



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:51 PM UTC

PDB ID : 3ZED / pdb_00003zed
Title : X-ray structure of the birnavirus VP1-VP3 complex
Authors : Bahar, M.W.; Sarin, L.P.; Graham, S.C.; Pang, J.; Bamford, D.H.; Stuart, D.I.; Grimes, J.M.
Deposited on : 2012-12-04
Resolution : 2.20 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 ⓘ 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

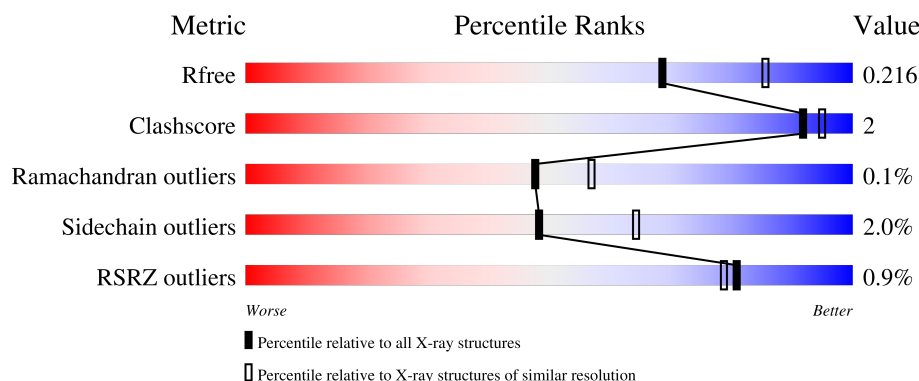
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



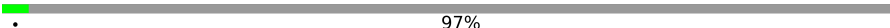
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	853	
1	B	853	
1	C	853	
2	D	242	
2	E	242	

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Mol	Chain	Length	Quality of chain
2	F	242	 97%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19298 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	2	0
			5996	3803	1006	1162	25			
1	B	766	Total	C	N	O	S	0	1	0
			5972	3788	996	1163	25			
1	C	765	Total	C	N	O	S	0	0	0
			5982	3794	1003	1160	25			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	846	VAL	-	expression tag	UNP P22173
A	847	GLU	-	expression tag	UNP P22173
A	848	HIS	-	expression tag	UNP P22173
A	849	HIS	-	expression tag	UNP P22173
A	850	HIS	-	expression tag	UNP P22173
A	851	HIS	-	expression tag	UNP P22173
A	852	HIS	-	expression tag	UNP P22173
A	853	HIS	-	expression tag	UNP P22173
B	846	VAL	-	expression tag	UNP P22173
B	847	GLU	-	expression tag	UNP P22173
B	848	HIS	-	expression tag	UNP P22173
B	849	HIS	-	expression tag	UNP P22173
B	850	HIS	-	expression tag	UNP P22173
B	851	HIS	-	expression tag	UNP P22173
B	852	HIS	-	expression tag	UNP P22173
B	853	HIS	-	expression tag	UNP P22173
C	846	VAL	-	expression tag	UNP P22173
C	847	GLU	-	expression tag	UNP P22173
C	848	HIS	-	expression tag	UNP P22173
C	849	HIS	-	expression tag	UNP P22173
C	850	HIS	-	expression tag	UNP P22173
C	851	HIS	-	expression tag	UNP P22173
C	852	HIS	-	expression tag	UNP P22173

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Chain	Residue	Modelled	Actual	Comment	Reference
C	853	HIS	-	expression tag	UNP P22173

- Molecule 2 is a protein called CAPSID PROTEIN VP3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	0	0	0
			89	52	15	22			
2	E	8	Total	C	N	O	0	0	0
			63	39	11	13			
2	F	8	Total	C	N	O	0	0	0
			63	39	11	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P05844
D	-2	PRO	-	expression tag	UNP P05844
D	-1	THR	-	expression tag	UNP P05844
D	0	ALA	-	expression tag	UNP P05844
E	-3	GLY	-	expression tag	UNP P05844
E	-2	PRO	-	expression tag	UNP P05844
E	-1	THR	-	expression tag	UNP P05844
E	0	ALA	-	expression tag	UNP P05844
F	-3	GLY	-	expression tag	UNP P05844
F	-2	PRO	-	expression tag	UNP P05844
F	-1	THR	-	expression tag	UNP P05844
F	0	ALA	-	expression tag	UNP P05844

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		
4	B	2	Total	K	0	0
			2	2		
4	C	2	Total	K	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	504	Total	O	0	0
			504	504		
5	B	303	Total	O	0	0
			303	303		
5	C	290	Total	O	0	0
			290	290		

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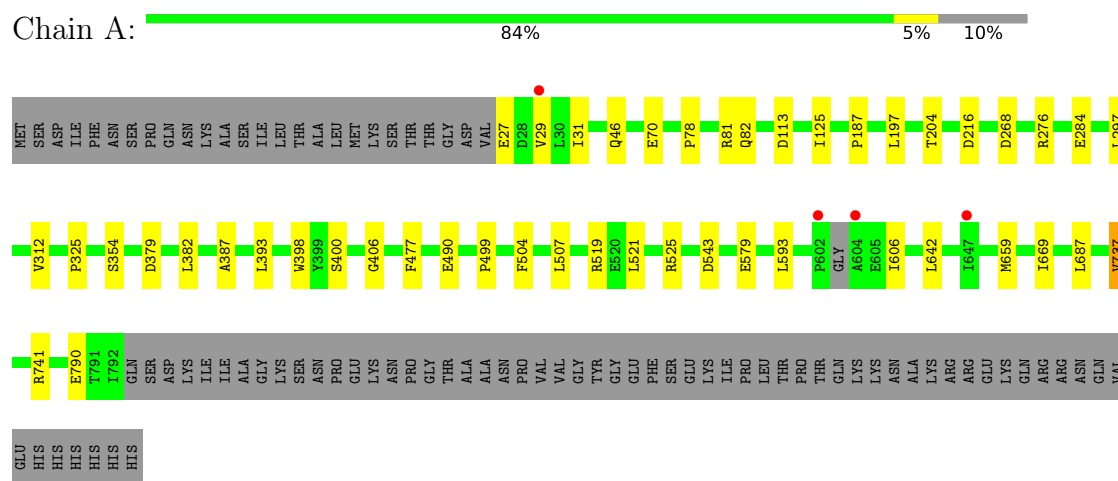
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	3	Total	O	0	0
			3	3		
5	E	6	Total	O	0	0
			6	6		
5	F	3	Total	O	0	0
			3	3		

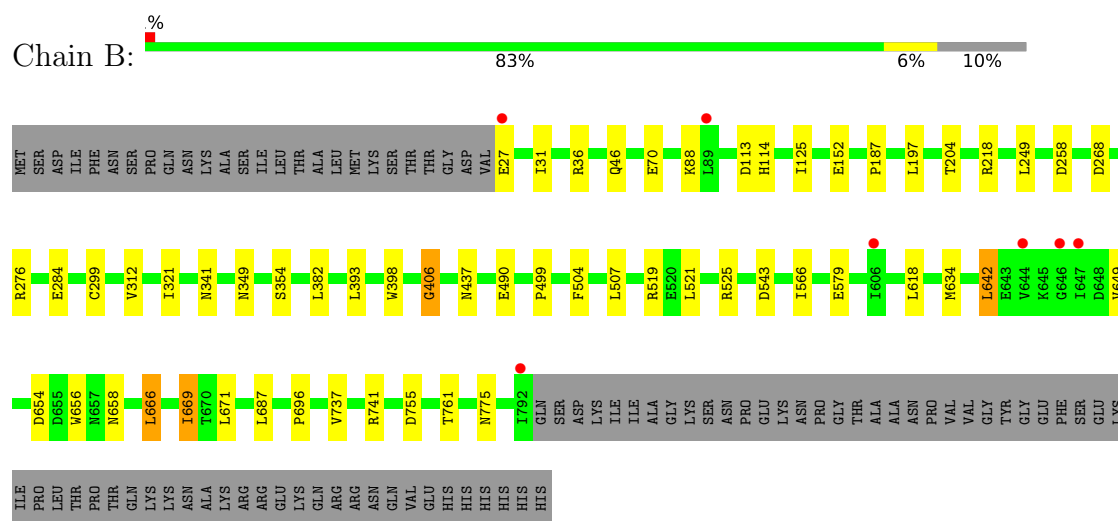
3 Residue-property plots [i](#)

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.

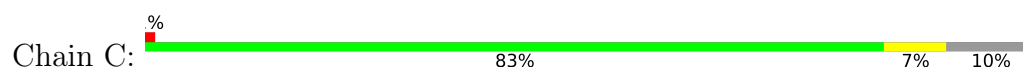
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

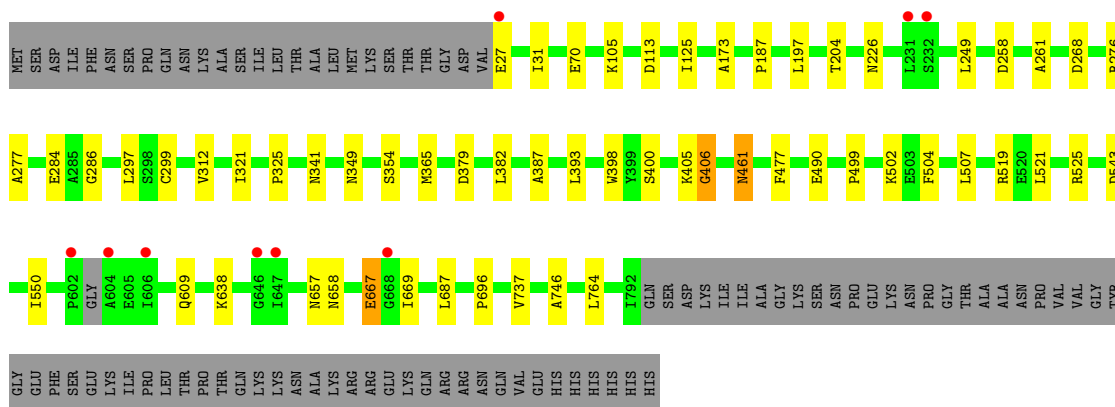


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



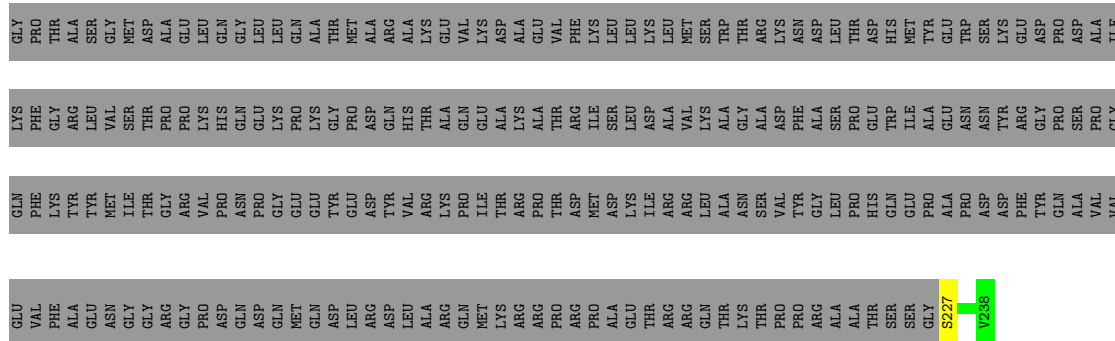
• Molecule 1: RNA-DIRECTED RNA POLYMERASE





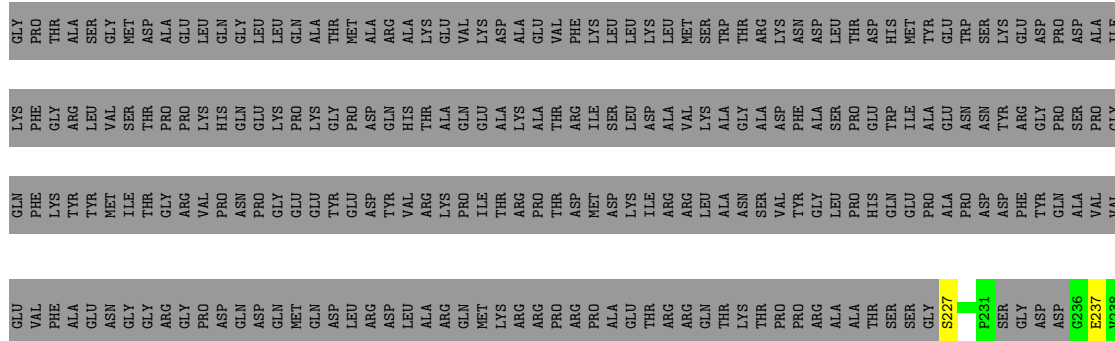
- Molecule 2: CAPSID PROTEIN VP3

Chain D: 5% 95%



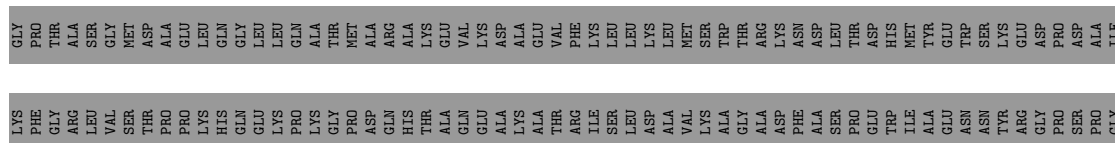
- Molecule 2: CAPSID PROTEIN VP3

Chain E: 97%



- Molecule 2: CAPSID PROTEIN VP3

Chain F: 97%



GLN PHE LYS LYS TYR TYR MET ILE THR GLY GLY ARG GLN VAL VAL PRO ASN ASP PRO PRO GLY GLY GLU GLU TYR TYR GLU ASP TYR VAL VAL ARG ARG LYS PRO PRO THR THR ASP MET MET LYS ASP LYS ILE ILE ARG ARG ARG LEU LEU LEU LEU HIS HIS GLN GLN GLU GLU PRO PRO ALA ALA ALA ALA ASP ASP ASP ASP PHE PHE TYR TYR GLN GLN VAL VAL VAL VAL

GLU	VAL	PHI	GLU	GLY	ASN	GLY	GLY	ARG	GLY	PRO	ASP	GLN	ASP	LEU	ARG	ASP	MET	LYS	THR	ALA	ALA	ARG	PRO	PRO	THR	THR	THR	PRO	PRO	ARG	ALA	ALA	THR	SER	SER	GLY	GLY	ASP	ASP	P31	G36	E37
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.27Å 341.87Å 59.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.13 – 2.20 59.13 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (59.13-2.20) 99.6 (59.13-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.179 , 0.214 0.179 , 0.216	Depositor DCC
R_{free} test set	6202 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19298	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.71% 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: GOL, K

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	0.86	0/6137	1.16	5/8359 (0.1%)
1	B	0.84	0/6111	1.20	14/8331 (0.2%)
1	C	0.83	1/6117 (0.0%)	1.20	14/8333 (0.2%)
2	D	0.89	0/90	1.19	0/119
2	E	0.87	0/63	0.93	0/81
2	F	0.86	0/63	0.90	0/81
All	All	0.85	1/18581 (0.0%)	1.18	33/25304 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	365	MET	SD-CE	-6.32	1.63	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CA-CB-CG	7.75	120.35	112.60
1	C	667	GLU	N-CA-C	6.88	119.62	111.71
1	B	437	ASN	CA-CB-CG	6.40	119.00	112.60
1	B	543	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	406	GLY	CA-C-N	5.94	128.52	120.38
1	B	406	GLY	C-N-CA	5.94	128.52	120.38
1	B	113	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	341	ASN	CA-CB-CG	5.85	118.45	112.60
1	C	543	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	113	ASP	CA-CB-CG	5.66	118.25	112.60
1	A	113	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	258	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	525	ARG	CA-C-N	5.46	127.54	120.44
1	B	525	ARG	C-N-CA	5.46	127.54	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	268	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	268	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	152	GLU	CB-CG-CD	5.30	121.61	112.60
1	A	543	ASP	CA-CB-CG	5.28	117.88	112.60
1	C	261	ALA	CA-C-N	5.28	127.35	120.28
1	C	261	ALA	C-N-CA	5.28	127.35	120.28
1	C	226	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	790	GLU	CB-CG-CD	5.24	121.52	112.60
1	C	461	ASN	CA-CB-CG	5.12	117.72	112.60
1	B	761	THR	CA-C-N	5.08	127.05	120.44
1	B	761	THR	C-N-CA	5.08	127.05	120.44
1	C	406	GLY	CA-C-N	5.04	127.29	120.38
1	C	406	GLY	C-N-CA	5.04	127.29	120.38
1	B	654	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	216	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	502	LYS	CA-C-N	5.01	127.50	120.28
1	C	502	LYS	C-N-CA	5.01	127.50	120.28
1	C	341	ASN	CA-CB-CG	5.00	117.60	112.60

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	5996	0	5912	17	0
1	B	5972	0	5859	20	0
1	C	5982	0	5893	22	0
2	D	89	0	74	0	0
2	E	63	0	57	1	0
2	F	63	0	57	0	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	2	0	0	0	0
5	A	504	0	0	0	0
5	B	303	0	0	0	0
5	C	290	0	0	0	0
5	D	3	0	0	0	0
5	E	6	0	0	0	0
5	F	3	0	0	0	0
All	All	19298	0	17876	58	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 2.

All (58) 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:A:606:ILE:HG21	1:A:642:LEU:HD21	1.61	0.80
1:B:666:LEU:HB3	1:B:669:ILE:HG12	1.79	0.64
1:A:78:PRO:O	1:A:81:ARG:HG3	1.99	0.62
1:C:284:GLU:HA	1:C:737:VAL:HG12	1.86	0.57
1:A:284:GLU:HA	1:A:737:VAL:HG12	1.86	0.57
1:B:284:GLU:HA	1:B:737:VAL:HG12	1.87	0.56
1:A:398:TRP:HB3	1:A:521:LEU:HB3	1.89	0.55
1:C:187:PRO:HB3	1:C:197:LEU:HD11	1.88	0.55
1:B:187:PRO:HB3	1:B:197:LEU:HD11	1.88	0.55
1:C:398:TRP:HB3	1:C:521:LEU:HB3	1.89	0.55
1:A:187:PRO:HB3	1:A:197:LEU:HD11	1.90	0.54
1:B:398:TRP:HB3	1:B:521:LEU:HB3	1.89	0.53
1:B:642:LEU:HD21	1:B:649:VAL:HG22	1.91	0.53
1:A:593:LEU:HD21	1:A:659:MET:HE2	1.91	0.53
1:C:173:ALA:HB1	1:C:405:LYS:HE2	1.91	0.51
1:B:218:ARG:O	2:E:237:GLU:HB2	2.10	0.50
1:B:204:THR:O	1:B:354:SER:HB2	2.12	0.49
1:B:775:ASN:CG	1:C:550:ILE:HG21	2.37	0.49
1:C:382:LEU:HB3	1:C:393:LEU:HB3	1.95	0.49
1:B:519:ARG:NH1	1:B:579[B]:GLU:OE2	2.46	0.49
1:A:606:ILE:CG2	1:A:642:LEU:HD21	2.36	0.48
1:B:382:LEU:HB3	1:B:393:LEU:HB3	1.95	0.48
1:B:499:PRO:HA	1:B:504:PHE:CG	2.48	0.48
1:A:499:PRO:HA	1:A:504:PHE:CG	2.49	0.48
1:C:499:PRO:HA	1:C:504:PHE:CG	2.49	0.47
1:A:382:LEU:HB3	1:A:393:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:O	1:A:354:SER:HB2	2.16	0.46
1:C:249:LEU:O	1:C:325:PRO:HB3	2.16	0.46
1:C:249:LEU:HD12	1:C:299:CYS:HB3	1.98	0.45
1:B:490:GLU:HB3	1:B:507:LEU:HD22	1.99	0.45
1:C:657:ASN:ND2	1:C:667:GLU:HA	2.32	0.45
1:A:31:ILE:HD12	1:A:125:ILE:HG23	1.99	0.45
1:C:31:ILE:HD12	1:C:125:ILE:HG23	2.00	0.44
1:A:519:ARG:NH1	1:A:579[B]:GLU:OE2	2.51	0.44
1:C:297:LEU:HA	1:C:325:PRO:HG2	2.00	0.44
1:B:634:MET:HA	1:B:634:MET:HE2	2.00	0.43
1:A:387:ALA:HB2	1:A:477:PHE:CD2	2.53	0.43
1:B:36:ARG:NH1	1:B:114:HIS:O	2.48	0.43
1:C:277:ALA:HB1	1:C:286:GLY:C	2.44	0.43
1:A:297:LEU:HA	1:A:325:PRO:HG2	2.01	0.43
1:B:31:ILE:HG23	1:B:125:ILE:HD12	2.01	0.42
1:B:249:LEU:HD12	1:B:299:CYS:HB3	2.02	0.42
1:C:31:ILE:HG23	1:C:125:ILE:HD12	2.01	0.42
1:C:746:ALA:HA	1:C:764:LEU:HD13	2.00	0.41
1:C:387:ALA:HB2	1:C:477:PHE:CD2	2.56	0.41
1:C:609:GLN:HB3	1:C:638:LYS:HD3	2.02	0.41
1:A:490:GLU:HB3	1:A:507:LEU:HD22	2.03	0.41
1:C:400:SER:HB3	1:C:519:ARG:HB3	2.03	0.41
1:A:31:ILE:HG23	1:A:125:ILE:HD12	2.01	0.41
1:B:31:ILE:HD12	1:B:125:ILE:HG23	2.03	0.41
1:C:349:ASN:O	1:C:696:PRO:HD2	2.20	0.41
1:A:400:SER:HB3	1:A:519:ARG:HB3	2.02	0.41
1:B:656:TRP:HZ2	1:B:666:LEU:HB2	1.85	0.40
1:C:490:GLU:HB3	1:C:507:LEU:HD22	2.02	0.40
1:B:349:ASN:O	1:B:696:PRO:HD2	2.20	0.40
1:C:105:LYS:HG2	1:C:461:ASN:HB3	2.04	0.40
1:B:618:LEU:HD11	1:B:671:LEU:HD21	2.02	0.40
1:C:204:THR:O	1:C:354:SER:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	763/853 (89%)	745 (98%)	17 (2%)	1 (0%)	48	57
1	B	765/853 (90%)	742 (97%)	22 (3%)	1 (0%)	48	57
1	C	761/853 (89%)	740 (97%)	20 (3%)	1 (0%)	48	57
2	D	10/242 (4%)	9 (90%)	1 (10%)	0	100	100
2	E	4/242 (2%)	4 (100%)	0	0	100	100
2	F	4/242 (2%)	4 (100%)	0	0	100	100
All	All	2307/3285 (70%)	2244 (97%)	60 (3%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLY
1	B	406	GLY
1	C	406	GLY

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	653/739 (88%)	640 (98%)	13 (2%)	48	64
1	B	648/739 (88%)	633 (98%)	15 (2%)	44	59
1	C	651/739 (88%)	641 (98%)	10 (2%)	57	73
2	D	10/202 (5%)	9 (90%)	1 (10%)	7	7
2	E	7/202 (4%)	6 (86%)	1 (14%)	3	3
2	F	7/202 (4%)	7 (100%)	0	100	100
All	All	1976/2823 (70%)	1936 (98%)	40 (2%)	48	64

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLU
1	A	29	VAL
1	A	46	GLN
1	A	70	GLU
1	A	82	GLN
1	A	276	ARG
1	A	312	VAL
1	A	379	ASP
1	A	525	ARG
1	A	669	ILE
1	A	687	LEU
1	A	737	VAL
1	A	741	ARG
1	B	27	GLU
1	B	46	GLN
1	B	70	GLU
1	B	88	LYS
1	B	276	ARG
1	B	312	VAL
1	B	321	ILE
1	B	566	ILE
1	B	642	LEU
1	B	658	ASN
1	B	666	LEU
1	B	669	ILE
1	B	687	LEU
1	B	741	ARG
1	B	755	ASP
1	C	27	GLU
1	C	70	GLU
1	C	276	ARG
1	C	312	VAL
1	C	321	ILE
1	C	379	ASP
1	C	525	ARG
1	C	658	ASN
1	C	669	ILE
1	C	687	LEU
2	D	227	SER
2	E	227	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	130	GLN
1	A	768	GLN
1	B	130	GLN
1	B	329	HIS
1	B	609	GLN
1	C	130	GLN
1	C	329	HIS
1	C	580	ASN
1	C	633	HIS
1	C	775	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	GOL	A	1004	-	5,5,5	0.17	0	5,5,5	0.24	0
3	GOL	C	1001	-	5,5,5	0.25	0	5,5,5	0.40	0
3	GOL	A	1001	-	5,5,5	0.23	0	5,5,5	0.42	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	GOL	A	1004	-	-	0/4/4/4	-
3	GOL	C	1001	-	-	0/4/4/4	-
3	GOL	A	1001	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	765/853 (89%)	-0.37	4 (0%) 87 85	26, 43, 71, 110	2 (0%)
1	B	766/853 (89%)	-0.07	7 (0%) 81 79	27, 56, 94, 128	1 (0%)
1	C	765/853 (89%)	-0.06	9 (1%) 76 74	35, 57, 98, 143	0
2	D	12/242 (4%)	0.47	0 100 100	45, 65, 85, 89	0
2	E	8/242 (3%)	0.86	0 100 100	58, 66, 77, 79	0
2	F	8/242 (3%)	1.10	1 (12%) 8 6	56, 76, 87, 90	0
All	All	2324/3285 (70%)	-0.15	21 (0%) 81 79	26, 52, 92, 143	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	792	ILE	4.1
1	C	604	ALA	3.9
1	C	602	PRO	3.6
1	B	644	VAL	3.4
1	A	647	ILE	3.1
1	C	668	GLY	2.9
1	B	89	LEU	2.8
1	A	602	PRO	2.8
1	C	647	ILE	2.7
1	B	647	ILE	2.6
1	B	646	GLY	2.5
1	C	606	ILE	2.5
1	C	232	SER	2.4
1	B	606	ILE	2.4
1	C	27	GLU	2.4
1	A	604	ALA	2.4
2	F	230	THR	2.3
1	C	646	GLY	2.3
1	B	27	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	231	LEU	2.1
1	A	29	VAL	2.1

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
3	GOL	C	1001	6/6	0.82	0.14	53,63,64,65	0
3	GOL	A	1001	6/6	0.84	0.14	48,61,63,65	0
3	GOL	A	1004	6/6	0.92	0.10	60,61,61,62	0
4	K	C	1003	1/1	0.98	0.05	70,70,70,70	0
4	K	B	1003	1/1	0.99	0.02	56,56,56,56	0
4	K	A	1003	1/1	0.99	0.05	37,37,37,37	0
4	K	A	1002	1/1	1.00	0.01	34,34,34,34	0
4	K	C	1002	1/1	1.00	0.04	38,38,38,38	0
4	K	B	1002	1/1	1.00	0.04	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.