



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:56 AM UTC

PDB ID : 6Y41 / pdb_00006y41
Title : Fibrinogen-like globe domain of human ANGPTL2
Authors : Coker, J.A.; Krojer, T.; Mutisya, J.M.; Arrowsmith, C.H.; Bountra, C.; Midwood, K.S.; Yue, W.W.; Marsden, B.D.; Structural Genomics Consortium (SGC)
Deposited on : 2020-02-19
Resolution : 1.79 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

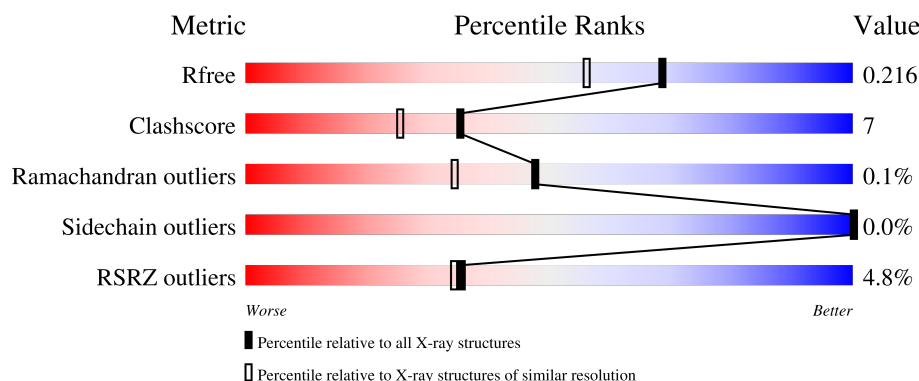
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	227	0% 88% 8% .
1	B	227	2% 83% 13% .
1	C	227	2% 88% 9% .
1	D	227	2% 87% 9% .
1	E	227	2% 85% 12% .

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Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	
1	K	227	
1	L	227	
1	M	227	
1	N	227	
1	O	227	
1	P	227	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	G	401	-	X	-	-
4	TRS	H	401	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 57945 atoms, of which 26401 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 Angiopoietin-related protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	H	N	O	S	0	0	0
			3490	1159	1666	326	331	8			
1	B	218	Total	C	H	N	O	S	0	0	0
			3469	1154	1656	323	328	8			
1	C	219	Total	C	H	N	O	S	0	0	0
			3458	1153	1647	322	328	8			
1	D	218	Total	C	H	N	O	S	0	0	0
			3442	1149	1638	318	329	8			
1	E	219	Total	C	H	N	O	S	0	0	0
			3492	1159	1669	328	328	8			
1	F	220	Total	C	H	N	O	S	0	0	0
			3495	1163	1669	324	331	8			
1	G	219	Total	C	H	N	O	S	0	0	0
			3456	1153	1644	320	331	8			
1	H	218	Total	C	H	N	O	S	0	0	0
			3470	1155	1656	322	329	8			
1	I	217	Total	C	H	N	O	S	0	0	0
			3456	1151	1648	321	328	8			
1	J	217	Total	C	H	N	O	S	0	0	0
			3414	1143	1622	314	327	8			
1	K	216	Total	C	H	N	O	S	0	0	0
			3434	1145	1638	319	324	8			
1	L	218	Total	C	H	N	O	S	0	0	0
			3479	1156	1661	325	329	8			
1	M	217	Total	C	H	N	O	S	0	0	0
			3440	1147	1640	320	325	8			
1	N	216	Total	C	H	N	O	S	0	0	0
			3451	1148	1649	322	324	8			
1	O	216	Total	C	H	N	O	S	0	0	0
			3426	1144	1632	316	326	8			
1	P	216	Total	C	H	N	O	S	0	0	0
			3420	1143	1630	317	322	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q9UKU9
A	0	MET	-	expression tag	UNP Q9UKU9
B	-1	SER	-	expression tag	UNP Q9UKU9
B	0	MET	-	expression tag	UNP Q9UKU9
C	-1	SER	-	expression tag	UNP Q9UKU9
C	0	MET	-	expression tag	UNP Q9UKU9
D	-1	SER	-	expression tag	UNP Q9UKU9
D	0	MET	-	expression tag	UNP Q9UKU9
E	-1	SER	-	expression tag	UNP Q9UKU9
E	0	MET	-	expression tag	UNP Q9UKU9
F	-1	SER	-	expression tag	UNP Q9UKU9
F	0	MET	-	expression tag	UNP Q9UKU9
G	-1	SER	-	expression tag	UNP Q9UKU9
G	0	MET	-	expression tag	UNP Q9UKU9
H	-1	SER	-	expression tag	UNP Q9UKU9
H	0	MET	-	expression tag	UNP Q9UKU9
I	-1	SER	-	expression tag	UNP Q9UKU9
I	0	MET	-	expression tag	UNP Q9UKU9
J	-1	SER	-	expression tag	UNP Q9UKU9
J	0	MET	-	expression tag	UNP Q9UKU9
K	-1	SER	-	expression tag	UNP Q9UKU9
K	0	MET	-	expression tag	UNP Q9UKU9
L	-1	SER	-	expression tag	UNP Q9UKU9
L	0	MET	-	expression tag	UNP Q9UKU9
M	-1	SER	-	expression tag	UNP Q9UKU9
M	0	MET	-	expression tag	UNP Q9UKU9
N	-1	SER	-	expression tag	UNP Q9UKU9
N	0	MET	-	expression tag	UNP Q9UKU9
O	-1	SER	-	expression tag	UNP Q9UKU9
O	0	MET	-	expression tag	UNP Q9UKU9
P	-1	SER	-	expression tag	UNP Q9UKU9
P	0	MET	-	expression tag	UNP Q9UKU9

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

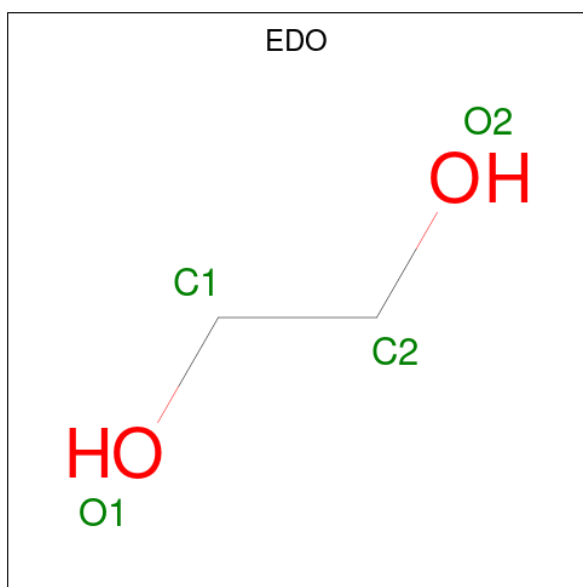
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

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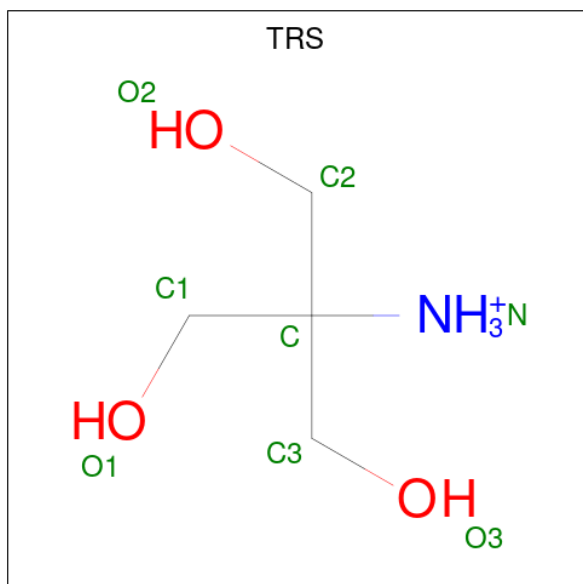
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Ca 1	0	0
2	E	1	Total 1	Ca 1	0	0
2	F	1	Total 1	Ca 1	0	0
2	G	1	Total 1	Ca 1	0	0
2	H	1	Total 1	Ca 1	0	0
2	I	1	Total 1	Ca 1	0	0
2	J	1	Total 1	Ca 1	0	0
2	K	1	Total 1	Ca 1	0	0
2	L	1	Total 1	Ca 1	0	0
2	M	1	Total 1	Ca 1	0	0
2	N	1	Total 1	Ca 1	0	0
2	O	1	Total 1	Ca 1	0	0
2	P	1	Total 1	Ca 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	I	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	H	N	O	0	0
			20	4	12	1	3		

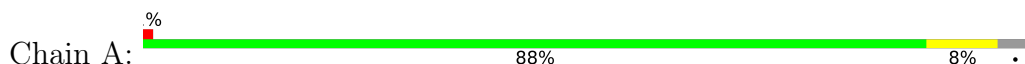
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	196	Total	O	0	0
			196	196		
5	C	187	Total	O	0	0
			187	187		
5	D	172	Total	O	0	0
			172	172		
5	E	178	Total	O	0	0
			178	178		
5	F	177	Total	O	0	0
			177	177		
5	G	214	Total	O	0	0
			214	214		
5	H	191	Total	O	0	0
			191	191		
5	I	138	Total	O	0	0
			138	138		
5	J	149	Total	O	0	0
			149	149		
5	K	130	Total	O	0	0
			130	130		
5	L	139	Total	O	0	0
			139	139		
5	M	149	Total	O	0	0
			149	149		
5	N	130	Total	O	0	0
			130	130		
5	O	117	Total	O	0	0
			117	117		
5	P	106	Total	O	0	0
			106	106		

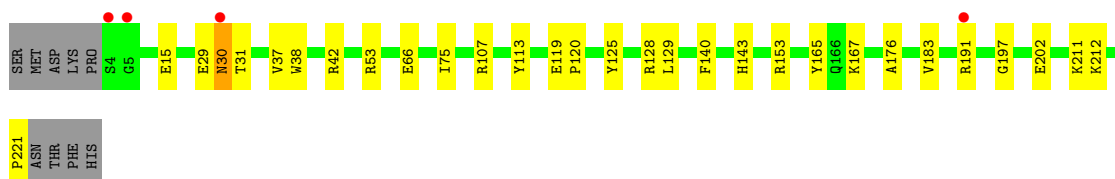
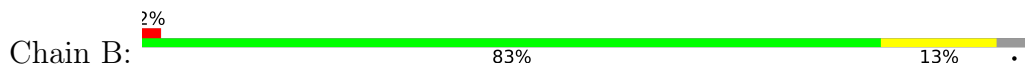
3 Residue-property plots [i](#)

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.

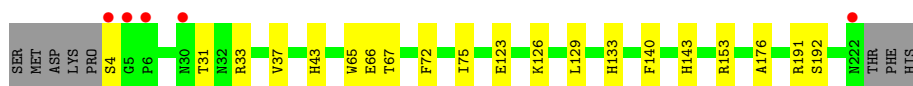
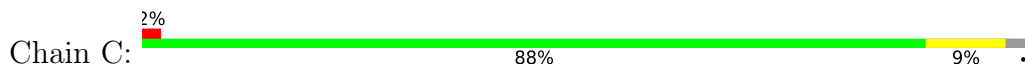
- Molecule 1: Angiotensin-related protein 2



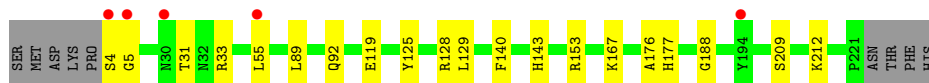
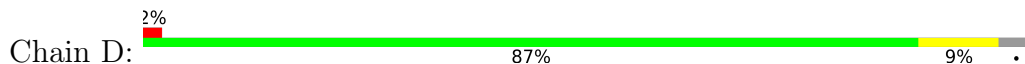
- Molecule 1: Angiotensin-related protein 2



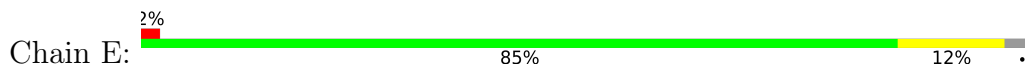
- Molecule 1: Angiotensin-related protein 2



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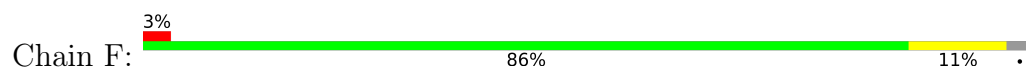


- Molecule 1: Angiotensin-related protein 2

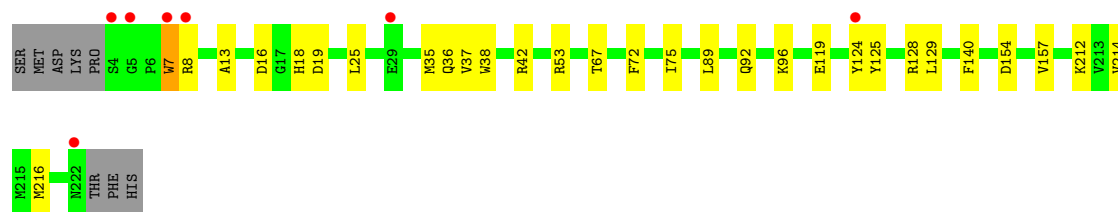
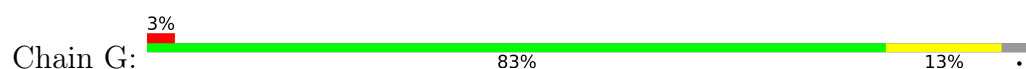




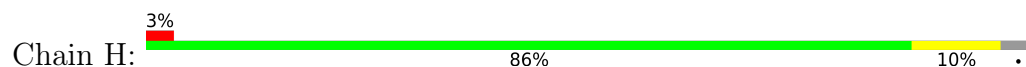
- Molecule 1: Angiotensinogen-related protein 2



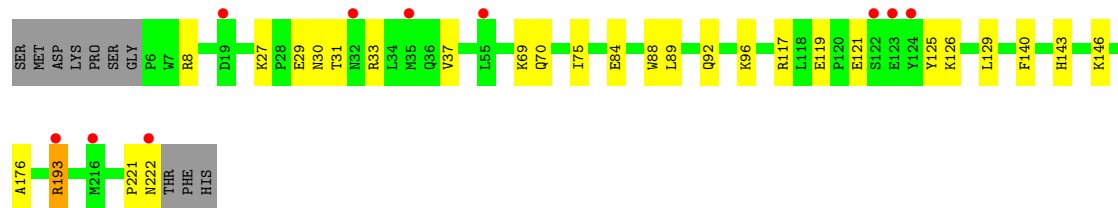
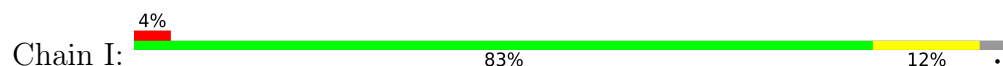
- Molecule 1: Angiotensinogen-related protein 2



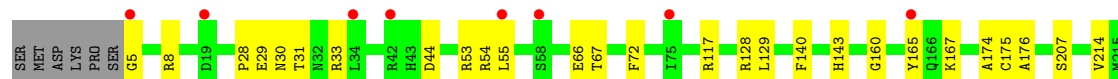
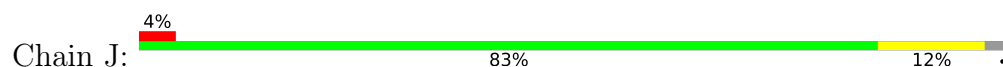
- Molecule 1: Angiotensinogen-related protein 2

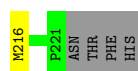


- Molecule 1: Angiotensinogen-related protein 2

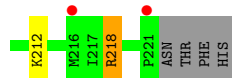
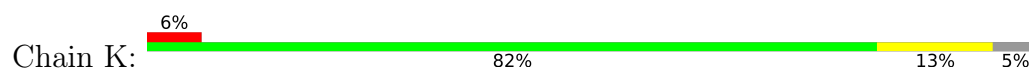


- Molecule 1: Angiotensinogen-related protein 2

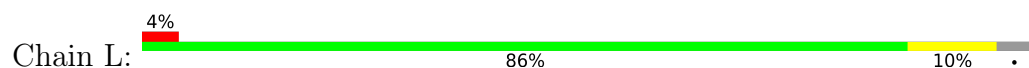




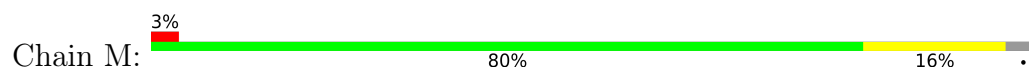
- Molecule 1: Angiopoietin-related protein 2



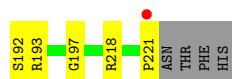
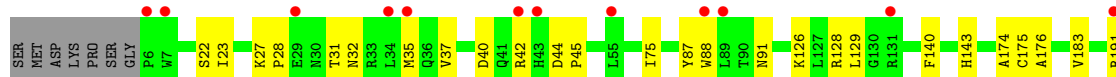
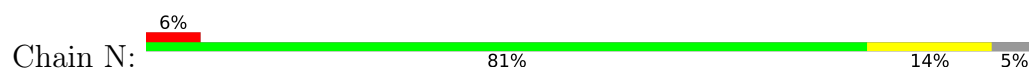
- Molecule 1: Angiopoietin-related protein 2



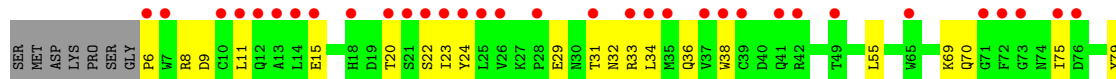
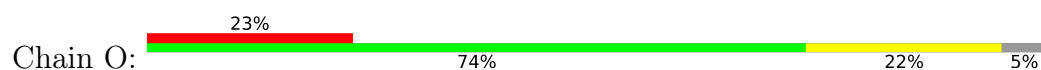
- Molecule 1: Angiopoietin-related protein 2



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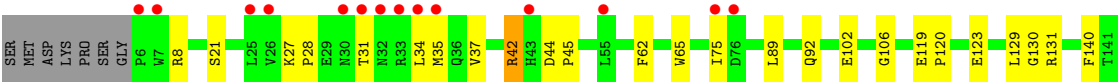
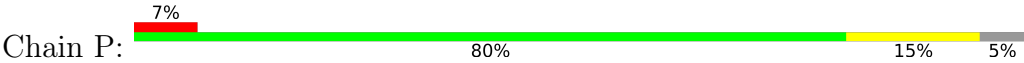


- Molecule 1: Angiopoietin-related protein 2





● Molecule 1: Angiopoietin-related protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	153.94Å 154.86Å 172.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.63 – 1.79 70.63 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.63-1.79) 99.9 (70.63-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.192 , 0.215 0.194 , 0.216	Depositor DCC
R_{free} test set	19275 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.069 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	57945	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6938e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, TRS

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	0.22	0/1886	0.51	0/2559
1	B	0.24	0/1875	0.52	0/2544
1	C	0.23	0/1873	0.52	0/2543
1	D	0.23	0/1866	0.51	0/2534
1	E	0.23	0/1885	0.53	0/2557
1	F	0.24	0/1889	0.50	1/2564 (0.0%)
1	G	0.68	7/1874 (0.4%)	0.57	2/2545 (0.1%)
1	H	0.35	1/1876 (0.1%)	0.50	0/2546
1	I	0.51	3/1870 (0.2%)	0.75	3/2538 (0.1%)
1	J	0.20	0/1854	0.46	0/2519
1	K	0.23	0/1858	0.47	0/2522
1	L	0.19	0/1880	0.45	0/2551
1	M	0.20	0/1862	0.47	0/2528
1	N	0.20	0/1864	0.45	0/2529
1	O	0.21	0/1856	0.51	0/2520
1	P	0.27	0/1852	0.52	2/2514 (0.1%)
All	All	0.31	11/29920 (0.0%)	0.52	8/40613 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	I	0	1
All	All	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	7	TRP	CZ3-CH2	-19.20	0.92	1.40
1	I	193	ARG	NE-CZ	-12.97	1.18	1.33
1	G	7	TRP	CE3-CZ3	12.40	1.75	1.38
1	H	131	ARG	CD-NE	11.53	1.62	1.46
1	I	193	ARG	CZ-NH2	-11.22	1.18	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	193	ARG	NE-CZ-NH2	-20.19	101.03	119.20
1	I	193	ARG	NE-CZ-NH1	17.39	138.89	121.50
1	I	193	ARG	CG-CD-NE	-6.60	97.48	112.00
1	G	7	TRP	CD2-CE2-CZ2	-6.30	116.10	122.40
1	P	42	ARG	NE-CZ-NH2	-5.81	113.97	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	5	GLY	Peptide
1	I	193	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1824	1666	1666	16	0
1	B	1813	1656	1656	25	0
1	C	1811	1647	1647	17	0
1	D	1804	1638	1638	16	0
1	E	1823	1669	1669	26	0
1	F	1826	1669	1669	19	1
1	G	1812	1644	1644	45	2
1	H	1814	1656	1654	21	0
1	I	1808	1648	1648	20	2
1	J	1792	1622	1622	25	0
1	K	1796	1638	1638	28	0
1	L	1818	1661	1661	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1800	1640	1640	28	2
1	N	1802	1649	1649	30	0
1	O	1794	1632	1631	44	0
1	P	1790	1630	1630	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	E	4	6	6	0	0
3	I	4	6	6	1	0
4	G	8	12	12	3	0
4	H	8	12	12	6	0
5	A	204	0	0	6	0
5	B	196	0	0	15	1
5	C	187	0	0	8	1
5	D	172	0	0	8	4
5	E	178	0	0	9	4
5	F	177	0	0	9	1
5	G	214	0	0	14	0
5	H	191	0	0	9	1
5	I	138	0	0	7	3
5	J	149	0	0	4	0
5	K	130	0	0	15	2
5	L	139	0	0	12	0
5	M	149	0	0	10	2
5	N	130	0	0	15	0
5	O	117	0	0	13	1
5	P	106	0	0	12	1
All	All	31544	26401	26398	407	15

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 7.

The worst 5 of 407 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:G:7:TRP:CE3	1:G:7:TRP:CZ3	1.75	1.71
1:G:7:TRP:CZ3	1:G:7:TRP:CZ2	2.13	1.36
1:H:191:ARG:NH1	5:H:501:HOH:O	1.57	1.28
1:G:7:TRP:CE3	1:G:13:ALA:HA	1.77	1.20
1:G:7:TRP:CZ3	1:G:13:ALA:HA	1.87	1.08

The worst 5 of 15 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:532:HOH:O	5:E:551:HOH:O[2_554]	1.22	0.98
5:D:423:HOH:O	5:E:540:HOH:O[2_554]	1.65	0.55
1:M:202:GLU:OE1	5:I:402:HOH:O[4_544]	1.91	0.29
5:I:529:HOH:O	5:M:530:HOH:O[4_545]	1.93	0.27
5:D:555:HOH:O	5:E:549:HOH:O[2_554]	1.94	0.26

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/227 (96%)	206 (95%)	11 (5%)	0	100	100
1	B	216/227 (95%)	206 (95%)	9 (4%)	1 (0%)	24	14
1	C	217/227 (96%)	205 (94%)	12 (6%)	0	100	100
1	D	216/227 (95%)	207 (96%)	9 (4%)	0	100	100
1	E	217/227 (96%)	208 (96%)	9 (4%)	0	100	100
1	F	218/227 (96%)	207 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	217/227 (96%)	206 (95%)	11 (5%)	0	100	100
1	H	216/227 (95%)	206 (95%)	10 (5%)	0	100	100
1	I	215/227 (95%)	204 (95%)	11 (5%)	0	100	100
1	J	215/227 (95%)	203 (94%)	12 (6%)	0	100	100
1	K	214/227 (94%)	202 (94%)	12 (6%)	0	100	100
1	L	216/227 (95%)	204 (94%)	12 (6%)	0	100	100
1	M	215/227 (95%)	204 (95%)	10 (5%)	1 (0%)	24	14
1	N	214/227 (94%)	204 (95%)	10 (5%)	0	100	100
1	O	214/227 (94%)	203 (95%)	11 (5%)	0	100	100
1	P	214/227 (94%)	202 (94%)	12 (6%)	0	100	100
All	All	3451/3632 (95%)	3277 (95%)	172 (5%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	ASN
1	M	55	LEU

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	186/195 (95%)	186 (100%)	0	100	100
1	B	184/195 (94%)	184 (100%)	0	100	100
1	C	183/195 (94%)	183 (100%)	0	100	100
1	D	183/195 (94%)	183 (100%)	0	100	100
1	E	185/195 (95%)	185 (100%)	0	100	100
1	F	186/195 (95%)	186 (100%)	0	100	100
1	G	184/195 (94%)	184 (100%)	0	100	100
1	H	184/195 (94%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	184/195 (94%)	184 (100%)	0	100	100
1	J	181/195 (93%)	181 (100%)	0	100	100
1	K	182/195 (93%)	181 (100%)	1 (0%)	81	80
1	L	185/195 (95%)	185 (100%)	0	100	100
1	M	182/195 (93%)	182 (100%)	0	100	100
1	N	183/195 (94%)	183 (100%)	0	100	100
1	O	182/195 (93%)	182 (100%)	0	100	100
1	P	180/195 (92%)	180 (100%)	0	100	100
All	All	2934/3120 (94%)	2933 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	222	ASN
1	P	18	HIS
1	M	36	GLN
1	N	147	GLN
1	F	36	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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	EDO	E	301	-	3,3,3	0.46	0	2,2,2	0.27	0
4	TRS	H	401	-	7,7,7	1.13	1 (14%)	9,9,9	3.24	6 (66%)
4	TRS	G	401	-	7,7,7	1.24	1 (14%)	9,9,9	4.53	6 (66%)
3	EDO	I	301	-	3,3,3	0.46	0	2,2,2	0.39	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	EDO	E	301	-	-	0/1/1/1	-
4	TRS	H	401	-	-	9/9/9/9	-
4	TRS	G	401	-	-	4/9/9/9	-
3	EDO	I	301	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	401	TRS	C-N	2.90	1.58	1.49
4	G	401	TRS	C-N	2.83	1.58	1.49

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	TRS	C2-C-N	8.29	129.31	108.17
4	H	401	TRS	C2-C-N	6.41	124.52	108.17
4	G	401	TRS	C1-C-N	5.64	122.56	108.17
4	G	401	TRS	C2-C-C1	-5.45	96.15	110.66
4	G	401	TRS	C3-C-C2	-5.28	96.59	110.66

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	401	TRS	C2-C-C1-O1
4	G	401	TRS	C3-C-C1-O1
4	H	401	TRS	N-C-C1-O1
4	H	401	TRS	N-C-C2-O2
4	H	401	TRS	C1-C-C3-O3

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	401	TRS	6	0
4	G	401	TRS	3	0
3	I	301	EDO	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	219/227 (96%)	-0.10	3 (1%) 73 73	23, 30, 49, 61	0
1	B	218/227 (96%)	-0.12	4 (1%) 67 68	23, 30, 49, 67	0
1	C	219/227 (96%)	-0.10	5 (2%) 61 61	23, 30, 52, 70	0
1	D	218/227 (96%)	-0.01	5 (2%) 61 61	23, 32, 48, 70	0
1	E	219/227 (96%)	-0.07	4 (1%) 67 68	23, 31, 52, 72	0
1	F	220/227 (96%)	0.12	6 (2%) 56 56	23, 32, 51, 71	0
1	G	219/227 (96%)	-0.13	7 (3%) 50 50	23, 29, 45, 64	0
1	H	218/227 (96%)	-0.00	7 (3%) 50 50	23, 32, 51, 68	0
1	I	217/227 (95%)	0.32	10 (4%) 37 36	25, 37, 64, 80	0
1	J	217/227 (95%)	0.26	8 (3%) 45 45	28, 38, 58, 71	0
1	K	216/227 (95%)	0.29	13 (6%) 27 26	25, 38, 65, 84	0
1	L	218/227 (96%)	0.39	9 (4%) 41 41	28, 40, 63, 80	0
1	M	217/227 (95%)	0.28	7 (3%) 50 50	28, 39, 65, 87	0
1	N	216/227 (95%)	0.60	13 (6%) 27 26	26, 41, 76, 103	0
1	O	216/227 (95%)	1.12	52 (24%) 2 1	24, 45, 77, 104	0
1	P	216/227 (95%)	0.69	15 (6%) 23 21	30, 44, 75, 106	0
All	All	3483/3632 (95%)	0.22	168 (4%) 35 34	23, 35, 62, 106	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5	GLY	7.8
1	G	7	TRP	7.6
1	H	5	GLY	6.2
1	C	5	GLY	5.7
1	D	5	GLY	5.6

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, 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($\text{\AA}^2$)	Q<0.9
4	TRS	G	401	8/8	0.62	0.17	39,63,74,75	0
4	TRS	H	401	8/8	0.66	0.18	43,57,72,75	0
3	EDO	I	301	4/4	0.77	0.19	36,57,69,80	0
3	EDO	E	301	4/4	0.80	0.12	45,63,76,77	0
2	CA	C	301	1/1	0.96	0.22	60,60,60,60	0
2	CA	O	301	1/1	0.97	0.05	36,36,36,36	0
2	CA	P	301	1/1	0.97	0.05	37,37,37,37	0
2	CA	N	301	1/1	0.97	0.06	35,35,35,35	0
2	CA	K	301	1/1	0.98	0.03	27,27,27,27	0
2	CA	D	301	1/1	0.98	0.03	28,28,28,28	0
2	CA	F	301	1/1	0.98	0.04	34,34,34,34	0
2	CA	I	302	1/1	0.98	0.05	33,33,33,33	0
2	CA	A	301	1/1	0.99	0.03	26,26,26,26	0
2	CA	H	402	1/1	0.99	0.03	24,24,24,24	0
2	CA	B	301	1/1	0.99	0.07	33,33,33,33	0
2	CA	J	301	1/1	0.99	0.03	32,32,32,32	0
2	CA	E	302	1/1	0.99	0.03	28,28,28,28	0
2	CA	L	301	1/1	0.99	0.04	34,34,34,34	0
2	CA	M	301	1/1	0.99	0.04	33,33,33,33	0
2	CA	G	402	1/1	1.00	0.04	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.