



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 01:58 PM BST

PDB ID : 5OM6
Title : Crystal structure of Alpha1-antichymotrypsin variant DBS-I-allo2: a MMP9-cleavable drug-binding serpin for doxycycline
Authors : Schmidt, K.; Muller, Y.A.
Deposited on : 2017-07-28
Resolution : 1.85 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 : 2.13.1
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) : 2.13.1

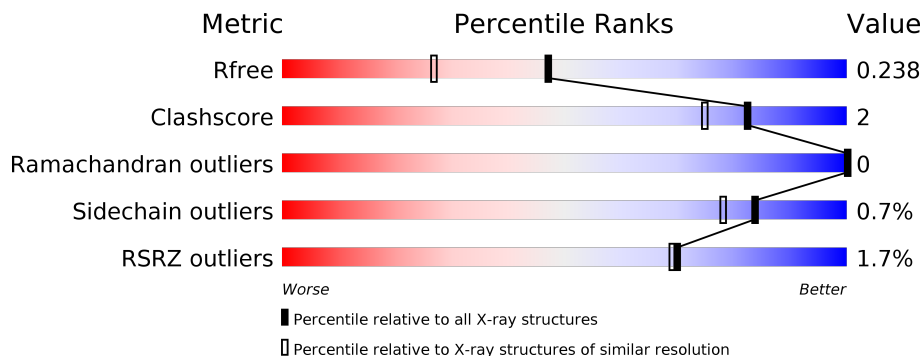
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	369	 0% 85% 7% 8%
1	C	369	 2% 85% 6% 9%
2	B	40	 3% 95% • •
2	D	40	 3% 93% 5% •

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6454 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 Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2719	1733	449	526	11	0	4	0
1	C	335	2661	1699	437	514	11	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP P01011
A	-7	LYS	-	expression tag	UNP P01011
A	-6	HIS	-	expression tag	UNP P01011
A	-5	HIS	-	expression tag	UNP P01011
A	-4	HIS	-	expression tag	UNP P01011
A	-3	HIS	-	expression tag	UNP P01011
A	-2	HIS	-	expression tag	UNP P01011
A	-1	HIS	-	expression tag	UNP P01011
A	0	MET	-	expression tag	UNP P01011
A	1	LYS	-	expression tag	UNP P01011
A	2	GLN	-	expression tag	UNP P01011
A	24	ARG	LEU	engineered mutation	UNP P01011
A	194	PHE	TRP	engineered mutation	UNP P01011
A	215	TYR	TRP	engineered mutation	UNP P01011
A	242	GLN	GLU	engineered mutation	UNP P01011
A	244	ASN	LYS	engineered mutation	UNP P01011
A	269	SER	LEU	engineered mutation	UNP P01011
A	270	GLN	PRO	engineered mutation	UNP P01011
A	274	SER	LYS	engineered mutation	UNP P01011
A	276	PHE	TRP	engineered mutation	UNP P01011
A	277	PHE	ARG	engineered mutation	UNP P01011
A	349	ARG	ALA	engineered mutation	UNP P01011
A	355	LEU	VAL	engineered mutation	UNP P01011
A	357	GLY	ILE	engineered mutation	UNP P01011
A	358	PRO	THR	engineered mutation	UNP P01011

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Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ARG	LEU	engineered mutation	UNP P01011
A	360	GLN	LEU	engineered mutation	UNP P01011
C	-8	MET	-	initiating methionine	UNP P01011
C	-7	LYS	-	expression tag	UNP P01011
C	-6	HIS	-	expression tag	UNP P01011
C	-5	HIS	-	expression tag	UNP P01011
C	-4	HIS	-	expression tag	UNP P01011
C	-3	HIS	-	expression tag	UNP P01011
C	-2	HIS	-	expression tag	UNP P01011
C	-1	HIS	-	expression tag	UNP P01011
C	0	MET	-	expression tag	UNP P01011
C	1	LYS	-	expression tag	UNP P01011
C	2	GLN	-	expression tag	UNP P01011
C	24	ARG	LEU	engineered mutation	UNP P01011
C	194	PHE	TRP	engineered mutation	UNP P01011
C	215	TYR	TRP	engineered mutation	UNP P01011
C	242	GLN	GLU	engineered mutation	UNP P01011
C	244	ASN	LYS	engineered mutation	UNP P01011
C	269	SER	LEU	engineered mutation	UNP P01011
C	270	GLN	PRO	engineered mutation	UNP P01011
C	274	SER	LYS	engineered mutation	UNP P01011
C	276	PHE	TRP	engineered mutation	UNP P01011
C	277	PHE	ARG	engineered mutation	UNP P01011
C	349	ARG	ALA	engineered mutation	UNP P01011
C	355	LEU	VAL	engineered mutation	UNP P01011
C	357	GLY	ILE	engineered mutation	UNP P01011
C	358	PRO	THR	engineered mutation	UNP P01011
C	359	ARG	LEU	engineered mutation	UNP P01011
C	360	GLN	LEU	engineered mutation	UNP P01011

- Molecule 2 is a protein called Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	39	335	223	56	53	3	0	1	0
2	D	39	330	219	56	53	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

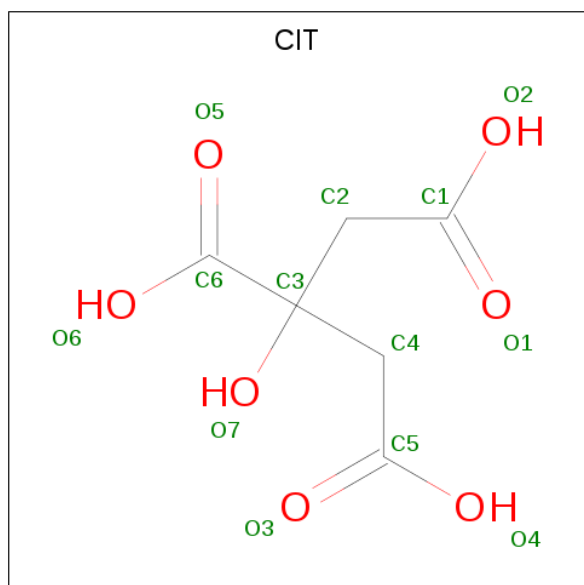
Chain	Residue	Modelled	Actual	Comment	Reference
B	361	ILE	SER	engineered mutation	UNP P01011

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Chain	Residue	Modelled	Actual	Comment	Reference
B	362	THR	ALA	engineered mutation	UNP P01011
B	363	ALA	LEU	engineered mutation	UNP P01011
B	382	ASP	PRO	engineered mutation	UNP P01011
B	383	HIS	THR	engineered mutation	UNP P01011
B	384	PHE	ASP	engineered mutation	UNP P01011
B	386	TRP	GLN	engineered mutation	UNP P01011
B	387	SER	ASN	engineered mutation	UNP P01011
D	361	ILE	SER	engineered mutation	UNP P01011
D	362	THR	ALA	engineered mutation	UNP P01011
D	363	ALA	LEU	engineered mutation	UNP P01011
D	382	ASP	PRO	engineered mutation	UNP P01011
D	383	HIS	THR	engineered mutation	UNP P01011
D	384	PHE	ASP	engineered mutation	UNP P01011
D	386	TRP	GLN	engineered mutation	UNP P01011
D	387	SER	ASN	engineered mutation	UNP P01011

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	211	Total O 211 211	0	0
6	B	23	Total O 23 23	0	0
6	C	133	Total O 133 133	0	0
6	D	7	Total O 7 7	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.80Å 73.92Å 78.32Å 90.00° 99.69° 90.00°	Depositor
Resolution (Å)	38.60 – 1.85 38.60 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.60-1.85) 98.7 (38.60-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.85Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.194 , 0.238 0.194 , 0.238	Depositor DCC
R_{free} test set	2100 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtrriage
Anisotropy	0.510	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.023 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6454	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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, EDO, CIT

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	0.43	0/2774	0.55	0/3742
1	C	0.43	0/2709	0.56	0/3655
2	B	0.40	0/347	0.54	0/469
2	D	0.42	0/339	0.53	0/459
All	All	0.43	0/6169	0.55	0/8325

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2719	0	2714	14	0
1	C	2661	0	2658	14	0
2	B	335	0	349	1	0
2	D	330	0	340	1	0
3	A	13	0	5	0	0
3	C	13	0	5	0	0
4	A	4	0	6	1	0
4	C	4	0	6	1	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	211	0	0	1	1
6	B	23	0	0	0	0
6	C	133	0	0	1	0
6	D	7	0	0	0	0
All	All	6454	0	6083	30	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (30) 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:223:LEU:HB3	1:C:226:LEU:HD11	1.71	0.71
1:A:212:LYS:NZ	1:A:258:GLN:HG2	2.15	0.61
1:A:51:ILE:HD12	1:A:297:ARG:HG2	1.87	0.56
1:A:191:LYS:HG3	1:A:348:GLU:HG2	1.86	0.56
1:C:296:SER:HB2	1:C:339:VAL:HG12	1.92	0.51
1:C:288:LEU:HD23	2:D:370:VAL:HB	1.93	0.50
1:A:110:LEU:HD23	1:A:192:ALA:HB2	1.94	0.49
1:C:91:GLU:HA	1:C:94:GLN:HB2	1.96	0.48
1:A:212:LYS:HZ1	1:A:258:GLN:HG2	1.79	0.46
4:C:402:EDO:H11	6:C:505:HOH:O	2.16	0.46
1:A:67:GLY:HA3	1:A:323:ILE:HG13	1.98	0.45
1:C:359:ARG:CZ	1:C:359:ARG:HB3	2.47	0.45
1:C:339:VAL:CG2	1:C:350:SER:HB2	2.47	0.45
1:C:168:LYS:NZ	1:C:348:GLU:OE2	2.35	0.45
1:A:334:VAL:HG22	1:A:355:LEU:HD22	1.98	0.44
1:C:168:LYS:HD3	1:C:168:LYS:HA	1.85	0.44
1:C:303:ASP:O	1:C:307:GLN:HG3	2.18	0.44
1:C:77:LEU:HD12	1:C:84:LEU:HD21	1.99	0.44
1:C:230:TYR:N	1:C:281:GLU:O	2.47	0.43
1:A:126:LEU:HD22	1:A:323:ILE:HG22	2.01	0.42
1:A:44:LYS:HE2	6:A:688:HOH:O	2.19	0.42
1:C:296:SER:CB	1:C:339:VAL:HG12	2.50	0.41
2:B:398:LYS:HA	2:B:398:LYS:HD3	1.93	0.41
1:A:100:LEU:HG	1:A:114:MET:SD	2.61	0.41
1:C:51:ILE:HD13	1:C:340:LEU:HD23	2.03	0.41
1:A:294:SER:OG	1:A:341[A]:ASP:OD1	2.31	0.41
1:A:52:PHE:CE1	1:A:54:PRO:HG3	2.56	0.41
1:A:330:ALA:O	1:A:358:PRO:HD2	2.21	0.41
1:A:96:PHE:CE2	4:A:402:EDO:H12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LYS:NZ	1:C:259:ASP:OD2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:501:HOH:O	6:A:635:HOH:O 2_556]	2.10	0.10

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	341/369 (92%)	337 (99%)	4 (1%)	0	100	100
1	C	333/369 (90%)	326 (98%)	7 (2%)	0	100	100
2	B	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
2	D	37/40 (92%)	37 (100%)	0	0	100	100
All	All	749/818 (92%)	737 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	302/327 (92%)	300 (99%)	2 (1%)	84	78
1	C	295/327 (90%)	293 (99%)	2 (1%)	84	78
2	B	39/38 (103%)	39 (100%)	0	100	100
2	D	38/38 (100%)	37 (97%)	1 (3%)	46	29
All	All	674/730 (92%)	669 (99%)	5 (1%)	84	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	63	PHE
1	C	100	LEU
1	C	359	ARG
2	D	391	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	CIT	C	401	-	3,12,12	0.78	0	3,17,17	0.64	0
4	EDO	A	402	-	3,3,3	0.43	0	2,2,2	0.64	0
4	EDO	C	402	-	3,3,3	0.47	0	2,2,2	0.28	0
3	CIT	A	401	-	3,12,12	1.36	1 (33%)	3,17,17	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	C	401	-	-	0/6/16/16	-
4	EDO	A	402	-	-	0/1/1/1	-
4	EDO	C	402	-	-	1/1/1/1	-
3	CIT	A	401	-	-	0/6/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	CIT	O7-C3	-2.00	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	402	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	EDO	1	0
4	C	402	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	339/369 (91%)	-0.27	3 (0%) 84 84	16, 28, 46, 61	0
1	C	335/369 (90%)	-0.04	8 (2%) 59 57	19, 33, 51, 68	0
2	B	39/40 (97%)	-0.11	1 (2%) 56 53	18, 27, 52, 56	0
2	D	39/40 (97%)	0.08	1 (2%) 56 53	21, 33, 50, 53	0
All	All	752/818 (91%)	-0.14	13 (1%) 70 69	16, 31, 50, 68	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	384	PHE	4.9
1	C	84	LEU	4.2
1	C	26	LEU	3.8
1	A	213	LYS	3.5
1	C	27	ALA	3.3
2	D	384	PHE	3.2
1	A	22	VAL	3.0
1	C	85	THR	2.7
1	C	201	GLN	2.6
1	C	225	HIS	2.6
1	A	24	ARG	2.5
1	C	87	THR	2.3
1	C	98	HIS	2.2

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(Å ²)	Q<0.9
4	EDO	A	402	4/4	0.91	0.14	31,33,39,45	0
4	EDO	C	402	4/4	0.92	0.13	22,27,34,36	0
3	CIT	A	401	13/13	0.93	0.09	29,34,39,48	0
3	CIT	C	401	13/13	0.94	0.08	26,31,36,37	0
5	CL	C	403	1/1	0.98	0.08	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.