



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:34 AM UTC

PDB ID : 3ZX3 / pdb_00003zx3
Title : Crystal Structure and Domain Rotation of NTPDase1 CD39
Authors : Zebisch, M.; Schaefer, P.; Straeter, N.
Deposited on : 2011-08-04
Resolution : 1.70 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

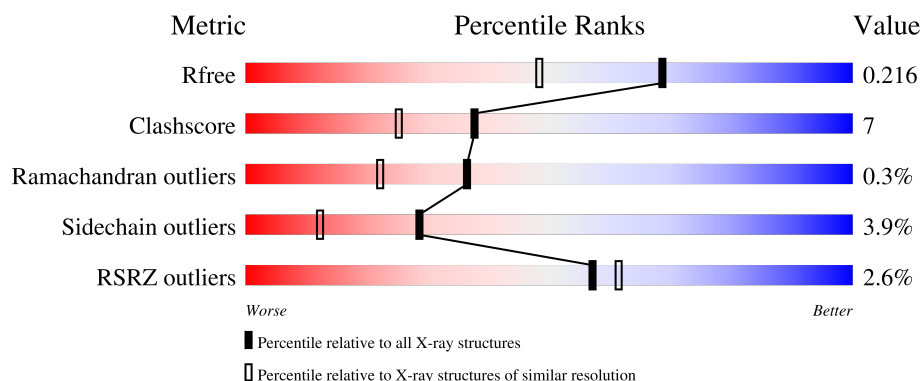
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	452	3% 71% 14% • 12%
1	B	452	2% 72% 15% • 12%
1	C	452	2% 71% 13% • 13%
1	D	452	2% 72% 15% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	511	-	-	X	-
3	ACY	B	512	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13625 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 ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	10	0
			3201	2070	515	596	20			
1	B	400	Total	C	N	O	S	0	8	0
			3209	2073	517	598	21			
1	C	393	Total	C	N	O	S	0	5	0
			3137	2031	503	583	20			
1	D	397	Total	C	N	O	S	0	12	0
			3196	2072	516	587	21			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	expression tag	UNP P97687
A	16	ALA	-	expression tag	UNP P97687
A	17	HIS	-	expression tag	UNP P97687
A	18	HIS	-	expression tag	UNP P97687
A	19	HIS	-	expression tag	UNP P97687
A	20	HIS	-	expression tag	UNP P97687
A	21	HIS	-	expression tag	UNP P97687
A	22	HIS	-	expression tag	UNP P97687
A	23	VAL	-	expression tag	UNP P97687
A	24	GLY	-	expression tag	UNP P97687
A	25	THR	-	expression tag	UNP P97687
A	26	GLY	-	expression tag	UNP P97687
A	27	SER	-	expression tag	UNP P97687
A	28	ASN	-	expression tag	UNP P97687
A	29	ASP	-	expression tag	UNP P97687
A	30	ASP	-	expression tag	UNP P97687
A	31	ASP	-	expression tag	UNP P97687
A	32	ASP	-	expression tag	UNP P97687
A	33	LYS	-	expression tag	UNP P97687
A	34	SER	-	expression tag	UNP P97687

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Chain	Residue	Modelled	Actual	Comment	Reference
A	35	PRO	-	expression tag	UNP P97687
A	36	ASP	-	expression tag	UNP P97687
A	37	PRO	-	expression tag	UNP P97687
A	80	GLN	LEU	SEE REMARK 999	UNP P97687
A	190	LYS	-	linker	UNP P97687
A	191	THR	-	linker	UNP P97687
A	192	PRO	-	linker	UNP P97687
A	204	GLY	-	linker	UNP P97687
A	205	GLY	-	linker	UNP P97687
A	206	SER	-	linker	UNP P97687
A	220	ILE	VAL	SEE REMARK 999	UNP P97687
A	227	SER	GLN	SEE REMARK 999	UNP P97687
A	331	ILE	PHE	conflict	UNP P97687
B	15	MET	-	expression tag	UNP P97687
B	16	ALA	-	expression tag	UNP P97687
B	17	HIS	-	expression tag	UNP P97687
B	18	HIS	-	expression tag	UNP P97687
B	19	HIS	-	expression tag	UNP P97687
B	20	HIS	-	expression tag	UNP P97687
B	21	HIS	-	expression tag	UNP P97687
B	22	HIS	-	expression tag	UNP P97687
B	23	VAL	-	expression tag	UNP P97687
B	24	GLY	-	expression tag	UNP P97687
B	25	THR	-	expression tag	UNP P97687
B	26	GLY	-	expression tag	UNP P97687
B	27	SER	-	expression tag	UNP P97687
B	28	ASN	-	expression tag	UNP P97687
B	29	ASP	-	expression tag	UNP P97687
B	30	ASP	-	expression tag	UNP P97687
B	31	ASP	-	expression tag	UNP P97687
B	32	ASP	-	expression tag	UNP P97687
B	33	LYS	-	expression tag	UNP P97687
B	34	SER	-	expression tag	UNP P97687
B	35	PRO	-	expression tag	UNP P97687
B	36	ASP	-	expression tag	UNP P97687
B	37	PRO	-	expression tag	UNP P97687
B	80	GLN	LEU	SEE REMARK 999	UNP P97687
B	190	LYS	-	linker	UNP P97687
B	191	THR	-	linker	UNP P97687
B	192	PRO	-	linker	UNP P97687
B	204	GLY	-	linker	UNP P97687
B	205	GLY	-	linker	UNP P97687

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Chain	Residue	Modelled	Actual	Comment	Reference
B	206	SER	-	linker	UNP P97687
B	220	ILE	VAL	SEE REMARK 999	UNP P97687
B	227	SER	GLN	SEE REMARK 999	UNP P97687
B	331	ILE	PHE	conflict	UNP P97687
C	15	MET	-	expression tag	UNP P97687
C	16	ALA	-	expression tag	UNP P97687
C	17	HIS	-	expression tag	UNP P97687
C	18	HIS	-	expression tag	UNP P97687
C	19	HIS	-	expression tag	UNP P97687
C	20	HIS	-	expression tag	UNP P97687
C	21	HIS	-	expression tag	UNP P97687
C	22	HIS	-	expression tag	UNP P97687
C	23	VAL	-	expression tag	UNP P97687
C	24	GLY	-	expression tag	UNP P97687
C	25	THR	-	expression tag	UNP P97687
C	26	GLY	-	expression tag	UNP P97687
C	27	SER	-	expression tag	UNP P97687
C	28	ASN	-	expression tag	UNP P97687
C	29	ASP	-	expression tag	UNP P97687
C	30	ASP	-	expression tag	UNP P97687
C	31	ASP	-	expression tag	UNP P97687
C	32	ASP	-	expression tag	UNP P97687
C	33	LYS	-	expression tag	UNP P97687
C	34	SER	-	expression tag	UNP P97687
C	35	PRO	-	expression tag	UNP P97687
C	36	ASP	-	expression tag	UNP P97687
C	37	PRO	-	expression tag	UNP P97687
C	80	GLN	LEU	SEE REMARK 999	UNP P97687
C	190	LYS	-	linker	UNP P97687
C	191	THR	-	linker	UNP P97687
C	192	PRO	-	linker	UNP P97687
C	204	GLY	-	linker	UNP P97687
C	205	GLY	-	linker	UNP P97687
C	206	SER	-	linker	UNP P97687
C	220	ILE	VAL	SEE REMARK 999	UNP P97687
C	227	SER	GLN	SEE REMARK 999	UNP P97687
C	331	ILE	PHE	conflict	UNP P97687
D	15	MET	-	expression tag	UNP P97687
D	16	ALA	-	expression tag	UNP P97687
D	17	HIS	-	expression tag	UNP P97687
D	18	HIS	-	expression tag	UNP P97687
D	19	HIS	-	expression tag	UNP P97687

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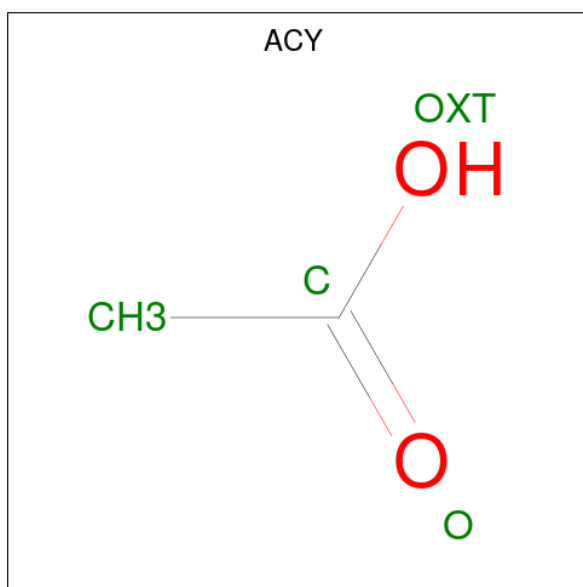
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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P97687
D	21	HIS	-	expression tag	UNP P97687
D	22	HIS	-	expression tag	UNP P97687
D	23	VAL	-	expression tag	UNP P97687
D	24	GLY	-	expression tag	UNP P97687
D	25	THR	-	expression tag	UNP P97687
D	26	GLY	-	expression tag	UNP P97687
D	27	SER	-	expression tag	UNP P97687
D	28	ASN	-	expression tag	UNP P97687
D	29	ASP	-	expression tag	UNP P97687
D	30	ASP	-	expression tag	UNP P97687
D	31	ASP	-	expression tag	UNP P97687
D	32	ASP	-	expression tag	UNP P97687
D	33	LYS	-	expression tag	UNP P97687
D	34	SER	-	expression tag	UNP P97687
D	35	PRO	-	expression tag	UNP P97687
D	36	ASP	-	expression tag	UNP P97687
D	37	PRO	-	expression tag	UNP P97687
D	80	GLN	LEU	SEE REMARK 999	UNP P97687
D	190	LYS	-	linker	UNP P97687
D	191	THR	-	linker	UNP P97687
D	192	PRO	-	linker	UNP P97687
D	204	GLY	-	linker	UNP P97687
D	205	GLY	-	linker	UNP P97687
D	206	SER	-	linker	UNP P97687
D	220	ILE	VAL	SEE REMARK 999	UNP P97687
D	227	SER	GLN	SEE REMARK 999	UNP P97687
D	331	ILE	PHE	conflict	UNP P97687

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Cl 6 6	0	0
2	B	6	Total Cl 6 6	0	0
2	C	6	Total Cl 6 6	0	0
2	D	9	Total Cl 9 9	0	0

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

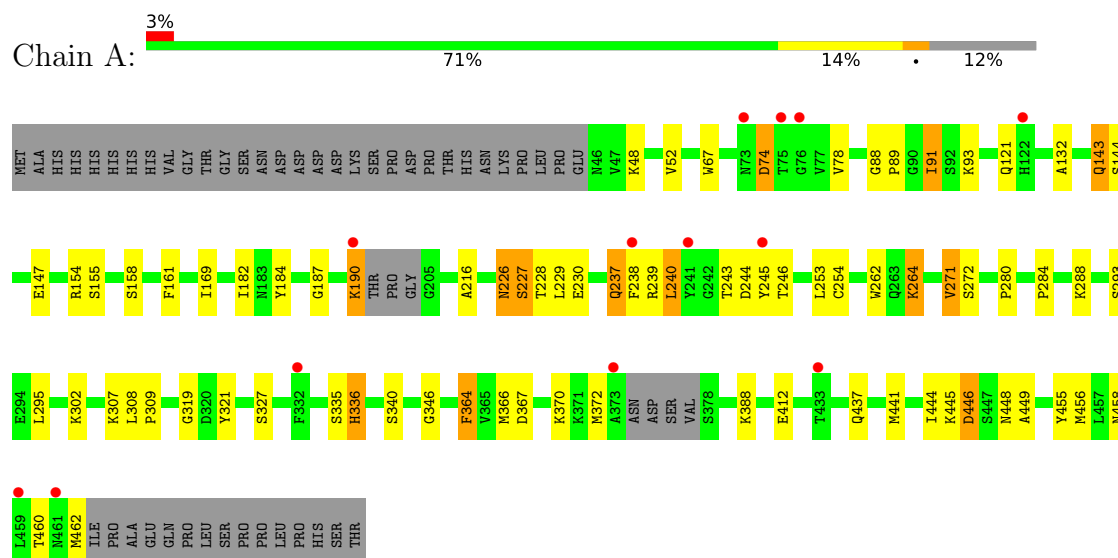
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	207	Total 210	O 210	0	3
5	B	159	Total 161	O 161	0	2
5	C	205	Total 206	O 206	0	1
5	D	245	Total 245	O 245	0	0

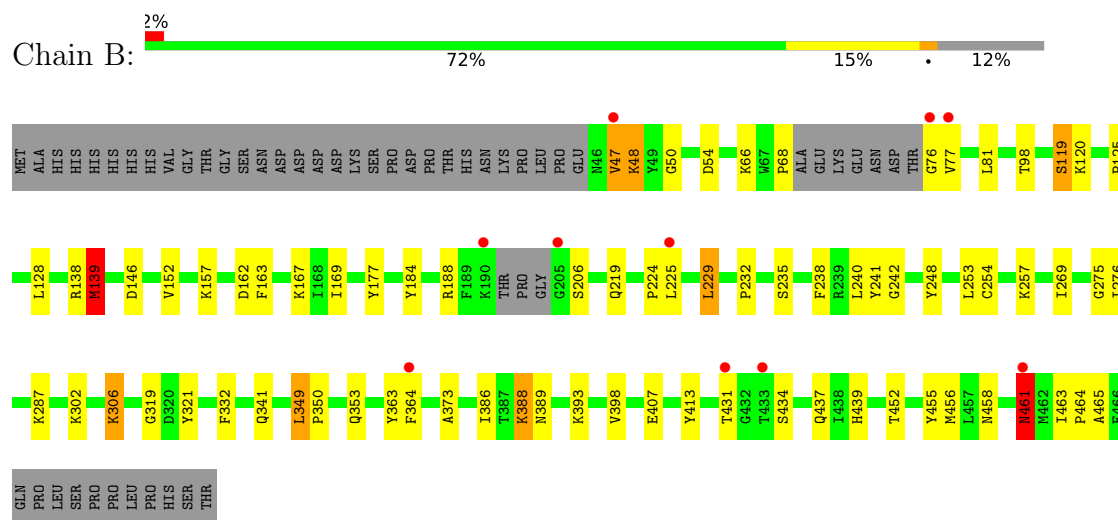
3 Residue-property plots [i](#)

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

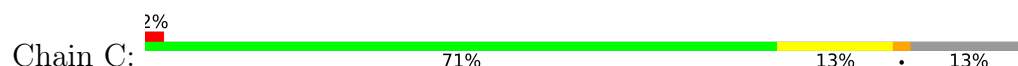
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

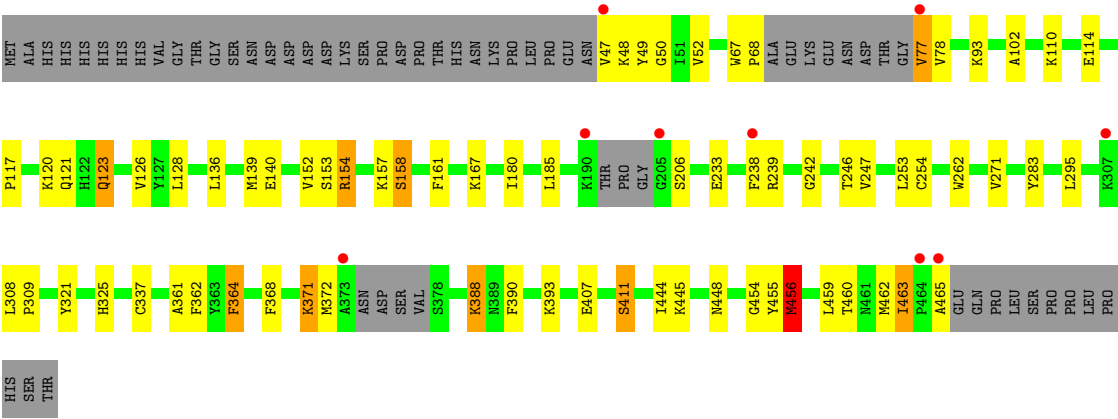


• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

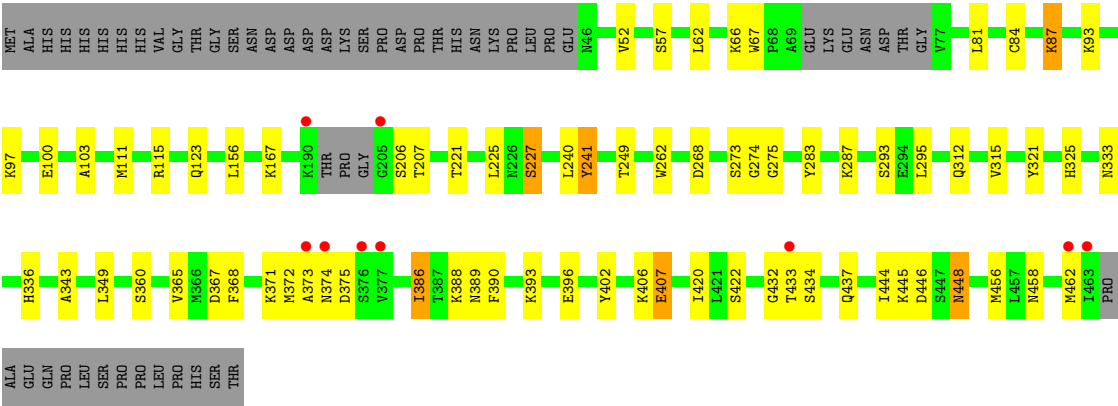


• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1





• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.13Å 81.14Å 165.47Å 90.00° 117.61° 90.00°	Depositor
Resolution (Å)	146.62 – 1.70 146.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	72.6 (146.62-1.70) 72.6 (146.62-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.233 (Not available) , 0.216	Depositor DCC
R_{free} test set	1139 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13625	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, ACY

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	1.32	6/3316 (0.2%)	1.23	11/4482 (0.2%)
1	B	1.25	3/3314 (0.1%)	1.26	14/4479 (0.3%)
1	C	1.31	7/3235 (0.2%)	1.28	11/4374 (0.3%)
1	D	1.34	4/3316 (0.1%)	1.25	21/4482 (0.5%)
All	All	1.31	20/13181 (0.2%)	1.26	57/17817 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	GLY	C-O	-5.99	1.17	1.24
1	A	448	ASN	CA-C	-5.91	1.45	1.52
1	B	439	HIS	CG-CD2	5.81	1.42	1.35
1	B	219	GLN	N-CA	5.77	1.52	1.45
1	A	367	ASP	N-CA	-5.59	1.39	1.46
1	D	240	LEU	CA-C	-5.59	1.45	1.52
1	D	336	HIS	CA-C	-5.54	1.46	1.52
1	C	247	VAL	N-CA	-5.42	1.40	1.46
1	A	449	ALA	CA-C	5.41	1.59	1.52
1	A	182	ILE	C-O	-5.39	1.17	1.24
1	C	52	VAL	C-O	-5.36	1.18	1.24
1	C	362	PHE	C-O	-5.34	1.18	1.24
1	A	336	HIS	CG-CD2	5.32	1.41	1.35
1	C	246	THR	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	PRO	C-O	-5.24	1.17	1.24
1	D	103	ALA	CA-C	5.22	1.59	1.52
1	B	388	LYS	N-CA	-5.20	1.40	1.46
1	C	454	GLY	N-CA	5.07	1.52	1.45
1	D	156	LEU	CA-C	-5.06	1.46	1.52
1	C	233	GLU	C-O	-5.01	1.17	1.24

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	CYS	CA-C-N	-8.10	112.57	120.83
1	C	337	CYS	C-N-CA	-8.10	112.57	120.83
1	C	463	ILE	CA-C-N	7.44	129.14	119.84
1	C	463	ILE	C-N-CA	7.44	129.14	119.84
1	D	433	THR	N-CA-C	7.01	118.61	110.97
1	D	275	GLY	N-CA-C	-6.89	104.48	115.08
1	D	462	MET	CB-CG-SD	6.79	133.08	112.70
1	B	139	MET	CA-C-N	6.78	129.36	120.28
1	B	139	MET	C-N-CA	6.78	129.36	120.28
1	B	77	VAL	CB-CA-C	-6.69	102.48	110.84
1	C	121	GLN	N-CA-C	6.66	119.89	111.69
1	D	207	THR	N-CA-C	6.55	120.71	110.17
1	B	393	LYS	CA-C-N	-6.39	113.19	119.78
1	B	393	LYS	C-N-CA	-6.39	113.19	119.78
1	D	432	GLY	CA-C-N	6.28	128.94	120.65
1	D	432	GLY	C-N-CA	6.28	128.94	120.65
1	D	448	ASN	N-CA-C	6.18	119.32	110.10
1	A	271	VAL	CB-CA-C	-6.17	103.04	112.05
1	B	431	THR	N-CA-C	6.04	119.42	110.48
1	A	364	PHE	CB-CA-C	6.03	120.80	110.79
1	A	74	ASP	N-CA-C	6.02	116.37	107.88
1	A	184	TYR	N-CA-C	-6.02	104.64	111.14
1	D	446	ASP	N-CA-C	6.00	120.40	113.38
1	C	444	ILE	N-CA-C	-5.96	99.76	108.11
1	B	398	VAL	N-CA-C	-5.83	105.05	110.53
1	B	363	TYR	N-CA-C	5.76	117.36	111.14
1	B	458	ASN	N-CA-C	5.75	117.22	111.07
1	D	349	LEU	CA-C-N	-5.74	114.46	120.38
1	D	349	LEU	C-N-CA	-5.74	114.46	120.38
1	D	389	ASN	N-CA-C	5.69	117.94	111.11
1	A	335	SER	N-CA-C	5.64	120.01	113.18
1	D	273	SER	CA-C-N	-5.64	112.68	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	273	SER	C-N-CA	-5.64	112.68	122.83
1	A	91	ILE	CB-CA-C	-5.61	103.47	112.16
1	B	238	PHE	N-CA-C	5.61	116.48	108.74
1	B	146	ASP	N-CA-C	5.61	117.39	111.28
1	D	67	TRP	N-CA-C	5.52	113.19	108.22
1	C	390	PHE	N-CA-C	5.47	117.33	111.36
1	C	180	ILE	N-CA-C	5.42	115.63	110.42
1	B	413	TYR	N-CA-C	5.42	117.19	111.28
1	D	407	GLU	CB-CG-CD	5.41	121.80	112.60
1	C	456	MET	N-CA-C	5.38	117.23	111.36
1	A	372	MET	N-CA-C	5.38	117.90	111.71
1	D	167	LYS	CB-CG-CD	-5.32	99.07	111.30
1	A	88	GLY	CA-C-N	5.30	126.46	119.84
1	A	88	GLY	C-N-CA	5.30	126.46	119.84
1	C	238	PHE	N-CA-C	5.29	117.42	109.23
1	B	349	LEU	CA-C-N	-5.26	114.96	120.38
1	B	349	LEU	C-N-CA	-5.26	114.96	120.38
1	C	448	ASN	N-CA-C	5.24	117.82	110.23
1	D	406	LYS	CD-CE-NZ	-5.18	95.31	111.90
1	D	268	ASP	N-CA-C	5.18	118.06	111.69
1	D	389	ASN	CB-CA-C	-5.12	102.61	110.81
1	A	144	SER	CB-CA-C	-5.06	102.94	110.88
1	D	360	SER	CB-CA-C	-5.05	110.73	116.54
1	D	386	ILE	N-CA-C	5.05	115.66	110.36
1	A	169	ILE	N-CA-C	-5.04	104.56	110.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	274	GLY	Peptide

5.2 Too-close contacts [i](#)

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	3201	0	3110	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3209	0	3131	50	0
1	C	3137	0	3060	42	0
1	D	3196	0	3145	39	0
2	A	6	0	0	0	0
2	B	6	0	0	1	0
2	C	6	0	0	0	0
2	D	9	0	0	3	0
3	A	4	0	3	6	0
3	B	8	0	6	2	0
3	C	8	0	6	0	0
3	D	8	0	6	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	210	0	0	2	0
5	B	161	0	0	4	0
5	C	206	0	0	4	0
5	D	245	0	0	4	0
All	All	13625	0	12467	176	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 7.

All (176) 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:366:MET:CE	3:A:511:ACY:H1	1.63	1.28
1:A:229:LEU:CB	1:B:139:MET:HE3	1.80	1.11
1:A:366:MET:HE2	3:A:511:ACY:H1	1.09	1.04
1:D:52:VAL:HG23	1:D:456:MET:HE3	1.37	1.04
1:D:52:VAL:HG23	1:D:456:MET:CE	1.88	1.03
1:B:50:GLY:HA3	1:B:456[A]:MET:HE1	1.39	1.02
1:A:229:LEU:CB	1:B:139:MET:CE	2.37	1.01
1:B:66:LYS:HD2	1:B:81:LEU:HD13	1.51	0.92
1:C:262[B]:TRP:HE3	1:C:295:LEU:HD12	1.35	0.91
1:A:366:MET:HE2	3:A:511:ACY:CH3	2.02	0.86
1:A:366:MET:HE1	3:A:511:ACY:H1	1.58	0.84
1:B:50:GLY:HA3	1:B:456[A]:MET:CE	2.09	0.82
1:D:52:VAL:CG2	1:D:456:MET:CE	2.58	0.81
1:A:228:THR:HG21	1:B:302:LYS:HZ3	1.45	0.79
1:C:239:ARG:HG2	1:C:465:ALA:HB1	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:HG21	1:B:302:LYS:NZ	1.98	0.77
1:A:456:MET:O	1:A:460:THR:HG23	1.85	0.77
1:A:226:ASN:C	1:A:226:ASN:HD22	1.94	0.75
1:C:185:LEU:O	1:C:445:LYS:HE3	1.87	0.74
1:A:271:VAL:HG13	1:A:309:PRO:HD3	1.68	0.73
1:A:238:PHE:HE1	1:A:240:LEU:HD11	1.54	0.72
1:A:437[A]:GLN:OE1	5:A:2170:HOH:O	2.07	0.72
1:D:373:ALA:O	1:D:374:ASN:HB2	1.90	0.71
1:C:407:GLU:O	1:C:411[A]:SER:HB2	1.90	0.71
1:B:138[B]:ARG:HH11	1:B:138[B]:ARG:HG2	1.54	0.71
1:C:325[B]:HIS:HD2	5:C:2128:HOH:O	1.73	0.71
1:D:87:LYS:HE2	5:D:2070:HOH:O	1.90	0.70
1:A:262[B]:TRP:HE3	1:A:295:LEU:HD12	1.56	0.70
1:C:136:LEU:O	1:C:140:GLU:HG3	1.92	0.69
1:B:241:TYR:CE1	1:B:464:PRO:HD2	2.28	0.68
1:A:455:TYR:C	1:A:455:TYR:CD1	2.70	0.68
1:D:52:VAL:CG2	1:D:456:MET:HE2	2.23	0.68
1:D:373:ALA:HB2	1:D:386:ILE:HD13	1.76	0.66
1:B:240:LEU:HD22	1:B:463:ILE:HG21	1.78	0.66
1:A:262[B]:TRP:HE3	1:A:295:LEU:CD1	2.09	0.66
1:A:237:GLN:HA	1:A:245:TYR:O	1.95	0.65
1:C:455:TYR:CZ	1:C:459:LEU:HD11	2.32	0.64
1:B:224:PRO:HG3	1:B:229:LEU:HD21	1.80	0.63
1:A:238:PHE:CE1	1:A:240:LEU:HD11	2.34	0.62
1:C:253:LEU:O	1:C:254:CYS:HB2	2.00	0.61
1:D:373:ALA:HB2	1:D:386:ILE:CD1	2.31	0.61
1:D:262[B]:TRP:HE3	1:D:295:LEU:HD12	1.67	0.60
1:A:52:VAL:CG2	1:A:456:MET:HE2	2.33	0.59
1:A:262[B]:TRP:CE3	1:A:295:LEU:HD12	2.36	0.59
1:B:434:SER:O	1:B:437:GLN:HG2	2.02	0.59
1:A:366:MET:CE	3:A:511:ACY:CH3	2.58	0.58
1:B:225:LEU:HD12	5:B:2074:HOH:O	2.03	0.58
1:D:367:ASP:O	1:D:371[B]:LYS:HG2	2.03	0.58
1:C:262[B]:TRP:CE3	1:C:295:LEU:HA	2.38	0.58
1:C:242:GLY:H	1:C:465:ALA:HA	1.66	0.58
1:D:437[A]:GLN:CD	5:D:2216:HOH:O	2.46	0.58
1:C:460:THR:OG1	1:C:462:MET:HG3	2.05	0.57
1:C:49:TYR:CZ	1:C:117:PRO:HD2	2.39	0.56
1:D:66:LYS:HE3	1:D:81:LEU:HD13	1.86	0.56
1:B:407:GLU:HG3	2:B:504:CL:CL	2.42	0.56
1:D:81:LEU:HD11	1:D:115[A]:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437[A]:GLN:OE1	5:D:2216:HOH:O	2.18	0.56
1:B:125:PRO:HA	1:B:162:ASP:HB3	1.87	0.55
5:C:2144:HOH:O	1:D:333:ASN:HB3	2.05	0.55
1:D:97:LYS:HD2	1:D:100:GLU:OE1	2.06	0.55
1:A:226:ASN:C	1:A:226:ASN:ND2	2.62	0.55
1:B:242:GLY:N	1:B:465:ALA:O	2.34	0.55
1:A:366:MET:HE1	3:A:511:ACY:CH3	2.34	0.54
1:D:372:MET:HE1	1:D:390:PHE:CD1	2.42	0.54
1:B:224:PRO:CG	1:B:229:LEU:HD21	2.37	0.54
1:D:87:LYS:CE	5:D:2070:HOH:O	2.53	0.54
1:B:138[B]:ARG:HH11	1:B:138[B]:ARG:CG	2.19	0.53
1:C:262[B]:TRP:CE3	1:C:295:LEU:HD12	2.27	0.53
1:A:67:TRP:HB3	1:A:78:VAL:HA	1.90	0.53
1:A:226:ASN:HD22	1:A:227:SER:N	2.06	0.53
1:B:157:LYS:HG3	1:B:163:PHE:CG	2.45	0.52
1:A:366:MET:HG3	1:A:370:LYS:HE2	1.92	0.52
1:A:445:LYS:O	1:A:446:ASP:HB2	2.08	0.52
1:B:275:GLY:O	1:B:276:ILE:HD13	2.10	0.52
1:D:84:CYS:HB2	1:D:111[A]:MET:HE2	1.93	0.51
1:B:128:LEU:HD13	1:B:152:VAL:HG11	1.93	0.51
1:D:321:TYR:HB3	1:D:388:LYS:HG3	1.93	0.51
1:B:232:PRO:HA	1:B:235:SER:HB3	1.93	0.51
1:B:373:ALA:HB2	1:B:386:ILE:CD1	2.41	0.51
1:D:365:VAL:HG11	1:D:420[A]:ILE:HD12	1.93	0.51
1:A:253:LEU:O	1:A:254:CYS:HB2	2.11	0.51
1:A:284:PRO:HD3	1:A:319:GLY:HA3	1.93	0.50
1:B:461:ASN:HA	5:B:2159:HOH:O	2.10	0.50
1:B:269:ILE:O	1:B:306:LYS:HE2	2.11	0.50
1:C:139:MET:O	1:D:227:SER:HA	2.11	0.50
1:D:434:SER:HA	1:D:437[A]:GLN:OE1	2.11	0.50
1:D:262[B]:TRP:HE3	1:D:295:LEU:CD1	2.24	0.50
1:C:321:TYR:HB2	1:C:388:LYS:HA	1.94	0.50
1:C:48:LYS:N	1:C:67:TRP:O	2.40	0.49
1:B:47:VAL:O	1:B:120:LYS:NZ	2.45	0.49
1:D:373:ALA:O	1:D:374:ASN:CB	2.61	0.49
1:A:230:GLU:OE2	1:A:340:SER:OG	2.28	0.48
1:B:253:LEU:O	1:B:254:CYS:HB2	2.13	0.48
1:A:228:THR:CG2	1:B:302:LYS:NZ	2.73	0.48
1:A:52:VAL:HG23	1:A:456:MET:CE	2.43	0.48
1:C:126:VAL:HG23	1:C:161:PHE:HB3	1.94	0.48
1:B:287[A]:LYS:HG3	5:B:2096:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:HB2	1:A:93:LYS:HG3	1.96	0.47
1:C:262[B]:TRP:CZ3	1:C:295:LEU:HA	2.49	0.47
1:C:325[B]:HIS:HE1	5:C:2134:HOH:O	1.98	0.47
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.29	0.47
1:D:262[B]:TRP:CE3	1:D:295:LEU:HA	2.50	0.47
1:D:241:TYR:CD1	1:D:241:TYR:N	2.83	0.47
1:A:91:ILE:HG21	1:A:91:ILE:HD13	1.59	0.47
1:A:321:TYR:HB2	1:A:388:LYS:HA	1.98	0.46
1:A:239:ARG:HA	1:A:243:THR:O	2.15	0.46
1:C:455:TYR:CE1	1:C:459:LEU:HD11	2.51	0.46
1:C:49:TYR:OH	1:C:117:PRO:CD	2.64	0.46
1:C:139:MET:HE3	1:C:139:MET:HB2	1.77	0.46
1:B:321:TYR:HB3	1:B:388:LYS:HG3	1.97	0.46
1:C:49:TYR:CE2	1:C:117:PRO:HD2	2.51	0.45
1:C:283:TYR:HB3	1:C:393:LYS:O	2.17	0.45
1:A:121:GLN:HG2	1:A:161:PHE:CE1	2.52	0.45
1:C:123:GLN:H	1:C:123:GLN:HG3	1.57	0.45
1:B:76:GLY:HA2	1:B:184:TYR:CE1	2.52	0.45
1:A:336:HIS:O	1:A:346:GLY:HA2	2.17	0.45
1:C:47:VAL:HA	1:C:68:PRO:HA	1.99	0.45
1:C:456:MET:HB3	1:C:456:MET:HE2	1.56	0.45
1:B:321:TYR:HB2	1:B:388:LYS:HA	1.99	0.45
1:A:243:THR:HG22	1:A:244:ASP:O	2.16	0.45
1:C:117:PRO:O	1:C:120:LYS:HB2	2.17	0.44
1:A:154:ARG:NH2	5:A:2044:HOH:O	2.50	0.44
1:D:221:THR:HG23	1:D:249:THR:HB	1.99	0.44
1:D:283:TYR:HB3	1:D:393:LYS:O	2.18	0.44
1:A:441:MET:SD	1:A:444:ILE:HD11	2.58	0.44
1:B:240:LEU:HD22	1:B:463:ILE:CG2	2.47	0.44
1:B:341:GLN:HG2	1:B:349:LEU:O	2.17	0.44
1:D:325:HIS:HD2	1:D:422:SER:OG	1.99	0.44
1:A:229:LEU:CB	1:B:139:MET:HE1	2.39	0.44
1:B:332:PHE:CD1	3:B:512:ACY:H3	2.53	0.44
1:D:374:ASN:O	1:D:375:ASP:HB3	2.18	0.44
1:B:54:ASP:HB2	1:B:452:THR:HG21	2.00	0.44
1:A:228:THR:CG2	1:B:302:LYS:HZ2	2.31	0.43
1:C:239:ARG:HG2	1:C:465:ALA:CB	2.43	0.43
1:D:444:ILE:O	1:D:445:LYS:HB2	2.19	0.43
1:A:187:GLY:O	1:A:190:LYS:HE2	2.18	0.43
1:A:132:ALA:HB3	1:A:216:ALA:HB3	2.00	0.43
1:B:157:LYS:HG3	1:B:163:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:CG	1:A:246:THR:OG1	2.67	0.43
1:B:389:ASN:ND2	5:B:2137[B]:HOH:O	2.50	0.43
1:C:102:ALA:HB3	5:C:2029:HOH:O	2.18	0.43
1:C:153:SER:O	1:C:157:LYS:HG3	2.19	0.43
1:B:177:TYR:CE2	1:B:455:TYR:HD1	2.35	0.43
1:B:257:LYS:HE2	1:B:364[B]:PHE:CZ	2.55	0.42
1:C:110:LYS:O	1:C:114:GLU:HG2	2.20	0.42
1:C:368:PHE:CE2	1:C:372:MET:CE	3.03	0.42
1:C:371:LYS:HD2	1:C:371:LYS:HA	1.58	0.42
1:C:361:ALA:HA	1:C:364:PHE:CD2	2.54	0.42
1:C:49:TYR:OH	1:C:117:PRO:HD2	2.19	0.42
1:A:302:LYS:HB3	1:A:302:LYS:HE2	1.63	0.42
1:B:167:LYS:HE2	1:B:169:ILE:HG22	2.02	0.42
1:D:287:LYS:HA	1:D:315:VAL:O	2.19	0.42
1:A:264[A]:LYS:HD2	1:A:327[A]:SER:OG	2.20	0.42
1:C:128:LEU:HD13	1:C:152:VAL:HG11	2.02	0.42
1:D:57:SER:HA	2:D:503:CL:CL	2.57	0.42
1:A:307:LYS:HG2	1:A:308:LEU:N	2.35	0.41
1:D:402:TYR:HA	2:D:505:CL:CL	2.57	0.41
1:A:237:GLN:HG2	1:A:246:THR:OG1	2.21	0.41
1:C:154:ARG:HE	1:C:154:ARG:HB2	1.39	0.41
1:A:437[B]:GLN:HA	1:A:437[B]:GLN:NE2	2.35	0.41
1:B:332:PHE:CE1	3:B:512:ACY:H3	2.55	0.41
1:C:271:VAL:HG13	1:C:309:PRO:HD3	2.02	0.41
1:B:456[B]:MET:HE3	1:B:456[B]:MET:HB2	1.82	0.41
1:C:77:VAL:HG23	1:C:78:VAL:N	2.36	0.41
1:D:62:LEU:C	1:D:62:LEU:HD23	2.46	0.41
1:D:368:PHE:CE2	1:D:372:MET:HE3	2.56	0.41
1:A:155:SER:O	1:A:158:SER:OG	2.35	0.41
1:B:248:TYR:CD1	1:B:248:TYR:C	2.99	0.41
1:D:396:GLU:HG2	2:D:508:CL:CL	2.57	0.41
1:C:308:LEU:HA	1:C:309:PRO:HD3	1.85	0.40
1:A:143:GLN:NE2	1:A:147:GLU:OE2	2.54	0.40
1:B:50:GLY:HA3	1:B:456[B]:MET:HE1	2.03	0.40
1:B:248:TYR:CE2	1:B:350:PRO:HD3	2.56	0.40
1:B:48:LYS:HB3	1:B:48:LYS:HE3	1.57	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	403/452 (89%)	389 (96%)	14 (4%)	0	100	100
1	B	402/452 (89%)	384 (96%)	15 (4%)	3 (1%)	18	7
1	C	390/452 (86%)	375 (96%)	15 (4%)	0	100	100
1	D	403/452 (89%)	382 (95%)	20 (5%)	1 (0%)	43	28
All	All	1598/1808 (88%)	1530 (96%)	64 (4%)	4 (0%)	36	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	SER
1	B	319	GLY
1	B	461	ASN
1	D	343	ALA

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	345/389 (89%)	327 (95%)	18 (5%)	21	7
1	B	349/389 (90%)	337 (97%)	12 (3%)	32	16
1	C	340/389 (87%)	326 (96%)	14 (4%)	27	11
1	D	348/389 (90%)	336 (97%)	12 (3%)	32	16
All	All	1382/1556 (89%)	1326 (96%)	56 (4%)	28	11

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	74	ASP
1	A	143	GLN
1	A	190	LYS
1	A	226	ASN
1	A	227	SER
1	A	237	GLN
1	A	240	LEU
1	A	264[A]	LYS
1	A	264[B]	LYS
1	A	272	SER
1	A	288	LYS
1	A	293	SER
1	A	364	PHE
1	A	412	GLU
1	A	446	ASP
1	A	458	ASN
1	A	462	MET
1	B	47	VAL
1	B	48	LYS
1	B	68	PRO
1	B	98	THR
1	B	119	SER
1	B	139	MET
1	B	188	ARG
1	B	206	SER
1	B	229	LEU
1	B	306	LYS
1	B	353	GLN
1	B	461	ASN
1	C	77	VAL
1	C	93	LYS
1	C	123	GLN
1	C	154	ARG
1	C	158	SER
1	C	167	LYS
1	C	206	SER
1	C	364	PHE
1	C	371	LYS
1	C	388	LYS
1	C	411[A]	SER
1	C	411[B]	SER

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Mol	Chain	Res	Type
1	C	456	MET
1	C	463	ILE
1	D	87	LYS
1	D	93[A]	LYS
1	D	93[B]	LYS
1	D	206	SER
1	D	225	LEU
1	D	227	SER
1	D	241	TYR
1	D	293	SER
1	D	312	GLN
1	D	407	GLU
1	D	448	ASN
1	D	458	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	96	GLN
1	A	143	GLN
1	A	226	ASN
1	A	312	GLN
1	A	326	GLN
1	B	61	ASN
1	B	85	GLN
1	B	164	GLN
1	B	219	GLN
1	B	458	ASN
1	C	61	ASN
1	C	85	GLN
1	C	123	GLN
1	C	291	ASN
1	C	314	GLN
1	C	316	GLN
1	C	323	GLN
1	C	333	ASN
1	C	336	HIS
1	C	341	GLN
1	C	353	GLN
1	C	458	ASN
1	C	461	ASN

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Mol	Chain	Res	Type
1	D	61	ASN
1	D	96	GLN
1	D	123	GLN
1	D	164	GLN
1	D	323	GLN
1	D	325	HIS
1	D	326	GLN
1	D	336	HIS
1	D	341	GLN
1	D	353	GLN
1	D	458	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 39 ligands modelled in this entry, 32 are monoatomic - leaving 7 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	ACY	D	512	-	3,3,3	1.28	1 (33%)	3,3,3	0.71	0
3	ACY	A	511	-	3,3,3	1.30	0	3,3,3	2.08	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	D	511	-	3,3,3	0.86	0	3,3,3	1.14	0
3	ACY	B	512	-	3,3,3	1.10	0	3,3,3	1.59	1 (33%)
3	ACY	C	511	-	3,3,3	0.97	0	3,3,3	0.53	0
3	ACY	B	511	-	3,3,3	0.70	0	3,3,3	1.86	1 (33%)
3	ACY	C	512	-	3,3,3	0.90	0	3,3,3	1.05	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	512	ACY	OXT-C	-2.07	1.21	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	511	ACY	OXT-C-CH3	2.78	126.70	115.05
3	B	511	ACY	OXT-C-CH3	2.60	125.95	115.05
3	B	512	ACY	OXT-C-CH3	2.22	124.38	115.05
3	A	511	ACY	OXT-C-O	-2.15	114.05	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	511	ACY	6	0
3	B	512	ACY	2	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	399/452 (88%)	-0.04	13 (3%) 49 53	19, 40, 74, 119	10 (2%)
1	B	400/452 (88%)	0.03	10 (2%) 58 62	21, 45, 75, 103	8 (2%)
1	C	393/452 (86%)	0.02	9 (2%) 61 65	21, 44, 80, 108	5 (1%)
1	D	397/452 (87%)	-0.17	9 (2%) 61 65	18, 37, 69, 99	12 (3%)
All	All	1589/1808 (87%)	-0.04	41 (2%) 57 61	18, 41, 76, 119	35 (2%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	ALA	5.5
1	D	205	GLY	4.7
1	D	463	ILE	4.7
1	C	190	LYS	4.5
1	B	76	GLY	3.9
1	B	205	GLY	3.9
1	A	373	ALA	3.6
1	B	190	LYS	3.6
1	C	373	ALA	3.5
1	A	122[A]	HIS	3.4
1	B	47	VAL	3.2
1	A	433	THR	3.2
1	B	364[A]	PHE	3.0
1	A	73	ASN	3.0
1	A	76	GLY	2.9
1	D	377	VAL	2.8
1	D	433	THR	2.7
1	A	241	TYR	2.7
1	B	433	THR	2.6
1	A	245	TYR	2.6
1	C	464	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	205	GLY	2.5
1	C	47	VAL	2.4
1	A	461	ASN	2.4
1	D	376	SER	2.4
1	D	462	MET	2.4
1	A	190	LYS	2.3
1	C	77	VAL	2.3
1	B	461	ASN	2.3
1	B	77	VAL	2.3
1	B	431	THR	2.2
1	D	374	ASN	2.2
1	A	459	LEU	2.2
1	D	190	LYS	2.2
1	A	75	THR	2.2
1	D	373	ALA	2.2
1	C	238	PHE	2.2
1	B	225	LEU	2.1
1	A	238	PHE	2.0
1	A	332	PHE	2.0
1	C	307	LYS	2.0

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(Å ²)	Q<0.9
3	ACY	A	511	4/4	0.81	0.13	36,46,48,48	0
3	ACY	B	512	4/4	0.85	0.14	47,50,57,58	0
4	NA	C	521	1/1	0.90	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	B	521	1/1	0.91	0.09	51,51,51,51	0
2	CL	A	506	1/1	0.93	0.21	62,62,62,62	0
2	CL	D	508	1/1	0.94	0.12	50,50,50,50	0
3	ACY	B	511	4/4	0.95	0.08	37,42,43,43	0
2	CL	D	504	1/1	0.95	0.08	53,53,53,53	0
2	CL	B	504	1/1	0.96	0.10	56,56,56,56	0
3	ACY	C	512	4/4	0.96	0.09	28,32,33,34	0
4	NA	D	522	1/1	0.96	0.08	52,52,52,52	0
2	CL	C	502	1/1	0.97	0.10	44,44,44,44	0
2	CL	C	503	1/1	0.97	0.08	42,42,42,42	0
2	CL	C	504	1/1	0.97	0.19	55,55,55,55	0
3	ACY	C	511	4/4	0.97	0.06	30,32,33,34	0
2	CL	B	505	1/1	0.97	0.07	46,46,46,46	0
3	ACY	D	511	4/4	0.97	0.06	36,39,39,40	0
2	CL	D	507	1/1	0.97	0.07	40,40,40,40	0
2	CL	B	506	1/1	0.97	0.14	53,53,53,53	0
2	CL	D	509	1/1	0.97	0.08	42,42,42,42	1
4	NA	D	521	1/1	0.97	0.04	35,35,35,35	0
2	CL	C	506	1/1	0.98	0.04	34,34,34,34	0
3	ACY	D	512	4/4	0.98	0.10	31,33,35,42	0
2	CL	A	505	1/1	0.98	0.06	41,41,41,41	0
2	CL	A	504	1/1	0.98	0.06	46,46,46,46	0
2	CL	B	503	1/1	0.98	0.08	44,44,44,44	0
2	CL	C	505	1/1	0.98	0.06	44,44,44,44	0
2	CL	A	503	1/1	0.99	0.04	35,35,35,35	0
2	CL	B	501	1/1	0.99	0.04	35,35,35,35	0
2	CL	D	501	1/1	0.99	0.02	31,31,31,31	0
2	CL	D	502	1/1	0.99	0.08	38,38,38,38	0
2	CL	D	503	1/1	0.99	0.05	36,36,36,36	0
2	CL	C	501	1/1	0.99	0.04	36,36,36,36	0
2	CL	D	505	1/1	0.99	0.08	43,43,43,43	0
2	CL	D	506	1/1	0.99	0.09	43,43,43,43	0
2	CL	B	502	1/1	0.99	0.06	43,43,43,43	0
4	NA	C	522	1/1	0.99	0.02	29,29,29,29	0
2	CL	A	501	1/1	0.99	0.07	34,34,34,34	0
2	CL	A	502	1/1	0.99	0.07	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.