



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:38 PM UTC

PDB ID : 6I7D / pdb_00006i7d
Title : Plasmodium falciparum Myosin A, post-rigor and rigor-like states
Authors : Robert-Paganin, J.; Auguin, D.; Moussaoui, D.; Jousset, G.; Baum, J.; Trybus, K.M.; Houdusse, A.
Deposited on : 2018-11-16
Resolution : 2.82 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

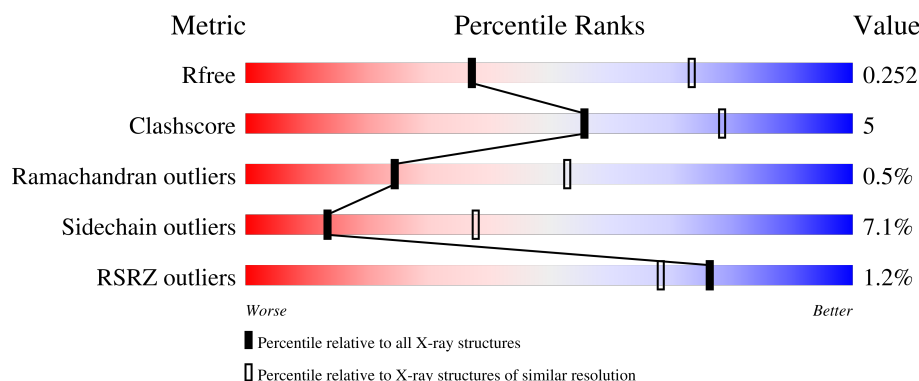
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	768	 82% 16% ..
1	B	768	 83% 14% ..
1	C	768	 80% 16% ..
1	D	768	 71% 23% 5% .

2 Entry composition [i](#)

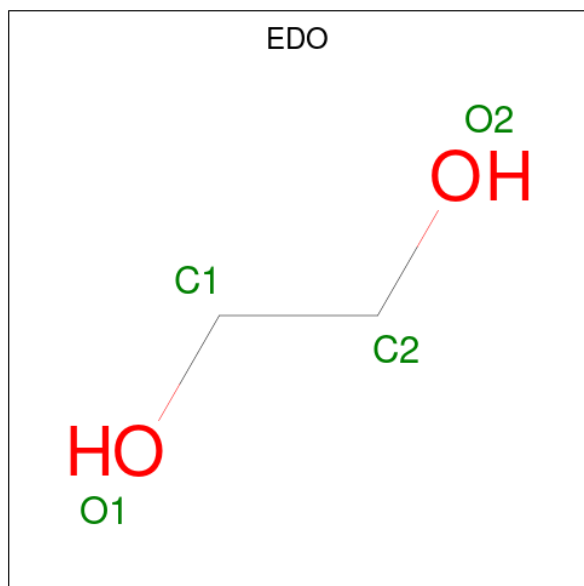
There are 4 unique types of molecules in this entry. The entry contains 24354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-A.

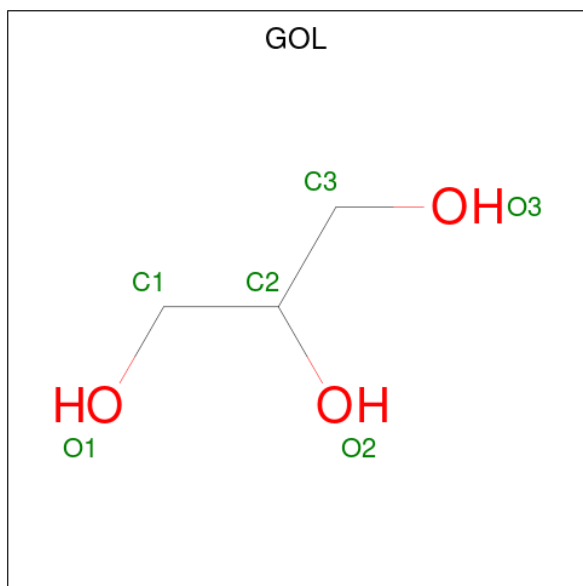
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	P	S	0	0	0
			6010	3819	1012	1147	1	31			
1	B	755	Total	C	N	O	P	S	0	1	0
			5952	3788	1002	1130	1	31			
1	C	755	Total	C	N	O	P	S	0	1	0
			5971	3798	1002	1139	1	31			
1	D	758	Total	C	N	O	P	S	0	1	0
			5984	3802	1007	1143	1	31			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

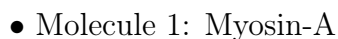


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

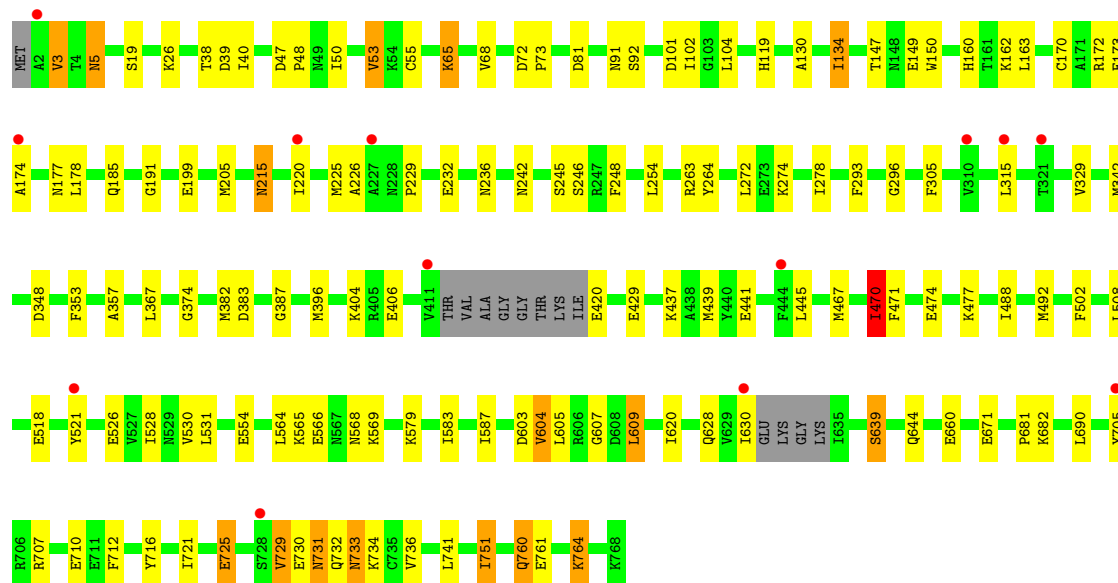
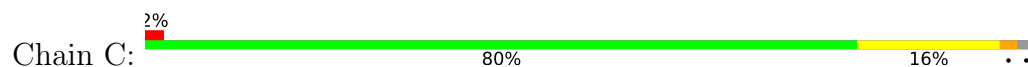
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	102	Total	O	0	0
			102	102		
4	C	67	Total	O	0	0
			67	67		
4	D	132	Total	O	0	0
			132	132		

- Molecule 1: Myosin-A

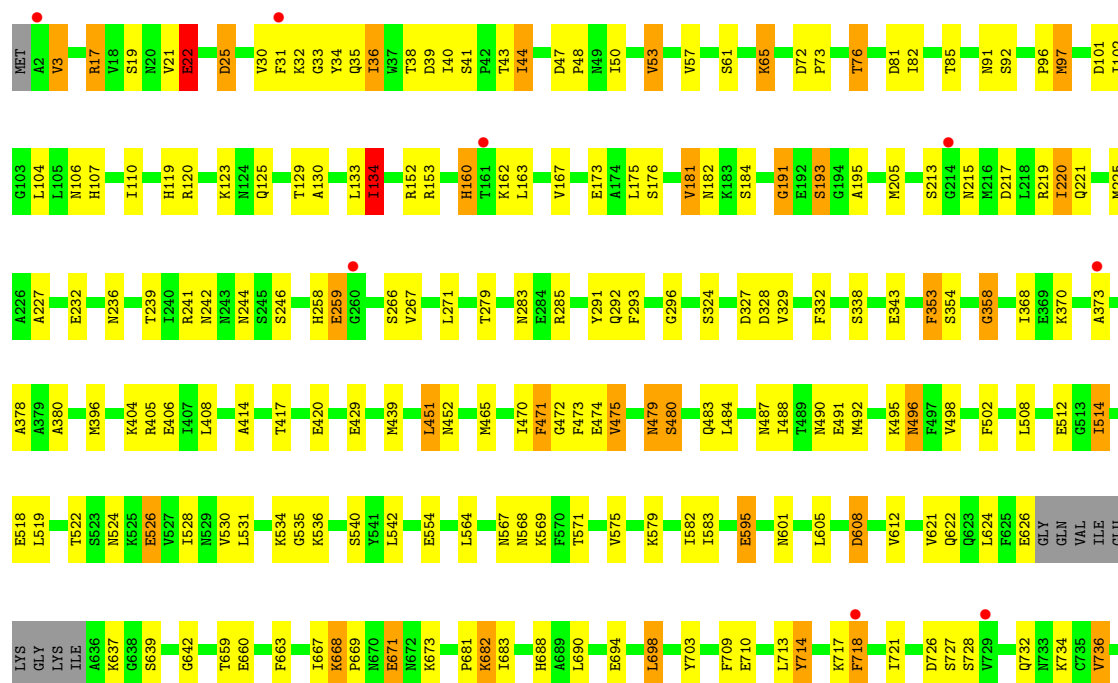


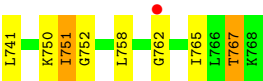


• Molecule 1: Myosin-A



• Molecule 1: Myosin-A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.52Å 258.73Å 103.09Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	49.19 – 2.82 49.19 – 2.82	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.19-2.82) 98.8 (49.19-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.187 , 0.241 0.197 , 0.252	Depositor DCC
R_{free} test set	3938 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24354	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: SEP, EDO, GOL

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	0/6104	1.39	31/8236 (0.4%)
1	B	0.86	2/6046 (0.0%)	1.38	25/8161 (0.3%)
1	C	0.86	3/6065 (0.0%)	1.41	41/8187 (0.5%)
1	D	0.93	5/6079 (0.1%)	1.52	65/8198 (0.8%)
All	All	0.88	10/24294 (0.0%)	1.43	162/32782 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	MET	SD-CE	-9.97	1.54	1.79
1	D	110	ILE	CA-CB	6.80	1.57	1.54
1	D	514	ILE	CG1-CD1	-6.38	1.26	1.51
1	C	470	ILE	CG1-CD1	6.15	1.75	1.51
1	D	191	GLY	C-N	5.81	1.41	1.33
1	C	225	MET	SD-CE	-5.74	1.65	1.79
1	B	110	ILE	CA-CB	5.42	1.56	1.54
1	C	587	ILE	CA-C	5.39	1.58	1.52
1	B	587	ILE	CA-C	5.32	1.58	1.52
1	D	465	MET	SD-CE	-5.22	1.66	1.79

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	76	THR	N-CA-C	-11.11	94.48	110.59
1	D	358	GLY	CA-C-N	7.89	131.11	120.77
1	D	358	GLY	C-N-CA	7.89	131.11	120.77
1	D	475	VAL	N-CA-CB	-7.80	102.20	112.26
1	D	33	GLY	CA-C-N	7.34	131.24	120.90
1	D	33	GLY	C-N-CA	7.34	131.24	120.90
1	C	293	PHE	CA-CB-CG	7.19	120.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	THR	CA-C-N	7.16	133.68	121.14
1	A	38	THR	C-N-CA	7.16	133.68	121.14
1	D	324	SER	N-CA-C	7.09	119.67	111.02
1	B	38	THR	CA-C-N	7.02	133.42	121.14
1	B	38	THR	C-N-CA	7.02	133.42	121.14
1	A	177	ASN	CA-CB-CG	7.00	119.60	112.60
1	C	39	ASP	CA-CB-CG	6.99	119.59	112.60
1	C	177	ASN	CA-CB-CG	6.95	119.55	112.60
1	D	681	PRO	CA-C-N	6.95	129.59	120.28
1	D	681	PRO	C-N-CA	6.95	129.59	120.28
1	A	353	PHE	CA-CB-CG	-6.87	106.93	113.80
1	A	416	GLY	CA-C-N	6.87	131.13	121.24
1	A	416	GLY	C-N-CA	6.87	131.13	121.24
1	A	25	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	293	PHE	CA-CB-CG	6.79	120.59	113.80
1	B	177	ASN	CA-CB-CG	6.78	119.38	112.60
1	C	564	LEU	CA-C-N	6.76	129.33	120.28
1	C	564	LEU	C-N-CA	6.76	129.33	120.28
1	C	764	LYS	CA-C-N	6.70	129.24	120.60
1	C	764	LYS	C-N-CA	6.70	129.24	120.60
1	B	293	PHE	CA-CB-CG	6.69	120.49	113.80
1	C	681	PRO	CA-C-N	6.69	129.25	120.28
1	C	681	PRO	C-N-CA	6.69	129.25	120.28
1	B	681	PRO	CA-C-N	6.60	129.12	120.28
1	B	681	PRO	C-N-CA	6.60	129.12	120.28
1	A	72	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	382	MET	CA-C-N	6.56	130.66	120.82
1	C	382	MET	C-N-CA	6.56	130.66	120.82
1	D	39	ASP	CA-CB-CG	6.49	119.08	112.60
1	A	39	ASP	CA-CB-CG	6.48	119.08	112.60
1	D	564	LEU	CA-C-N	6.46	128.94	120.28
1	D	564	LEU	C-N-CA	6.46	128.94	120.28
1	C	38	THR	CA-C-N	6.40	132.34	121.14
1	C	38	THR	C-N-CA	6.40	132.34	121.14
1	B	39	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	25	ASP	CA-CB-CG	6.38	118.97	112.60
1	D	25	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	353	PHE	CA-CB-CG	-6.26	107.54	113.80
1	C	353	PHE	CA-CB-CG	-6.25	107.55	113.80
1	D	353	PHE	CA-CB-CG	-6.24	107.56	113.80
1	A	565	LYS	CA-C-N	6.22	128.62	120.28
1	A	565	LYS	C-N-CA	6.22	128.62	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	SER	N-CA-C	6.15	118.47	108.76
1	D	595	GLU	CB-CG-CD	6.14	123.04	112.60
1	D	134	ILE	N-CA-CB	6.12	119.17	111.46
1	D	473	PHE	CA-CB-CG	6.10	119.90	113.80
1	C	764	LYS	N-CA-C	-6.09	104.27	111.03
1	B	564	LEU	CA-C-N	6.03	128.36	120.28
1	B	564	LEU	C-N-CA	6.03	128.36	120.28
1	D	668	LYS	CB-CA-C	6.00	117.05	110.15
1	D	717	LYS	CA-C-N	5.87	128.40	120.65
1	D	717	LYS	C-N-CA	5.87	128.40	120.65
1	D	479	ASN	CA-CB-CG	5.84	118.44	112.60
1	D	217	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	521	TYR	CA-C-N	5.82	129.54	120.75
1	C	521	TYR	C-N-CA	5.82	129.54	120.75
1	D	698	LEU	CA-C-N	5.81	128.38	120.54
1	D	698	LEU	C-N-CA	5.81	128.38	120.54
1	D	181	VAL	CA-C-N	-5.80	113.46	122.16
1	D	181	VAL	C-N-CA	-5.80	113.46	122.16
1	A	242	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	681	PRO	CA-C-N	5.72	127.88	120.44
1	A	681	PRO	C-N-CA	5.72	127.88	120.44
1	D	480	SER	CA-C-N	5.71	128.21	120.38
1	D	480	SER	C-N-CA	5.71	128.21	120.38
1	C	565	LYS	CA-C-N	5.69	127.90	120.28
1	C	565	LYS	C-N-CA	5.69	127.90	120.28
1	D	205	MET	CA-C-N	5.67	127.81	120.44
1	D	205	MET	C-N-CA	5.67	127.81	120.44
1	C	383	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	215	ASN	CA-CB-CG	5.53	118.13	112.60
1	B	553	ASP	CA-C-N	5.52	127.68	120.28
1	B	553	ASP	C-N-CA	5.52	127.68	120.28
1	C	357	ALA	CA-C-N	5.52	126.11	119.98
1	C	357	ALA	C-N-CA	5.52	126.11	119.98
1	B	242	ASN	CA-CB-CG	5.52	118.12	112.60
1	D	30	VAL	CA-C-N	5.50	130.42	121.74
1	D	30	VAL	C-N-CA	5.50	130.42	121.74
1	A	564	LEU	CA-C-N	5.49	128.65	120.31
1	A	564	LEU	C-N-CA	5.49	128.65	120.31
1	B	387	GLY	CA-C-N	5.46	127.54	120.56
1	B	387	GLY	C-N-CA	5.46	127.54	120.56
1	B	394	GLU	CA-C-N	5.45	127.59	120.28
1	B	394	GLU	C-N-CA	5.45	127.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	671	GLU	CB-CG-CD	5.43	121.83	112.60
1	C	502	PHE	CA-C-N	5.40	127.46	120.44
1	C	502	PHE	C-N-CA	5.40	127.46	120.44
1	D	703	TYR	CA-C-N	5.37	127.73	120.38
1	D	703	TYR	C-N-CA	5.37	127.73	120.38
1	D	22	GLU	N-CA-C	-5.35	102.56	110.48
1	C	305	PHE	CA-CB-CG	5.35	119.15	113.80
1	C	119	HIS	CA-C-N	5.33	127.68	120.44
1	C	119	HIS	C-N-CA	5.33	127.68	120.44
1	D	491	GLU	CB-CG-CD	5.33	121.65	112.60
1	B	91	ASN	CA-C-N	5.32	127.94	120.28
1	B	91	ASN	C-N-CA	5.32	127.94	120.28
1	A	387	GLY	CA-C-N	5.31	127.36	120.56
1	A	387	GLY	C-N-CA	5.31	127.36	120.56
1	D	502	PHE	CA-C-N	5.30	127.70	120.54
1	D	502	PHE	C-N-CA	5.30	127.70	120.54
1	C	716	TYR	CA-C-N	5.30	127.64	120.38
1	C	716	TYR	C-N-CA	5.30	127.64	120.38
1	D	688	HIS	CA-C-N	5.28	127.88	120.28
1	D	688	HIS	C-N-CA	5.28	127.88	120.28
1	D	595	GLU	CA-C-N	5.27	131.54	123.47
1	D	595	GLU	C-N-CA	5.27	131.54	123.47
1	C	488	ILE	N-CA-C	-5.27	105.57	110.53
1	A	277	ILE	CA-C-N	5.27	128.28	120.74
1	A	277	ILE	C-N-CA	5.27	128.28	120.74
1	D	714	TYR	CA-C-N	5.25	127.77	120.63
1	D	714	TYR	C-N-CA	5.25	127.77	120.63
1	D	567	ASN	CA-C-N	5.24	129.46	120.72
1	D	567	ASN	C-N-CA	5.24	129.46	120.72
1	D	125	GLN	CA-C-N	5.23	129.22	120.64
1	D	125	GLN	C-N-CA	5.23	129.22	120.64
1	B	348	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	622	GLN	CA-C-N	5.21	128.24	120.31
1	D	622	GLN	C-N-CA	5.21	128.24	120.31
1	D	354	SER	N-CA-C	-5.20	105.69	111.36
1	D	542	LEU	CA-C-N	5.20	127.56	120.54
1	D	542	LEU	C-N-CA	5.20	127.56	120.54
1	A	92	SER	N-CA-C	-5.19	103.18	110.50
1	D	718	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	382	MET	CA-C-N	5.19	127.49	120.38
1	A	382	MET	C-N-CA	5.19	127.49	120.38
1	D	496	ASN	CA-CB-CG	5.18	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	328	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	488	ILE	N-CA-C	-5.12	105.71	110.53
1	D	152	ARG	CA-C-N	5.12	127.45	120.54
1	D	152	ARG	C-N-CA	5.12	127.45	120.54
1	C	348	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	348	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	327	ASP	CA-C-O	-5.07	115.48	120.70
1	D	498	VAL	CA-C-N	5.07	127.38	120.54
1	D	498	VAL	C-N-CA	5.07	127.38	120.54
1	C	729	VAL	CA-C-N	5.06	128.40	120.75
1	C	729	VAL	C-N-CA	5.06	128.40	120.75
1	A	43	THR	CA-C-N	5.06	127.03	120.56
1	A	43	THR	C-N-CA	5.06	127.03	120.56
1	C	91	ASN	CA-C-N	5.05	127.56	120.28
1	C	91	ASN	C-N-CA	5.05	127.56	120.28
1	C	603	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	109	ASN	CA-C-N	5.04	124.36	120.33
1	A	109	ASN	C-N-CA	5.04	124.36	120.33
1	C	387	GLY	CA-C-N	5.04	127.01	120.56
1	C	387	GLY	C-N-CA	5.04	127.01	120.56
1	D	225	MET	CB-CG-SD	5.04	127.82	112.70
1	C	639	SER	CA-C-N	5.04	130.68	122.07
1	C	639	SER	C-N-CA	5.04	130.68	122.07
1	A	625	PHE	CA-C-N	5.03	128.25	121.05
1	A	625	PHE	C-N-CA	5.03	128.25	121.05
1	D	338	SER	CA-C-N	5.02	127.42	120.29
1	D	338	SER	C-N-CA	5.02	127.42	120.29
1	B	42	PRO	CA-C-N	5.02	127.00	120.28
1	B	42	PRO	C-N-CA	5.02	127.00	120.28

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	6010	0	6050	48	0
1	B	5952	0	5973	42	0
1	C	5971	0	5996	57	0
1	D	5984	0	5999	83	0
2	B	4	0	6	1	0
2	D	4	0	6	0	0
3	D	6	0	8	0	0
4	A	122	0	0	0	0
4	B	102	0	0	0	0
4	C	67	0	0	1	0
4	D	132	0	0	1	0
All	All	24354	0	24038	224	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 5.

All (224) 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:470:ILE:CD1	1:C:470:ILE:CG1	1.75	1.64
1:A:153:ARG:HD3	1:D:76:THR:HB	1.49	0.93
1:D:474:GLU:H	1:D:487:ASN:HD21	1.20	0.90
1:A:32:LYS:HG2	1:D:714:TYR:O	1.75	0.87
1:D:479:ASN:HD22	1:D:483:GLN:HG2	1.41	0.84
1:D:97:MET:HE1	1:D:120:ARG:HA	1.60	0.84
1:D:97:MET:CE	1:D:120:ARG:HA	2.08	0.84
1:C:604:VAL:HG11	1:C:644:GLN:HE22	1.44	0.82
1:D:396:MET:HE2	1:D:439:MET:HG3	1.63	0.80
1:D:3:VAL:HG11	1:D:48:PRO:HB2	1.67	0.76
1:B:109:ASN:OD1	1:B:111:PRO:HD2	1.87	0.74
1:D:38:THR:HG22	1:D:40:ILE:H	1.52	0.74
1:D:91:ASN:HD21	1:D:107:HIS:H	1.36	0.73
1:D:239:THR:HG22	1:D:241:ARG:H	1.52	0.73
1:C:530:VAL:HG21	1:C:569:LYS:HB2	1.70	0.72
1:D:41:SER:HB3	1:D:44:ILE:HD12	1.71	0.72
1:A:530:VAL:HG21	1:A:569:LYS:HB2	1.70	0.72
1:B:530:VAL:HG21	1:B:569:LYS:HB2	1.72	0.72
1:C:205:MET:CE	1:C:467:MET:SD	2.77	0.72
1:D:530:VAL:HG21	1:D:569:LYS:HB2	1.72	0.72
1:D:474:GLU:H	1:D:487:ASN:ND2	1.87	0.71
1:B:242:ASN:HD21	2:B:801:EDO:H12	1.56	0.70
1:C:3:VAL:HG11	1:C:48:PRO:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:VAL:HG22	1:C:73:PRO:HD2	1.75	0.69
1:D:470:ILE:HG13	1:D:471:PHE:H	1.58	0.69
1:D:751:ILE:HG22	1:D:752:GLY:H	1.57	0.69
1:A:53:VAL:HG22	1:A:73:PRO:HD2	1.77	0.66
1:B:396:MET:HE3	1:B:439:MET:HG3	1.76	0.66
1:D:236:ASN:HD22	1:D:244:ASN:ND2	1.94	0.66
1:B:232:GLU:O	1:B:236:ASN:HB2	1.96	0.66
1:C:205:MET:HE1	1:C:254:LEU:HD11	1.77	0.66
1:C:220[B]:ILE:HD11	1:C:264:TYR:HA	1.78	0.65
1:A:607:GLY:HA2	1:A:632:LYS:HA	1.78	0.65
1:D:53:VAL:HG22	1:D:73:PRO:HD2	1.78	0.65
1:B:58:GLN:NE2	1:B:69:VAL:HG22	2.12	0.65
1:C:396:MET:HE2	1:C:439:MET:HG3	1.79	0.65
1:D:474:GLU:N	1:D:487:ASN:HD21	1.91	0.65
1:A:396:MET:HE2	1:A:439:MET:HG3	1.76	0.64
1:C:761:GLU:HA	1:C:764:LYS:HE2	1.80	0.64
1:D:713:LEU:HD21	1:D:734:LYS:HB3	1.78	0.64
1:B:53:VAL:HG22	1:B:73:PRO:HD2	1.80	0.64
1:C:205:MET:HE2	1:C:467:MET:SD	2.37	0.64
1:D:106:ASN:HD21	1:D:767:THR:HG21	1.63	0.64
1:C:518:GLU:HB2	4:C:810:HOH:O	1.97	0.63
1:D:242:ASN:HA	4:D:918:HOH:O	1.97	0.63
1:A:369:GLU:HG3	1:A:425:LYS:HB2	1.82	0.62
1:D:184:SER:HB3	1:D:659:THR:HG22	1.81	0.62
1:D:751:ILE:CG2	1:D:752:GLY:H	2.14	0.60
1:B:102:ILE:HD12	1:B:130:ALA:HB2	1.85	0.59
1:C:707:ARG:HG3	1:C:712:PHE:HB2	1.84	0.58
1:C:604:VAL:HG21	1:C:639:SER:O	2.04	0.57
1:D:526:GLU:O	1:D:530:VAL:HG23	2.04	0.57
1:D:671:GLU:HG2	1:D:682:LYS:HE2	1.84	0.57
1:A:630:ILE:HG12	1:C:5:ASN:HB3	1.85	0.57
1:A:102:ILE:HD12	1:A:130:ALA:HB2	1.86	0.57
1:B:41:SER:HB3	1:B:44:ILE:HD12	1.87	0.57
1:D:31:PHE:CZ	1:D:61:SER:HB3	2.39	0.57
1:D:195:ALA:HA	1:D:668:LYS:HB3	1.86	0.57
1:D:285:ARG:HB3	1:D:291:TYR:CZ	2.40	0.57
1:D:484:LEU:O	1:D:488:ILE:HG13	2.04	0.56
1:B:369:GLU:HG3	1:B:425:LYS:HB2	1.88	0.56
1:D:3:VAL:CG1	1:D:48:PRO:HB2	2.36	0.56
1:D:414:ALA:HB3	1:D:417:THR:HG23	1.87	0.55
1:B:492:MET:HE1	1:B:528:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:HIS:HA	1:C:163:LEU:HD12	1.89	0.55
1:D:751:ILE:HG22	1:D:752:GLY:N	2.21	0.55
1:A:134:ILE:HD13	1:A:170:CYS:SG	2.47	0.55
1:C:134:ILE:HD13	1:C:170:CYS:SG	2.47	0.54
1:B:134:ILE:HD13	1:B:170:CYS:SG	2.47	0.54
1:C:232:GLU:O	1:C:236:ASN:HB2	2.08	0.54
1:A:748:MET:HE1	1:A:761:GLU:HG3	1.89	0.54
1:C:3:VAL:CG1	1:C:48:PRO:HB2	2.38	0.53
1:B:346:GLU:CD	1:B:346:GLU:H	2.16	0.53
1:D:267:VAL:H	1:D:452:ASN:HD21	1.57	0.53
1:D:370:LYS:HZ2	1:D:380:ALA:HB2	1.72	0.53
1:A:422:ARG:HH11	1:A:422:ARG:HB3	1.74	0.53
1:B:3:VAL:HG22	1:B:679:CYS:SG	2.49	0.52
1:D:129:THR:HG22	1:D:134:ILE:HG22	1.92	0.52
1:D:102:ILE:HD12	1:D:130:ALA:HB2	1.91	0.52
1:D:232:GLU:O	1:D:236:ASN:HB2	2.10	0.52
1:A:605:LEU:HD11	1:A:609:LEU:HD13	1.91	0.52
1:D:267:VAL:H	1:D:452:ASN:ND2	2.09	0.51
1:C:721:ILE:O	1:C:725:GLU:HG3	2.11	0.51
1:C:736:VAL:HG22	1:C:751:ILE:HG12	1.92	0.51
1:B:608:ASP:O	1:B:612:VAL:HG23	2.11	0.51
1:D:293:PHE:CE1	1:D:353:PHE:HB3	2.46	0.51
1:C:102:ILE:HD12	1:C:130:ALA:HB2	1.92	0.51
1:C:492:MET:HE1	1:C:528:ILE:HG23	1.92	0.50
1:D:227:ALA:HB2	1:D:451:LEU:HD13	1.93	0.50
1:A:416:GLY:HA3	1:C:40:ILE:HD11	1.92	0.50
1:A:3:VAL:HG22	1:A:679:CYS:SG	2.52	0.50
1:B:748:MET:HE1	1:B:761:GLU:HG3	1.94	0.49
1:D:492:MET:HE1	1:D:528:ILE:HG23	1.94	0.49
1:C:526:GLU:O	1:C:530:VAL:HG23	2.12	0.49
1:D:514:ILE:HG23	1:D:750:LYS:HD3	1.93	0.49
1:D:65:LYS:HD3	1:D:81:ASP:HB3	1.94	0.49
1:A:101:ASP:HB3	1:A:104:LEU:HG	1.94	0.49
1:B:371:GLN:HE21	1:B:376:SER:HA	1.77	0.49
1:C:65:LYS:HD3	1:C:81:ASP:HB3	1.95	0.49
1:B:707:ARG:HG3	1:B:711:GLU:HB3	1.94	0.49
1:C:278:ILE:HA	1:C:315:LEU:HD22	1.94	0.48
1:A:630:ILE:HG13	1:C:5:ASN:HD22	1.79	0.48
1:A:242:ASN:HB3	1:A:245:SER:HB2	1.94	0.48
1:A:608:ASP:O	1:A:612:VAL:HG23	2.13	0.48
1:A:492:MET:HE1	1:A:528:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:PRO:HG2	1:D:119:HIS:CG	2.49	0.48
1:A:65:LYS:HD3	1:A:81:ASP:HB3	1.95	0.48
1:A:278:ILE:HA	1:A:315:LEU:HD22	1.96	0.48
1:C:160:HIS:HB3	1:C:172:ARG:CZ	2.44	0.47
1:B:65:LYS:HD3	1:B:81:ASP:HB3	1.96	0.47
1:B:242:ASN:HB3	1:B:245:SER:HB2	1.96	0.47
1:D:236:ASN:HD22	1:D:244:ASN:HD21	1.60	0.47
1:D:726:ASP:C	1:D:728:SER:H	2.23	0.47
1:D:669:PRO:HA	1:D:683:ILE:HD11	1.96	0.47
1:D:17:ARG:HH21	1:D:85:THR:HG22	1.80	0.47
1:D:160:HIS:HA	1:D:163:LEU:HD12	1.96	0.47
1:C:705:TYR:HE2	1:C:760:GLN:HA	1.79	0.47
1:B:101:ASP:HB3	1:B:104:LEU:HG	1.98	0.46
1:B:526:GLU:O	1:B:530:VAL:HG23	2.15	0.46
1:C:160:HIS:HB2	1:C:163:LEU:HD12	1.97	0.46
1:C:296:GLY:HA2	1:C:329:VAL:HG13	1.97	0.46
1:A:406:GLU:HB3	1:A:609:LEU:HG	1.98	0.46
1:C:242:ASN:HB3	1:C:245:SER:HB2	1.96	0.46
1:D:119:HIS:O	1:D:123:LYS:HG3	2.16	0.46
1:C:470:ILE:HD12	1:C:471:PHE:H	1.81	0.46
1:C:531:LEU:HD21	1:C:583:ILE:HG21	1.97	0.46
1:D:495:LYS:HA	1:D:524[B]:ASN:HD21	1.81	0.46
1:D:709:PHE:CZ	1:D:732:GLN:HG3	2.50	0.46
1:B:55:CYS:HB3	1:B:68:VAL:HB	1.96	0.46
1:D:133:LEU:HD23	1:D:663:PHE:HB2	1.98	0.46
1:D:97:MET:HE2	1:D:120:ARG:HA	1.96	0.46
1:A:526:GLU:O	1:A:530:VAL:HG23	2.16	0.46
1:B:332:PHE:HA	1:B:335:VAL:HG12	1.97	0.46
1:D:608:ASP:O	1:D:612:VAL:HG23	2.16	0.46
1:A:724:ALA:O	1:A:728:SER:HB3	2.16	0.45
1:C:226:ALA:O	1:C:229:PRO:HD2	2.15	0.45
1:C:730:GLU:HB3	1:C:733:ASN:HB2	1.97	0.45
1:C:705:TYR:CE2	1:C:760:GLN:HA	2.51	0.45
1:B:706:ARG:O	1:B:707:ARG:HD3	2.17	0.45
1:D:762:GLY:HA2	1:D:765:ILE:HD12	1.97	0.45
1:D:296:GLY:HA2	1:D:329:VAL:HG13	1.99	0.45
1:B:406:GLU:HB3	1:B:609:LEU:HG	1.98	0.45
1:D:751:ILE:CG2	1:D:752:GLY:N	2.79	0.45
1:C:101:ASP:HB3	1:C:104:LEU:HG	1.99	0.45
1:B:226:ALA:O	1:B:229:PRO:HD2	2.17	0.45
1:B:296:GLY:HA2	1:B:329:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:LEU:HD21	1:B:583:ILE:HG21	1.98	0.44
1:B:762:GLY:HA2	1:B:765:ILE:HD12	2.00	0.44
1:D:292:GLN:HB2	1:D:332:PHE:HB2	1.98	0.44
1:A:554:GLU:HG3	1:A:579:LYS:HE3	1.99	0.44
1:B:278:ILE:HA	1:B:315:LEU:HD22	1.98	0.44
1:D:219:ARG:HG3	1:D:220:ILE:HD12	1.99	0.44
1:C:554:GLU:HG3	1:C:579:LYS:HE3	1.99	0.44
1:D:259:GLU:H	1:D:259:GLU:HG3	1.65	0.44
1:A:713:LEU:HD21	1:A:734:LYS:HB3	2.00	0.44
1:D:101:ASP:HB3	1:D:104:LEU:HG	1.99	0.44
1:C:47:ASP:HB3	1:C:50:ILE:HG12	2.00	0.44
1:C:220[B]:ILE:CD1	1:C:264:TYR:HA	2.46	0.44
1:A:226:ALA:O	1:A:229:PRO:HD2	2.18	0.44
1:B:47:ASP:HB3	1:B:50:ILE:HG12	1.98	0.44
1:C:174:ALA:O	1:C:185:GLN:HG3	2.18	0.44
1:D:571:THR:HB	1:D:582:ILE:HB	2.00	0.44
1:A:604:VAL:HG21	1:A:644:GLN:HE22	1.83	0.43
1:C:406:GLU:HB3	1:C:609:LEU:HG	1.98	0.43
1:D:175:LEU:HD23	1:D:175:LEU:HA	1.87	0.43
1:B:230:VAL:HG22	1:B:335:VAL:HG23	1.99	0.43
1:C:147:THR:HG22	1:C:150:TRP:HD1	1.84	0.43
1:A:413:VAL:HG12	1:A:413:VAL:O	2.19	0.43
1:A:174:ALA:O	1:A:185:GLN:HG3	2.18	0.43
1:D:31:PHE:CD2	1:D:31:PHE:N	2.86	0.43
1:D:732:GLN:O	1:D:736:VAL:HG13	2.19	0.43
1:A:274:LYS:HD2	1:A:437:LYS:HB3	2.01	0.42
1:C:729:VAL:HG13	1:C:734:LYS:HG3	2.01	0.42
1:A:508:LEU:HD23	1:A:509:TYR:HD1	1.84	0.42
1:B:554:GLU:HG3	1:B:579:LYS:HE3	2.00	0.42
1:C:72:ASP:HA	1:C:73:PRO:C	2.44	0.42
1:A:47:ASP:HB3	1:A:50:ILE:HG12	2.00	0.42
1:A:762:GLY:HA2	1:A:765:ILE:HD12	2.01	0.42
1:A:531:LEU:HD21	1:A:583:ILE:HG21	2.01	0.42
1:C:55:CYS:HB3	1:C:68:VAL:HB	2.02	0.42
1:D:370:LYS:HB2	1:D:378:ALA:HB3	2.01	0.42
1:C:732:GLN:O	1:C:736:VAL:HG23	2.20	0.42
1:D:601:ASN:HD21	1:D:642:GLY:H	1.67	0.42
1:D:47:ASP:HB3	1:D:50:ILE:HG22	2.01	0.42
1:D:554:GLU:CD	1:D:579:LYS:HE3	2.44	0.42
1:A:296:GLY:HA2	1:A:329:VAL:HG13	2.00	0.42
1:C:274:LYS:HD2	1:C:437:LYS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLU:O	1:C:445:LEU:HG	2.19	0.42
1:D:472:GLY:HA2	1:D:490:ASN:OD1	2.20	0.42
1:B:605:LEU:HD11	1:B:609:LEU:HD13	2.02	0.42
1:D:22:GLU:O	1:D:34:TYR:CZ	2.73	0.42
1:D:72:ASP:HA	1:D:73:PRO:C	2.44	0.42
1:A:41:SER:HB3	1:A:44:ILE:HD12	2.02	0.42
1:A:451:LEU:O	1:A:455:ILE:HG12	2.19	0.42
1:A:698:LEU:HA	1:A:701:LEU:HD12	2.02	0.41
1:D:21:VAL:HG21	1:D:36:ILE:HG22	2.02	0.41
1:A:633:GLY:HA2	1:A:634:LYS:HA	1.83	0.41
1:C:248:PHE:HB3	1:C:272:LEU:HD12	2.02	0.41
1:D:358:GLY:HA3	1:D:396:MET:HG3	2.02	0.41
1:A:59:GLN:HB3	1:D:714:TYR:CZ	2.55	0.41
1:A:359:ILE:HG13	1:A:396:MET:HE3	2.01	0.41
1:B:174:ALA:O	1:B:185:GLN:HG3	2.20	0.41
1:B:470:ILE:HD12	1:B:471:PHE:H	1.85	0.41
1:C:147:THR:HG22	1:C:150:TRP:CD1	2.55	0.41
1:D:512:GLU:HB2	1:D:514:ILE:HD12	2.01	0.41
1:B:400:PRO:O	1:B:404:LYS:HB2	2.21	0.41
1:D:191:GLY:HA2	1:D:690:LEU:HD21	2.03	0.41
1:A:55:CYS:HB3	1:A:68:VAL:HB	2.02	0.41
1:C:220[B]:ILE:HG12	1:C:263:ARG:O	2.21	0.41
1:A:224:ILE:HG22	1:A:225:MET:HE2	2.03	0.41
1:C:191:GLY:HA2	1:C:690:LEU:HD21	2.03	0.41
1:A:147:THR:HG22	1:A:150:TRP:HD1	1.86	0.40
1:A:239:THR:HA	1:A:284:GLU:HG2	2.02	0.40
1:B:451:LEU:O	1:B:455:ILE:HG12	2.21	0.40
1:C:160:HIS:CA	1:C:163:LEU:HD12	2.51	0.40
1:D:106:ASN:ND2	1:D:767:THR:HG21	2.32	0.40
1:A:317:ASN:HB3	1:A:320:SER:OG	2.21	0.40
1:B:147:THR:HG22	1:B:150:TRP:HD1	1.84	0.40
1:C:731:ASN:HA	1:C:734:LYS:HE3	2.03	0.40
1:B:147:THR:HG22	1:B:150:TRP:CD1	2.55	0.40
1:B:171:ALA:HB1	1:B:207:TYR:CD1	2.56	0.40
1:D:193:SER:HB3	1:D:242:ASN:ND2	2.36	0.40
1:D:621:VAL:HA	1:D:624:LEU:HG	2.03	0.40
1:D:488:ILE:HG12	1:D:531:LEU:HD13	2.04	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	757/768 (99%)	723 (96%)	32 (4%)	2 (0%)	36	64
1	B	749/768 (98%)	723 (96%)	25 (3%)	1 (0%)	48	75
1	C	749/768 (98%)	714 (95%)	32 (4%)	3 (0%)	30	58
1	D	754/768 (98%)	711 (94%)	35 (5%)	8 (1%)	11	34
All	All	3009/3072 (98%)	2871 (95%)	124 (4%)	14 (0%)	24	53

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	631	GLU
1	C	607	GLY
1	C	751	ILE
1	D	213	SER
1	D	215	ASN
1	D	373	ALA
1	D	519	LEU
1	A	630	ILE
1	C	374	GLY
1	D	637	LYS
1	B	603	ASP
1	D	727	SER
1	D	535	GLY
1	D	751	ILE

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	670/679 (99%)	630 (94%)	40 (6%)	17	45
1	B	661/679 (97%)	625 (95%)	36 (5%)	20	50
1	C	666/679 (98%)	626 (94%)	40 (6%)	17	45
1	D	668/679 (98%)	594 (89%)	74 (11%)	6	19
All	All	2665/2716 (98%)	2475 (93%)	190 (7%)	13	38

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	53	VAL
1	A	65	LYS
1	A	134	ILE
1	A	149	GLU
1	A	162	LYS
1	A	173	GLU
1	A	178	LEU
1	A	199	GLU
1	A	216	MET
1	A	342	MET
1	A	368	ILE
1	A	371	GLN
1	A	375	LEU
1	A	376	SER
1	A	401	GLU
1	A	404	LYS
1	A	417	THR
1	A	420	GLU
1	A	422	ARG
1	A	429	GLU
1	A	470	ILE
1	A	474	GLU
1	A	508	LEU
1	A	522	THR
1	A	540	SER
1	A	566	GLU
1	A	568	ASN
1	A	609	LEU
1	A	628	GLN
1	A	630	ILE
1	A	660	GLU
1	A	671	GLU

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Mol	Chain	Res	Type
1	A	682	LYS
1	A	699	ARG
1	A	704	SER
1	A	710	GLU
1	A	714	TYR
1	A	740	LYS
1	A	741	LEU
1	B	25	ASP
1	B	35	GLN
1	B	36	ILE
1	B	53	VAL
1	B	63	LYS
1	B	65	LYS
1	B	92	SER
1	B	134	ILE
1	B	149	GLU
1	B	173	GLU
1	B	178	LEU
1	B	199	GLU
1	B	246	SER
1	B	302	LYS
1	B	314	LYS
1	B	342	MET
1	B	368	ILE
1	B	370	LYS
1	B	371	GLN
1	B	404	LYS
1	B	420	GLU
1	B	429	GLU
1	B	470	ILE
1	B	474	GLU
1	B	508	LEU
1	B	511	ASP
1	B	568	ASN
1	B	609	LEU
1	B	630	ILE
1	B	660	GLU
1	B	671	GLU
1	B	682	LYS
1	B	707	ARG
1	B	710	GLU
1	B	741	LEU

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Mol	Chain	Res	Type
1	B	761	GLU
1	C	3	VAL
1	C	5	ASN
1	C	26	LYS
1	C	53	VAL
1	C	65	LYS
1	C	92	SER
1	C	134	ILE
1	C	149	GLU
1	C	162	LYS
1	C	173	GLU
1	C	178	LEU
1	C	199	GLU
1	C	215	ASN
1	C	246	SER
1	C	342	MET
1	C	367	LEU
1	C	404	LYS
1	C	420	GLU
1	C	429	GLU
1	C	470	ILE
1	C	474	GLU
1	C	477	LYS
1	C	508	LEU
1	C	566	GLU
1	C	568	ASN
1	C	604	VAL
1	C	605	LEU
1	C	609	LEU
1	C	620	ILE
1	C	628	GLN
1	C	630	ILE
1	C	660	GLU
1	C	671	GLU
1	C	682	LYS
1	C	710	GLU
1	C	725	GLU
1	C	731	ASN
1	C	733	ASN
1	C	741	LEU
1	C	760	GLN
1	D	3	VAL

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Mol	Chain	Res	Type
1	D	17	ARG
1	D	22	GLU
1	D	25	ASP
1	D	32	LYS
1	D	35	GLN
1	D	36	ILE
1	D	43	THR
1	D	44	ILE
1	D	53	VAL
1	D	57	VAL
1	D	65	LYS
1	D	82	ILE
1	D	92	SER
1	D	134	ILE
1	D	153	ARG
1	D	160	HIS
1	D	162	LYS
1	D	167	VAL
1	D	173	GLU
1	D	176	SER
1	D	181	VAL
1	D	182	ASN
1	D	193	SER
1	D	220	ILE
1	D	221	GLN
1	D	246	SER
1	D	258	HIS
1	D	259	GLU
1	D	266	SER
1	D	271	LEU
1	D	279	THR
1	D	283	ASN
1	D	343	GLU
1	D	368	ILE
1	D	404	LYS
1	D	405	ARG
1	D	406	GLU
1	D	408	LEU
1	D	420	GLU
1	D	429	GLU
1	D	451	LEU
1	D	471	PHE

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Mol	Chain	Res	Type
1	D	475	VAL
1	D	480	SER
1	D	496	ASN
1	D	508	LEU
1	D	518	GLU
1	D	522	THR
1	D	526	GLU
1	D	534	LYS
1	D	536	LYS
1	D	540	SER
1	D	568	ASN
1	D	575	VAL
1	D	583	ILE
1	D	595	GLU
1	D	605	LEU
1	D	608	ASP
1	D	626	GLU
1	D	639	SER
1	D	660	GLU
1	D	667	ILE
1	D	673	LYS
1	D	682	LYS
1	D	694	GLU
1	D	698	LEU
1	D	710	GLU
1	D	718	PHE
1	D	721	ILE
1	D	736	VAL
1	D	741	LEU
1	D	758	LEU
1	D	767	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	49	ASN
1	A	59	GLN
1	A	70	GLN
1	A	107	HIS
1	A	317	ASN
1	A	319	ASN

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Mol	Chain	Res	Type
1	A	490	ASN
1	A	644	GLN
1	A	731	ASN
1	A	732	GLN
1	B	20	ASN
1	B	49	ASN
1	B	70	GLN
1	B	107	HIS
1	B	242	ASN
1	B	258	HIS
1	B	317	ASN
1	B	319	ASN
1	B	371	GLN
1	B	648	GLN
1	B	700	GLN
1	B	760	GLN
1	C	5	ASN
1	C	20	ASN
1	C	49	ASN
1	C	86	HIS
1	C	107	HIS
1	C	160	HIS
1	C	258	HIS
1	C	317	ASN
1	C	319	ASN
1	C	371	GLN
1	C	644	GLN
1	C	731	ASN
1	D	58	GLN
1	D	70	GLN
1	D	91	ASN
1	D	93	GLN
1	D	106	ASN
1	D	182	ASN
1	D	215	ASN
1	D	221	GLN
1	D	242	ASN
1	D	244	ASN
1	D	253	GLN
1	D	317	ASN
1	D	319	ASN
1	D	390	ASN

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Mol	Chain	Res	Type
1	D	452	ASN
1	D	479	ASN
1	D	487	ASN
1	D	567	ASN
1	D	601	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	SEP	A	19	1	8,9,10	1.08	0	7,12,14	2.36	1 (14%)
1	SEP	B	19	1	8,9,10	0.99	0	7,12,14	3.22	4 (57%)
1	SEP	D	19	1	8,9,10	1.32	1 (12%)	7,12,14	5.88	3 (42%)
1	SEP	C	19	1	8,9,10	1.18	1 (12%)	7,12,14	3.36	4 (57%)

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
1	SEP	A	19	1	-	1/6/8/10	-
1	SEP	B	19	1	-	1/6/8/10	-
1	SEP	D	19	1	-	5/6/8/10	-
1	SEP	C	19	1	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	19	SEP	CB-CA	2.61	1.59	1.52
1	C	19	SEP	P-OG	-2.13	1.53	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	SEP	OG-CB-CA	14.94	122.68	108.14
1	A	19	SEP	OG-CB-CA	5.51	113.50	108.14
1	C	19	SEP	OG-CB-CA	5.42	113.42	108.14
1	C	19	SEP	O2P-P-OG	-5.14	93.27	106.67
1	B	19	SEP	OG-CB-CA	5.05	113.06	108.14
1	B	19	SEP	OG-P-O1P	-4.95	93.06	106.44
1	C	19	SEP	OG-P-O1P	4.29	118.05	106.44
1	B	19	SEP	O2P-P-OG	3.81	116.60	106.67
1	D	19	SEP	O3P-P-OG	3.33	115.35	106.67
1	B	19	SEP	O3P-P-OG	2.10	112.14	106.67
1	C	19	SEP	O3P-P-O2P	2.07	115.58	107.80
1	D	19	SEP	OG-P-O1P	2.07	112.04	106.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	19	SEP	N-CA-CB-OG
1	D	19	SEP	C-CA-CB-OG
1	D	19	SEP	CB-OG-P-O1P
1	D	19	SEP	CB-OG-P-O2P
1	A	19	SEP	CA-CB-OG-P
1	B	19	SEP	CA-CB-OG-P
1	C	19	SEP	CA-CB-OG-P
1	D	19	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 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	EDO	B	801	-	3,3,3	0.92	0	2,2,2	0.42	0
2	EDO	D	801	-	3,3,3	0.32	0	2,2,2	0.75	0
3	GOL	D	802	-	5,5,5	0.16	0	5,5,5	0.45	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
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	D	801	-	-	0/1/1/1	-
3	GOL	D	802	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	802	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	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	761/768 (99%)	-0.14	3 (0%) 88 84	36, 60, 95, 138	0
1	B	754/768 (98%)	0.12	11 (1%) 72 63	37, 70, 160, 182	1 (0%)
1	C	754/768 (98%)	0.15	13 (1%) 69 60	34, 76, 122, 144	1 (0%)
1	D	757/768 (98%)	-0.09	9 (1%) 76 68	30, 61, 106, 132	1 (0%)
All	All	3026/3072 (98%)	0.01	36 (1%) 76 68	30, 66, 117, 182	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502[A]	PHE	3.5
1	B	741	LEU	3.0
1	D	373	ALA	3.0
1	B	630	ILE	2.9
1	C	227	ALA	2.8
1	C	705	TYR	2.8
1	C	411	VAL	2.7
1	C	220[A]	ILE	2.7
1	C	521	TYR	2.5
1	B	645	PHE	2.5
1	B	713	LEU	2.4
1	B	570	PHE	2.4
1	C	2	ALA	2.4
1	C	321	THR	2.4
1	D	718	PHE	2.4
1	D	729	VAL	2.3
1	D	161	THR	2.3
1	B	729	VAL	2.3
1	D	762	GLY	2.3
1	A	570	PHE	2.3
1	C	310	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	704	SER	2.2
1	D	214	GLY	2.2
1	B	519	LEU	2.2
1	C	315	LEU	2.2
1	C	630	ILE	2.2
1	C	444	PHE	2.2
1	C	728	SER	2.2
1	C	174	ALA	2.1
1	A	629	VAL	2.1
1	B	407	ILE	2.1
1	A	645	PHE	2.1
1	B	576	ALA	2.1
1	D	31	PHE	2.0
1	D	260	GLY	2.0
1	D	2	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	SEP	B	19	10/11	0.91	0.09	68,72,80,81	0
1	SEP	C	19	10/11	0.94	0.08	63,67,74,76	0
1	SEP	D	19	10/11	0.94	0.06	76,79,80,80	0
1	SEP	A	19	10/11	0.95	0.07	58,61,66,67	0

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
2	EDO	B	801	4/4	0.85	0.15	40,47,52,53	0
3	GOL	D	802	6/6	0.93	0.12	54,64,66,67	0
2	EDO	D	801	4/4	0.98	0.07	54,56,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.