



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:23 PM BST

PDB ID : 4B6Z
Title : Crystal structure of metallo-carboxypeptidase from Burkholderia cenocepacia
Authors : Rimsa, V.; Eadsforth, T.C.; Joosten, R.P.; Hunter, W.N.
Deposited on : 2012-08-16
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

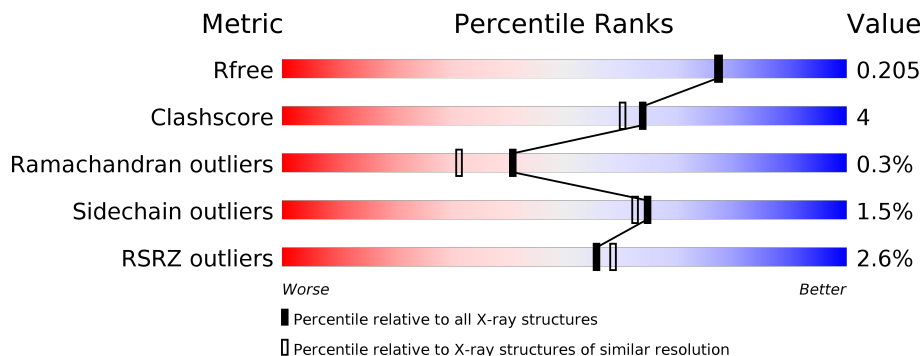
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	405	<p>3% 85% 9% 6%</p>
1	B	405	<p>3% 84% 10% 6%</p>
1	C	405	<p>2% 86% 6% 7%</p>
1	D	405	<p>2% 85% 9% 6%</p>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	B	1390	-	-	X	-
4	ACT	C	1390	-	-	X	-
7	PEG	D	1390	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 13485 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 FAMILY M14 UNASSIGNED PEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	Total 3096	C 1962	N 526	O 590	S 18	0	14	0
1	B	382	Total 3083	C 1958	N 521	O 585	S 19	0	15	0
1	C	376	Total 3045	C 1934	N 522	O 573	S 16	0	13	0
1	D	380	Total 3100	C 1969	N 534	O 580	S 17	0	13	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP B4EEQ5
A	-19	GLY	-	expression tag	UNP B4EEQ5
A	-18	SER	-	expression tag	UNP B4EEQ5
A	-17	SER	-	expression tag	UNP B4EEQ5
A	-16	HIS	-	expression tag	UNP B4EEQ5
A	-15	HIS	-	expression tag	UNP B4EEQ5
A	-14	HIS	-	expression tag	UNP B4EEQ5
A	-13	HIS	-	expression tag	UNP B4EEQ5
A	-12	HIS	-	expression tag	UNP B4EEQ5
A	-11	HIS	-	expression tag	UNP B4EEQ5
A	-10	SER	-	expression tag	UNP B4EEQ5
A	-9	SER	-	expression tag	UNP B4EEQ5
A	-8	GLY	-	expression tag	UNP B4EEQ5
A	-7	GLU	-	expression tag	UNP B4EEQ5
A	-6	ASN	-	expression tag	UNP B4EEQ5
A	-5	LEU	-	expression tag	UNP B4EEQ5
A	-4	TYR	-	expression tag	UNP B4EEQ5
A	-3	PHE	-	expression tag	UNP B4EEQ5
A	-2	GLN	-	expression tag	UNP B4EEQ5
A	-1	GLY	-	expression tag	UNP B4EEQ5
A	0	HIS	-	expression tag	UNP B4EEQ5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASP	GLU	engineered mutation	UNP B4EEQ5
A	21	SER	ARG	engineered mutation	UNP B4EEQ5
A	73	SER	HIS	engineered mutation	UNP B4EEQ5
A	158	GLY	ASP	engineered mutation	UNP B4EEQ5
A	210	HIS	TYR	engineered mutation	UNP B4EEQ5
A	296	THR	ALA	engineered mutation	UNP B4EEQ5
A	300	GLU	ASP	engineered mutation	UNP B4EEQ5
B	-20	MET	-	expression tag	UNP B4EEQ5
B	-19	GLY	-	expression tag	UNP B4EEQ5
B	-18	SER	-	expression tag	UNP B4EEQ5
B	-17	SER	-	expression tag	UNP B4EEQ5
B	-16	HIS	-	expression tag	UNP B4EEQ5
B	-15	HIS	-	expression tag	UNP B4EEQ5
B	-14	HIS	-	expression tag	UNP B4EEQ5
B	-13	HIS	-	expression tag	UNP B4EEQ5
B	-12	HIS	-	expression tag	UNP B4EEQ5
B	-11	HIS	-	expression tag	UNP B4EEQ5
B	-10	SER	-	expression tag	UNP B4EEQ5
B	-9	SER	-	expression tag	UNP B4EEQ5
B	-8	GLY	-	expression tag	UNP B4EEQ5
B	-7	GLU	-	expression tag	UNP B4EEQ5
B	-6	ASN	-	expression tag	UNP B4EEQ5
B	-5	LEU	-	expression tag	UNP B4EEQ5
B	-4	TYR	-	expression tag	UNP B4EEQ5
B	-3	PHE	-	expression tag	UNP B4EEQ5
B	-2	GLN	-	expression tag	UNP B4EEQ5
B	-1	GLY	-	expression tag	UNP B4EEQ5
B	0	HIS	-	expression tag	UNP B4EEQ5
B	20	ASP	GLU	engineered mutation	UNP B4EEQ5
B	21	SER	ARG	engineered mutation	UNP B4EEQ5
B	73	SER	HIS	engineered mutation	UNP B4EEQ5
B	158	GLY	ASP	engineered mutation	UNP B4EEQ5
B	210	HIS	TYR	engineered mutation	UNP B4EEQ5
B	296	THR	ALA	engineered mutation	UNP B4EEQ5
B	300	GLU	ASP	engineered mutation	UNP B4EEQ5
C	-20	MET	-	expression tag	UNP B4EEQ5
C	-19	GLY	-	expression tag	UNP B4EEQ5
C	-18	SER	-	expression tag	UNP B4EEQ5
C	-17	SER	-	expression tag	UNP B4EEQ5
C	-16	HIS	-	expression tag	UNP B4EEQ5
C	-15	HIS	-	expression tag	UNP B4EEQ5
C	-14	HIS	-	expression tag	UNP B4EEQ5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP B4EEQ5
C	-12	HIS	-	expression tag	UNP B4EEQ5
C	-11	HIS	-	expression tag	UNP B4EEQ5
C	-10	SER	-	expression tag	UNP B4EEQ5
C	-9	SER	-	expression tag	UNP B4EEQ5
C	-8	GLY	-	expression tag	UNP B4EEQ5
C	-7	GLU	-	expression tag	UNP B4EEQ5
C	-6	ASN	-	expression tag	UNP B4EEQ5
C	-5	LEU	-	expression tag	UNP B4EEQ5
C	-4	TYR	-	expression tag	UNP B4EEQ5
C	-3	PHE	-	expression tag	UNP B4EEQ5
C	-2	GLN	-	expression tag	UNP B4EEQ5
C	-1	GLY	-	expression tag	UNP B4EEQ5
C	0	HIS	-	expression tag	UNP B4EEQ5
C	20	ASP	GLU	engineered mutation	UNP B4EEQ5
C	21	SER	ARG	engineered mutation	UNP B4EEQ5
C	73	SER	HIS	engineered mutation	UNP B4EEQ5
C	158	GLY	ASP	engineered mutation	UNP B4EEQ5
C	210	HIS	TYR	engineered mutation	UNP B4EEQ5
C	296	THR	ALA	engineered mutation	UNP B4EEQ5
C	300	GLU	ASP	engineered mutation	UNP B4EEQ5
D	-20	MET	-	expression tag	UNP B4EEQ5
D	-19	GLY	-	expression tag	UNP B4EEQ5
D	-18	SER	-	expression tag	UNP B4EEQ5
D	-17	SER	-	expression tag	UNP B4EEQ5
D	-16	HIS	-	expression tag	UNP B4EEQ5
D	-15	HIS	-	expression tag	UNP B4EEQ5
D	-14	HIS	-	expression tag	UNP B4EEQ5
D	-13	HIS	-	expression tag	UNP B4EEQ5
D	-12	HIS	-	expression tag	UNP B4EEQ5
D	-11	HIS	-	expression tag	UNP B4EEQ5
D	-10	SER	-	expression tag	UNP B4EEQ5
D	-9	SER	-	expression tag	UNP B4EEQ5
D	-8	GLY	-	expression tag	UNP B4EEQ5
D	-7	GLU	-	expression tag	UNP B4EEQ5
D	-6	ASN	-	expression tag	UNP B4EEQ5
D	-5	LEU	-	expression tag	UNP B4EEQ5
D	-4	TYR	-	expression tag	UNP B4EEQ5
D	-3	PHE	-	expression tag	UNP B4EEQ5
D	-2	GLN	-	expression tag	UNP B4EEQ5
D	-1	GLY	-	expression tag	UNP B4EEQ5
D	0	HIS	-	expression tag	UNP B4EEQ5

Continued on next page...

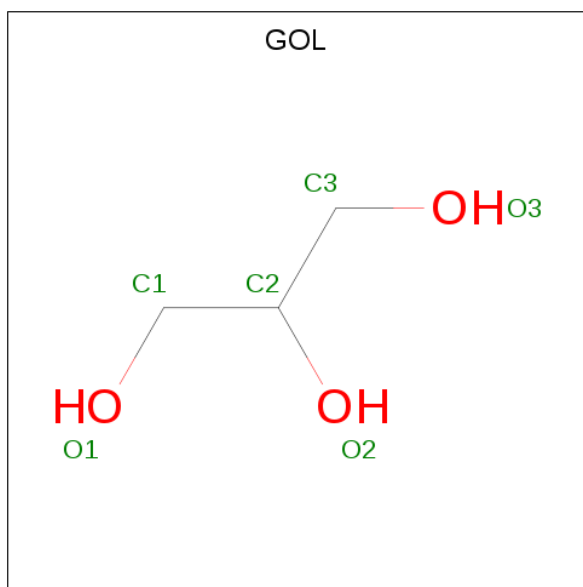
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	20	ASP	GLU	engineered mutation	UNP B4EEQ5
D	21	SER	ARG	engineered mutation	UNP B4EEQ5
D	73	SER	HIS	engineered mutation	UNP B4EEQ5
D	158	GLY	ASP	engineered mutation	UNP B4EEQ5
D	210	HIS	TYR	engineered mutation	UNP B4EEQ5
D	296	THR	ALA	engineered mutation	UNP B4EEQ5
D	300	GLU	ASP	engineered mutation	UNP B4EEQ5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



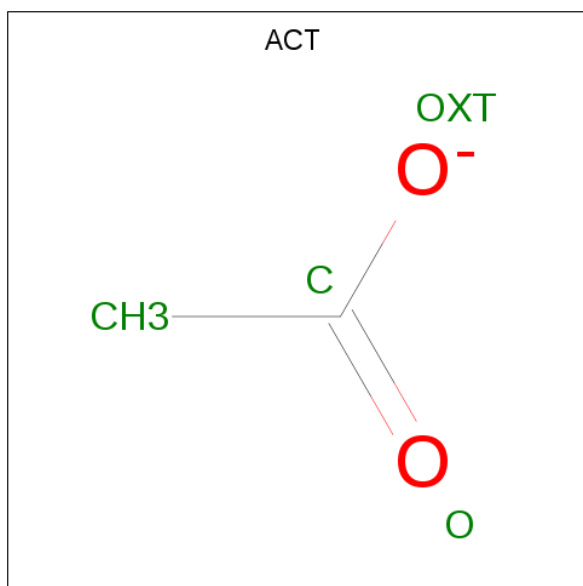
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



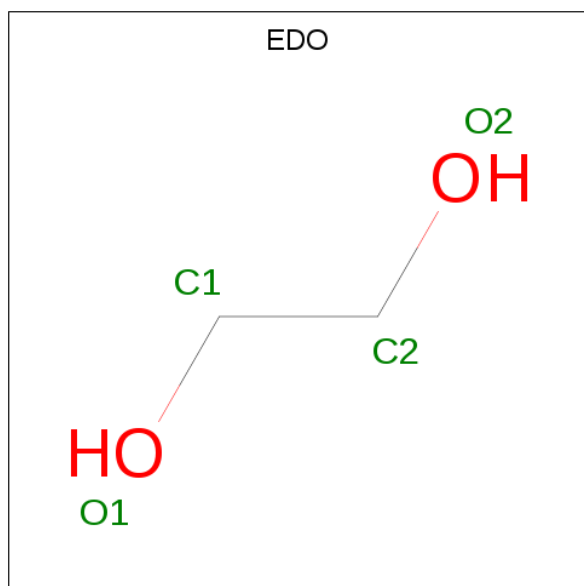
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

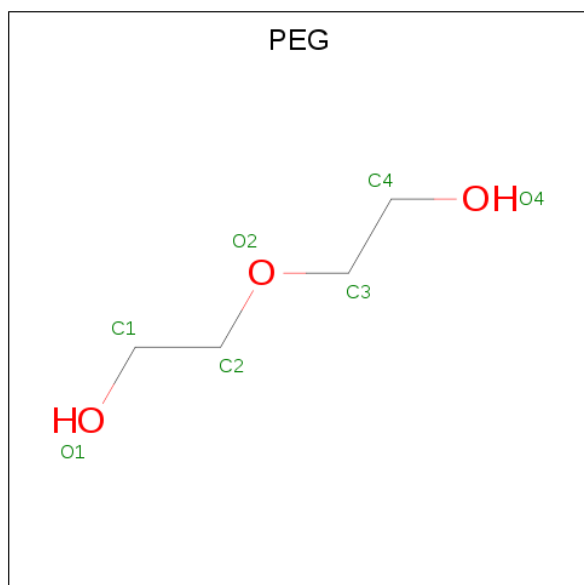
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 7 4 3	0	0

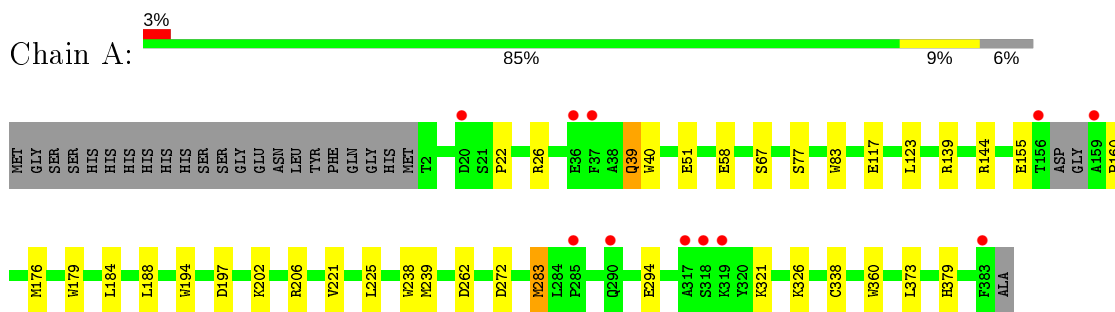
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	267	Total O 267 267	0	0
8	B	256	Total O 256 256	0	0
8	C	271	Total O 271 271	0	0
8	D	255	Total O 255 255	0	0

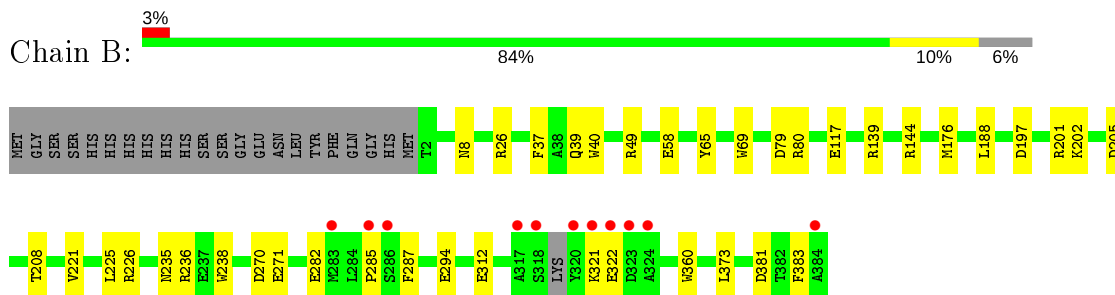
3 Residue-property plots [i](#)

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.

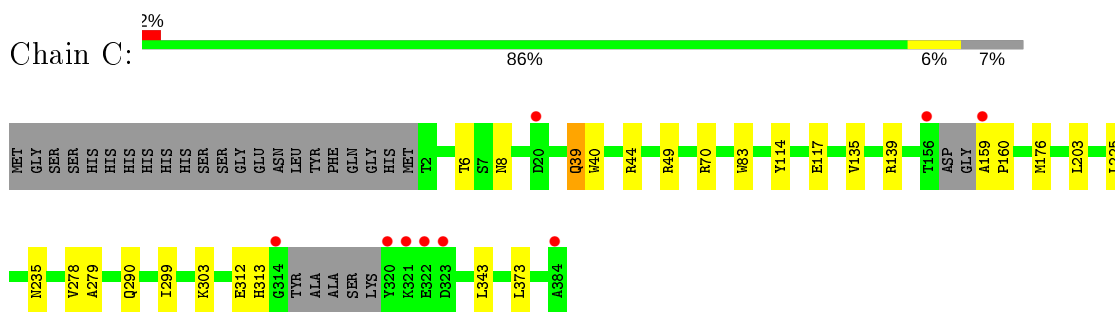
- Molecule 1: FAMILY M14 UNASSIGNED PEPTIDASE



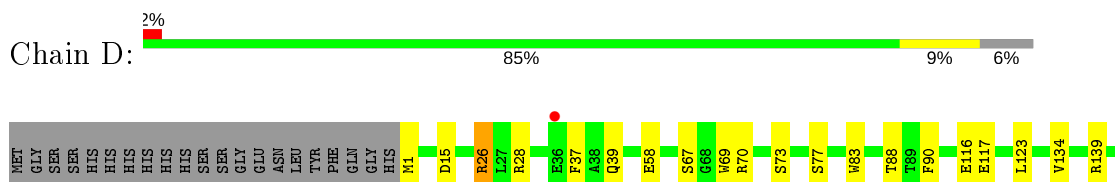
- Molecule 1: FAMILY M14 UNASSIGNED PEPTIDASE



- Molecule 1: FAMILY M14 UNASSIGNED PEPTIDASE



- Molecule 1: FAMILY M14 UNASSIGNED PEPTIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 85.95Å 289.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 38.24 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.90) 99.8 (38.24-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.205 0.165 , 0.205	Depositor DCC
R_{free} test set	6246 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13485	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GOL, ZN, CL, EDO, ACT, PEG

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	0.58	5/3186 (0.2%)	0.58	0/4326
1	B	0.59	4/3200 (0.1%)	0.61	0/4346
1	C	0.58	2/3148 (0.1%)	0.60	0/4271
1	D	0.58	3/3198 (0.1%)	0.59	0/4338
All	All	0.58	14/12732 (0.1%)	0.59	0/17281

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	TRP	CD2-CE2	5.88	1.48	1.41
1	A	179	TRP	CD2-CE2	5.81	1.48	1.41
1	D	69	TRP	CD2-CE2	5.68	1.48	1.41
1	A	360	TRP	CD2-CE2	5.47	1.48	1.41
1	B	40	TRP	CD2-CE2	5.43	1.47	1.41
1	C	40	TRP	CD2-CE2	5.39	1.47	1.41
1	C	83	TRP	CD2-CE2	5.25	1.47	1.41
1	B	238	TRP	CD2-CE2	5.21	1.47	1.41
1	A	238	TRP	CD2-CE2	5.17	1.47	1.41
1	A	194	TRP	CD2-CE2	5.17	1.47	1.41
1	B	69	TRP	CD2-CE2	5.11	1.47	1.41
1	D	165	TRP	CD2-CE2	5.11	1.47	1.41
1	D	191	TRP	CD2-CE2	5.02	1.47	1.41
1	B	360	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	2937	19	0
1	B	3083	0	2952	28	0
1	C	3045	0	2920	24	0
1	D	3100	0	2962	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	18	0	24	0	0
3	B	12	0	16	1	0
3	C	6	0	8	0	0
3	D	18	0	24	0	0
4	A	4	0	3	0	0
4	B	4	0	3	4	0
4	C	4	0	3	5	0
4	D	4	0	3	0	0
5	B	8	0	12	3	0
5	C	12	0	18	1	0
5	D	8	0	12	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	D	7	0	10	12	0
8	A	267	0	0	3	0
8	B	256	0	0	7	0
8	C	271	0	0	3	0
8	D	255	0	0	1	0
All	All	13485	0	11907	103	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 4.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ASN:HD22	4:C:1390:ACT:H1	0.99	1.08
1:B:8:ASN:HA	3:B:1385:GOL:H11	1.47	0.97
1:C:235:ASN:ND2	4:C:1390:ACT:H1	1.78	0.97
1:A:123[B]:LEU:O	1:A:123[B]:LEU:HD23	1.68	0.94
1:A:123[B]:LEU:C	1:A:123[B]:LEU:HD23	1.95	0.88
1:B:197[A]:ASP:OD2	8:B:2167:HOH:O	1.93	0.85
4:C:1390:ACT:H3	8:C:2225:HOH:O	1.81	0.80
1:C:49:ARG:NH2	8:C:2067:HOH:O	2.23	0.72
1:A:123[B]:LEU:C	1:A:123[B]:LEU:CD2	2.59	0.71
1:A:197[A]:ASP:OD2	8:A:2189:HOH:O	2.10	0.69
1:D:26[A]:ARG:HH11	1:D:26[A]:ARG:HG2	1.57	0.69
1:D:311:THR:HG22	1:D:312:GLU:H	1.59	0.68
1:D:144:ARG:HA	7:D:1390:PEG:H21	1.76	0.67
1:C:159:ALA:HB3	1:C:160:PRO:HD3	1.76	0.67
1:A:26:ARG:HD2	1:A:58:GLU:OE2	1.95	0.67
1:D:37[B]:PHE:CE2	1:D:226:ARG:HD2	2.30	0.67
1:C:114:TYR:HA	5:C:1385:EDO:H22	1.77	0.65
1:D:26[A]:ARG:HH11	1:D:26[A]:ARG:CG	2.08	0.65
1:C:8:ASN:O	7:D:1390:PEG:H22	1.98	0.64
1:D:123[B]:LEU:HD11	1:D:134:VAL:HG11	1.80	0.64
1:D:116[A]:GLU:OE2	7:D:1390:PEG:H32	2.00	0.61
1:D:311:THR:HG22	1:D:312:GLU:N	2.16	0.61
1:C:290[B]:GLN:HA	1:C:290[B]:GLN:OE1	2.00	0.61
1:D:145:PRO:HD2	7:D:1390:PEG:H42	1.83	0.61
1:B:205:ASP:HB2	5:B:1387:EDO:H11	1.84	0.58
1:B:294:GLU:HG3	1:B:383:PHE:CE2	2.38	0.58
1:C:235:ASN:HD22	4:C:1390:ACT:CH3	1.93	0.57
1:B:26:ARG:HD2	1:B:58[B]:GLU:OE2	2.06	0.56
1:C:203:LEU:CD1	1:C:373[B]:LEU:HG	2.36	0.55
1:D:144:ARG:HG2	7:D:1390:PEG:C2	2.37	0.55
1:C:44:ARG:HH12	7:D:1390:PEG:C1	2.20	0.55
1:A:39:GLN:HB3	1:A:225:LEU:HD22	1.88	0.55
1:D:144:ARG:HG2	7:D:1390:PEG:H22	1.89	0.54
1:B:117[B]:GLU:HG3	8:B:2121:HOH:O	2.08	0.54
1:D:225:LEU:HD21	1:D:271:GLU:OE2	2.08	0.53
1:B:235:ASN:HD22	4:B:1390:ACT:CH3	2.21	0.53
1:A:117[B]:GLU:HG3	8:A:2133:HOH:O	2.09	0.53
1:A:294[A]:GLU:HG3	1:A:379:HIS:CE1	2.43	0.53
1:C:39:GLN:HB3	1:C:225:LEU:HD22	1.92	0.52
1:A:283[A]:MET:N	1:A:283[A]:MET:SD	2.78	0.52
1:B:37:PHE:CE2	1:B:226:ARG:HD2	2.45	0.51
1:A:22:PRO:HG2	1:A:51[B]:GLU:HG2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASP:OD1	5:B:1387:EDO:H22	2.11	0.51
1:B:37:PHE:CE2	1:B:226:ARG:CD	2.93	0.51
1:C:6:THR:HB	7:D:1390:PEG:H12	1.93	0.51
1:D:26[A]:ARG:NH1	1:D:26[A]:ARG:CG	2.71	0.51
1:C:299:ILE:HD13	1:C:312:GLU:HG3	1.92	0.50
1:C:343[B]:LEU:C	1:C:343[B]:LEU:HD23	2.31	0.50
1:A:188:LEU:HG	1:A:373:LEU:HD11	1.93	0.50
1:A:184:LEU:HG	1:A:373:LEU:HG	1.94	0.49
1:B:312:GLU:OE2	8:B:2240:HOH:O	2.20	0.49
1:C:44:ARG:HH12	7:D:1390:PEG:H12	1.78	0.48
1:D:278:VAL:HG21	1:D:299:ILE:HD12	1.94	0.48
1:C:6:THR:HB	7:D:1390:PEG:C1	2.44	0.48
1:C:278:VAL:HG23	1:C:312:GLU:HG2	1.96	0.47
1:B:188:LEU:HG	1:B:373:LEU:HD11	1.95	0.47
1:D:278:VAL:HG21	1:D:299:ILE:CD1	2.44	0.47
1:C:44:ARG:NH1	7:D:1390:PEG:H12	2.30	0.47
1:C:279:ALA:HA	1:C:313:HIS:O	2.15	0.46
1:D:37[B]:PHE:CE2	1:D:226:ARG:CD	2.98	0.46
1:D:15:ASP:HB2	1:D:28:ARG:HB2	1.97	0.46
1:B:144:ARG:NH2	1:B:221:VAL:HG21	2.30	0.46
1:B:270:ASP:HB3	8:B:2212:HOH:O	2.14	0.46
1:B:37:PHE:CE2	1:B:226:ARG:HD3	2.51	0.46
1:C:117[B]:GLU:HG3	8:C:2136:HOH:O	2.16	0.46
1:D:278:VAL:HG23	1:D:312:GLU:HG2	1.97	0.45
1:D:331:TYR:CZ	1:D:335:GLN:HG3	2.52	0.45
1:B:202:LYS:HD2	5:B:1387:EDO:H12	1.98	0.45
1:B:235:ASN:HD22	4:B:1390:ACT:H3	1.82	0.45
1:D:77:SER:HB2	1:D:83:TRP:CD2	2.52	0.44
1:D:70[B]:ARG:HE	1:D:90:PHE:HE2	1.64	0.44
1:D:144:ARG:NH2	1:D:221[B]:VAL:HG11	2.31	0.44
1:A:144:ARG:NH2	1:A:221[A]:VAL:HG21	2.33	0.44
1:D:26[A]:ARG:NH1	1:D:58:GLU:OE2	2.51	0.44
1:D:311:THR:CG2	1:D:312:GLU:H	2.27	0.44
1:D:117[B]:GLU:HG3	8:D:2114:HOH:O	2.17	0.44
1:A:262:ASP:O	1:A:338:CYS:HB2	2.18	0.44
1:B:236:ARG:NH1	4:B:1390:ACT:O	2.49	0.44
1:B:225:LEU:HD11	1:B:271:GLU:OE2	2.18	0.44
1:D:73:SER:HA	1:D:88:THR:HB	1.99	0.43
1:A:67:SER:HB3	1:A:272[B]:ASP:OD1	2.17	0.43
1:C:235:ASN:ND2	4:C:1390:ACT:CH3	2.68	0.43
1:A:155:GLU:OE1	1:A:160:PRO:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:THR:CG2	1:D:312:GLU:N	2.82	0.42
1:B:235:ASN:HD22	4:B:1390:ACT:H2	1.84	0.42
1:C:135:VAL:HG13	1:D:1:MET:HE1	2.01	0.42
1:B:37:PHE:CD2	1:B:226:ARG:HD3	2.55	0.42
1:D:67:SER:HA	1:D:70[B]:ARG:HD2	2.02	0.42
1:A:202:LYS:HE2	1:A:206:ARG:HH12	1.84	0.42
1:A:239[B]:MET:HG3	1:A:326:LYS:HA	2.02	0.42
8:A:2151:HOH:O	1:B:49:ARG:NH1	2.53	0.42
1:B:79:ASP:O	1:B:80:ARG:HB2	2.19	0.41
1:C:117[A]:GLU:HG3	1:D:117[A]:GLU:HG3	2.02	0.41
1:B:208[A]:THR:HG22	8:B:2145:HOH:O	2.20	0.41
1:B:282:GLU:HA	1:B:287:PHE:CD2	2.55	0.41
1:B:37:PHE:HZ	1:B:65:TYR:HE2	1.67	0.41
1:D:37[B]:PHE:HE1	1:D:225:LEU:CD2	2.33	0.41
1:B:208[A]:THR:HG21	8:B:2150:HOH:O	2.21	0.41
1:C:299:ILE:CD1	1:C:312:GLU:HG3	2.51	0.41
1:A:77:SER:HB2	1:A:83:TRP:CD2	2.56	0.40
1:B:285:PRO:HD2	8:B:2222:HOH:O	2.21	0.40
1:D:144:ARG:HG2	7:D:1390:PEG:H21	2.02	0.40
1:D:310:GLN:HB3	1:D:310:GLN:HE21	1.62	0.40

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	390/405 (96%)	380 (97%)	9 (2%)	1 (0%)	41 31
1	B	393/405 (97%)	382 (97%)	10 (2%)	1 (0%)	41 31
1	C	383/405 (95%)	369 (96%)	13 (3%)	1 (0%)	41 31
1	D	389/405 (96%)	373 (96%)	15 (4%)	1 (0%)	41 31
All	All	1555/1620 (96%)	1504 (97%)	47 (3%)	4 (0%)	41 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	C	39	GLN
1	B	39	GLN
1	D	39	GLN

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	322/328 (98%)	316 (98%)	6 (2%)	57 53
1	B	323/328 (98%)	317 (98%)	6 (2%)	57 53
1	C	318/328 (97%)	313 (98%)	5 (2%)	62 60
1	D	321/328 (98%)	315 (98%)	6 (2%)	57 53
All	All	1284/1312 (98%)	1261 (98%)	23 (2%)	65 55

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ARG
1	A	176	MET
1	A	283[A]	MET
1	A	283[B]	MET
1	A	321[A]	LYS
1	A	321[B]	LYS
1	B	139	ARG
1	B	176	MET
1	B	201[A]	ARG
1	B	201[B]	ARG
1	B	321	LYS
1	B	322	GLU
1	C	70[A]	ARG
1	C	70[B]	ARG
1	C	139	ARG
1	C	176	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	303	LYS
1	D	26[A]	ARG
1	D	26[B]	ARG
1	D	139	ARG
1	D	176	MET
1	D	283	MET
1	D	310	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	291	GLN
1	D	310	GLN

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 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	1385	-	5,5,5	0.39	0	5,5,5	0.21	0
4	ACT	A	1387	-	1,3,3	1.35	0	0,3,3	0.00	-
3	GOL	D	1387	-	5,5,5	0.32	0	5,5,5	0.37	0
5	EDO	B	1388	-	3,3,3	0.41	0	2,2,2	0.54	0
5	EDO	D	1388	-	3,3,3	0.46	0	2,2,2	0.33	0
3	GOL	C	1386	-	5,5,5	0.40	0	5,5,5	0.31	0
5	EDO	C	1387	-	3,3,3	0.46	0	2,2,2	0.50	0
4	ACT	B	1390	-	1,3,3	0.64	0	0,3,3	0.00	-
5	EDO	D	1389	-	3,3,3	0.43	0	2,2,2	0.45	0
3	GOL	A	1385	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	B	1385	-	5,5,5	0.33	0	5,5,5	0.45	0
5	EDO	B	1387	-	3,3,3	0.43	0	2,2,2	0.34	0
7	PEG	D	1390	-	6,6,6	0.29	0	5,5,5	0.49	0
3	GOL	A	1386	-	5,5,5	0.33	0	5,5,5	0.32	0
3	GOL	B	1386	-	5,5,5	0.40	0	5,5,5	0.26	0
5	EDO	C	1388	-	3,3,3	0.40	0	2,2,2	0.46	0
5	EDO	C	1385	-	3,3,3	0.48	0	2,2,2	0.38	0
3	GOL	A	1384	-	5,5,5	0.37	0	5,5,5	0.37	0
4	ACT	D	1391	-	1,3,3	0.64	0	0,3,3	0.00	-
3	GOL	D	1386	-	5,5,5	0.34	0	5,5,5	0.34	0
4	ACT	C	1390	-	1,3,3	0.10	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	1385	-	-	2/4/4/4	-
3	GOL	D	1387	-	-	4/4/4/4	-
5	EDO	B	1388	-	-	1/1/1/1	-
5	EDO	C	1387	-	-	1/1/1/1	-
3	GOL	C	1386	-	-	0/4/4/4	-
5	EDO	D	1388	-	-	1/1/1/1	-
5	EDO	D	1389	-	-	1/1/1/1	-
3	GOL	A	1385	-	-	2/4/4/4	-
3	GOL	B	1385	-	-	2/4/4/4	-
5	EDO	B	1387	-	-	1/1/1/1	-
7	PEG	D	1390	-	-	2/4/4/4	-
3	GOL	A	1386	-	-	2/4/4/4	-
3	GOL	B	1386	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	1388	-	-	0/1/1/1	-
5	EDO	C	1385	-	-	1/1/1/1	-
3	GOL	A	1384	-	-	0/4/4/4	-
3	GOL	D	1386	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1385	GOL	O1-C1-C2-C3
3	D	1387	GOL	C1-C2-C3-O3
3	A	1385	GOL	C1-C2-C3-O3
7	D	1390	PEG	O2-C3-C4-O4
3	D	1385	GOL	C1-C2-C3-O3
3	B	1386	GOL	C1-C2-C3-O3
3	B	1385	GOL	O1-C1-C2-O2
3	D	1385	GOL	O2-C2-C3-O3
3	D	1387	GOL	O2-C2-C3-O3
3	A	1385	GOL	O2-C2-C3-O3
5	C	1385	EDO	O1-C1-C2-O2
5	D	1388	EDO	O1-C1-C2-O2
3	A	1386	GOL	O1-C1-C2-C3
3	A	1386	GOL	O1-C1-C2-O2
5	C	1387	EDO	O1-C1-C2-O2
5	B	1387	EDO	O1-C1-C2-O2
3	D	1386	GOL	C1-C2-C3-O3
7	D	1390	PEG	C4-C3-O2-C2
5	B	1388	EDO	O1-C1-C2-O2
3	B	1386	GOL	O1-C1-C2-C3
3	D	1387	GOL	O1-C1-C2-O2
3	B	1386	GOL	O2-C2-C3-O3
5	D	1389	EDO	O1-C1-C2-O2
3	D	1387	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1390	ACT	4	0
3	B	1385	GOL	1	0
5	B	1387	EDO	3	0
7	D	1390	PEG	12	0
5	C	1385	EDO	1	0
4	C	1390	ACT	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	380/405 (93%)	-0.18	11 (2%) 51 54	7, 14, 37, 67	0
1	B	382/405 (94%)	-0.22	11 (2%) 51 54	6, 12, 28, 74	0
1	C	376/405 (92%)	-0.23	9 (2%) 59 62	6, 13, 35, 65	0
1	D	380/405 (93%)	-0.24	9 (2%) 59 62	7, 12, 31, 75	0
All	All	1518/1620 (93%)	-0.22	40 (2%) 56 58	6, 13, 34, 75	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	TYR	8.7
1	A	156	THR	6.3
1	D	156	THR	5.5
1	B	317	ALA	4.7
1	C	320	TYR	4.6
1	B	322	GLU	4.5
1	D	384	ALA	4.3
1	B	285	PRO	4.0
1	C	156	THR	3.8
1	D	157	ASP	3.4
1	D	321	LYS	3.4
1	D	320	TYR	3.3
1	A	20	ASP	3.2
1	A	159	ALA	3.2
1	C	159	ALA	2.9
1	A	290	GLN	2.8
1	C	384	ALA	2.8
1	B	318	SER	2.8
1	B	286	SER	2.8
1	A	318	SER	2.7
1	A	317	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	322	GLU	2.7
1	A	285	PRO	2.7
1	C	314	GLY	2.7
1	B	283[A]	MET	2.6
1	B	321	LYS	2.6
1	C	321	LYS	2.5
1	D	310	GLN	2.4
1	C	20	ASP	2.4
1	A	319	LYS	2.3
1	D	323	ASP	2.3
1	A	383	PHE	2.3
1	A	37	PHE	2.2
1	A	36	GLU	2.2
1	C	322	GLU	2.2
1	B	323	ASP	2.2
1	B	384	ALA	2.2
1	B	324	ALA	2.1
1	D	36	GLU	2.1
1	C	323	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
5	EDO	D	1388	4/4	0.83	0.24	24,30,36,43	0
5	EDO	D	1389	4/4	0.84	0.31	28,32,41,46	0
3	GOL	C	1386	6/6	0.85	0.31	29,46,51,52	0
3	GOL	B	1385	6/6	0.86	0.17	26,32,36,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	D	1386	6/6	0.87	0.22	35,38,41,42	0
3	GOL	D	1385	6/6	0.88	0.15	26,40,46,54	0
5	EDO	B	1388	4/4	0.89	0.14	38,38,39,41	0
3	GOL	B	1386	6/6	0.89	0.27	35,38,48,51	0
6	CL	D	1999	1/1	0.91	0.07	55,55,55,55	0
6	CL	B	1389	1/1	0.91	0.13	44,44,44,44	0
4	ACT	D	1391	4/4	0.92	0.22	24,29,30,38	0
4	ACT	C	1390	4/4	0.93	0.18	23,28,33,34	0
5	EDO	C	1387	4/4	0.93	0.13	17,32,38,42	0
3	GOL	A	1385	6/6	0.93	0.16	20,37,43,45	0
5	EDO	C	1388	4/4	0.93	0.15	20,26,28,33	0
5	EDO	C	1385	4/4	0.93	0.13	20,21,21,26	0
4	ACT	A	1387	4/4	0.93	0.19	23,32,35,35	0
6	CL	C	1389	1/1	0.93	0.06	54,54,54,54	0
4	ACT	B	1390	4/4	0.93	0.14	23,27,27,35	0
5	EDO	B	1387	4/4	0.93	0.13	28,31,32,43	0
3	GOL	D	1387	6/6	0.93	0.12	18,31,32,42	0
7	PEG	D	1390	7/7	0.94	0.22	14,17,24,32	0
3	GOL	A	1386	6/6	0.95	0.13	21,31,38,38	0
3	GOL	A	1384	6/6	0.95	0.09	22,27,30,34	0
2	ZN	D	385	1/1	0.99	0.04	40,40,40,40	0
2	ZN	C	385	1/1	0.99	0.06	39,39,39,39	0
2	ZN	A	385	1/1	0.99	0.04	32,32,32,32	0
2	ZN	B	385	1/1	1.00	0.05	40,40,40,40	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.