wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 12:18 PM EDT

PDB ID	:	3ZX3
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

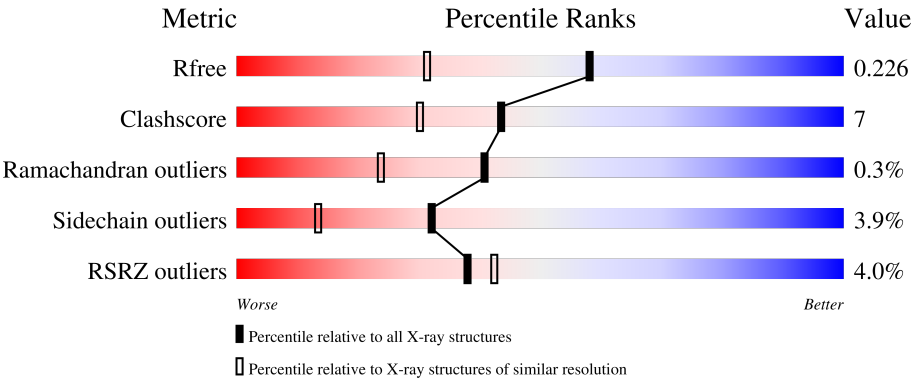
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	4% 73% 13% • 12%
1	B	452	3% 73% 14% • 12%
1	C	452	5% 72% 13% • 13%
1	D	452	3% 75% 12% • 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 (i)

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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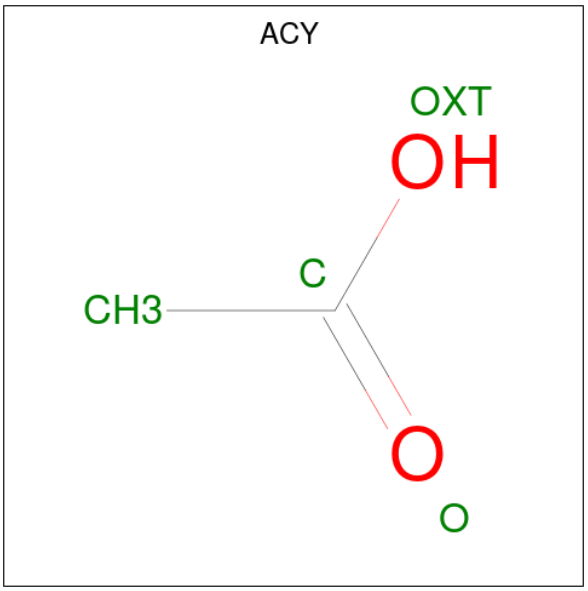
Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P97687
D	21	HIS	-	expression tag	UNP P97687
D	22	HIS	-	expression tag	UNP P97687
D	23	VAL	-	expression tag	UNP P97687
D	24	GLY	-	expression tag	UNP P97687
D	25	THR	-	expression tag	UNP P97687
D	26	GLY	-	expression tag	UNP P97687
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 (three-letter code: 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 (three-letter code: ACY) (formula: $C_2H_4O_2$).



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 (three-letter code: 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.

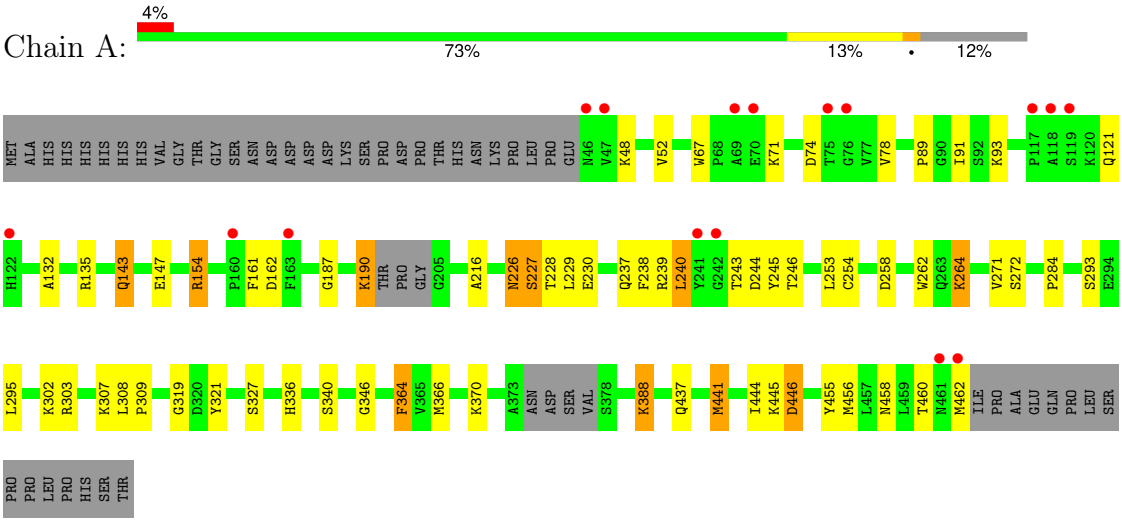
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	207	Total O 210 210	0	3
5	B	159	Total O 161 161	0	2
5	C	205	Total O 206 206	0	1
5	D	245	Total O 245 245	0	0

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.

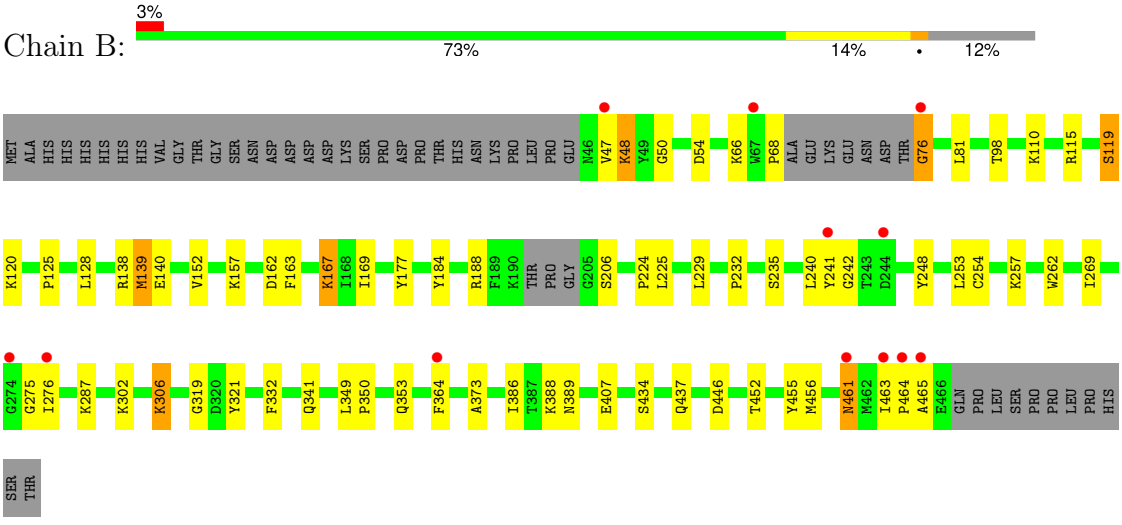
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain A:



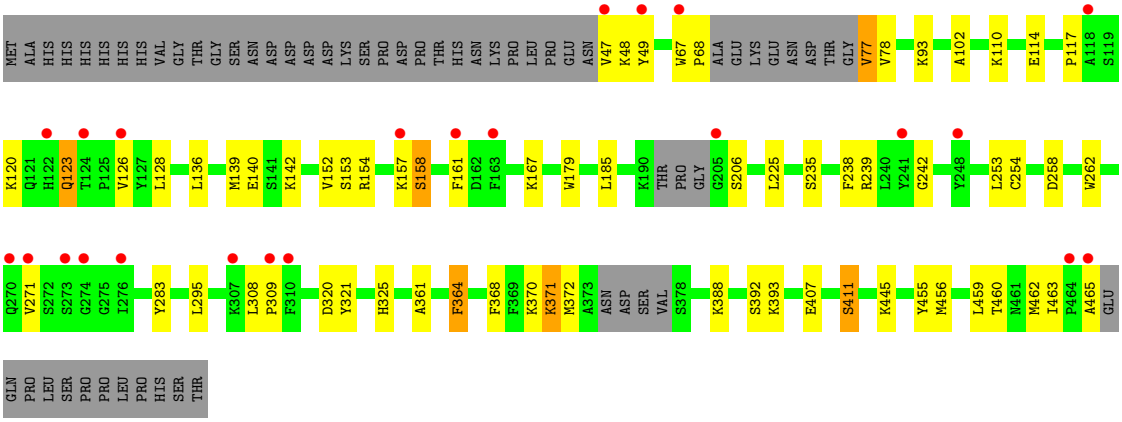
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain B:



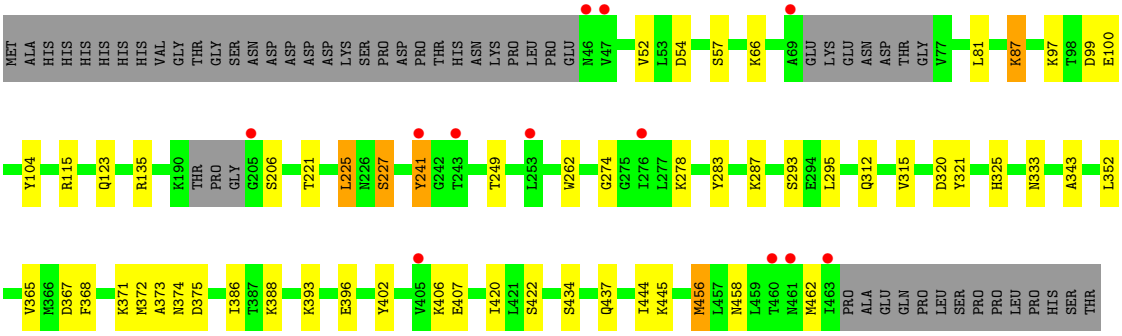
• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain C:



• Molecule 1: ECTONUCLEOSIDE TRIPHOSPHATE DIPHOSPHOHYDROLASE 1

Chain D:



4 Data and refinement statistics (i)

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 41.43 – 1.70	Depositor EDS
% Data completeness (in resolution range)	72.6 (146.62-1.70) 72.6 (41.43-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.233 0.170 , 0.226	Depositor DCC
R_{free} test set	1139 reflections (0.75%)	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 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.03	0/3316	1.01	8/4482 (0.2%)
1	B	0.99	2/3314 (0.1%)	1.00	2/4479 (0.0%)
1	C	1.01	3/3235 (0.1%)	1.01	4/4374 (0.1%)
1	D	1.05	1/3316 (0.0%)	1.04	9/4482 (0.2%)
All	All	1.02	6/13181 (0.0%)	1.02	23/17817 (0.1%)

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	SER	CB-OG	-6.92	1.33	1.42
1	B	262	TRP	CD2-CE2	6.84	1.49	1.41
1	C	179	TRP	CD2-CE2	5.85	1.48	1.41
1	B	140	GLU	CG-CD	5.78	1.60	1.51
1	D	99	ASP	CB-CG	5.65	1.63	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	135	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	C	320	ASP	CB-CG-OD1	8.18	125.66	118.30
1	D	99	ASP	CB-CG-OD1	7.47	125.03	118.30
1	D	406	LYS	CD-CE-NZ	-7.13	95.31	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	462	MET	CB-CG-SD	6.89	133.08	112.40

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
1	B	3209	0	3131	49	0
1	C	3137	0	3060	40	0
1	D	3196	0	3145	36	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	5	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	3	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	170	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.

The worst 5 of 170 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:D:52:VAL:HG23	1:D:456:MET:HE3	1.36	1.06
1:D:52:VAL:HG23	1:D:456:MET:CE	1.88	1.03
1:A:366:MET:HE2	3:A:511:ACY:H1	1.06	1.03
1:A:229:LEU:CB	1:B:139:MET:CE	2.37	1.01

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	403/452 (89%)	389 (96%)	14 (4%)	0	100 100
1	B	402/452 (89%)	384 (96%)	15 (4%)	3 (1%)	22 8
1	C	390/452 (86%)	375 (96%)	15 (4%)	0	100 100
1	D	403/452 (89%)	382 (95%)	20 (5%)	1 (0%)	47 30
All	All	1598/1808 (88%)	1530 (96%)	64 (4%)	4 (0%)	41 24

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 (i)

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%)	329 (95%)	16 (5%)	27	10
1	B	349/389 (90%)	336 (96%)	13 (4%)	34	15
1	C	340/389 (87%)	326 (96%)	14 (4%)	30	12
1	D	348/389 (90%)	337 (97%)	11 (3%)	39	20
All	All	1382/1556 (89%)	1328 (96%)	54 (4%)	32	13

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	446	ASP
1	C	206	SER
1	D	278	LYS
1	C	77	VAL
1	C	142	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	458	ASN
1	D	323	GLN
1	D	123	GLN
1	D	325	HIS
1	B	439	HIS

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 monosaccharides 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	511	-	3,3,3	0.86	0	3,3,3	1.14	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
3	ACY	A	511	-	3,3,3	1.30	0	3,3,3	2.08	2 (66%)
3	ACY	D	512	-	3,3,3	1.28	1 (33%)	3,3,3	0.71	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

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(^{o})	Ideal(^{o})
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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	511	ACY	5	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, 95^{th} 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%)	-0.19	16 (4%)	38	42	27, 41, 74, 119	0
1	B	400/452 (88%)	-0.17	12 (3%)	50	54	28, 45, 75, 103	0
1	C	393/452 (86%)	0.21	23 (5%)	22	24	25, 44, 80, 108	0
1	D	397/452 (87%)	-0.05	12 (3%)	50	54	25, 38, 69, 99	0
All	All	1589/1808 (87%)	-0.05	63 (3%)	38	42	25, 42, 76, 119	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	VAL	6.9
1	D	463	ILE	6.1
1	D	241	TYR	5.5
1	A	47	VAL	5.2
1	C	465	ALA	5.0

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 monosaccharides 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, 95^{th} 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	0.86	0.14	36,46,48,48	0
4	NA	C	521	1/1	0.88	0.12	52,52,52,52	0
3	ACY	B	512	4/4	0.90	0.24	47,50,57,58	0
2	CL	D	508	1/1	0.94	0.06	50,50,50,50	0
4	NA	B	521	1/1	0.95	0.07	51,51,51,51	0
2	CL	B	504	1/1	0.95	0.06	56,56,56,56	0
2	CL	C	504	1/1	0.96	0.04	55,55,55,55	0
2	CL	A	506	1/1	0.96	0.06	62,62,62,62	0
2	CL	C	503	1/1	0.97	0.07	42,42,42,42	0
3	ACY	C	512	4/4	0.97	0.06	28,32,33,34	0
2	CL	D	504	1/1	0.97	0.06	53,53,53,53	0
3	ACY	B	511	4/4	0.97	0.09	37,42,43,43	0
2	CL	B	505	1/1	0.98	0.07	46,46,46,46	0
2	CL	D	509	1/1	0.98	0.07	42,42,42,42	1
2	CL	B	506	1/1	0.98	0.08	53,53,53,53	0
2	CL	C	502	1/1	0.98	0.05	44,44,44,44	0
2	CL	A	502	1/1	0.98	0.04	42,42,42,42	0
3	ACY	C	511	4/4	0.98	0.06	30,32,33,34	0
2	CL	B	503	1/1	0.98	0.04	44,44,44,44	0
2	CL	A	504	1/1	0.98	0.06	46,46,46,46	0
2	CL	D	507	1/1	0.98	0.08	40,40,40,40	0
4	NA	D	522	1/1	0.98	0.11	52,52,52,52	0
4	NA	D	521	1/1	0.98	0.05	35,35,35,35	0
2	CL	C	506	1/1	0.99	0.14	34,34,34,34	0
2	CL	D	503	1/1	0.99	0.06	36,36,36,36	0
2	CL	C	501	1/1	0.99	0.09	36,36,36,36	0
2	CL	D	505	1/1	0.99	0.06	43,43,43,43	0
3	ACY	D	511	4/4	0.99	0.05	36,39,39,40	0
3	ACY	D	512	4/4	0.99	0.10	31,33,35,42	0
2	CL	A	501	1/1	0.99	0.06	34,34,34,34	0
2	CL	B	502	1/1	0.99	0.06	43,43,43,43	0
4	NA	C	522	1/1	0.99	0.11	29,29,29,29	0
2	CL	A	505	1/1	0.99	0.08	41,41,41,41	0
2	CL	C	505	1/1	0.99	0.07	44,44,44,44	0
2	CL	D	502	1/1	1.00	0.05	38,38,38,38	0
2	CL	B	501	1/1	1.00	0.08	35,35,35,35	0
2	CL	A	503	1/1	1.00	0.06	35,35,35,35	0
2	CL	D	501	1/1	1.00	0.12	31,31,31,31	0
2	CL	D	506	1/1	1.00	0.07	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.