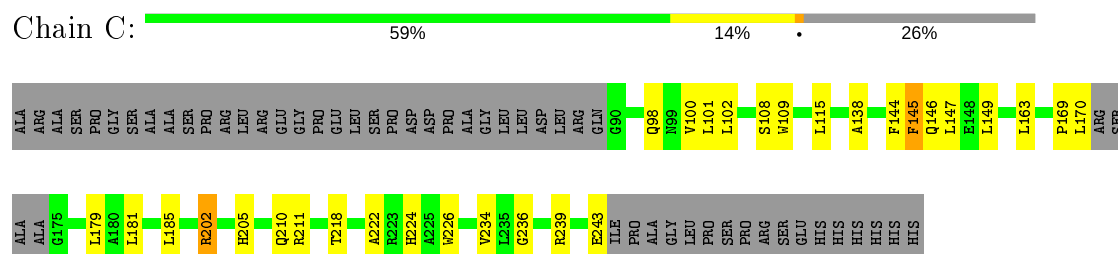
3 Residue-property plots [i](#)

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.

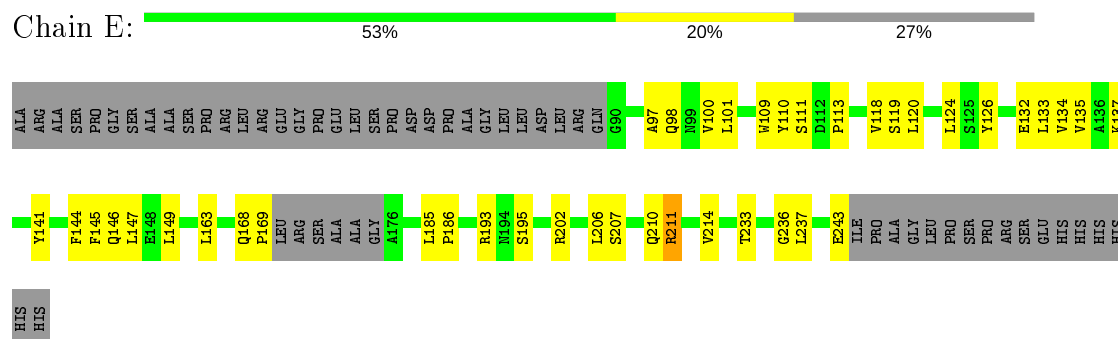
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



- Molecule 1: Tumor necrosis factor ligand superfamily member 9

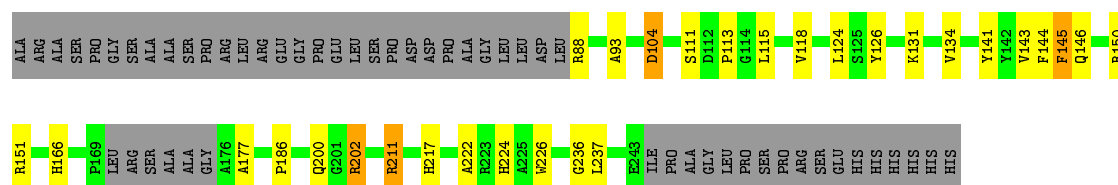


- Molecule 1: Tumor necrosis factor ligand superfamily member 9



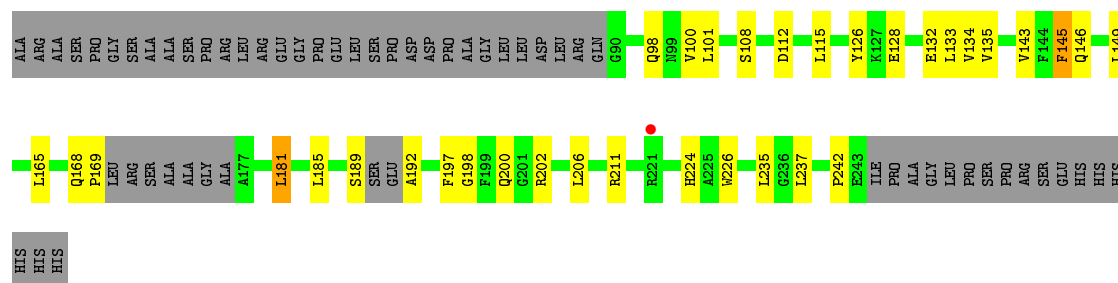
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain G: 



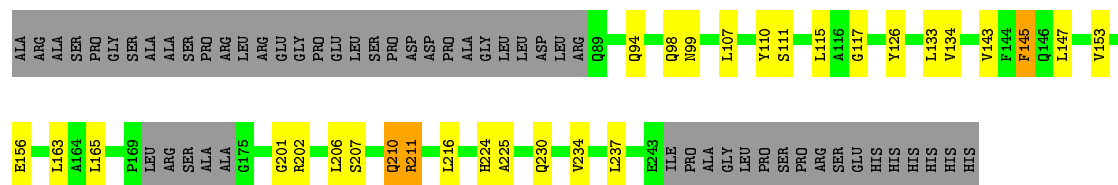
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain I: 



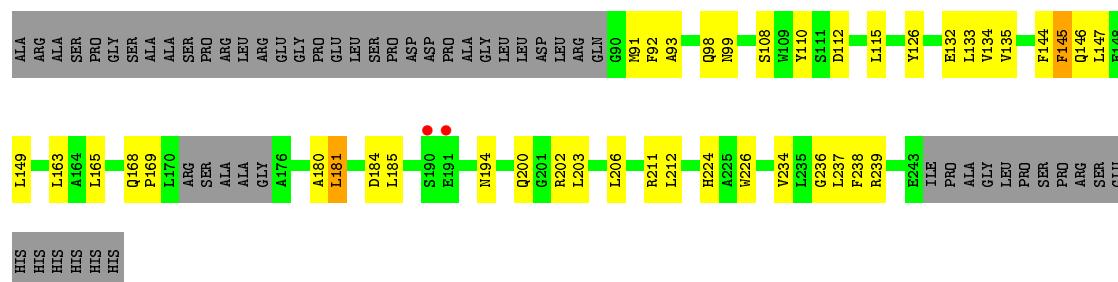
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain K: 



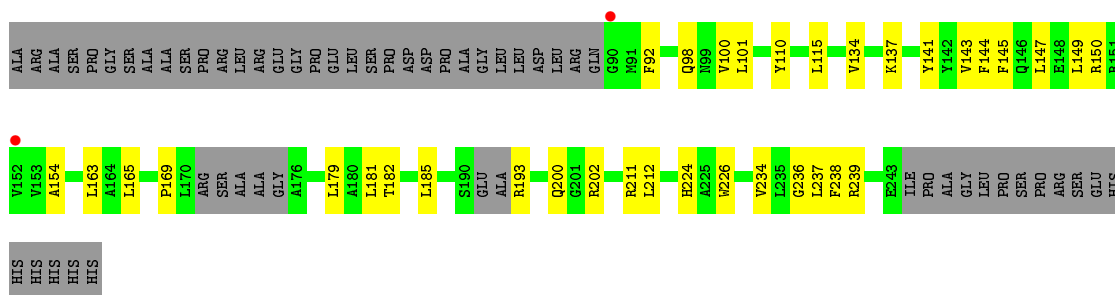
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain M: 



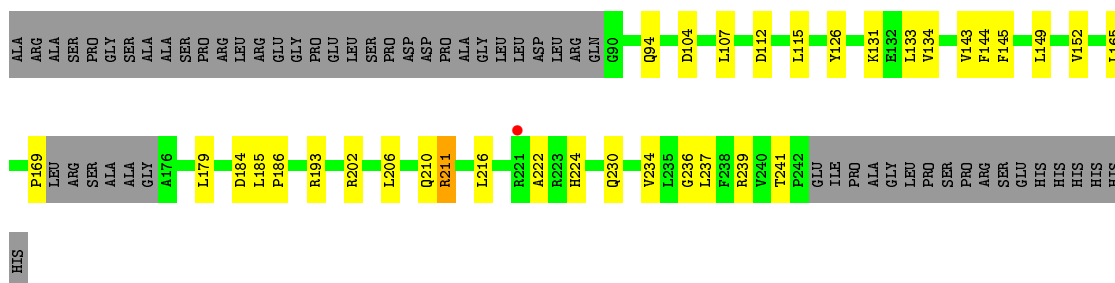
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain O: 



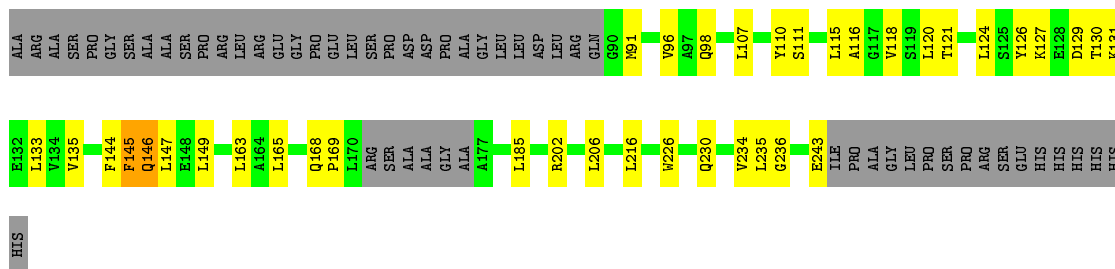
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain Q: 56% 16% 28%



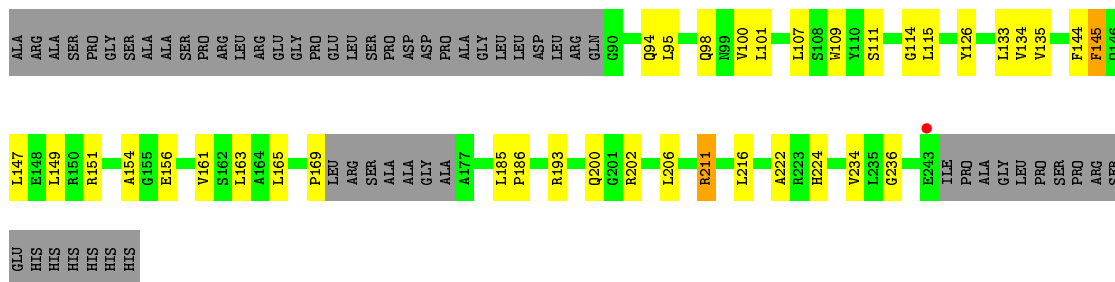
- Molecule 1: Tumor necrosis factor ligand superfamily member 9

Chain S: 54% 18% 27%

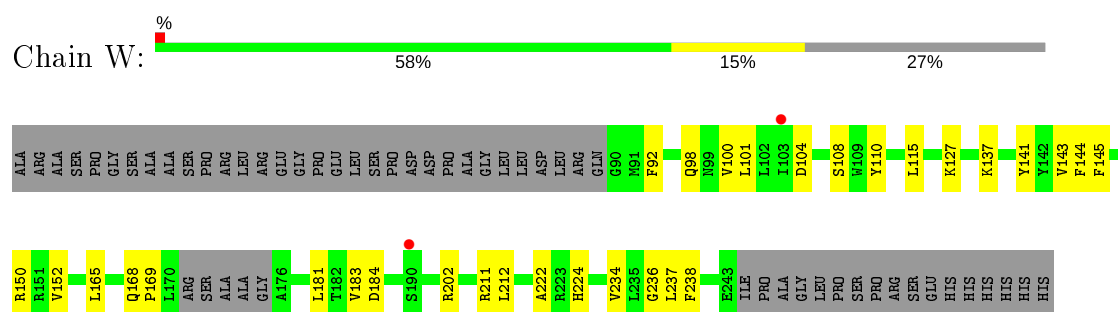


- Molecule 1: Tumor necrosis factor ligand superfamily member 9

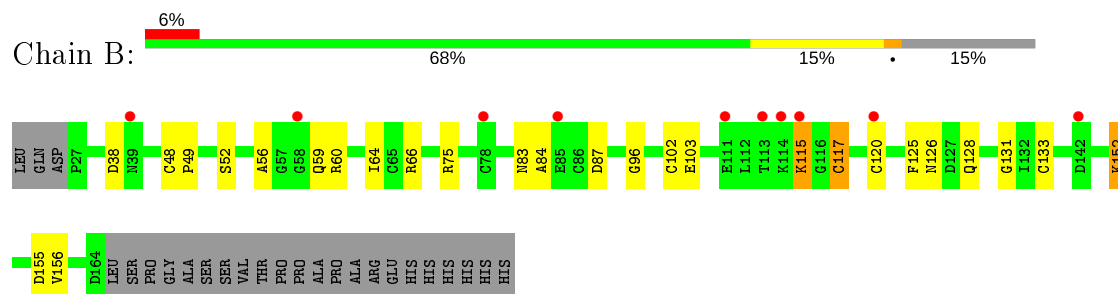
Chain U: 54% 17% 28%



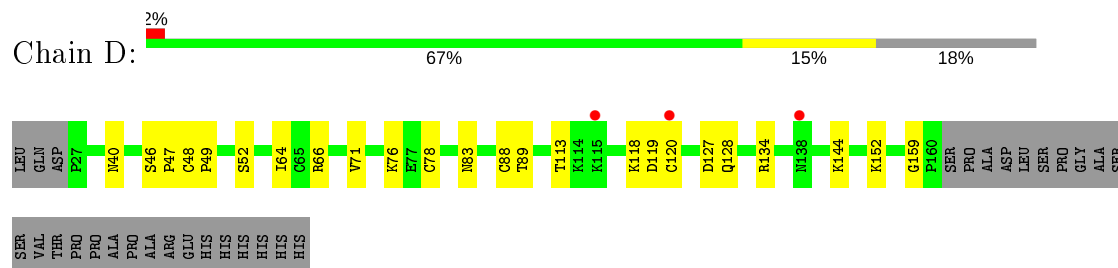
- Molecule 1: Tumor necrosis factor ligand superfamily member 9



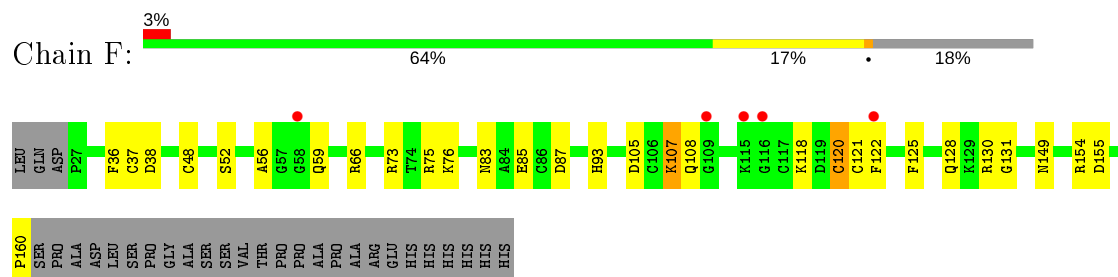
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



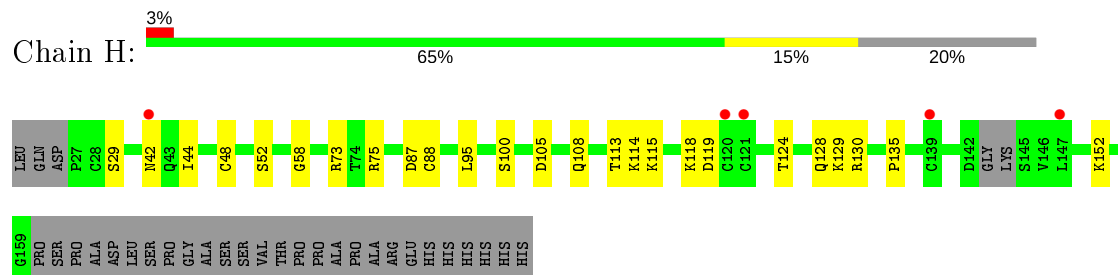
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



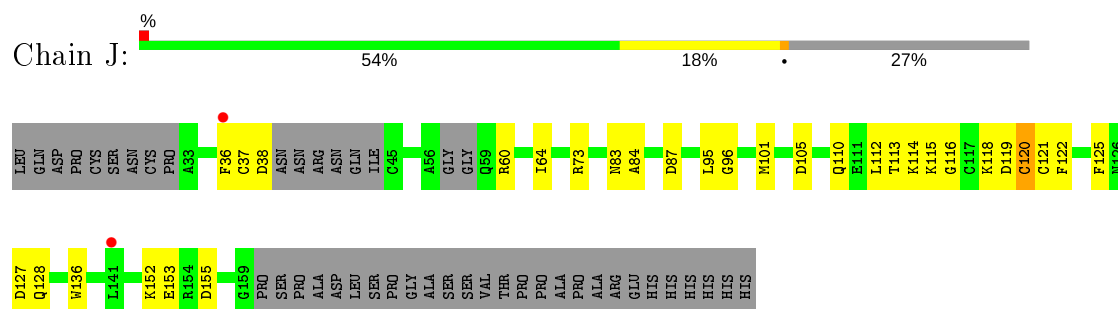
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



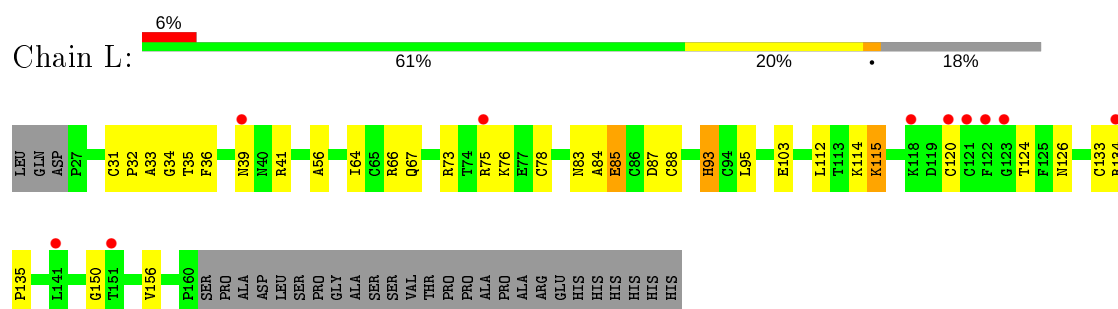
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



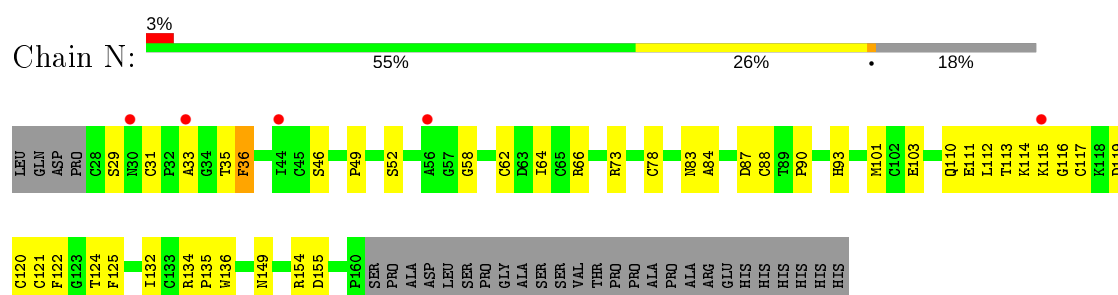
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



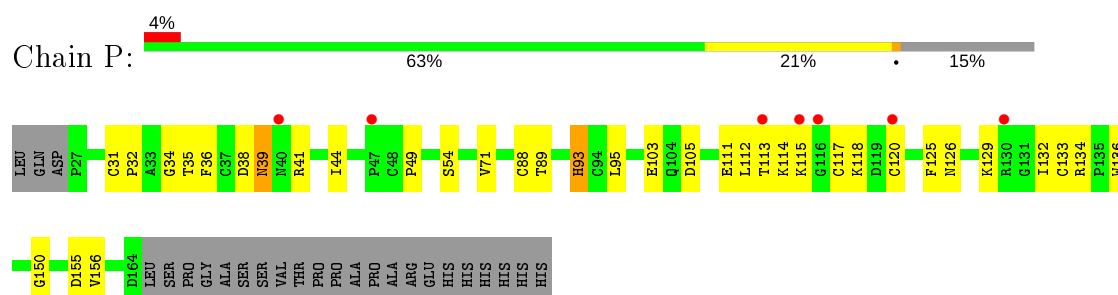
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



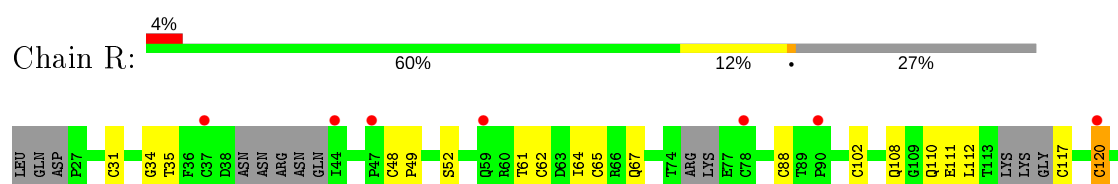
- Molecule 2: Tumor necrosis factor receptor superfamily member 9

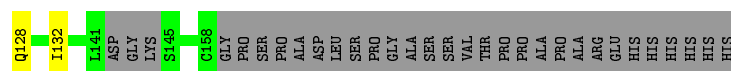


- Molecule 2: Tumor necrosis factor receptor superfamily member 9

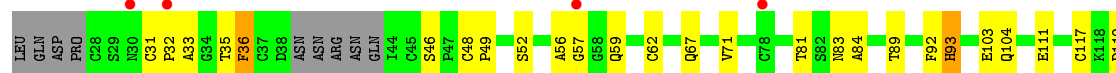


- Molecule 2: Tumor necrosis factor receptor superfamily member 9

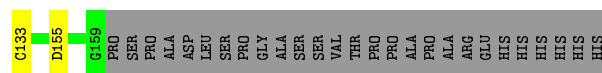
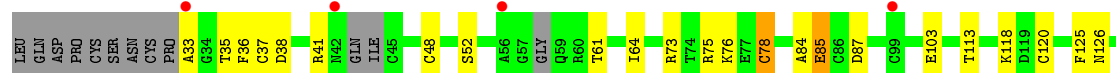




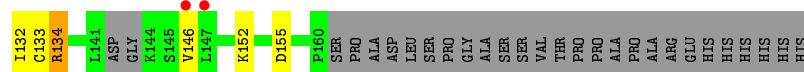
- Molecule 2: Tumor necrosis factor receptor superfamily member 9



- Molecule 2: Tumor necrosis factor receptor superfamily member 9



- Molecule 2: Tumor necrosis factor receptor superfamily member 9



4 Data and refinement statistics

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 44.66 – 3.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.67-3.39) 98.8 (44.66-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.264 , 0.293 0.263 , 0.293	Depositor DCC
R_{free} test set	3099 reflections (5.09%)	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)	0.26 , 24.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	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.*

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: 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	0.25	0/1143	0.47	0/1553
1	C	0.26	0/1147	0.50	0/1558
1	E	0.25	0/1135	0.48	0/1542
1	G	0.25	0/1155	0.48	0/1568
1	I	0.25	0/1114	0.46	0/1512
1	K	0.25	0/1148	0.48	0/1559
1	M	0.25	0/1143	0.45	0/1553
1	O	0.25	0/1128	0.45	0/1531
1	Q	0.25	0/1126	0.46	0/1530
1	S	0.29	0/1138	0.48	0/1546
1	U	0.25	0/1130	0.46	0/1535
1	W	0.25	0/1143	0.46	0/1553
2	B	0.30	0/1032	0.53	0/1387
2	D	0.26	0/1004	0.51	0/1348
2	F	0.25	0/1005	0.52	0/1349
2	H	0.27	0/983	0.55	0/1318
2	J	0.25	0/893	0.49	0/1193
2	L	0.25	0/1005	0.56	0/1349
2	N	0.27	0/997	0.56	0/1338
2	P	0.26	0/1032	0.54	0/1387
2	R	0.30	0/882	0.59	0/1182
2	T	0.26	0/944	0.53	0/1264
2	V	0.26	0/932	0.50	0/1245
2	X	0.26	0/992	0.53	0/1330
All	All	0.26	0/25351	0.50	0/34230

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	1120	0	1130	32	0
1	C	1124	0	1133	23	0
1	E	1112	0	1119	26	0
1	G	1132	0	1140	20	0
1	I	1092	0	1102	21	0
1	K	1125	0	1130	18	0
1	M	1120	0	1130	30	0
1	O	1106	0	1118	23	0
1	Q	1103	0	1113	23	0
1	S	1115	0	1125	26	0
1	U	1107	0	1114	28	0
1	W	1120	0	1130	19	0
2	B	1015	0	936	17	0
2	D	988	0	915	11	0
2	F	989	0	915	16	0
2	H	969	0	891	15	0
2	J	882	0	818	22	0
2	L	989	0	915	25	0
2	N	982	0	907	29	0
2	P	1015	0	936	22	0
2	R	871	0	787	17	0
2	T	931	0	860	24	0
2	V	921	0	852	15	0
2	X	977	0	907	26	0
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	472	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.

The worst 5 of 472 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	111 (97%)	3 (3%)	46	72
1	C	114/155 (74%)	110 (96%)	4 (4%)	36	65
1	E	113/155 (73%)	108 (96%)	5 (4%)	28	58
1	G	115/155 (74%)	111 (96%)	4 (4%)	36	65
1	I	111/155 (72%)	108 (97%)	3 (3%)	44	70
1	K	114/155 (74%)	109 (96%)	5 (4%)	28	58
1	M	114/155 (74%)	112 (98%)	2 (2%)	59	79
1	O	113/155 (73%)	111 (98%)	2 (2%)	59	79
1	Q	112/155 (72%)	107 (96%)	5 (4%)	27	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	114/155 (74%)	108 (95%)	6 (5%)	22	52
1	U	113/155 (73%)	110 (97%)	3 (3%)	44	70
1	W	114/155 (74%)	111 (97%)	3 (3%)	46	72
2	B	119/140 (85%)	115 (97%)	4 (3%)	37	65
2	D	116/140 (83%)	111 (96%)	5 (4%)	29	59
2	F	116/140 (83%)	111 (96%)	5 (4%)	29	59
2	H	114/140 (81%)	113 (99%)	1 (1%)	78	90
2	J	103/140 (74%)	101 (98%)	2 (2%)	57	78
2	L	116/140 (83%)	109 (94%)	7 (6%)	19	49
2	N	115/140 (82%)	110 (96%)	5 (4%)	29	59
2	P	119/140 (85%)	114 (96%)	5 (4%)	30	59
2	R	104/140 (74%)	102 (98%)	2 (2%)	57	78
2	T	109/140 (78%)	104 (95%)	5 (5%)	27	57
2	V	107/140 (76%)	103 (96%)	4 (4%)	34	62
2	X	115/140 (82%)	110 (96%)	5 (4%)	29	59
All	All	2714/3540 (77%)	2619 (96%)	95 (4%)	36	65

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	85	GLU
2	N	120	CYS
1	W	104	ASP
2	L	93	HIS
1	M	145	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	X	301	2	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	B	301	2	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	V	301	2	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	P	301	2	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	T	301	2	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	N	301	2	14,14,15	0.48	0	17,19,21	0.52	0
3	NAG	H	301	2	14,14,15	0.30	0	17,19,21	0.51	0
3	NAG	R	301	2	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	L	301	2	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	F	301	2	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	J	301	2	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	D	301	2	14,14,15	0.31	0	17,19,21	0.46	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	X	301	2	-	0/6/23/26	0/1/1/1
3	NAG	B	301	2	-	2/6/23/26	0/1/1/1
3	NAG	V	301	2	-	2/6/23/26	0/1/1/1
3	NAG	P	301	2	-	2/6/23/26	0/1/1/1
3	NAG	T	301	2	-	3/6/23/26	0/1/1/1
3	NAG	N	301	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	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	L	301	2	-	1/6/23/26	0/1/1/1
3	NAG	F	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	D	301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 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	N	301	NAG	C8-C7-N2-C2
3	N	301	NAG	O7-C7-N2-C2
3	J	301	NAG	C8-C7-N2-C2

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, 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	149/203 (73%)	-0.02	1 (0%) 87 87	16, 41, 89, 111	0
1	C	150/203 (73%)	-0.03	0 100 100	14, 39, 83, 121	0
1	E	148/203 (72%)	0.03	0 100 100	17, 47, 92, 114	0
1	G	150/203 (73%)	0.07	0 100 100	15, 41, 95, 130	0
1	I	145/203 (71%)	0.00	1 (0%) 87 87	17, 41, 85, 112	0
1	K	150/203 (73%)	-0.01	0 100 100	18, 48, 85, 119	0
1	M	149/203 (73%)	0.10	2 (1%) 77 76	18, 50, 88, 128	0
1	O	147/203 (72%)	-0.03	2 (1%) 75 74	21, 48, 81, 103	0
1	Q	147/203 (72%)	0.04	1 (0%) 87 87	17, 51, 88, 143	0
1	S	148/203 (72%)	0.09	0 100 100	21, 46, 92, 107	0
1	U	147/203 (72%)	0.03	1 (0%) 87 87	21, 50, 91, 109	0
1	W	149/203 (73%)	0.06	2 (1%) 77 76	23, 50, 101, 138	0
2	B	138/163 (84%)	0.54	10 (7%) 15 17	20, 68, 112, 141	0
2	D	134/163 (82%)	0.29	3 (2%) 62 60	21, 57, 105, 135	0
2	F	134/163 (82%)	0.41	5 (3%) 41 40	30, 70, 106, 129	0
2	H	131/163 (80%)	0.33	5 (3%) 40 39	27, 68, 107, 147	0
2	J	119/163 (73%)	0.21	2 (1%) 70 68	25, 58, 97, 122	0
2	L	134/163 (82%)	0.54	10 (7%) 14 16	34, 74, 120, 148	0
2	N	133/163 (81%)	0.36	5 (3%) 40 39	23, 67, 125, 157	0
2	P	138/163 (84%)	0.59	7 (5%) 28 28	31, 73, 112, 135	0
2	R	119/163 (73%)	0.65	7 (5%) 22 23	37, 76, 118, 150	0
2	T	127/163 (77%)	0.31	4 (3%) 49 48	23, 67, 103, 148	0
2	V	124/163 (76%)	0.27	4 (3%) 47 46	24, 66, 117, 132	0
2	X	132/163 (80%)	0.51	8 (6%) 21 22	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%)	0.21	80 (2%) 59 57	14, 56, 105, 157	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	GLY	5.4
2	T	30	ASN	4.5
2	X	127	ASP	4.5
2	L	141	LEU	3.9
2	N	56	ALA	3.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 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	B-factors(Å ²)	Q<0.9
3	NAG	R	301	14/15	0.58	0.28	98,115,120,120	0
3	NAG	H	301	14/15	0.61	0.27	68,91,100,100	0
3	NAG	X	301	14/15	0.63	0.26	99,116,127,130	0
3	NAG	F	301	14/15	0.66	0.27	73,103,109,114	0
3	NAG	P	301	14/15	0.78	0.21	78,91,100,106	0
3	NAG	V	301	14/15	0.78	0.19	77,93,100,100	0
3	NAG	J	301	14/15	0.78	0.19	83,93,100,101	0
3	NAG	T	301	14/15	0.79	0.24	70,78,87,89	0
3	NAG	L	301	14/15	0.80	0.25	69,86,90,91	0
3	NAG	B	301	14/15	0.82	0.23	43,56,70,76	0
3	NAG	N	301	14/15	0.83	0.27	69,77,90,90	0
3	NAG	D	301	14/15	0.84	0.20	55,71,75,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.