



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:12 pm BST

PDB ID : 3QGJ  
Title : 1.3A Structure of alpha-Lytic Protease Bound to Ac-AlaAlaPro-Alanal  
Authors : Everill, P.; Meinke, G.; Bohm, A.; Bachovchin, W.  
Deposited on : 2011-01-24  
Resolution : 1.30 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](mailto: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 : 2.11  
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) : 2.11

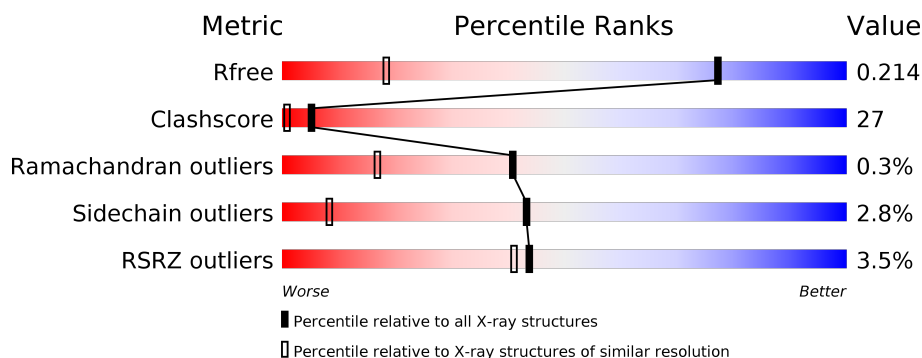
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\geq 3$ , 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	198	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	198	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	5	<div> <div></div> <div>100%</div> </div>
2	D	5	<div> <div></div> <div>80%</div> <div>20%</div> </div>

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
3	EDO	A	201	-	-	X	-
3	EDO	C	201	-	-	-	X
4	SO4	A	207	-	-	-	X
4	SO4	C	202	-	-	X	X
5	TFA	A	208[A]	-	-	X	-
5	TFA	A	208[B]	-	X	X	-
5	TFA	A	210[B]	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3757 atoms, of which 33 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.

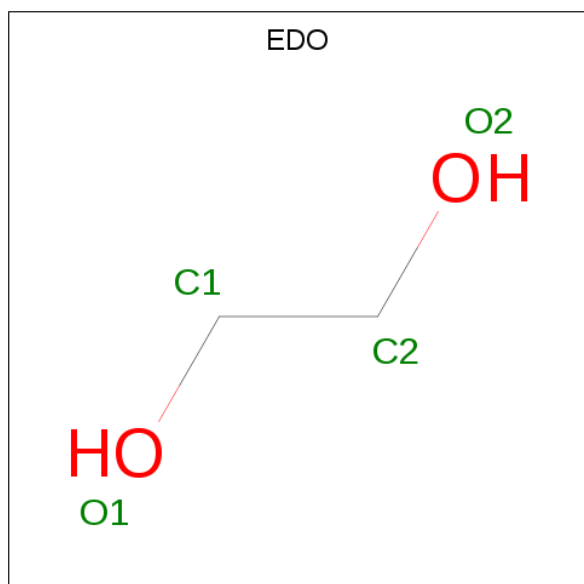
- Molecule 1 is a protein called Alpha-lytic protease.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	30	0
			1566	962	4	292	300	8			
1	C	198	Total	C	H	N	O	S	0	19	0
			1500	917	4	281	290	8			

- Molecule 2 is a protein called Ac-AlaAlaPro-Alanal peptide.

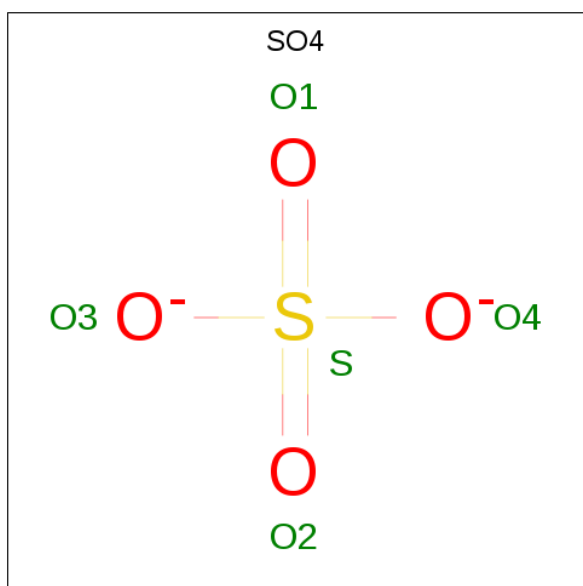
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	H	N	O	0	0	0
			36	16	11	4	5			
2	D	5	Total	C	H	N	O	0	0	0
			35	16	10	4	5			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



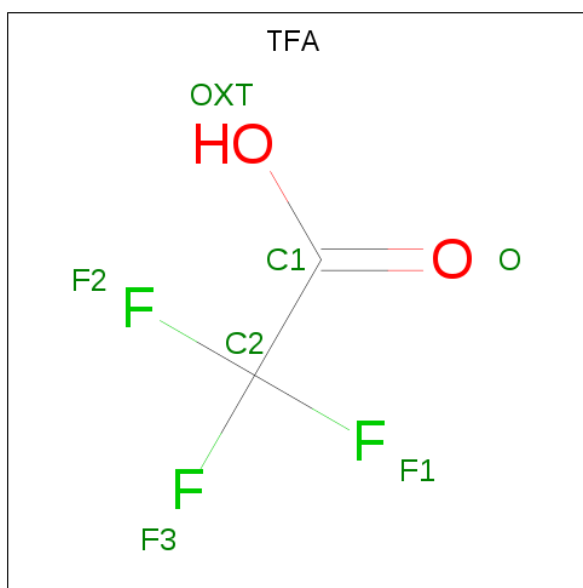
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C H O 6 2 2 2	0	0
3	C	1	Total C H O 6 2 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is trifluoroacetic acid (three-letter code: TFA) (formula:  $C_2HF_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	1
			12	4	6	2		
5	A	1	Total	C	F	O	0	0
			6	2	3	1		
5	A	1	Total	C	F	O	0	1
			12	4	6	2		
5	C	1	Total	C	F	O	0	0
			6	2	3	1		

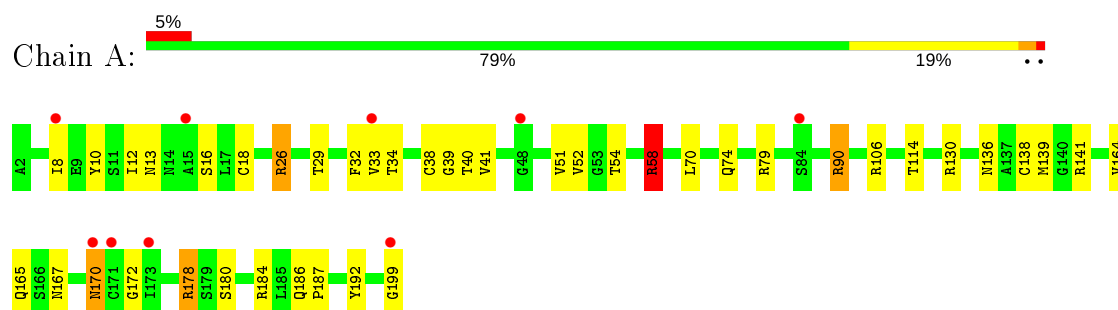
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	269	Total	O	0	0
			269	269		
6	B	8	Total	O	0	0
			8	8		
6	C	244	Total	O	0	0
			244	244		
6	D	4	Total	O	0	0
			4	4		

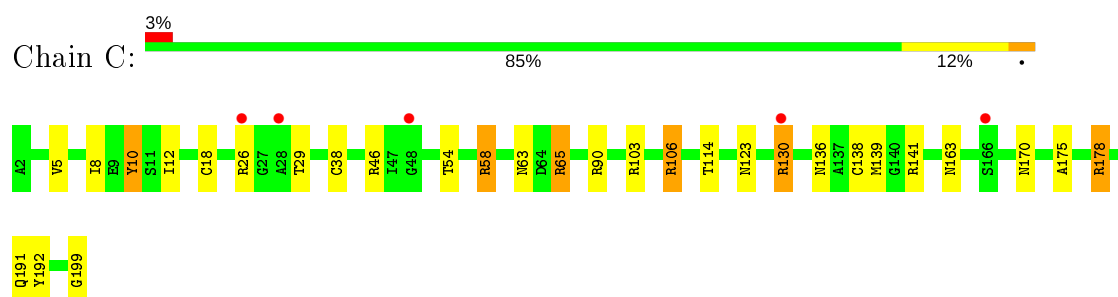
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Alpha-lytic protease



- Molecule 1: Alpha-lytic protease

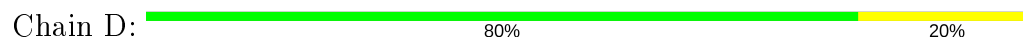


- Molecule 2: Ac-AlaAlaPro-Alanal peptide



There are no outlier residues recorded for this chain.

- Molecule 2: Ac-AlaAlaPro-Alanal peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.94Å 63.94Å 316.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.10 – 1.30 26.14 – 1.30	Depositor EDS
% Data completeness (in resolution range)	89.4 (26.10-1.30) 89.4 (26.14-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.167 , 0.192 0.188 , 0.214	Depositor DCC
$R_{free}$ test set	4332 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 2A1, TFA, EDO, ACE, SO4

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	1.38	8/1643 (0.5%)	1.43	23/2225 (1.0%)
1	C	1.24	2/1571 (0.1%)	1.22	7/2125 (0.3%)
2	B	0.98	0/18	1.12	0/25
2	D	1.37	0/18	0.96	0/25
All	All	1.31	10/3250 (0.3%)	1.33	30/4400 (0.7%)

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	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	ARG	CZ-NH2	8.76	1.44	1.33
1	A	58[A]	ARG	CZ-NH2	-8.21	1.22	1.33
1	A	58[B]	ARG	CZ-NH2	-8.21	1.22	1.33
1	A	164	VAL	CB-CG2	-7.84	1.36	1.52
1	A	180	SER	CB-OG	5.59	1.49	1.42
1	A	33[A]	VAL	CB-CG1	-5.47	1.41	1.52
1	A	33[B]	VAL	CB-CG1	-5.47	1.41	1.52
1	A	192	TYR	CE1-CZ	-5.32	1.31	1.38
1	C	192	TYR	CE2-CZ	-5.31	1.31	1.38
1	C	10	TYR	CG-CD2	5.19	1.45	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH1	-19.34	110.63	120.30
1	A	141	ARG	NE-CZ-NH2	15.64	128.12	120.30
1	C	90	ARG	NE-CZ-NH2	14.36	127.48	120.30
1	A	184[A]	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	A	184[B]	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	C	178	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	A	184[A]	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	A	184[B]	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	C	106	ARG	NE-CZ-NH1	-8.27	116.16	120.30
1	C	90	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	10	TYR	CB-CG-CD1	-7.69	116.38	121.00
1	A	141	ARG	CD-NE-CZ	7.42	133.99	123.60
1	A	130	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	58[A]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	58[B]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	178[A]	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	178[B]	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	58[A]	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	58[B]	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	79	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	A	10	TYR	CB-CG-CD2	5.63	124.38	121.00
1	C	46	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	90[A]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	90[B]	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	58	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	65	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	58[A]	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	58[B]	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	A	26[A]	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	26[B]	ARG	NE-CZ-NH2	5.21	122.91	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	103	ARG	Sidechain

## 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	1562	4	1606	83	0
1	C	1496	4	1529	66	1
2	B	25	11	26	0	0
2	D	25	10	26	2	0
3	A	12	0	18	6	0
3	C	8	4	12	3	0
4	A	20	0	0	0	0
4	C	15	0	0	31	1
5	A	30	0	0	12	1
5	C	6	0	0	0	0
6	A	269	0	0	40	8
6	B	8	0	0	0	0
6	C	244	0	0	20	4
6	D	4	0	0	2	0
All	All	3724	33	3217	168	9

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 27.

All (168) 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:90[B]:ARG:HH11	1:A:90[B]:ARG:CG	1.27	1.41
1:C:8:ILE:HD13	6:C:327:HOH:O	1.31	1.30
1:C:136:ASN:O	4:C:202:SO4:O3	1.52	1.27
1:C:114[A]:THR:CG2	6:C:313:HOH:O	1.83	1.26
1:C:130[B]:ARG:HD3	6:C:413:HOH:O	1.31	1.26
1:C:136:ASN:O	4:C:202:SO4:S	1.93	1.26
1:A:136[B]:ASN:C	1:A:178[B]:ARG:HD3	1.59	1.20
1:C:175:ALA:HA	4:C:202:SO4:S	1.83	1.18
1:C:175:ALA:CA	4:C:202:SO4:O1	1.90	1.18
1:C:178:ARG:CD	4:C:202:SO4:O3	1.92	1.17
1:C:136:ASN:HB2	4:C:202:SO4:O2	1.44	1.16
1:C:175:ALA:HA	4:C:202:SO4:O1	0.98	1.16
1:A:136[B]:ASN:O	1:A:178[B]:ARG:NH1	1.77	1.15
5:A:208[B]:TFA:F1	6:A:330:HOH:O	1.56	1.13
1:A:114[B]:THR:HG21	6:A:329:HOH:O	1.48	1.13
1:C:178:ARG:HD2	4:C:202:SO4:S	1.87	1.13
1:C:178:ARG:HD2	4:C:202:SO4:O3	0.96	1.13
5:A:210[B]:TFA:F3	6:A:301:HOH:O	1.57	1.12

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:208[B]:TFA:F1	6:A:348:HOH:O	1.59	1.08
1:A:136[B]:ASN:O	1:A:178[B]:ARG:HD3	1.57	1.04
1:C:10:TYR:CE1	1:C:12[B]:ILE:HD11	1.93	1.04
1:A:178[B]:ARG:HG2	1:A:178[B]:ARG:O	1.62	0.99
1:A:52[B]:VAL:HG23	1:A:74:GLN:CD	1.83	0.99
1:A:90[B]:ARG:HH11	1:A:90[B]:ARG:HG3	0.82	0.97
1:A:41:VAL:H	1:A:58[B]:ARG:NH1	1.61	0.97
1:C:199:GLY:C	6:C:308:HOH:O	2.02	0.96
1:A:90[B]:ARG:HG3	1:A:90[B]:ARG:NH1	1.61	0.96
3:A:201:EDO:C2	6:A:310:HOH:O	2.12	0.95
3:A:201:EDO:C1	6:A:310:HOH:O	2.15	0.95
1:C:10:TYR:HE1	1:C:12[B]:ILE:HD11	1.30	0.95
1:C:114[A]:THR:HG22	6:C:313:HOH:O	1.51	0.93
3:A:201:EDO:H22	6:A:310:HOH:O	1.66	0.93
1:C:54:THR:HG22	6:C:532:HOH:O	1.71	0.90
1:A:90[B]:ARG:CG	1:A:90[B]:ARG:NH1	2.06	0.89
1:A:165:GLN:HB2	6:A:313:HOH:O	1.73	0.89
1:C:178:ARG:HB2	4:C:202:SO4:O2	1.73	0.89
1:A:90[B]:ARG:HD3	1:A:199:GLY:O	1.72	0.89
1:A:90[B]:ARG:HH11	1:A:90[B]:ARG:HG2	1.36	0.88
1:A:172:GLY:C	6:A:494:HOH:O	2.11	0.88
5:A:208[A]:TFA:C1	6:A:330:HOH:O	2.22	0.87
6:C:349:HOH:O	2:D:1:ACE:H3	1.74	0.87
5:A:210[B]:TFA:C2	6:A:301:HOH:O	2.19	0.86
1:C:178:ARG:CD	4:C:202:SO4:S	2.60	0.86
1:C:54:THR:CG2	6:C:532:HOH:O	2.23	0.86
1:A:167:ASN:OD1	6:A:313:HOH:O	1.93	0.85
1:C:123:ASN:HD22	3:C:200:EDO:H22	1.39	0.84
1:C:178:ARG:CZ	4:C:202:SO4:O1	2.26	0.83
1:A:136[B]:ASN:CA	1:A:178[B]:ARG:HD3	2.08	0.83
1:C:18:CYS:HG	1:C:38:CYS:HG	1.05	0.83
1:C:136:ASN:CB	4:C:202:SO4:O2	2.25	0.83
1:C:178:ARG:NH1	4:C:202:SO4:S	2.51	0.83
1:A:12[B]:ILE:HD13	1:A:38:CYS:O	1.78	0.82
1:A:186[A]:GLN:HG2	1:A:187:PRO:HD3	1.63	0.81
3:A:201:EDO:H12	6:A:310:HOH:O	1.76	0.81
1:A:41:VAL:HG23	1:A:58[B]:ARG:NH1	1.96	0.81
1:C:141[B]:ARG:HG2	6:D:102:HOH:O	1.79	0.81
1:C:136:ASN:O	4:C:202:SO4:O4	1.99	0.81
1:C:175:ALA:CA	4:C:202:SO4:S	2.64	0.80
3:C:201:EDO:O1	6:C:323:HOH:O	1.74	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:VAL:HG23	1:A:58[B]:ARG:HH11	1.46	0.78
1:A:18:CYS:HG	1:A:38:CYS:HG	1.23	0.78
1:A:136[B]:ASN:O	1:A:178[B]:ARG:CD	2.31	0.78
1:A:165:GLN:C	6:A:313:HOH:O	2.21	0.77
1:A:54[B]:THR:HG22	3:A:201:EDO:H11	1.67	0.77
1:A:26[B]:ARG:CZ	6:A:301:HOH:O	2.34	0.76
1:A:172:GLY:O	6:A:494:HOH:O	2.04	0.75
1:C:175:ALA:CB	4:C:202:SO4:O4	2.36	0.73
5:A:208[A]:TFA:F1	6:A:348:HOH:O	1.94	0.73
1:C:114[A]:THR:HG21	6:C:313:HOH:O	1.65	0.72
1:C:199:GLY:CA	6:C:308:HOH:O	2.35	0.71
1:C:5:VAL:HB	6:C:327:HOH:O	1.90	0.71
1:C:5:VAL:N	6:C:327:HOH:O	2.23	0.71
1:A:90[B]:ARG:NH1	1:A:90[B]:ARG:HG2	1.98	0.71
1:A:32:PHE:HE1	1:A:34[B]:THR:HG21	1.56	0.71
1:C:136:ASN:HB2	4:C:202:SO4:S	2.31	0.70
1:C:178:ARG:NE	4:C:202:SO4:O1	2.23	0.70
1:A:90[B]:ARG:CD	6:A:315:HOH:O	2.41	0.68
1:A:136[B]:ASN:HB2	1:A:178[B]:ARG:HD2	1.75	0.67
1:A:54[B]:THR:HG22	3:A:201:EDO:C1	2.24	0.67
1:C:175:ALA:HB1	4:C:202:SO4:O4	1.93	0.67
1:A:136[B]:ASN:C	1:A:178[B]:ARG:HH11	1.91	0.67
1:C:178:ARG:CD	4:C:202:SO4:O1	2.42	0.67
1:A:90[B]:ARG:HD2	6:A:315:HOH:O	1.94	0.66
1:C:199:GLY:O	6:C:308:HOH:O	2.09	0.66
1:A:136[B]:ASN:CA	1:A:178[B]:ARG:CD	2.73	0.66
5:A:208[A]:TFA:C2	6:A:348:HOH:O	2.45	0.64
1:A:54[B]:THR:HG21	6:A:479:HOH:O	1.96	0.64
1:A:186[A]:GLN:CG	1:A:187:PRO:HD3	2.27	0.64
1:C:65:ARG:HH11	1:C:191:GLN:HE21	1.43	0.64
1:A:12[B]:ILE:HG22	1:A:16[B]:SER:O	1.98	0.63
1:A:52[B]:VAL:HG22	1:A:70:LEU:HD22	1.81	0.63
1:C:114[B]:THR:HG21	6:C:501:HOH:O	1.98	0.63
3:C:201:EDO:O1	6:C:311:HOH:O	2.16	0.63
1:C:163:ASN:HA	2:D:1:ACE:H1	1.80	0.63
1:C:12[B]:ILE:N	1:C:12[B]:ILE:HD13	2.14	0.63
1:A:165:GLN:CB	6:A:313:HOH:O	2.39	0.62
1:A:54[B]:THR:HG21	6:A:316:HOH:O	1.99	0.62
5:A:208[B]:TFA:C1	6:A:330:HOH:O	2.41	0.61
1:A:26[B]:ARG:NH1	6:A:301:HOH:O	2.31	0.61
1:C:65:ARG:HH11	1:C:191:GLN:NE2	1.99	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90[B]:ARG:NH1	6:A:562:HOH:O	2.21	0.60
1:A:165:GLN:CA	6:A:313:HOH:O	2.50	0.60
1:C:175:ALA:O	4:C:202:SO4:O2	2.19	0.59
5:A:208[A]:TFA:F2	6:A:348:HOH:O	2.02	0.58
5:A:208[B]:TFA:C2	6:A:330:HOH:O	2.39	0.58
1:A:32:PHE:CD1	1:A:34[B]:THR:HG23	2.39	0.57
1:A:136[B]:ASN:C	1:A:178[B]:ARG:CD	2.54	0.57
1:A:52[B]:VAL:CG2	1:A:74:GLN:CD	2.68	0.57
1:A:32:PHE:CE1	1:A:34[B]:THR:HG21	2.40	0.57
1:C:178:ARG:CZ	4:C:202:SO4:S	2.93	0.56
1:A:136[B]:ASN:HA	1:A:178[B]:ARG:CG	2.35	0.56
1:C:54:THR:HG23	6:C:521:HOH:O	2.05	0.56
1:A:136[B]:ASN:HA	1:A:178[B]:ARG:CD	2.35	0.56
1:A:52[B]:VAL:HG22	1:A:74:GLN:HG3	1.88	0.56
5:A:209:TFA:O	6:A:554:HOH:O	2.18	0.55
1:A:52[B]:VAL:CG2	1:A:74:GLN:HG3	2.37	0.54
1:A:186[B]:GLN:CD	6:A:326:HOH:O	2.46	0.54
1:A:18:CYS:HG	1:A:38:CYS:CB	2.20	0.54
1:A:52[B]:VAL:HG23	1:A:74:GLN:OE1	2.05	0.54
1:C:178:ARG:NH1	4:C:202:SO4:O3	2.39	0.54
1:A:32:PHE:CE1	1:A:34[B]:THR:CG2	2.92	0.53
1:A:186[B]:GLN:CG	6:A:326:HOH:O	2.57	0.53
1:A:138:CYS:HA	1:A:170:ASN:HD21	1.74	0.52
1:A:32:PHE:HD1	1:A:34[B]:THR:HG23	1.74	0.52
1:A:114[A]:THR:HG21	6:A:329:HOH:O	2.09	0.51
1:A:26[B]:ARG:HG3	1:A:29:THR:HB	1.93	0.50
1:C:10:TYR:CD1	1:C:12[B]:ILE:HD11	2.45	0.50
1:A:12[B]:ILE:CD1	1:A:39:GLY:CA	2.90	0.50
1:A:51:VAL:HG23	6:A:514:HOH:O	2.11	0.50
5:A:208[A]:TFA:C2	6:A:330:HOH:O	2.58	0.50
1:C:175:ALA:CB	4:C:202:SO4:S	2.99	0.50
1:A:136[B]:ASN:HA	1:A:178[B]:ARG:HG2	1.93	0.49
1:A:186[B]:GLN:HG2	6:A:326:HOH:O	2.12	0.49
1:A:178[B]:ARG:O	1:A:178[B]:ARG:CG	2.45	0.48
1:A:58[B]:ARG:HG2	1:A:58[B]:ARG:HH11	1.79	0.48
1:A:114[B]:THR:CG2	6:A:329:HOH:O	2.28	0.48
1:C:141[A]:ARG:HG2	6:C:309:HOH:O	2.15	0.47
1:C:138:CYS:HA	1:C:170[B]:ASN:HD21	1.79	0.47
1:A:12[B]:ILE:CD1	1:A:39:GLY:HA3	2.45	0.46
1:C:178:ARG:NH1	4:C:202:SO4:O4	2.48	0.46
1:C:54:THR:HG21	6:C:532:HOH:O	2.03	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141[B]:ARG:CG	6:D:102:HOH:O	2.53	0.45
1:C:136:ASN:CA	4:C:202:SO4:O2	2.64	0.45
1:C:178:ARG:HB2	4:C:202:SO4:S	2.56	0.45
1:A:52[B]:VAL:CG2	1:A:74:GLN:CG	2.95	0.45
1:C:178:ARG:CG	4:C:202:SO4:O1	2.65	0.45
1:C:18:CYS:CB	1:C:38:CYS:HG	2.29	0.45
1:C:26[B]:ARG:HB3	1:C:29:THR:HB	1.99	0.44
1:A:41:VAL:CG2	1:A:58[B]:ARG:NH1	2.76	0.44
1:A:12[B]:ILE:CD1	1:A:39:GLY:HA2	2.48	0.43
1:A:40:THR:HA	1:A:58[B]:ARG:HD3	2.00	0.43
1:A:136[B]:ASN:HB2	1:A:178[B]:ARG:CD	2.46	0.43
1:A:8[B]:ILE:HG13	6:A:497:HOH:O	2.19	0.42
1:A:136[B]:ASN:HA	1:A:178[B]:ARG:HD3	1.91	0.42
1:A:167:ASN:N	6:A:313:HOH:O	2.52	0.42
1:A:41:VAL:N	1:A:58[B]:ARG:NH1	2.46	0.42
1:C:178:ARG:HG3	4:C:202:SO4:O1	2.19	0.41
1:A:58[B]:ARG:CG	1:A:58[B]:ARG:HH11	2.33	0.41
1:C:63:ASN:HD21	1:C:130[A]:ARG:HH21	1.67	0.41
1:A:170:ASN:HD22	1:A:170:ASN:C	2.23	0.40
1:C:178:ARG:CG	4:C:202:SO4:S	3.09	0.40
1:A:114[A]:THR:HG22	6:A:328:HOH:O	2.22	0.40
1:C:5:VAL:CB	6:C:327:HOH:O	2.58	0.40

All (9) 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)
5:A:210[A]:TFA:O	6:A:392:HOH:O[11_655]	1.60	0.60
6:A:549:HOH:O	6:A:559:HOH:O[11_655]	1.64	0.56
6:A:433:HOH:O	6:C:535:HOH:O[6_655]	1.68	0.52
6:A:451:HOH:O	6:A:494:HOH:O[11_555]	1.89	0.31
6:A:480:HOH:O	6:A:480:HOH:O[11_655]	1.93	0.27
6:A:560:HOH:O	6:C:525:HOH:O[6_655]	1.97	0.23
6:A:343:HOH:O	6:C:324:HOH:O[6_655]	2.04	0.16
6:A:382:HOH:O	6:C:363:HOH:O[6_655]	2.05	0.15
1:C:141[A]:ARG:NH2	4:C:204:SO4:O4[7_555]	2.16	0.04

## 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	226/198 (114%)	219 (97%)	5 (2%)	2 (1%)	17	2
1	C	217/198 (110%)	209 (96%)	8 (4%)	0	100	100
2	B	2/5 (40%)	2 (100%)	0	0	100	100
2	D	2/5 (40%)	2 (100%)	0	0	100	100
All	All	447/406 (110%)	432 (97%)	13 (3%)	2 (0%)	41	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13[A]	ASN
1	A	13[B]	ASN

### 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	170/142 (120%)	165 (97%)	5 (3%)	42	7
1	C	163/142 (115%)	156 (96%)	7 (4%)	29	2
2	B	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	335/286 (117%)	323 (96%)	12 (4%)	43	4

All (12) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	58[A]	ARG
1	A	58[B]	ARG
1	A	106	ARG
1	A	139	MET
1	A	170	ASN
1	C	58	ARG
1	C	106	ARG
1	C	130[A]	ARG
1	C	130[B]	ARG
1	C	130[C]	ARG
1	C	130[D]	ARG
1	C	139	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	170	ASN
1	C	37	HIS
1	C	63	ASN
1	C	123	ASN
1	C	191	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	EDO	A	201	-	3,3,3	0.79	0	2,2,2	1.14	0
4	SO4	C	204	-	4,4,4	1.00	0	6,6,6	0.82	0
5	TFA	A	208[A]	-	5,5,6	1.81	1 (20%)	6,7,9	1.29	1 (16%)
4	SO4	C	203	-	4,4,4	0.20	0	6,6,6	0.64	0
3	EDO	C	200	-	3,3,3	0.90	0	2,2,2	1.26	0
4	SO4	A	207	-	4,4,4	0.99	0	6,6,6	1.11	1 (16%)
5	TFA	C	205	-	5,5,6	1.69	1 (20%)	6,7,9	1.63	2 (33%)
3	EDO	A	203	-	3,3,3	0.76	0	2,2,2	0.98	0
5	TFA	A	209	-	5,5,6	0.96	0	6,7,9	2.96	5 (83%)
4	SO4	A	206	-	4,4,4	0.35	0	6,6,6	0.28	0
5	TFA	A	208[B]	-	5,5,6	2.14	2 (40%)	6,7,9	7.16	5 (83%)
5	TFA	A	210[B]	-	5,5,6	1.16	0	6,7,9	13.10	4 (66%)
5	TFA	A	210[A]	-	5,5,6	1.66	2 (40%)	6,7,9	1.80	2 (33%)
3	EDO	A	202	-	3,3,3	0.67	0	2,2,2	1.05	0
4	SO4	C	202	-	4,4,4	0.10	0	6,6,6	0.26	0
4	SO4	A	205	-	4,4,4	0.55	0	6,6,6	0.93	0
3	EDO	C	201	-	3,3,3	0.74	0	2,2,2	0.75	0
4	SO4	A	204	-	4,4,4	0.97	0	6,6,6	0.73	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	EDO	A	201	-	-	1/1/1/1	-
5	TFA	A	208[A]	-	-	0/0/3/6	-
3	EDO	C	200	-	-	1/1/1/1	-
5	TFA	C	205	-	-	0/0/3/6	-
3	EDO	A	203	-	-	0/1/1/1	-
5	TFA	A	209	-	-	0/0/3/6	-
5	TFA	A	210[A]	-	-	0/0/3/6	-
5	TFA	A	208[B]	-	-	0/0/3/6	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TFA	A	210[B]	-	-	0/0/3/6	-
3	EDO	A	202	-	-	0/1/1/1	-
3	EDO	C	201	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	208[B]	TFA	C2-C1	4.09	1.56	1.47
5	A	208[A]	TFA	C2-C1	3.37	1.54	1.47
5	C	205	TFA	C2-C1	2.82	1.53	1.47
5	A	208[B]	TFA	O-C1	2.45	1.28	1.19
5	A	210[A]	TFA	F3-C2	2.35	1.42	1.32
5	A	210[A]	TFA	C2-C1	2.18	1.52	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	210[B]	TFA	F2-C2-C1	-30.57	14.37	112.66
5	A	208[B]	TFA	F1-C2-C1	-10.79	77.98	112.66
5	A	208[B]	TFA	F2-C2-C1	9.57	143.43	112.66
5	A	208[B]	TFA	F2-C2-F1	-8.82	65.78	105.47
5	A	210[B]	TFA	F1-C2-C1	-6.80	90.79	112.66
5	A	210[B]	TFA	F2-C2-F1	-5.34	81.43	105.47
5	A	209	TFA	F2-C2-C1	-5.09	96.29	112.66
5	A	210[B]	TFA	F3-C2-F2	4.37	125.11	105.47
5	A	208[B]	TFA	F3-C2-C1	-3.84	100.31	112.66
5	A	210[A]	TFA	F3-C2-C1	3.24	123.08	112.66
5	A	209	TFA	F1-C2-C1	-3.23	102.27	112.66
5	C	205	TFA	F2-C2-C1	-2.70	103.97	112.66
5	A	209	TFA	F2-C2-F1	2.68	117.51	105.47
5	A	208[A]	TFA	F1-C2-C1	-2.52	104.57	112.66
5	C	205	TFA	F3-C2-F1	2.38	116.17	105.47
5	A	210[A]	TFA	F1-C2-C1	-2.26	105.38	112.66
4	A	207	SO4	O4-S-O3	2.21	118.48	109.06
5	A	208[B]	TFA	F3-C2-F1	2.18	115.28	105.47
5	A	209	TFA	F3-C2-F1	2.14	115.10	105.47
5	A	209	TFA	F3-C2-C1	2.13	119.51	112.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	EDO	O1-C1-C2-O2
3	C	200	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	EDO	6	0
4	C	204	SO4	0	1
5	A	208[A]	TFA	5	0
3	C	200	EDO	1	0
5	A	209	TFA	1	0
5	A	208[B]	TFA	4	0
5	A	210[B]	TFA	2	0
5	A	210[A]	TFA	0	1
4	C	202	SO4	31	0
3	C	201	EDO	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	198/198 (100%)	0.16	9 (4%)	33	31	8, 14, 23, 34	7 (3%)
1	C	198/198 (100%)	0.07	5 (2%)	57	56	9, 16, 27, 36	3 (1%)
2	B	3/5 (60%)	-0.37	0	100	100	14, 14, 15, 16	0
2	D	3/5 (60%)	-0.43	0	100	100	16, 16, 16, 18	0
All	All	402/406 (99%)	0.11	14 (3%)	44	41	8, 15, 25, 36	10 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ILE	10.5
1	A	170	ASN	5.5
1	C	130[A]	ARG	3.3
1	C	28	ALA	3.0
1	A	8[A]	ILE	2.6
1	A	48	GLY	2.6
1	C	166[A]	SER	2.5
1	A	33[A]	VAL	2.3
1	A	84	SER	2.3
1	C	26[A]	ARG	2.3
1	A	15	ALA	2.3
1	C	48	GLY	2.1
1	A	171	CYS	2.1
1	A	199	GLY	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	A	207	5/5	0.53	1.14	325,325,325,325	5
5	TFA	C	205	6/7	0.55	0.29	46,54,55,56	0
4	SO4	C	202	5/5	0.68	0.42	434,434,434,434	5
3	EDO	C	201	4/4	0.71	0.41	25,27,28,28	6
3	EDO	C	200	4/4	0.77	0.19	19,28,36,40	0
5	TFA	A	209	6/7	0.78	0.21	47,48,53,55	0
5	TFA	A	208[A]	6/7	0.82	0.38	72,74,75,76	6
5	TFA	A	208[B]	6/7	0.82	0.38	5,18,21,22	6
5	TFA	A	210[B]	6/7	0.90	0.15	2,3,11,12	6
4	SO4	A	205	5/5	0.90	0.12	27,29,33,37	4
5	TFA	A	210[A]	6/7	0.90	0.15	12,22,25,33	6
3	EDO	A	201	4/4	0.91	0.15	19,20,28,37	0
4	SO4	C	204	5/5	0.93	0.24	30,32,34,36	0
4	SO4	A	206	5/5	0.94	0.24	48,50,52,52	4
4	SO4	C	203	5/5	0.95	0.16	24,24,27,34	5
3	EDO	A	203	4/4	0.96	0.08	16,19,19,22	0
3	EDO	A	202	4/4	0.97	0.07	15,17,19,24	0
4	SO4	A	204	5/5	0.99	0.05	13,14,19,22	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.