



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:56 PM UTC

PDB ID : 8W52 / pdb_00008w52
Title : p17 protein structure of HIV2 when OLA1 existing
Authors : Dang, L.L.
Deposited on : 2023-08-25
Resolution : 2.38 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

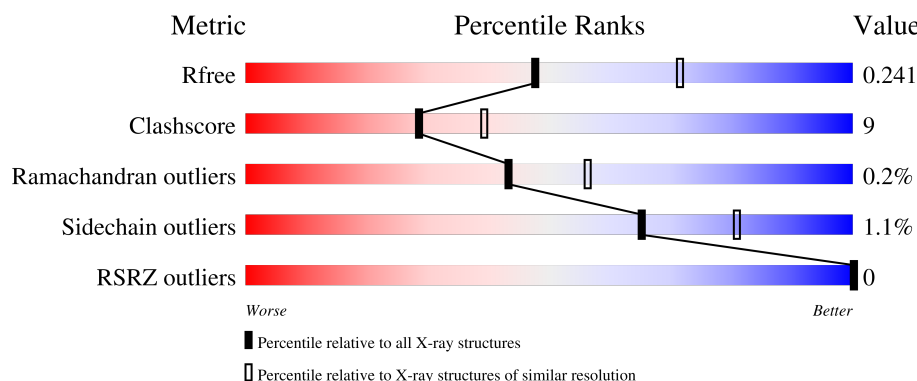
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

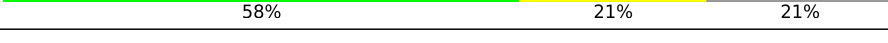
The reported resolution of this entry is 2.38 Å.

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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 $\leq 5\%$. 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	135	
1	B	135	
1	C	135	
1	D	135	
1	E	135	

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Mol	Chain	Length	Quality of chain
1	F	135	
1	G	135	
1	H	135	
1	I	135	
1	J	135	
1	K	135	
1	L	135	
1	M	135	
1	N	135	
1	O	135	
1	P	135	

2 Entry composition

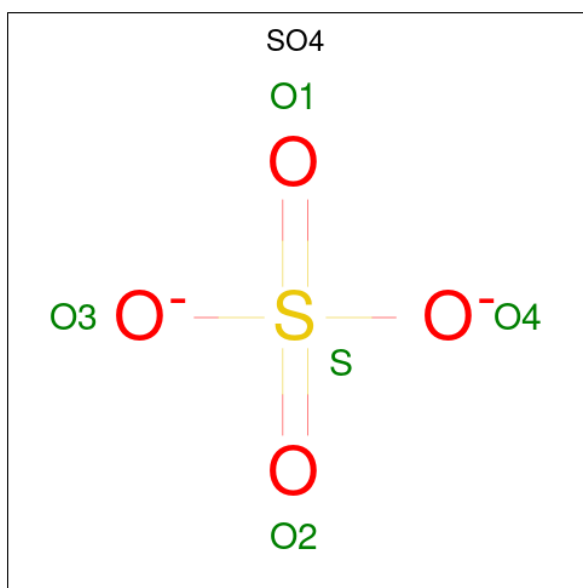
There are 3 unique types of molecules in this entry. The entry contains 14103 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Gag polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			879	556	161	159	3			
1	B	111	Total	C	N	O	S	0	0	0
			879	556	161	159	3			
1	C	109	Total	C	N	O	S	0	0	0
			868	550	159	156	3			
1	D	107	Total	C	N	O	S	0	0	0
			854	542	157	152	3			
1	E	111	Total	C	N	O	S	0	0	0
			879	556	161	159	3			
1	F	111	Total	C	N	O	S	0	0	0
			879	556	161	159	3			
1	G	106	Total	C	N	O	S	0	0	0
			842	535	152	152	3			
1	H	107	Total	C	N	O	S	0	0	0
			849	540	153	153	3			
1	I	105	Total	C	N	O	S	0	0	0
			838	534	151	150	3			
1	J	102	Total	C	N	O	S	0	0	0
			817	521	148	145	3			
1	K	108	Total	C	N	O	S	0	0	0
			859	545	155	156	3			
1	L	106	Total	C	N	O	S	0	0	0
			845	538	152	152	3			
1	M	103	Total	C	N	O	S	0	0	0
			823	524	149	147	3			
1	N	105	Total	C	N	O	S	0	0	0
			838	534	151	150	3			
1	O	108	Total	C	N	O	S	0	0	0
			864	548	158	155	3			
1	P	107	Total	C	N	O	S	0	0	0
			854	542	157	152	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	29	Total	O	0	0
			29	29		
3	C	10	Total	O	0	0
			10	10		
3	D	17	Total	O	0	0
			17	17		
3	E	24	Total	O	0	0
			24	24		
3	F	28	Total	O	0	0
			28	28		
3	G	22	Total	O	0	0
			22	22		
3	H	28	Total	O	0	0
			28	28		
3	I	25	Total	O	0	0
			25	25		
3	J	19	Total	O	0	0
			19	19		
3	K	25	Total	O	0	0
			25	25		
3	L	17	Total	O	0	0
			17	17		

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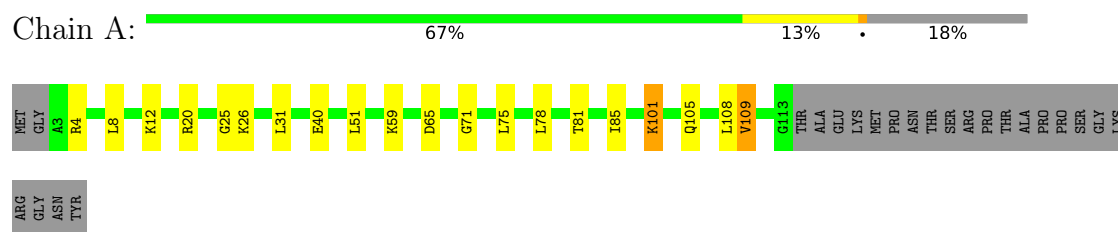
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	14	Total 14	O 14	0	0
3	N	27	Total 27	O 27	0	0
3	O	21	Total 21	O 21	0	0
3	P	13	Total 13	O 13	0	0

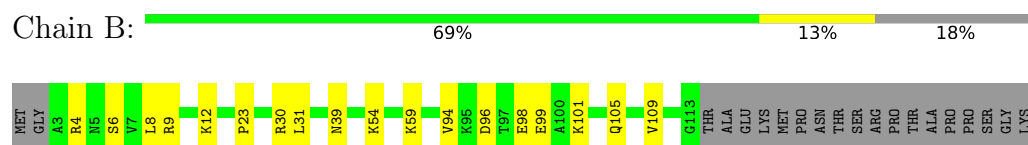
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

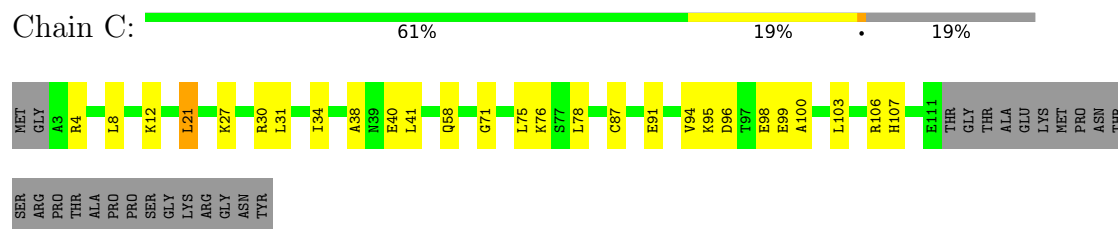
- Molecule 1: Gag polypeptide



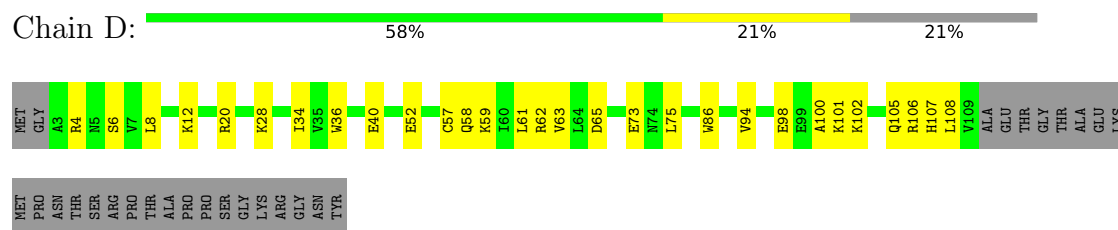
- Molecule 1: Gag polypeptide



- Molecule 1: Gag polypeptide

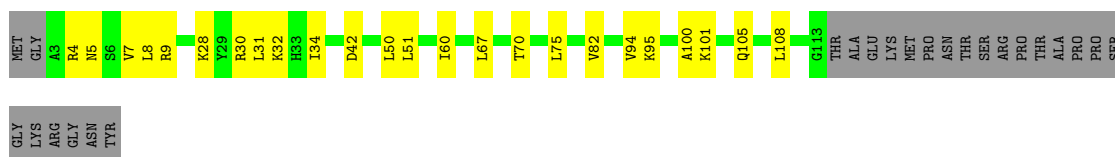


- Molecule 1: Gag polypeptide



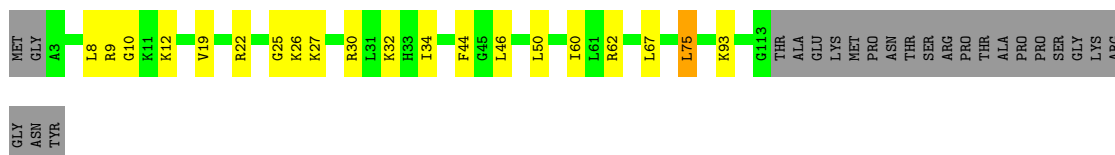
- Molecule 1: Gag polypeptide





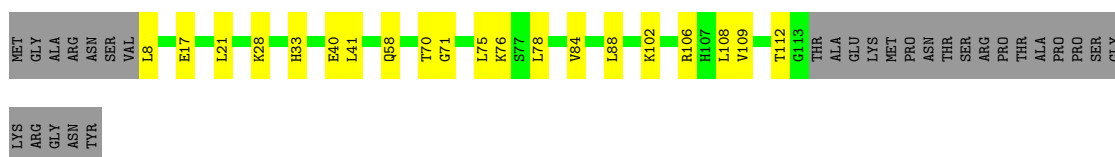
• Molecule 1: Gag polyprotein

Chain F: 67% 14% 18%



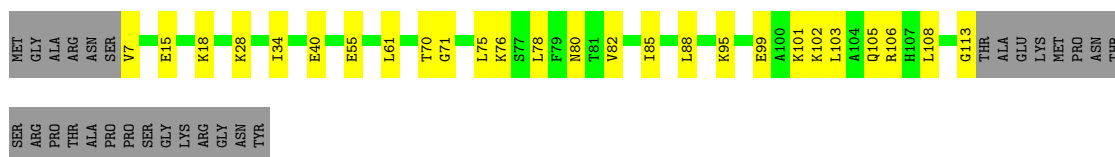
• Molecule 1: Gag polyprotein

Chain G: 64% 15% 21%



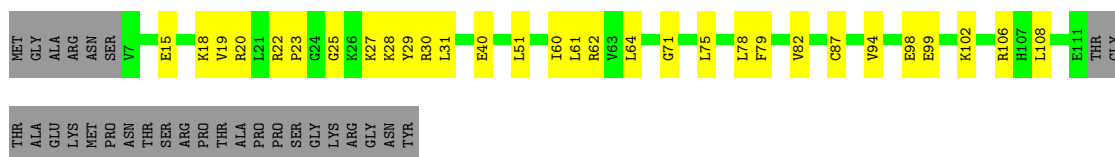
• Molecule 1: Gag polyprotein

Chain H: 60% 19% 21%



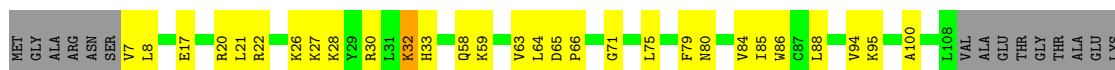
• Molecule 1: Gag polyprotein

Chain I: 56% 22% 22%



• Molecule 1: Gag polyprotein

Chain J: 54% 21% 24%



MET
PRO
ASN
THR
ARG
SER
ARG
PRO
THR
ALA
PRO
PRO
SER
GLY
LYS
ARG
ASN
TYR

- Molecule 1: Gag polypeptide

Chain K:  67% 13% 20%

MET
GLY
ALA
ARG
N5
S6
V7
L8
L21
K27
K28
L31
I34
E40
G71
L75
L78
I85
V94
A100
Q105
V109
T112
GLY
THR
ALA
GLU
LYS
MET
PRO
ASN
THR
SER
ARG
PRO
THR
ALA
PRO
PRO
SER
MET
GLY
LYS
ARG
GLY
ASN
TYR

- Molecule 1: Gag polypeptide

Chain L:  61% 17% 21%

MET
GLY
ALA
ARG
ASN
SER
V7
L8
R9
L16
L17
K18
L21
R22
P23
K27
R30
L31
K32
H33
I34
Q58
G71
L75
N80
V84
I85
W86
C87
L88
T97
E98
K101
L108
T112
GLY
THR
ALA
GLU
LYS
MET
PRO
ASN
THR
SER
ARG
PRO

THR
ALA
PRO
PRO
GLY
LYS
GLY
TYR

- Molecule 1: Gag polypeptide

Chain M:  56% 19% 24%

MET
GLY
ALA
ARG
ASN
S6
V7
L8
R20
L21
R22
P23
G24
G25
K26
E40
L50
S53
G56
I60
V63
L64
T70
E73
N74
L75
K76
S77
L78
F79
N80
I85
L88
V94
E98
E99
A100
K101
K102
R106
H107
L108
VAL
ALA
GLU
THR

GLY
THR
ALA
GLU
LYS
MET
PRO
ASN
THR
SER
PRO
THR
ALA
PRO
SER
GLY
LYS
ARG
ASN
TYR

- Molecule 1: Gag polypeptide

Chain N:  61% 17% 22%

MET
GLY
ALA
ARG
ASN
SER
V7
L8
L16
R20
L21
K27
K28
H33
W36
K54
E55
K59
I60
L61
R62
T70
S77
N80
I85
L88
V94
A100
K101
Q105
L108
E111
THR
GLY
THR
ALA
GLU
LYS
MET
PRO
ASN
THR
SER

ARG
PRO
THR
ALA
LYS
PRO
PRO
SER
GLY
LYS
ARG
ASN
TYR

- Molecule 1: Gag polypeptide

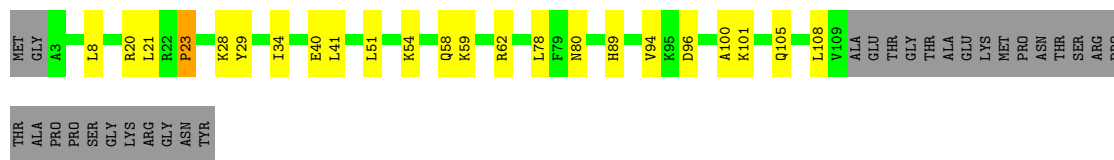
Chain O:  57% 21% 20%

MET
GLY
A3
R4
V7
L8
R9
G10
K11
K12
P23
GLY
G25
K26
K27
K28
E40
L50
L51
K54
Q58
K59
I60
L61
R62
G71
L75
L78
F79
W86
H89
E92
K93
V94
K95
D96
A100
L103
R106
H107
L108
E111
GLY

THR
ALA
GLU
LYS
MET
PRO
PRO
THR
THR
ARG
PRO
THR
ALA
PRO
SER
SER
GLY
LYS
ARG
GLY
ASN
TYR

- Molecule 1: Gag polypeptide

Response	Percentage
Yes	62%
No	16%
Don't know	21%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.78Å 123.78Å 108.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 2.38 46.19 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.19-2.38) 99.8 (46.19-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.248 0.209 , 0.241	Depositor DCC
R_{free} test set	3371 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	14103	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 75.96 % 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 1.1429e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.09	0/891	0.23	0/1194
1	B	0.11	0/891	0.26	0/1194
1	C	0.12	0/880	0.32	0/1179
1	D	0.10	0/866	0.27	0/1160
1	E	0.09	0/891	0.28	0/1194
1	F	0.09	0/891	0.24	0/1194
1	G	0.13	0/854	0.28	0/1144
1	H	0.10	0/861	0.28	0/1154
1	I	0.10	0/850	0.29	0/1139
1	J	0.16	0/829	0.31	0/1110
1	K	0.08	0/871	0.22	0/1168
1	L	0.10	0/857	0.27	0/1149
1	M	0.12	0/835	0.34	1/1118 (0.1%)
1	N	0.13	0/850	0.32	0/1139
1	O	0.12	0/875	0.29	0/1171
1	P	0.11	0/866	0.31	0/1160
All	All	0.11	0/13858	0.28	1/18567 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	74	ASN	N-CA-C	-6.13	104.52	111.14

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	879	0	926	13	0
1	B	879	0	926	14	0
1	C	868	0	916	16	0
1	D	854	0	905	19	0
1	E	879	0	926	20	0
1	F	879	0	926	14	0
1	G	842	0	888	16	0
1	H	849	0	897	20	0
1	I	838	0	887	20	0
1	J	817	0	867	21	0
1	K	859	0	905	11	0
1	L	845	0	894	16	0
1	M	823	0	872	15	0
1	N	838	0	887	15	0
1	O	864	0	912	24	0
1	P	854	0	905	12	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	E	10	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	10	0	0	1	0
2	J	10	0	0	0	0
2	K	10	0	0	0	0
2	L	15	0	0	1	0
2	N	5	0	0	0	0
2	P	5	0	0	0	0
3	A	17	0	0	1	0
3	B	29	0	0	2	0
3	C	10	0	0	0	0
3	D	17	0	0	1	0
3	E	24	0	0	3	0
3	F	28	0	0	2	0
3	G	22	0	0	0	0
3	H	28	0	0	3	0
3	I	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	19	0	0	0	0
3	K	25	0	0	1	0
3	L	17	0	0	4	0
3	M	14	0	0	1	0
3	N	27	0	0	0	0
3	O	21	0	0	2	0
3	P	13	0	0	0	0
All	All	14103	0	14439	247	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 9.

The worst 5 of 247 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:O:103:LEU:HA	1:O:106:ARG:HD3	1.60	0.82
1:I:62:ARG:HG3	1:I:108:LEU:HD11	1.61	0.80
1:D:8:LEU:HD12	1:D:34:ILE:HD11	1.67	0.77
1:C:103:LEU:HG	1:C:106:ARG:HH12	1.49	0.76
1:C:71:GLY:HA3	1:C:75:LEU:HD23	1.69	0.74

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	109/135 (81%)	108 (99%)	1 (1%)	0	100	100
1	B	109/135 (81%)	107 (98%)	2 (2%)	0	100	100
1	C	107/135 (79%)	106 (99%)	0	1 (1%)	14	20
1	D	105/135 (78%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	109/135 (81%)	107 (98%)	2 (2%)	0	100	100
1	F	109/135 (81%)	107 (98%)	2 (2%)	0	100	100
1	G	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
1	H	105/135 (78%)	104 (99%)	1 (1%)	0	100	100
1	I	103/135 (76%)	98 (95%)	5 (5%)	0	100	100
1	J	100/135 (74%)	99 (99%)	1 (1%)	0	100	100
1	K	106/135 (78%)	105 (99%)	1 (1%)	0	100	100
1	L	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
1	M	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
1	N	103/135 (76%)	102 (99%)	1 (1%)	0	100	100
1	O	104/135 (77%)	101 (97%)	2 (2%)	1 (1%)	12	17
1	P	105/135 (78%)	103 (98%)	1 (1%)	1 (1%)	12	17
All	All	1683/2160 (78%)	1650 (98%)	30 (2%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	21	LEU
1	P	23	PRO
1	O	7	VAL

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	95/114 (83%)	92 (97%)	3 (3%)	34	53
1	B	95/114 (83%)	94 (99%)	1 (1%)	65	81
1	C	94/114 (82%)	93 (99%)	1 (1%)	65	81
1	D	93/114 (82%)	91 (98%)	2 (2%)	45	65
1	E	95/114 (83%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	95/114 (83%)	93 (98%)	2 (2%)	47	67
1	G	91/114 (80%)	90 (99%)	1 (1%)	65	81
1	H	92/114 (81%)	91 (99%)	1 (1%)	65	81
1	I	91/114 (80%)	91 (100%)	0	100	100
1	J	89/114 (78%)	88 (99%)	1 (1%)	65	81
1	K	94/114 (82%)	93 (99%)	1 (1%)	65	81
1	L	92/114 (81%)	92 (100%)	0	100	100
1	M	90/114 (79%)	89 (99%)	1 (1%)	65	81
1	N	91/114 (80%)	90 (99%)	1 (1%)	65	81
1	O	94/114 (82%)	93 (99%)	1 (1%)	65	81
1	P	93/114 (82%)	93 (100%)	0	100	100
All	All	1484/1824 (81%)	1468 (99%)	16 (1%)	65	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	16	LEU
1	M	53	SER
1	F	75	LEU
1	K	6	SER
1	F	19	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	5	ASN
1	O	58	GLN
1	P	5	ASN
1	I	107	HIS
1	J	80	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 ⓘ

20 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	$\# Z > 2$
2	SO4	K	201	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	N	201	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	202	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	L	201	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	E	201	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	L	203	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	L	202	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	201	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	202	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	I	201	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	201	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	I	202	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	202	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	H	201	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	P	201	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	G	201	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	K	202	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	201	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	J	202	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	J	201	-	4,4,4	0.23	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	203	SO4	1	0
2	I	201	SO4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	111/135 (82%)	-1.52	0 100 100	20, 40, 56, 62	0
1	B	111/135 (82%)	-1.54	0 100 100	22, 39, 57, 63	0
1	C	109/135 (80%)	-1.28	0 100 100	32, 50, 67, 84	0
1	D	107/135 (79%)	-1.32	0 100 100	28, 48, 70, 86	0
1	E	111/135 (82%)	-1.48	0 100 100	24, 39, 60, 77	0
1	F	111/135 (82%)	-1.52	0 100 100	24, 38, 58, 75	0
1	G	106/135 (78%)	-1.47	0 100 100	25, 38, 61, 99	0
1	H	107/135 (79%)	-1.48	0 100 100	26, 39, 60, 98	0
1	I	105/135 (77%)	-1.35	0 100 100	30, 49, 66, 84	0
1	J	102/135 (75%)	-1.30	0 100 100	30, 48, 73, 87	0
1	K	108/135 (80%)	-1.44	0 100 100	26, 40, 60, 75	0
1	L	106/135 (78%)	-1.46	0 100 100	24, 42, 61, 86	0
1	M	103/135 (76%)	-1.33	0 100 100	27, 48, 69, 96	0
1	N	105/135 (77%)	-1.34	0 100 100	25, 46, 70, 90	0
1	O	108/135 (80%)	-1.26	0 100 100	30, 52, 74, 88	0
1	P	107/135 (79%)	-1.26	0 100 100	31, 51, 72, 83	0
All	All	1717/2160 (79%)	-1.40	0 100 100	20, 44, 66, 99	0

There are no RSRZ outliers to report.

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 ⓘ

There are no oligosaccharides 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
2	SO4	P	201	5/5	0.97	0.05	76,89,102,105	0
2	SO4	I	202	5/5	0.98	0.03	43,61,71,90	0
2	SO4	L	203	5/5	0.98	0.03	77,91,103,108	0
2	SO4	C	201	5/5	0.98	0.05	67,70,91,130	0
2	SO4	J	201	5/5	0.99	0.02	38,42,57,79	0
2	SO4	K	201	5/5	0.99	0.02	39,39,55,60	0
2	SO4	L	201	5/5	0.99	0.02	30,37,58,82	0
2	SO4	I	201	5/5	0.99	0.03	45,50,56,70	0
2	SO4	N	201	5/5	0.99	0.06	40,47,54,71	0
2	SO4	E	202	5/5	0.99	0.04	73,85,97,98	0
2	SO4	B	202	5/5	1.00	0.02	18,43,58,69	0
2	SO4	A	201	5/5	1.00	0.03	35,50,76,76	0
2	SO4	J	202	5/5	1.00	0.02	35,38,46,49	0
2	SO4	E	201	5/5	1.00	0.03	34,48,58,69	0
2	SO4	K	202	5/5	1.00	0.02	16,33,57,66	0
2	SO4	A	202	5/5	1.00	0.02	21,28,57,62	0
2	SO4	L	202	5/5	1.00	0.03	27,39,55,61	0
2	SO4	G	201	5/5	1.00	0.02	38,44,55,64	0
2	SO4	H	201	5/5	1.00	0.02	39,42,64,76	0
2	SO4	B	201	5/5	1.00	0.02	20,42,54,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.