



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:40 PM UTC

PDB ID : 3CPX / pdb_00003cpx
Title : Crystal structure of putative M42 glutamyl aminopeptidase (YP_676701.1)
from *Cytophaga hutchinsonii* ATCC 33406 at 2.39 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2008-04-01
Resolution : 2.39 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

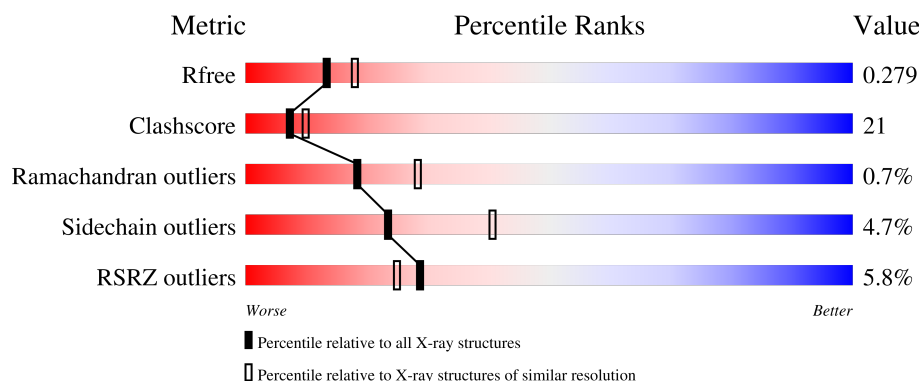
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	321	5% 65% 27% ...
1	B	321	2% 70% 23% ...
1	C	321	9% 64% 27% 5% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7728 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 Aminopeptidase, M42 family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	Se	0	1	0
			2438	1561	403	461	6	7			
1	B	311	Total	C	N	O	S	Se	0	0	0
			2473	1582	409	469	6	7			
1	C	309	Total	C	N	O	S	Se	0	2	0
			2439	1560	406	460	6	7			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	expression tag	UNP Q11Z05
A	-17	GLY	-	expression tag	UNP Q11Z05
A	-16	SER	-	expression tag	UNP Q11Z05
A	-15	ASP	-	expression tag	UNP Q11Z05
A	-14	LYS	-	expression tag	UNP Q11Z05
A	-13	ILE	-	expression tag	UNP Q11Z05
A	-12	HIS	-	expression tag	UNP Q11Z05
A	-11	HIS	-	expression tag	UNP Q11Z05
A	-10	HIS	-	expression tag	UNP Q11Z05
A	-9	HIS	-	expression tag	UNP Q11Z05
A	-8	HIS	-	expression tag	UNP Q11Z05
A	-7	HIS	-	expression tag	UNP Q11Z05
A	-6	GLU	-	expression tag	UNP Q11Z05
A	-5	ASN	-	expression tag	UNP Q11Z05
A	-4	LEU	-	expression tag	UNP Q11Z05
A	-3	TYR	-	expression tag	UNP Q11Z05
A	-2	PHE	-	expression tag	UNP Q11Z05
A	-1	GLN	-	expression tag	UNP Q11Z05
A	0	GLY	-	expression tag	UNP Q11Z05
B	-18	MSE	-	expression tag	UNP Q11Z05
B	-17	GLY	-	expression tag	UNP Q11Z05
B	-16	SER	-	expression tag	UNP Q11Z05
B	-15	ASP	-	expression tag	UNP Q11Z05

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	LYS	-	expression tag	UNP Q11Z05
B	-13	ILE	-	expression tag	UNP Q11Z05
B	-12	HIS	-	expression tag	UNP Q11Z05
B	-11	HIS	-	expression tag	UNP Q11Z05
B	-10	HIS	-	expression tag	UNP Q11Z05
B	-9	HIS	-	expression tag	UNP Q11Z05
B	-8	HIS	-	expression tag	UNP Q11Z05
B	-7	HIS	-	expression tag	UNP Q11Z05
B	-6	GLU	-	expression tag	UNP Q11Z05
B	-5	ASN	-	expression tag	UNP Q11Z05
B	-4	LEU	-	expression tag	UNP Q11Z05
B	-3	TYR	-	expression tag	UNP Q11Z05
B	-2	PHE	-	expression tag	UNP Q11Z05
B	-1	GLN	-	expression tag	UNP Q11Z05
B	0	GLY	-	expression tag	UNP Q11Z05
C	-18	MSE	-	expression tag	UNP Q11Z05
C	-17	GLY	-	expression tag	UNP Q11Z05
C	-16	SER	-	expression tag	UNP Q11Z05
C	-15	ASP	-	expression tag	UNP Q11Z05
C	-14	LYS	-	expression tag	UNP Q11Z05
C	-13	ILE	-	expression tag	UNP Q11Z05
C	-12	HIS	-	expression tag	UNP Q11Z05
C	-11	HIS	-	expression tag	UNP Q11Z05
C	-10	HIS	-	expression tag	UNP Q11Z05
C	-9	HIS	-	expression tag	UNP Q11Z05
C	-8	HIS	-	expression tag	UNP Q11Z05
C	-7	HIS	-	expression tag	UNP Q11Z05
C	-6	GLU	-	expression tag	UNP Q11Z05
C	-5	ASN	-	expression tag	UNP Q11Z05
C	-4	LEU	-	expression tag	UNP Q11Z05
C	-3	TYR	-	expression tag	UNP Q11Z05
C	-2	PHE	-	expression tag	UNP Q11Z05
C	-1	GLN	-	expression tag	UNP Q11Z05
C	0	GLY	-	expression tag	UNP Q11Z05

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total	Fe	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

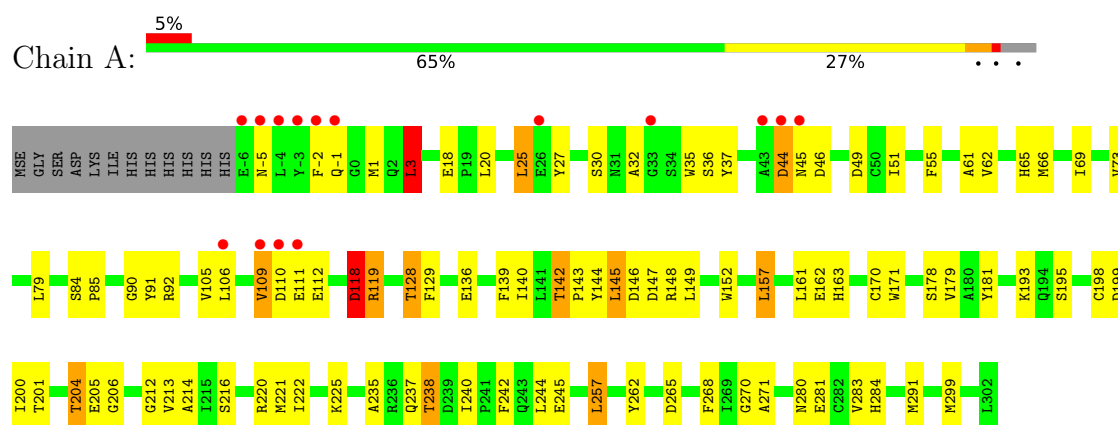
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	119	Total	O	0	1
			120	120		
5	C	98	Total	O	0	1
			98	98		

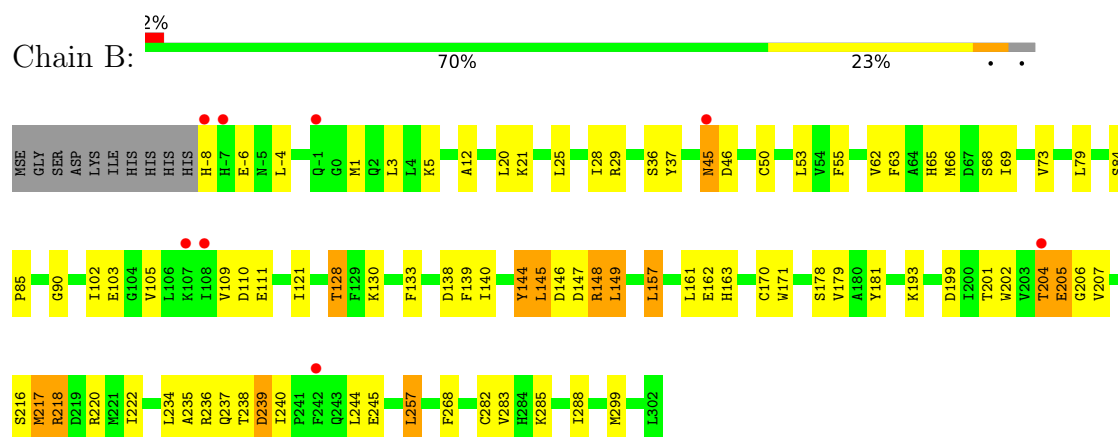
3 Residue-property plots [i](#)

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.

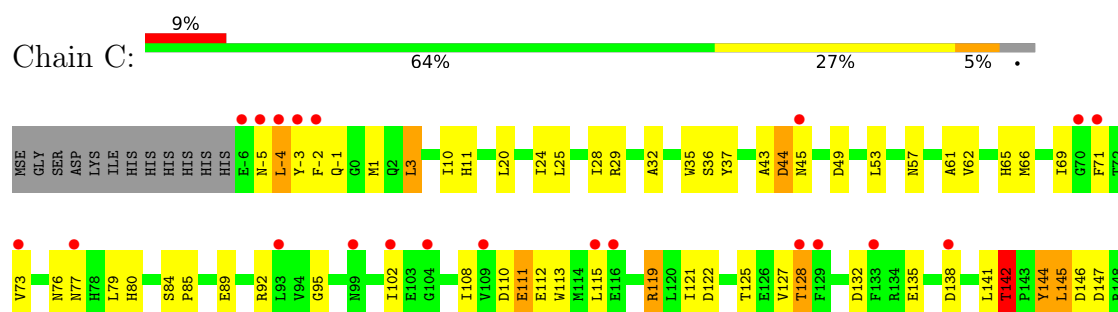
• Molecule 1: Aminopeptidase, M42 family

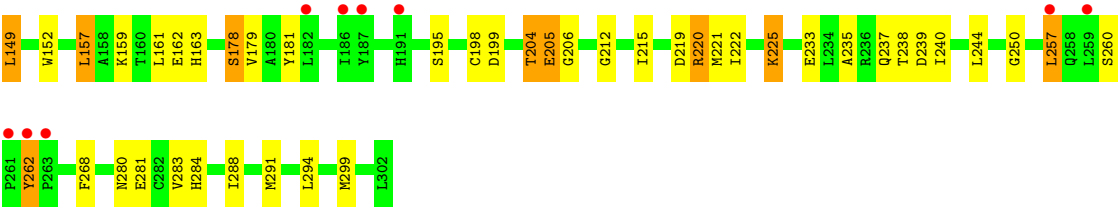


• Molecule 1: Aminopeptidase, M42 family



• Molecule 1: Aminopeptidase, M42 family





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	83.84Å 83.84Å 682.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.66 – 2.39 29.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.66-2.39) 89.3 (29.66-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.4.0067, PHENIX	Depositor
R, R_{free}	0.187 , 0.223 (Not available) , 0.279	Depositor DCC
R_{free} test set	2650 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: FE, EDO, CL

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	0.92	2/2497 (0.1%)	1.22	19/3383 (0.6%)
1	B	0.93	1/2531 (0.0%)	1.19	19/3427 (0.6%)
1	C	1.06	4/2502 (0.2%)	1.28	21/3394 (0.6%)
All	All	0.97	7/7530 (0.1%)	1.23	59/10204 (0.6%)

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	C	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	132	ASP	N-CA	8.43	1.58	1.47
1	C	80	HIS	CG-ND1	6.85	1.45	1.38
1	A	44	ASP	CA-C	-6.58	1.44	1.53
1	B	45	ASN	C-O	6.48	1.32	1.24
1	C	89	GLU	C-N	6.08	1.40	1.34
1	C	10	ILE	C-O	-5.56	1.18	1.24
1	A	45	ASN	C-O	5.50	1.31	1.24

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLY	N-CA-C	9.26	120.74	111.95
1	A	145	LEU	N-CA-C	-8.75	101.65	111.71
1	A	44	ASP	CB-CA-C	-8.60	94.04	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	LEU	N-CA-C	-8.32	102.21	111.28
1	B	205	GLU	N-CA-C	-7.78	103.06	112.54
1	C	89	GLU	O-C-N	7.63	133.52	123.07
1	C	220	ARG	N-CA-C	-7.52	103.16	111.36
1	A	142	THR	CA-C-N	-7.23	112.55	119.85
1	A	142	THR	C-N-CA	-7.23	112.55	119.85
1	C	89	GLU	CA-C-O	-7.23	112.99	120.80
1	B	84	SER	CA-C-N	-7.16	113.30	120.31
1	B	84	SER	C-N-CA	-7.16	113.30	120.31
1	A	222	ILE	CA-C-N	-7.01	113.48	120.98
1	A	222	ILE	C-N-CA	-7.01	113.48	120.98
1	C	237	GLN	N-CA-C	-6.94	104.55	113.16
1	C	205	GLU	N-CA-C	-6.91	104.72	113.01
1	B	145	LEU	N-CA-C	-6.91	103.75	111.28
1	B	237	GLN	N-CA-C	-6.87	104.89	113.20
1	B	288	ILE	N-CA-C	-6.86	103.79	110.72
1	C	144	TYR	N-CA-C	6.81	120.89	112.58
1	C	212	GLY	N-CA-C	6.64	118.26	111.95
1	C	222	ILE	CA-C-N	-6.51	114.02	120.98
1	C	222	ILE	C-N-CA	-6.51	114.02	120.98
1	A	84	SER	CA-C-N	-6.38	114.06	120.31
1	A	84	SER	C-N-CA	-6.38	114.06	120.31
1	C	142	THR	CA-C-N	-6.30	113.48	119.85
1	C	142	THR	C-N-CA	-6.30	113.48	119.85
1	B	109	VAL	N-CA-C	6.27	117.51	109.30
1	C	262	TYR	CA-C-N	6.13	127.50	119.84
1	C	262	TYR	C-N-CA	6.13	127.50	119.84
1	C	80	HIS	CA-C-N	-6.10	113.69	119.85
1	C	80	HIS	C-N-CA	-6.10	113.69	119.85
1	A	139	PHE	N-CA-C	5.87	119.25	110.14
1	A	262	TYR	CA-C-N	5.84	127.15	119.84
1	A	262	TYR	C-N-CA	5.84	127.15	119.84
1	B	12	ALA	CA-C-N	-5.80	114.64	120.21
1	B	12	ALA	C-N-CA	-5.80	114.64	120.21
1	A	18	GLU	CA-C-N	-5.76	112.94	119.28
1	A	18	GLU	C-N-CA	-5.76	112.94	119.28
1	B	222	ILE	CA-C-N	-5.52	112.94	119.84
1	B	222	ILE	C-N-CA	-5.52	112.94	119.84
1	A	3	LEU	N-CA-C	-5.43	105.39	112.23
1	A	237	GLN	N-CA-C	-5.38	106.48	113.16
1	B	109	VAL	CB-CA-C	-5.34	103.27	111.71
1	C	84	SER	CA-C-N	-5.33	114.49	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	SER	C-N-CA	-5.33	114.49	120.14
1	B	217	MSE	N-CA-C	-5.29	106.83	113.28
1	B	144	TYR	N-CA-C	5.28	119.03	112.58
1	B	239	ASP	N-CA-C	-5.22	106.15	112.88
1	C	288	ILE	N-CA-C	-5.18	105.66	110.53
1	A	118	ASP	CB-CA-C	-5.17	102.73	110.90
1	A	265	ASP	N-CA-C	-5.17	102.10	110.32
1	B	220	ARG	N-CA-C	-5.12	105.70	111.28
1	B	149	LEU	N-CA-C	-5.11	105.79	111.36
1	A	136	GLU	CB-CA-C	-5.09	105.03	111.70
1	C	149	LEU	N-CA-C	-5.09	105.82	112.23
1	C	178	SER	N-CA-C	-5.08	107.16	113.55
1	B	46	ASP	N-CA-C	-5.06	107.08	113.20
1	B	148	ARG	N-CA-C	-5.04	106.39	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	135	GLU	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	2438	0	2310	107	0
1	B	2473	0	2347	91	0
1	C	2439	0	2307	106	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	24	0	36	4	0
3	B	4	0	6	0	0
3	C	20	0	30	1	0
4	B	1	0	0	0	0
5	A	105	0	0	1	1
5	B	120	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	98	0	0	1	1
All	All	7728	0	7036	297	1

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 21.

All (297) 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:238:THR:CG2	1:A:240:ILE:H	1.51	1.23
1:B:238:THR:CG2	1:B:240:ILE:H	1.60	1.13
1:C:220:ARG:HG2	1:C:221:MSE:CE	1.77	1.13
1:A:220:ARG:HG2	1:A:221:MSE:CE	1.78	1.13
1:B:238:THR:HG22	1:B:240:ILE:N	1.66	1.11
1:C:204:THR:HG22	1:C:206:GLY:N	1.66	1.10
1:C:238:THR:HG22	1:C:240:ILE:H	1.05	1.09
1:B:204:THR:HG22	1:B:206:GLY:H	1.11	1.09
1:A:204:THR:HG22	1:A:206:GLY:H	0.93	1.08
1:B:204:THR:CG2	1:B:206:GLY:H	1.67	1.07
1:A:220:ARG:CD	1:A:221:MSE:HE3	1.87	1.05
1:C:1:MSE:HE2	1:C:1:MSE:HA	1.37	1.03
1:A:204:THR:HG22	1:A:206:GLY:N	1.76	1.01
1:C:220:ARG:CG	1:C:221:MSE:HE3	1.91	1.00
1:B:204:THR:HG22	1:B:206:GLY:N	1.74	1.00
1:A:238:THR:HG23	1:A:240:ILE:H	1.25	0.99
1:A:238:THR:HG21	1:A:240:ILE:HB	1.42	0.98
1:A:238:THR:HG22	1:A:240:ILE:H	1.29	0.97
1:C:204:THR:HG22	1:C:206:GLY:H	0.82	0.96
1:A:220:ARG:HD3	1:A:221:MSE:HE3	1.46	0.96
1:A:220:ARG:CG	1:A:221:MSE:HE3	1.96	0.96
1:A:221:MSE:HE1	3:A:403:EDO:H11	1.48	0.94
1:B:238:THR:HG22	1:B:240:ILE:H	0.80	0.94
1:A:220:ARG:CG	1:A:221:MSE:CE	2.46	0.93
1:C:238:THR:CG2	1:C:240:ILE:H	1.80	0.93
1:C:220:ARG:CD	1:C:221:MSE:HE3	1.97	0.93
1:B:1:MSE:SE	1:B:140:ILE:CD1	2.68	0.92
1:A:204:THR:CG2	1:A:206:GLY:H	1.83	0.92
1:A:1:MSE:SE	1:A:140:ILE:HD11	2.20	0.91
1:A:238:THR:CG2	1:A:240:ILE:N	2.33	0.90
1:B:238:THR:HG21	1:B:240:ILE:HB	1.50	0.90
1:A:119:ARG:CG	1:A:119:ARG:HH11	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:THR:CG2	1:C:206:GLY:H	1.79	0.88
1:C:43:ALA:O	1:C:44:ASP:HB3	1.70	0.88
1:C:238:THR:HG22	1:C:240:ILE:N	1.88	0.87
1:A:220:ARG:C	1:A:221:MSE:HE2	1.99	0.86
1:A:220:ARG:HG2	1:A:221:MSE:HE2	1.60	0.84
1:C:1:MSE:HA	1:C:1:MSE:CE	2.10	0.82
1:A:235:ALA:O	1:A:238:THR:HB	1.79	0.82
1:B:193:LYS:NZ	1:C:45:ASN:HB3	1.94	0.81
1:C:235:ALA:O	1:C:238:THR:HB	1.81	0.81
1:B:1:MSE:SE	1:B:140:ILE:HD13	2.31	0.80
1:C:-5:ASN:OD1	1:C:-4:LEU:HD12	1.81	0.80
1:C:220:ARG:HG2	1:C:221:MSE:HE2	1.65	0.79
1:A:238:THR:HG22	1:A:240:ILE:N	1.96	0.79
1:B:238:THR:HG21	1:B:240:ILE:CB	2.13	0.78
1:B:103:GLU:OE2	1:B:130:LYS:HE2	1.83	0.78
1:C:199:ASP:HB3	1:C:268:PHE:CE2	2.20	0.76
1:B:1:MSE:SE	1:B:140:ILE:HD11	2.33	0.76
1:B:-8:HIS:O	1:B:-6:GLU:OE1	2.03	0.76
1:A:110:ASP:C	1:A:112:GLU:H	1.92	0.76
1:B:138:ASP:O	1:B:285:LYS:HG3	1.86	0.75
1:A:162:GLU:HG2	1:A:163:HIS:CD2	2.23	0.73
1:A:238:THR:HG21	1:A:240:ILE:CB	2.18	0.73
1:A:193:LYS:NZ	1:B:45:ASN:HB3	2.04	0.73
1:B:193:LYS:HZ1	1:C:45:ASN:HB3	1.53	0.73
1:A:119:ARG:HH11	1:A:119:ARG:HG3	1.52	0.73
1:C:220:ARG:CG	1:C:221:MSE:CE	2.54	0.72
1:B:235:ALA:O	1:B:238:THR:HB	1.90	0.72
1:C:-5:ASN:C	1:C:-3:TYR:H	1.96	0.72
1:A:1:MSE:HE2	1:A:1:MSE:HA	1.73	0.71
1:C:-5:ASN:HA	1:C:-2:PHE:CE1	2.26	0.71
1:A:238:THR:CG2	1:A:240:ILE:HB	2.20	0.71
1:C:220:ARG:HD3	1:C:221:MSE:HE3	1.73	0.70
1:B:204:THR:HG22	1:B:207:VAL:H	1.56	0.70
1:A:1:MSE:SE	1:A:140:ILE:CD1	2.90	0.69
1:B:37:TYR:CE2	1:B:162:GLU:HG3	2.28	0.69
1:C:1:MSE:HE2	1:C:1:MSE:CA	2.17	0.69
1:B:162:GLU:HG2	1:B:163:HIS:CD2	2.28	0.69
1:C:110:ASP:C	1:C:111:GLU:OE1	2.35	0.69
1:C:220:ARG:C	1:C:221:MSE:HE2	2.18	0.68
1:A:73:VAL:HA	1:A:79:LEU:HD23	1.75	0.68
1:A:220:ARG:CD	1:A:221:MSE:CE	2.68	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:THR:CG2	1:B:239:ASP:N	2.57	0.68
1:A:193:LYS:HZ2	1:B:45:ASN:HB3	1.58	0.68
1:B:36:SER:HB2	1:B:37:TYR:HD1	1.58	0.67
1:B:179:VAL:CG1	1:B:257:LEU:HD13	2.25	0.67
1:A:220:ARG:O	1:A:221:MSE:HE2	1.94	0.66
1:C:238:THR:HG21	1:C:240:ILE:HD12	1.78	0.66
1:C:110:ASP:C	1:C:112:GLU:H	2.02	0.65
1:C:65:HIS:NE2	1:C:147:ASP:HB2	2.11	0.65
1:B:238:THR:HG21	1:B:240:ILE:CG1	2.26	0.65
1:B:-8:HIS:C	1:B:-6:GLU:OE1	2.39	0.65
1:C:204:THR:CG2	1:C:205:GLU:N	2.59	0.65
1:B:157:LEU:HD22	1:B:161:LEU:HB2	1.80	0.64
1:A:110:ASP:C	1:A:112:GLU:N	2.56	0.64
1:B:238:THR:CG2	1:B:240:ILE:N	2.42	0.64
1:B:204:THR:HG22	1:B:206:GLY:CA	2.28	0.63
1:B:238:THR:CG2	1:B:240:ILE:HB	2.24	0.63
1:A:221:MSE:HE1	3:A:403:EDO:C1	2.26	0.62
1:A:238:THR:CG2	1:A:240:ILE:CB	2.78	0.62
1:A:238:THR:HG23	1:A:240:ILE:N	2.05	0.62
1:B:238:THR:CG2	1:B:240:ILE:CB	2.77	0.62
1:A:145:LEU:CD1	1:A:283:VAL:HG12	2.30	0.61
1:A:69:ILE:HD12	1:A:85:PRO:HB3	1.83	0.61
1:B:204:THR:HG22	1:B:207:VAL:N	2.15	0.60
1:A:204:THR:CG2	1:A:205:GLU:N	2.64	0.60
1:C:37:TYR:CE2	1:C:162:GLU:HG3	2.36	0.60
1:C:-5:ASN:HA	1:C:-2:PHE:CD1	2.36	0.60
1:C:-5:ASN:OD1	1:C:-4:LEU:N	2.35	0.60
1:C:119:ARG:CG	1:C:119:ARG:HH11	2.15	0.60
1:A:90:GLY:C	1:A:105:VAL:HG13	2.27	0.59
1:A:179:VAL:CG1	1:A:257:LEU:HD13	2.32	0.59
1:A:119:ARG:HH11	1:A:119:ARG:HG2	1.66	0.59
1:A:65:HIS:NE2	1:A:147:ASP:HB2	2.19	0.58
1:B:193:LYS:HZ2	1:C:45:ASN:C	2.12	0.58
1:B:193:LYS:HZ2	1:C:45:ASN:HB3	1.69	0.58
1:C:238:THR:HG21	1:C:240:ILE:HB	1.85	0.57
1:B:36:SER:HB2	1:B:37:TYR:CD1	2.40	0.57
1:B:204:THR:HG23	1:B:206:GLY:H	1.62	0.57
1:C:3:LEU:HD22	1:C:3:LEU:O	2.05	0.56
1:B:238:THR:CG2	1:B:240:ILE:CG1	2.83	0.56
1:A:145:LEU:HD13	1:A:283:VAL:HG12	1.86	0.56
1:C:283:VAL:HG22	1:C:284:HIS:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASP:O	1:A:112:GLU:N	2.38	0.55
1:C:73:VAL:HA	1:C:79:LEU:HD23	1.87	0.55
1:C:157:LEU:HD22	1:C:161:LEU:HB2	1.89	0.55
1:C:110:ASP:O	1:C:112:GLU:N	2.40	0.54
1:A:157:LEU:HD22	1:A:161:LEU:HB2	1.89	0.54
1:A:142:THR:OG1	1:A:143:PRO:HD2	2.07	0.54
1:C:110:ASP:C	1:C:112:GLU:N	2.65	0.54
1:C:3:LEU:HD13	1:C:152:TRP:CD1	2.43	0.54
1:B:238:THR:CG2	1:B:240:ILE:HG13	2.38	0.54
1:B:238:THR:HG22	1:B:239:ASP:N	2.09	0.54
1:A:157:LEU:HD11	1:A:299:MSE:HG3	1.90	0.54
1:A:128:THR:HG23	1:A:144:TYR:HE2	1.73	0.53
1:C:61:ALA:O	1:C:195:SER:HA	2.07	0.53
1:C:179:VAL:CG1	1:C:257:LEU:HD13	2.38	0.53
1:A:128:THR:HG22	1:A:129:PHE:O	2.08	0.53
1:A:37:TYR:CE2	1:A:162:GLU:HG3	2.43	0.53
1:C:204:THR:HG22	1:C:205:GLU:N	2.18	0.53
1:C:138:ASP:HB3	1:C:284:HIS:CD2	2.44	0.53
1:A:25:LEU:HD13	1:A:51:ILE:HD13	1.91	0.53
1:A:216:SER:HA	1:A:245:GLU:HB3	1.91	0.52
1:C:-5:ASN:HA	1:C:-2:PHE:CZ	2.43	0.52
1:C:119:ARG:HH11	1:C:119:ARG:HG2	1.74	0.52
1:B:145:LEU:HD13	1:B:283:VAL:HG12	1.90	0.52
1:B:178:SER:HA	1:B:181:TYR:CE2	2.44	0.52
1:B:69:ILE:HD12	1:B:85:PRO:HA	1.92	0.52
1:C:108:ILE:CB	1:C:113:TRP:CZ3	2.92	0.52
1:A:36:SER:C	1:A:37:TYR:CD1	2.88	0.52
1:B:36:SER:C	1:B:37:TYR:CD1	2.88	0.52
1:C:220:ARG:O	1:C:221:MSE:HE2	2.10	0.52
1:A:90:GLY:HA2	1:A:105:VAL:CG1	2.40	0.51
1:A:193:LYS:NZ	1:B:45:ASN:CB	2.72	0.51
1:B:-6:GLU:CD	1:B:-6:GLU:H	2.18	0.51
1:A:44:ASP:HB3	1:A:46:ASP:H	1.76	0.51
3:A:406:EDO:H22	5:A:468:HOH:O	2.10	0.51
1:A:145:LEU:HD13	1:A:283:VAL:CG1	2.40	0.51
1:B:216:SER:HA	1:B:245:GLU:HB3	1.93	0.51
1:B:217:MSE:O	1:B:218:ARG:HB3	2.10	0.51
1:A:199:ASP:O	1:A:270:GLY:HA3	2.11	0.51
1:A:-5:ASN:HA	1:A:-2:PHE:CZ	2.46	0.50
1:C:3:LEU:HD13	1:C:152:TRP:HD1	1.76	0.50
1:C:178:SER:HA	1:C:181:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:O	1:A:66:MSE:HE1	2.11	0.50
1:C:25:LEU:O	1:C:29:ARG:HG3	2.10	0.50
1:C:65:HIS:CE1	1:C:147:ASP:HB2	2.47	0.50
1:C:238:THR:CG2	1:C:239:ASP:N	2.75	0.50
1:B:238:THR:HG21	1:B:240:ILE:HD12	1.95	0.49
1:A:118:ASP:HB2	1:A:119:ARG:HD2	1.94	0.49
1:B:199:ASP:HB3	1:B:268:PHE:CZ	2.47	0.49
1:A:238:THR:HG23	1:A:240:ILE:HG13	1.94	0.49
1:B:145:LEU:HD13	1:B:283:VAL:CG1	2.43	0.49
1:B:21:LYS:O	1:B:25:LEU:HB2	2.13	0.49
1:B:199:ASP:HB3	1:B:268:PHE:CE2	2.48	0.49
1:A:20:LEU:HD23	1:A:66:MSE:HB3	1.95	0.49
1:C:102:ILE:CD1	1:C:125:THR:HG21	2.43	0.48
1:B:170:CYS:O	1:B:171:TRP:HB2	2.13	0.48
1:C:36:SER:HB2	1:C:37:TYR:HD1	1.77	0.48
1:C:44:ASP:C	1:C:44:ASP:OD1	2.56	0.48
1:C:199:ASP:HB3	1:C:268:PHE:CZ	2.49	0.48
1:A:109:VAL:O	1:A:112:GLU:O	2.31	0.48
1:C:71:PHE:HB2	1:C:127:VAL:HG23	1.95	0.48
1:C:69:ILE:HD12	1:C:85:PRO:HB3	1.96	0.48
1:A:283:VAL:HG22	1:A:284:HIS:N	2.27	0.48
1:C:1:MSE:CE	1:C:1:MSE:CA	2.85	0.48
1:C:238:THR:CG2	1:C:240:ILE:HB	2.44	0.48
1:B:128:THR:HG23	1:B:144:TYR:HE2	1.79	0.47
1:A:1:MSE:HA	1:A:1:MSE:CE	2.43	0.47
1:C:-5:ASN:C	1:C:-3:TYR:N	2.62	0.47
1:A:69:ILE:HD12	1:A:85:PRO:CB	2.43	0.47
1:A:146:ASP:HA	1:A:147:ASP:HA	1.72	0.47
1:C:36:SER:C	1:C:37:TYR:CD1	2.92	0.47
1:C:238:THR:CG2	1:C:240:ILE:N	2.62	0.47
1:A:193:LYS:HZ2	1:B:45:ASN:C	2.22	0.47
1:A:268:PHE:CD1	1:A:268:PHE:C	2.92	0.47
1:B:102:ILE:HD13	1:B:121:ILE:HD12	1.97	0.47
1:A:118:ASP:HB2	1:A:119:ARG:CD	2.45	0.47
1:C:24:ILE:O	1:C:28:ILE:HG13	2.14	0.47
1:B:1:MSE:HA	1:B:1:MSE:HE2	1.96	0.47
1:B:5:LYS:HD2	1:B:133:PHE:HB3	1.97	0.47
1:B:216:SER:HB3	1:B:268:PHE:HB3	1.97	0.47
1:C:49:ASP:O	1:C:66:MSE:HE1	2.15	0.47
1:A:3:LEU:HD13	1:A:152:TRP:CD1	2.51	0.46
1:C:95:GLY:O	1:C:102:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:HD11	1:A:283:VAL:HG12	1.98	0.46
1:A:198:CYS:SG	1:A:291:MSE:HE2	2.54	0.46
1:B:65:HIS:NE2	1:B:147:ASP:HB2	2.31	0.46
1:B:145:LEU:CD1	1:B:283:VAL:HG12	2.45	0.46
1:C:28:ILE:HD13	1:C:53:LEU:HD11	1.97	0.46
1:C:44:ASP:HA	5:C:460:HOH:O	2.15	0.46
1:A:119:ARG:HG3	1:A:119:ARG:NH1	2.23	0.46
1:B:204:THR:CG2	1:B:205:GLU:N	2.78	0.46
1:A:90:GLY:HA2	1:A:105:VAL:HG11	1.97	0.45
1:A:105:VAL:HG12	1:A:106:LEU:N	2.31	0.45
1:B:179:VAL:HG11	1:B:257:LEU:HD13	1.99	0.45
1:C:238:THR:CG2	1:C:240:ILE:CG1	2.94	0.45
1:A:200:ILE:HG23	1:A:271:ALA:O	2.17	0.45
1:B:50:CYS:SG	1:B:178:SER:HB2	2.57	0.45
1:B:90:GLY:HA2	1:B:105:VAL:CG1	2.47	0.45
1:B:236:ARG:C	1:B:238:THR:H	2.22	0.45
1:C:128:THR:HG23	1:C:144:TYR:HE2	1.82	0.45
1:A:61:ALA:O	1:A:195:SER:HA	2.16	0.45
1:A:73:VAL:HG22	1:A:79:LEU:HD21	1.99	0.44
1:A:-5:ASN:HA	1:A:-2:PHE:CE2	2.52	0.44
1:A:225:LYS:HA	1:A:225:LYS:HD3	1.85	0.44
1:B:20:LEU:HD23	1:B:66:MSE:HB3	1.99	0.44
1:A:-5:ASN:HA	1:A:-2:PHE:CE1	2.52	0.44
1:A:199:ASP:HB3	1:A:268:PHE:CE2	2.52	0.44
1:B:103:GLU:OE2	1:B:130:LYS:CE	2.59	0.44
1:C:157:LEU:HD11	1:C:299:MSE:HG3	2.00	0.44
1:A:119:ARG:H	1:A:119:ARG:HD3	1.82	0.44
1:B:146:ASP:HA	1:B:147:ASP:HA	1.80	0.44
1:B:148:ARG:HA	1:B:148:ARG:HD3	1.82	0.44
1:A:-1:GLN:NE2	1:A:27:TYR:OH	2.50	0.44
1:B:238:THR:HG23	1:B:240:ILE:HG13	1.98	0.44
1:C:128:THR:HG23	1:C:144:TYR:CE2	2.53	0.44
1:C:146:ASP:HA	1:C:147:ASP:HA	1.79	0.44
1:C:238:THR:HG21	1:C:240:ILE:CD1	2.46	0.44
1:C:36:SER:HB2	1:C:37:TYR:CD1	2.53	0.43
1:C:220:ARG:CD	1:C:221:MSE:CE	2.85	0.43
1:C:238:THR:HG21	1:C:240:ILE:CB	2.48	0.43
1:B:68:SER:HB2	1:B:144:TYR:CD1	2.53	0.43
1:B:201:THR:HG23	1:B:202:TRP:N	2.32	0.43
1:C:198:CYS:SG	1:C:291:MSE:HE2	2.58	0.43
1:A:270:GLY:HA2	1:A:291:MSE:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:THR:CG2	1:C:240:ILE:CB	2.95	0.43
1:C:11:HIS:ND1	1:C:128:THR:HB	2.32	0.43
1:C:141:LEU:N	1:C:141:LEU:HD12	2.34	0.43
1:A:55:PHE:CD1	1:A:161:LEU:HD23	2.54	0.43
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.88	0.43
1:C:238:THR:HG21	1:C:240:ILE:CG1	2.47	0.43
1:B:55:PHE:CD1	1:B:161:LEU:HD23	2.54	0.43
1:B:63:PHE:CE1	1:B:257:LEU:HD21	2.54	0.43
1:A:280:ASN:O	1:A:281:GLU:C	2.62	0.43
1:C:57[A]:ASN:HB3	1:C:163:HIS:CE1	2.54	0.43
1:C:121:ILE:HG22	1:C:122:ASP:O	2.19	0.43
1:B:73:VAL:HA	1:B:79:LEU:HD23	2.00	0.42
1:B:139:PHE:CD2	1:B:282:CYS:SG	3.13	0.42
1:C:32:ALA:HA	1:C:35:TRP:CD2	2.54	0.42
1:A:178:SER:HA	1:A:181:TYR:CE2	2.54	0.42
1:C:221:MSE:HE1	3:C:404:EDO:O1	2.20	0.42
1:C:-5:ASN:O	1:C:-3:TYR:N	2.53	0.42
1:B:28:ILE:HD13	1:B:53:LEU:HD11	2.02	0.42
1:A:90:GLY:O	1:A:91:TYR:C	2.61	0.42
1:A:213:VAL:O	1:A:242:PHE:HA	2.19	0.42
1:B:238:THR:HG21	1:B:240:ILE:CD1	2.49	0.42
1:C:79:LEU:HD11	1:C:115:LEU:HB2	2.02	0.42
1:A:3:LEU:HD22	1:A:3:LEU:O	2.20	0.42
1:C:-1:GLN:OE1	1:C:159:LYS:NZ	2.31	0.42
1:A:216:SER:HB3	1:A:268:PHE:HB3	2.01	0.41
1:C:280:ASN:O	1:C:281:GLU:C	2.60	0.41
1:C:20:LEU:HD23	1:C:66:MSE:HB3	2.01	0.41
1:C:215:ILE:HD11	1:C:294:LEU:HD21	2.01	0.41
1:C:225:LYS:HD3	1:C:225:LYS:HA	1.66	0.41
1:B:37:TYR:CD2	1:B:162:GLU:HG3	2.54	0.41
1:B:204:THR:HG23	1:B:205:GLU:N	2.34	0.41
1:C:76:ASN:O	1:C:77:ASN:HB2	2.20	0.41
1:A:213:VAL:HG22	1:A:214:ALA:N	2.35	0.41
1:C:238:THR:CG2	1:C:240:ILE:HG13	2.49	0.41
1:A:105:VAL:CG1	1:A:106:LEU:N	2.83	0.41
3:A:405:EDO:O1	3:A:406:EDO:H11	2.19	0.41
1:B:69:ILE:HD12	1:B:85:PRO:HB3	2.01	0.41
1:C:219:ASP:HB2	1:C:250:GLY:O	2.21	0.41
1:B:25:LEU:O	1:B:29:ARG:HG3	2.20	0.41
1:B:110:ASP:O	1:B:111:GLU:HB2	2.20	0.41
1:C:142:THR:CG2	1:C:145:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:CG2	1:B:206:GLY:N	2.48	0.41
1:C:-5:ASN:OD1	1:C:-4:LEU:CD1	2.62	0.41
1:C:102:ILE:HD12	1:C:125:THR:HG21	2.03	0.41
1:A:170:CYS:O	1:A:171:TRP:HB2	2.20	0.41
1:A:201:THR:OG1	1:A:245:GLU:OE1	2.24	0.41
1:A:283:VAL:CG2	1:A:284:HIS:N	2.84	0.41
1:B:157:LEU:HD11	1:B:299:MSE:HG3	2.03	0.41
1:C:-2:PHE:C	1:C:-1:GLN:HG2	2.46	0.41
1:C:283:VAL:CG2	1:C:284:HIS:N	2.84	0.41
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.83	0.41
1:A:148:ARG:HA	1:A:148:ARG:HD3	1.92	0.41
1:B:36:SER:CB	1:B:37:TYR:CD1	3.04	0.41
1:A:25:LEU:HD13	1:A:51:ILE:CD1	2.50	0.40
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.91	0.40
1:C:260:SER:C	1:C:262:TYR:H	2.28	0.40
1:A:32:ALA:HA	1:A:35:TRP:CD2	2.56	0.40
1:A:193:LYS:HZ2	1:B:45:ASN:CB	2.31	0.40

All (1) 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:A:409:HOH:O	5:C:431:HOH:O[10_665]	2.04	0.16

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	308/321 (96%)	288 (94%)	18 (6%)	2 (1%)	21	32
1	B	309/321 (96%)	291 (94%)	17 (6%)	1 (0%)	36	50
1	C	309/321 (96%)	288 (93%)	18 (6%)	3 (1%)	12	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	926/963 (96%)	867 (94%)	53 (6%)	6 (1%)	18	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	ASP
1	A	111	GLU
1	C	-4	LEU
1	C	111	GLU
1	B	218	ARG
1	A	109	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	252/269 (94%)	238 (94%)	14 (6%)	19	33
1	B	258/269 (96%)	249 (96%)	9 (4%)	32	53
1	C	253/269 (94%)	240 (95%)	13 (5%)	21	37
All	All	763/807 (94%)	727 (95%)	36 (5%)	23	41

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	25	LEU
1	A	30	SER
1	A	62	VAL
1	A	92	ARG
1	A	118	ASP
1	A	119	ARG
1	A	128	THR
1	A	149	LEU
1	A	157	LEU

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Mol	Chain	Res	Type
1	A	204	THR
1	A	238	THR
1	A	244	LEU
1	A	257	LEU
1	B	-4	LEU
1	B	3	LEU
1	B	62	VAL
1	B	128	THR
1	B	149	LEU
1	B	157	LEU
1	B	204	THR
1	B	244	LEU
1	B	257	LEU
1	C	3	LEU
1	C	62	VAL
1	C	92	ARG
1	C	119	ARG
1	C	128	THR
1	C	142	THR
1	C	149	LEU
1	C	157	LEU
1	C	204	THR
1	C	225	LYS
1	C	233	GLU
1	C	244	LEU
1	C	257	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	99	ASN
1	B	48	GLN
1	C	2	GLN
1	C	48	GLN
1	C	280	ASN

5.3.3 RNA ⓘ

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 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	C	405	-	3,3,3	0.42	0	2,2,2	0.54	0
3	EDO	A	406	-	3,3,3	0.70	0	2,2,2	0.25	0
3	EDO	A	404	-	3,3,3	0.41	0	2,2,2	1.24	0
3	EDO	A	403	-	3,3,3	1.12	0	2,2,2	0.94	0
3	EDO	B	403	-	3,3,3	0.66	0	2,2,2	0.16	0
3	EDO	C	403	-	3,3,3	0.42	0	2,2,2	0.21	0
3	EDO	A	402	-	3,3,3	0.48	0	2,2,2	0.77	0
3	EDO	A	407	-	3,3,3	0.45	0	2,2,2	0.51	0
3	EDO	C	404	-	3,3,3	0.44	0	2,2,2	0.25	0
3	EDO	C	402	-	3,3,3	0.36	0	2,2,2	0.93	0
3	EDO	C	406	-	3,3,3	0.47	0	2,2,2	0.21	0
3	EDO	A	405	-	3,3,3	0.55	0	2,2,2	0.04	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	C	405	-	-	0/1/1/1	-
3	EDO	A	406	-	-	1/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	C	403	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	A	407	-	-	1/1/1/1	-
3	EDO	C	404	-	-	1/1/1/1	-
3	EDO	C	402	-	-	1/1/1/1	-
3	EDO	C	406	-	-	1/1/1/1	-
3	EDO	A	405	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	406	EDO	O1-C1-C2-O2
3	A	405	EDO	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2
3	C	403	EDO	O1-C1-C2-O2
3	C	402	EDO	O1-C1-C2-O2
3	A	406	EDO	O1-C1-C2-O2
3	B	403	EDO	O1-C1-C2-O2
3	A	404	EDO	O1-C1-C2-O2
3	C	404	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	EDO	2	0
3	A	403	EDO	2	0
3	C	404	EDO	1	0
3	A	405	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	302/321 (94%)	0.66	15 (4%) 34 30	27, 43, 49, 66	1 (0%)
1	B	304/321 (94%)	0.44	8 (2%) 57 53	37, 43, 51, 86	0
1	C	302/321 (94%)	0.99	30 (9%) 13 9	24, 43, 49, 63	2 (0%)
All	All	908/963 (94%)	0.70	53 (5%) 29 25	24, 43, 50, 86	3 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-2	PHE	6.8
1	A	-3	TYR	5.5
1	C	-2	PHE	4.6
1	C	-3	TYR	4.5
1	A	-4	LEU	4.5
1	A	-6	GLU	4.4
1	A	109	VAL	4.3
1	A	-5	ASN	3.6
1	C	109	VAL	3.6
1	B	-8	HIS	3.5
1	C	138	ASP	3.4
1	C	-4	LEU	3.4
1	C	261	PRO	3.1
1	C	104	GLY	3.1
1	B	45	ASN	2.9
1	C	-6	GLU	2.9
1	A	-1	GLN	2.8
1	C	70	GLY	2.8
1	C	-5	ASN	2.7
1	B	-1	GLN	2.7
1	C	116	GLU	2.7
1	C	186	ILE	2.6
1	C	191[A]	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	45	ASN	2.5
1	C	115	LEU	2.5
1	B	242	PHE	2.5
1	B	-7	HIS	2.3
1	C	77	ASN	2.3
1	C	128	THR	2.3
1	A	44	ASP	2.3
1	C	73	VAL	2.3
1	C	133	PHE	2.2
1	B	204	THR	2.2
1	C	187	TYR	2.2
1	C	262	TYR	2.2
1	C	259	LEU	2.2
1	C	99	ASN	2.2
1	A	111	GLU	2.2
1	A	33	GLY	2.2
1	C	129	PHE	2.1
1	B	108	ILE	2.1
1	C	102	ILE	2.1
1	A	26	GLU	2.1
1	A	43	ALA	2.1
1	A	45	ASN	2.1
1	A	110	ASP	2.1
1	C	71	PHE	2.1
1	B	107	LYS	2.0
1	C	182	LEU	2.0
1	C	257	LEU	2.0
1	C	263	PRO	2.0
1	A	106	LEU	2.0
1	C	93	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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
3	EDO	A	402	4/4	0.71	0.19	51,51,51,52	0
3	EDO	C	405	4/4	0.75	0.22	67,67,68,68	0
3	EDO	A	407	4/4	0.77	0.21	74,74,74,74	0
3	EDO	A	403	4/4	0.84	0.19	39,39,41,41	0
3	EDO	C	406	4/4	0.84	0.21	64,64,65,65	0
3	EDO	A	406	4/4	0.86	0.23	52,53,53,53	0
3	EDO	A	404	4/4	0.86	0.19	42,42,43,43	0
3	EDO	C	404	4/4	0.88	0.18	64,65,66,66	0
3	EDO	C	402	4/4	0.90	0.22	55,55,55,55	0
3	EDO	A	405	4/4	0.90	0.21	62,62,63,63	0
3	EDO	C	403	4/4	0.92	0.17	47,48,48,50	0
3	EDO	B	403	4/4	0.92	0.16	33,34,34,36	0
4	CL	B	402	1/1	0.93	0.09	62,62,62,62	0
2	FE	C	400	1/1	0.96	0.09	54,54,54,54	0
2	FE	B	401	1/1	0.98	0.07	35,35,35,35	0
2	FE	A	401	1/1	0.98	0.08	50,50,50,50	0
2	FE	C	401	1/1	0.98	0.12	38,38,38,38	0
2	FE	B	400	1/1	0.98	0.09	44,44,44,44	0
2	FE	A	400	1/1	0.99	0.13	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.