



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:49 PM BST

PDB ID : 6DAT
Title : ETS1 in complex with synthetic SRR mimic
Authors : Perez-Borrajero, C.; Okon, M.; Lin, C.S.; Scheu, K.; Murphy, M.E.P.; Graves, B.J.; McIntosh, L.P.
Deposited on : 2018-05-02
Resolution : 2.35 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

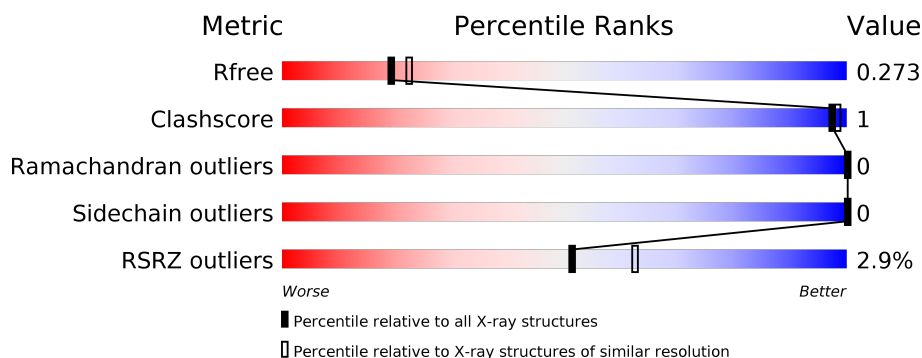
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	140	<div> <div>3%</div> <div>95%</div> <div>• •</div> </div>
1	B	140	<div> <div>94%</div> <div>• •</div> </div>
1	C	140	<div> <div>5%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
1	D	140	<div> <div>3%</div> <div>96%</div> <div>• •</div> </div>
2	E	17	<div> <div>6%</div> <div>71%</div> <div>29%</div> </div>
2	F	17	<div> <div>65%</div> <div>35%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9422 atoms, of which 4563 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 Protein C-ets-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	135	Total	C	H	N	O	S	0	0	0
			2200	712	1096	189	199	4			
1	B	135	Total	C	H	N	O	S	0	0	0
			2215	715	1105	192	199	4			
1	C	135	Total	C	H	N	O	S	0	0	0
			2202	712	1096	191	199	4			
1	D	135	Total	C	H	N	O	S	0	0	0
			2200	712	1096	189	199	4			

- Molecule 2 is a protein called serine-rich region (SRR) peptide.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	E	17	Total	C	F	H	N	O	P	0	0	1
			249	92	20	85	18	32	2			
2	F	17	Total	C	F	H	N	O	P	0	0	1
			249	92	20	85	18	32	2			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	18	Total	O	0	0
			18	18		
4	C	9	Total	O	0	0
			9	9		

Continued on next page...

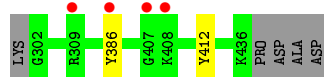
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	16	Total	O	0	0
			16	16		
4	E	1	Total	O	0	0
			1	1		

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.

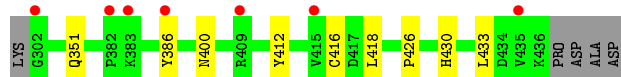
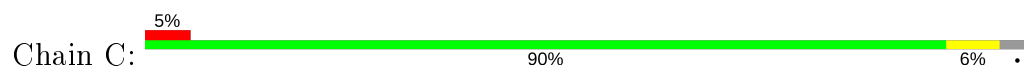
- Molecule 1: Protein C-ets-1



- Molecule 1: Protein C-ets-1



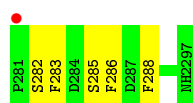
- Molecule 1: Protein C-ets-1



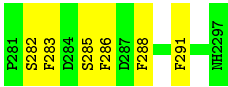
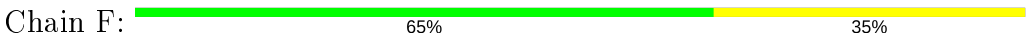
- Molecule 1: Protein C-ets-1



- Molecule 2: serine-rich region (SRR) peptide



- Molecule 2: serine-rich region (SRR) peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.11Å 89.11Å 215.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.19 – 2.35 39.19 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.19-2.35) 99.8 (39.19-2.35)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.233 , 0.268 0.238 , 0.273	Depositor DCC
R_{free} test set	2000 reflections (5.40%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9422	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1652e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NH2, PF5, SO4, SEP

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	0.26	0/1133	0.40	0/1529
1	B	0.25	0/1139	0.41	0/1536
1	C	0.26	0/1135	0.41	0/1532
1	D	0.25	0/1133	0.40	0/1529
2	E	0.20	0/78	0.31	0/100
2	F	0.19	0/78	0.36	0/100
All	All	0.25	0/4696	0.40	0/6326

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	1104	1096	1094	1	0
1	B	1110	1105	1105	1	1
1	C	1106	1096	1094	5	0
1	D	1104	1096	1094	0	1
2	E	164	85	82	0	0
2	F	164	85	82	0	0
3	A	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	0	0
4	A	18	0	0	0	0
4	B	18	0	0	0	0
4	C	9	0	0	0	0
4	D	16	0	0	0	0
4	E	1	0	0	0	0
All	All	4859	4563	4551	7	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 1.

All (7) 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:426:PRO:O	1:C:430:HIS:ND1	2.32	0.62
1:C:400:ASN:ND2	3:C:502:SO4:O4	2.32	0.62
1:C:386:TYR:OH	1:C:412:TYR:OH	2.20	0.59
1:A:386:TYR:OH	1:A:412:TYR:OH	2.32	0.48
1:C:416:CYS:O	1:C:418:LEU:N	2.51	0.43
1:B:318:LYS:N	1:B:319:PRO:CD	2.83	0.41
1:C:351:GLN:NE2	1:C:433:LEU:O	2.48	0.41

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)
1:B:410:TYR:OH	1:D:410:TYR:OH[3_444]	2.07	0.13

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	133/140 (95%)	129 (97%)	4 (3%)	0	100	100
1	B	133/140 (95%)	130 (98%)	3 (2%)	0	100	100
1	C	133/140 (95%)	129 (97%)	4 (3%)	0	100	100
1	D	133/140 (95%)	130 (98%)	3 (2%)	0	100	100
2	E	9/17 (53%)	7 (78%)	2 (22%)	0	100	100
2	F	9/17 (53%)	7 (78%)	2 (22%)	0	100	100
All	All	550/594 (93%)	532 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	116/121 (96%)	116 (100%)	0	100	100
1	B	117/121 (97%)	117 (100%)	0	100	100
1	C	116/121 (96%)	116 (100%)	0	100	100
1	D	116/121 (96%)	116 (100%)	0	100	100
2	E	8/8 (100%)	8 (100%)	0	100	100
2	F	8/8 (100%)	8 (100%)	0	100	100
All	All	481/500 (96%)	481 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	SEP	E	285	2	8,9,10	2.25	1 (12%)	8,12,14	1.40	1 (12%)
2	SEP	F	282	2	8,9,10	2.64	1 (12%)	8,12,14	1.48	0
2	PF5	E	288	2	15,16,17	1.04	1 (6%)	19,23,25	0.67	0
2	PF5	F	288	2	15,16,17	1.07	1 (6%)	19,23,25	0.74	1 (5%)
2	PF5	E	283	2	15,16,17	0.89	1 (6%)	19,23,25	0.65	0
2	SEP	E	282	2	8,9,10	2.67	1 (12%)	8,12,14	1.48	1 (12%)
2	PF5	E	286	2	15,16,17	0.93	1 (6%)	19,23,25	0.50	0
2	PF5	F	286	2	15,16,17	0.99	1 (6%)	19,23,25	0.46	0
2	PF5	F	283	2	15,16,17	0.96	1 (6%)	19,23,25	0.69	0
2	SEP	F	285	2	8,9,10	2.34	1 (12%)	8,12,14	1.41	1 (12%)
2	PF5	E	291	2	15,16,17	0.80	0	19,23,25	0.58	0
2	PF5	F	291	2	15,16,17	0.89	1 (6%)	19,23,25	0.56	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
2	SEP	E	285	2	-	1/5/8/10	-
2	SEP	F	282	2	-	4/5/8/10	-
2	PF5	E	288	2	-	0/5/6/8	0/1/1/1
2	PF5	F	288	2	-	0/5/6/8	0/1/1/1
2	PF5	E	283	2	-	0/5/6/8	0/1/1/1
2	SEP	E	282	2	-	4/5/8/10	-
2	PF5	E	286	2	-	0/5/6/8	0/1/1/1
2	PF5	F	286	2	-	0/5/6/8	0/1/1/1
2	PF5	F	283	2	-	0/5/6/8	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	F	285	2	-	2/5/8/10	-
2	PF5	E	291	2	-	1/5/6/8	0/1/1/1
2	PF5	F	291	2	-	1/5/6/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	282	SEP	P-OG	6.81	1.82	1.60
2	F	282	SEP	P-OG	6.74	1.81	1.60
2	F	285	SEP	P-OG	5.80	1.78	1.60
2	E	285	SEP	P-OG	5.61	1.78	1.60
2	F	288	PF5	CB-CG	-3.62	1.47	1.51
2	E	288	PF5	CB-CG	-3.34	1.47	1.51
2	F	286	PF5	CB-CG	-3.03	1.47	1.51
2	F	283	PF5	CB-CG	-2.91	1.48	1.51
2	E	283	PF5	CB-CG	-2.58	1.48	1.51
2	F	291	PF5	CB-CG	-2.45	1.48	1.51
2	E	286	PF5	CB-CG	-2.29	1.48	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	288	PF5	CB-CA-C	-2.11	107.52	111.47
2	F	285	SEP	O3P-P-O2P	2.05	115.47	107.64
2	E	282	SEP	O3P-P-OG	-2.03	101.32	106.73
2	E	285	SEP	O3P-P-OG	-2.01	101.37	106.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	285	SEP	CB-OG-P-O2P
2	F	282	SEP	N-CA-CB-OG
2	F	282	SEP	CB-OG-P-O2P
2	F	282	SEP	CB-OG-P-O3P
2	E	282	SEP	CB-OG-P-O2P
2	E	282	SEP	CB-OG-P-O3P
2	F	282	SEP	CB-OG-P-O1P
2	E	282	SEP	CB-OG-P-O1P
2	F	285	SEP	CB-OG-P-O1P
2	E	282	SEP	N-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	285	SEP	N-CA-CB-OG
2	E	291	PF5	CA-CB-CG-CD1
2	F	291	PF5	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

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	SO4	A	502	-	4,4,4	0.18	0	6,6,6	0.07	0
3	SO4	C	502	-	4,4,4	0.16	0	6,6,6	0.05	0
3	SO4	A	503	-	4,4,4	0.16	0	6,6,6	0.04	0
3	SO4	B	502	-	4,4,4	0.19	0	6,6,6	0.04	0
3	SO4	D	502	-	4,4,4	0.18	0	6,6,6	0.09	0
3	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	D	501	-	4,4,4	0.19	0	6,6,6	0.08	0
3	SO4	B	501	-	4,4,4	0.17	0	6,6,6	0.08	0
3	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	SO4	1	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	135/140 (96%)	0.41	4 (2%) 50 61	46, 57, 77, 88	0
1	B	135/140 (96%)	0.32	0 100 100	45, 58, 75, 105	0
1	C	135/140 (96%)	0.51	7 (5%) 27 39	50, 62, 80, 103	0
1	D	135/140 (96%)	0.37	4 (2%) 50 61	49, 60, 78, 94	0
2	E	10/17 (58%)	0.34	1 (10%) 7 11	48, 53, 82, 87	0
2	F	10/17 (58%)	0.30	0 100 100	52, 53, 79, 89	0
All	All	560/594 (94%)	0.40	16 (2%) 51 62	45, 59, 79, 105	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	TYR	3.4
1	A	309	ARG	3.1
1	A	407	GLY	2.8
1	C	435	VAL	2.6
1	D	415	VAL	2.4
1	D	436	LYS	2.4
2	E	281	PRO	2.3
1	C	409	ARG	2.3
1	D	342	LEU	2.2
1	A	386	TYR	2.2
1	C	415	VAL	2.2
1	C	302	GLY	2.2
1	A	408	LYS	2.1
1	D	397	TYR	2.1
1	C	382	PRO	2.1
1	C	383	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	SEP	E	285	10/11	0.78	0.20	61,81,92,97	0
2	PF5	E	288	16/17	0.90	0.19	49,50,64,64	0
2	SEP	F	285	10/11	0.90	0.17	66,75,90,91	0
2	SEP	F	282	10/11	0.91	0.12	78,90,101,105	0
2	PF5	F	286	16/17	0.92	0.19	57,60,70,70	0
2	PF5	E	286	16/17	0.93	0.20	54,61,69,69	0
2	PF5	F	288	16/17	0.94	0.14	46,50,61,61	0
2	PF5	E	283	16/17	0.94	0.15	60,68,81,87	0
2	SEP	E	282	10/11	0.94	0.09	76,95,109,115	0
2	PF5	F	283	16/17	0.95	0.13	56,64,77,83	0
2	PF5	F	291	16/17	0.95	0.16	48,50,60,61	0
2	PF5	E	291	16/17	0.96	0.12	42,46,58,65	0

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
3	SO4	A	501	5/5	0.68	0.26	68,69,72,86	5
3	SO4	B	502	5/5	0.80	0.20	73,73,80,90	5
3	SO4	D	501	5/5	0.83	0.17	54,68,75,80	5
3	SO4	C	501	5/5	0.85	0.17	68,68,77,85	5
3	SO4	A	503	5/5	0.92	0.46	77,81,96,102	0
3	SO4	A	502	5/5	0.93	0.21	82,92,109,111	0
3	SO4	C	502	5/5	0.94	0.23	82,88,96,100	0
3	SO4	B	501	5/5	0.97	0.17	53,55,60,63	0
3	SO4	D	502	5/5	0.98	0.18	47,50,58,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.