



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:42 am GMT

PDB ID : 1P8J
Title : CRYSTAL STRUCTURE OF THE PROPROTEIN CONVERTASE FURIN
Authors : Henrich, S.; Cameron, A.; Bourenkov, G.P.; Kiefersauer, R.; Huber, R.; Lindberg, I.; Bode, W.; Than, M.E.
Deposited on : 2003-05-07
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

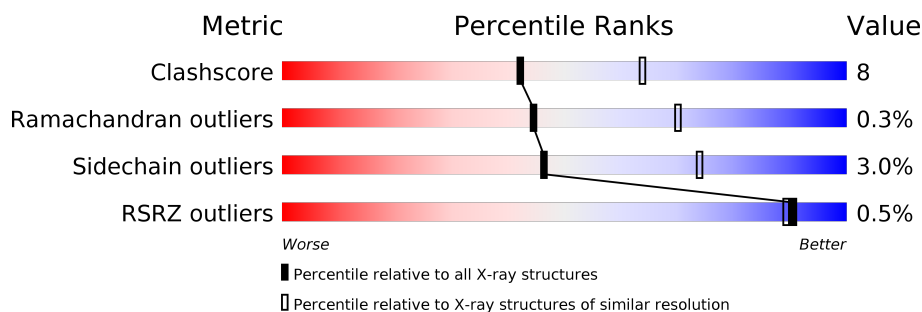
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	471	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	471	<div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	C	471	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	471	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	E	471	<div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	F	471	<div> <div>81%</div> <div>18%</div> <div>..</div> </div>
1	G	471	<div> <div>82%</div> <div>17%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	471	 % 81% 17% **
2	J	6	 100%
2	K	6	 67% 33%
2	L	6	 67% 33%
2	M	6	 83% 17%
2	N	6	 100%
2	P	6	 100%
2	Q	6	 50% 50%
2	R	6	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	4004	-	-	-	X
6	SO4	A	4014	-	-	-	X
6	SO4	A	4064	-	-	-	X
6	SO4	A	4069	-	-	-	X
6	SO4	B	4027	-	-	-	X
6	SO4	C	4013	-	-	-	X
6	SO4	D	4012	-	-	-	X
6	SO4	D	4015	-	-	-	X
6	SO4	E	4039	-	-	-	X
6	SO4	E	4060	-	-	-	X
6	SO4	F	4070	-	-	-	X
6	SO4	G	4030	-	-	-	X
6	SO4	G	4032	-	-	-	X
7	FUC	G	953	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31923 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 Furin precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	44	0	0
			3591	2227	640	710	14			
1	B	468	Total	C	N	O	S	39	0	0
			3578	2219	638	707	14			
1	C	467	Total	C	N	O	S	56	0	0
			3569	2214	637	704	14			
1	D	467	Total	C	N	O	S	51	0	0
			3569	2214	637	704	14			
1	E	467	Total	C	N	O	S	45	0	0
			3569	2214	637	704	14			
1	F	468	Total	C	N	O	S	40	0	0
			3577	2218	638	707	14			
1	G	467	Total	C	N	O	S	43	0	0
			3569	2214	637	704	14			
1	H	466	Total	C	N	O	S	60	0	0
			3562	2209	636	703	14			

- Molecule 2 is a protein called DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR.

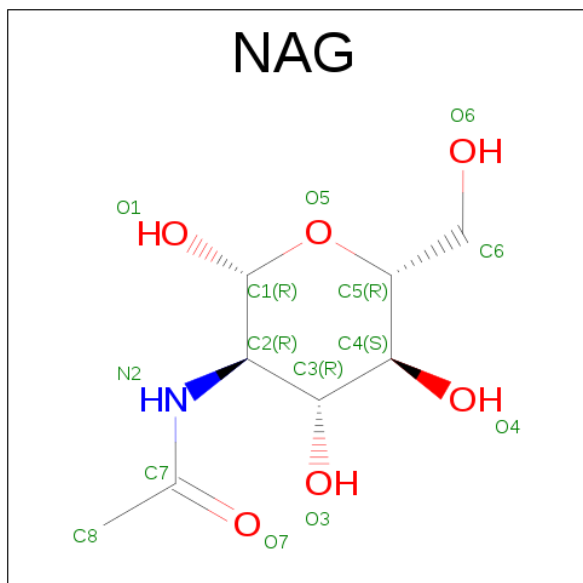
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	K	6	Total	C	N	O	2	0	1
			50	34	11	5			
2	L	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	M	6	Total	C	N	O	1	0	1
			50	34	11	5			
2	N	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	P	6	Total	C	N	O	0	0	1
			50	34	11	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	R	6	Total	C	N	O	0	0	1
			50	34	11	5			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	3	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

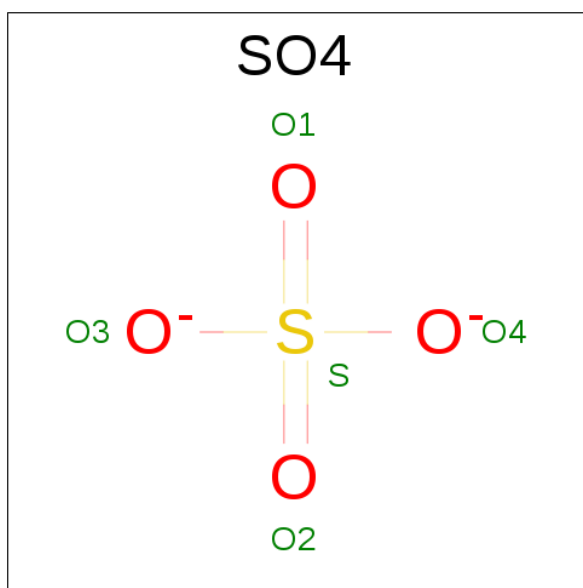
- Molecule 4 is a polymer of unknown type called SUGAR (11-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	11	Total	C	N	O	4	0
			135	76	5	54		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	2	Total	Ca	0	0
			2	2		
5	D	2	Total	Ca	0	0
			2	2		
5	E	2	Total	Ca	0	0
			2	2		
5	H	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		
5	C	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		
5	F	2	Total	Ca	0	0
			2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	N	1	Total	O	S	0	0
			5	4	1		
6	P	1	Total	O	S	0	0
			5	4	1		
6	Q	1	Total	O	S	0	0
			5	4	1		
6	R	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	352	Total	O	0	0
			352	352		
8	B	291	Total	O	0	0
			291	291		
8	C	292	Total	O	0	0
			292	292		
8	D	181	Total	O	0	0
			181	181		
8	E	270	Total	O	0	0
			270	270		
8	F	325	Total	O	0	0
			325	325		
8	G	319	Total	O	0	0
			319	319		
8	H	231	Total	O	0	0
			231	231		
8	J	6	Total	O	0	0
			6	6		
8	K	7	Total	O	0	0
			7	7		
8	L	5	Total	O	0	0
			5	5		
8	M	5	Total	O	0	0
			5	5		

Continued on next page...

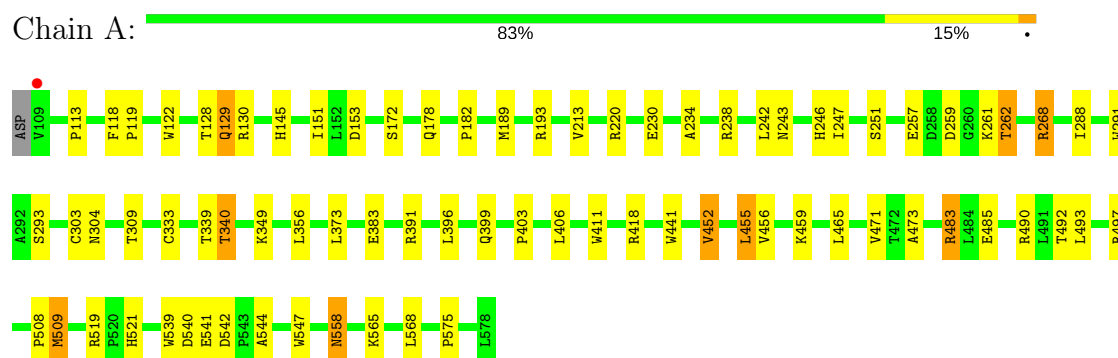
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	8	Total 8	O 8	0	0
8	P	6	Total 6	O 6	0	0
8	Q	3	Total 3	O 3	0	0
8	R	4	Total 4	O 4	0	0

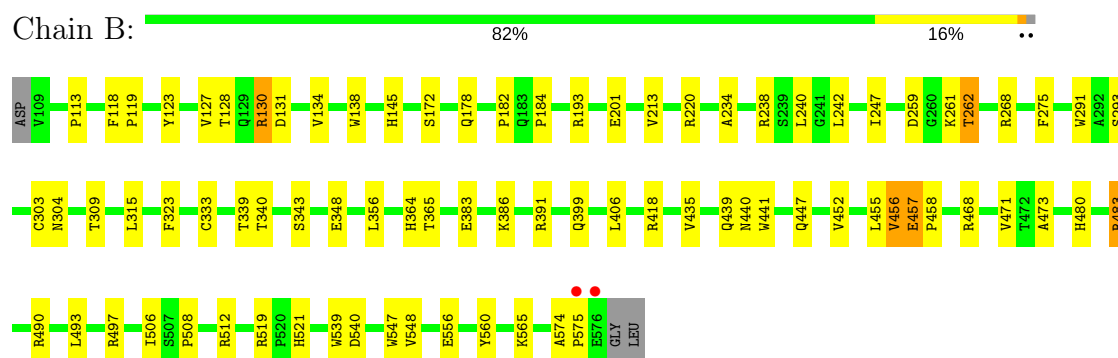
3 Residue-property plots

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.

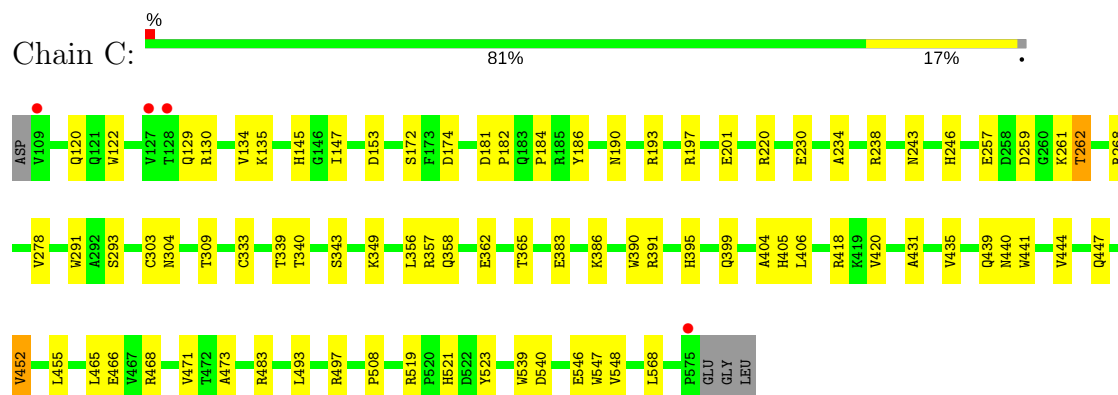
• Molecule 1: Furin precursor



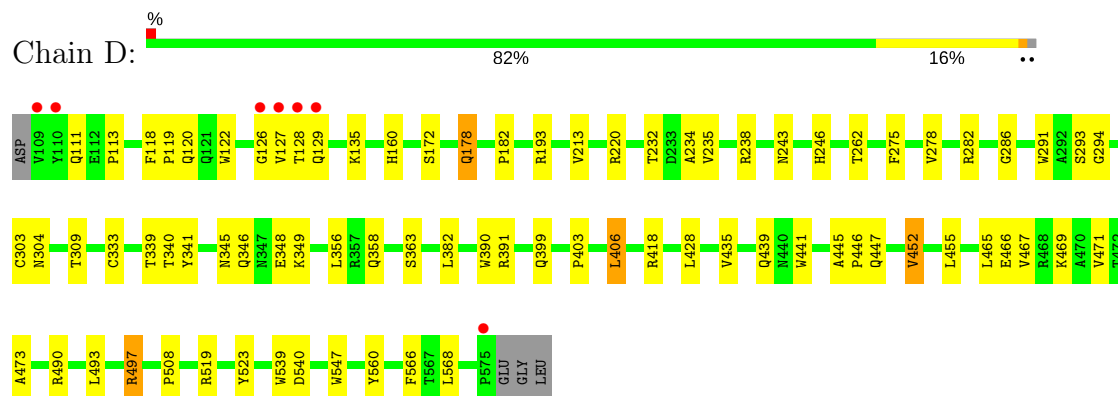
• Molecule 1: Furin precursor



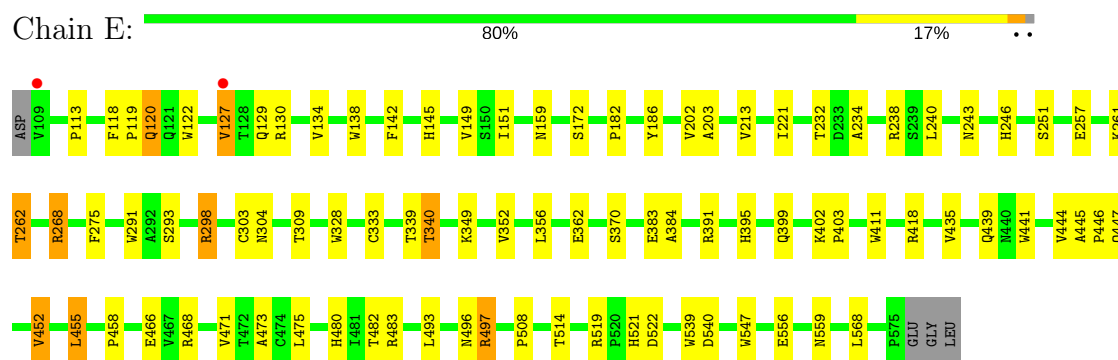
• Molecule 1: Furin precursor



- Molecule 1: Furin precursor



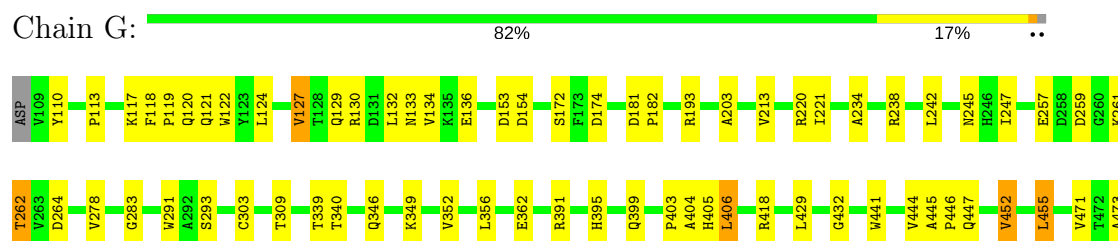
- Molecule 1: Furin precursor

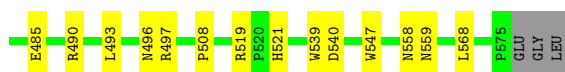


- Molecule 1: Furin precursor

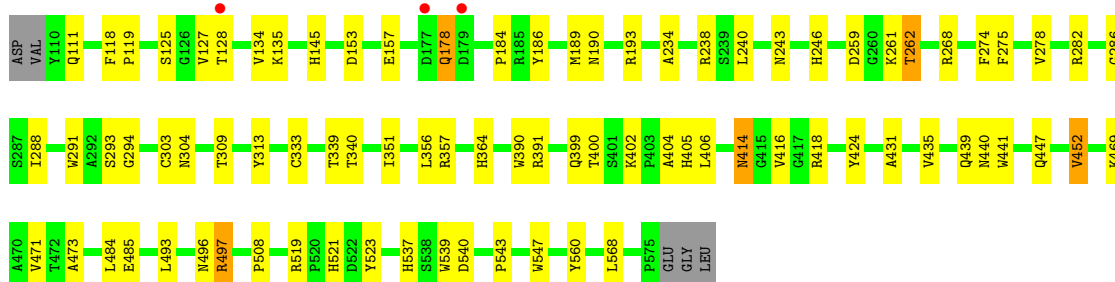
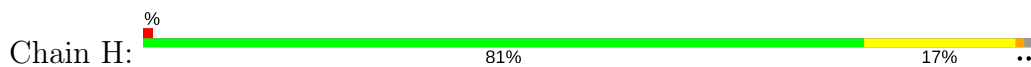


- Molecule 1: Furin precursor





- Molecule 1: Furin precursor



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR



There are no outlier residues recorded for this chain.

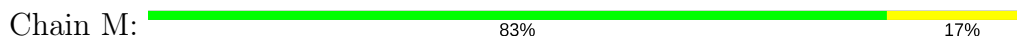
- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR



There are no outlier residues recorded for this chain.

- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain Q:  50% 50%



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain R:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.31Å 135.39Å 137.81Å 103.56° 98.98° 107.09°	Depositor
Resolution (Å)	18.82 – 2.60 18.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (18.82-2.60) 87.7 (18.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.219 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31923	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0QE, BMA, NAG, AR7, CA, GAL, SO4, DKA, FUL, MAN, FUC

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	0.38	0/3674	0.65	0/5007
1	B	0.38	0/3661	0.65	0/4991
1	C	0.38	0/3652	0.64	0/4979
1	D	0.38	0/3652	0.63	0/4979
1	E	0.38	0/3652	0.63	0/4979
1	F	0.38	0/3660	0.65	0/4990
1	G	0.39	0/3652	0.66	0/4979
1	H	0.38	0/3645	0.63	0/4969
2	J	0.45	0/26	0.63	0/32
2	K	0.45	0/26	0.63	0/32
2	L	0.41	0/26	0.76	0/32
2	M	0.38	0/26	0.83	0/32
2	N	0.37	0/26	0.63	0/32
2	P	0.38	0/26	0.70	0/32
2	Q	0.38	0/26	0.65	0/32
2	R	0.46	0/26	0.67	0/32
All	All	0.38	0/29456	0.64	0/40129

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
7	G	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	953	FUC	C1

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	3591	0	3406	62	0
1	B	3578	0	3393	51	0
1	C	3569	0	3388	54	0
1	D	3569	0	3388	48	0
1	E	3569	0	3387	69	0
1	F	3577	0	3389	53	0
1	G	3569	0	3387	52	0
1	H	3562	0	3378	53	0
2	J	50	0	66	0	0
2	K	50	0	66	2	0
2	L	50	0	66	2	0
2	M	50	0	66	1	0
2	N	50	0	66	0	0
2	P	50	0	66	0	0
2	Q	50	0	66	3	0
2	R	50	0	66	2	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	E	14	0	13	0	0
3	F	28	0	26	1	0
3	H	14	0	13	0	0
4	A	135	0	115	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
6	A	55	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	30	0	0	1	0
6	C	30	0	0	0	0
6	D	45	0	0	1	0
6	E	45	0	0	2	0
6	F	45	0	0	1	0
6	G	30	0	0	1	0
6	H	30	0	0	0	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	1	0
6	M	5	0	0	0	0
6	N	5	0	0	0	0
6	P	5	0	0	0	0
6	Q	5	0	0	0	0
6	R	5	0	0	0	0
7	G	49	0	43	2	0
8	A	352	0	0	12	0
8	B	291	0	0	9	0
8	C	292	0	0	6	0
8	D	181	0	0	6	0
8	E	270	0	0	5	0
8	F	325	0	0	10	0
8	G	319	0	0	6	0
8	H	231	0	0	4	0
8	J	6	0	0	0	0
8	K	7	0	0	1	0
8	L	5	0	0	0	0
8	M	5	0	0	0	0
8	N	8	0	0	0	0
8	P	6	0	0	0	0
8	Q	3	0	0	0	0
8	R	4	0	0	1	0
All	All	31923	0	27880	447	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 8.

The worst 5 of 447 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:E:298:ARG:HB2	1:E:298:ARG:HH21	1.02	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ARG:HH21	1:E:298:ARG:CB	1.74	0.99
1:E:475:LEU:HA	1:E:480:HIS:CD2	1.99	0.98
1:E:475:LEU:HA	1:E:480:HIS:HD2	1.28	0.95
1:F:125:SER:HA	1:F:135:LYS:HE2	1.49	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	468/471 (99%)	450 (96%)	16 (3%)	2 (0%)	38	63
1	B	466/471 (99%)	441 (95%)	22 (5%)	3 (1%)	28	53
1	C	465/471 (99%)	445 (96%)	19 (4%)	1 (0%)	51	76
1	D	465/471 (99%)	448 (96%)	16 (3%)	1 (0%)	51	76
1	E	465/471 (99%)	447 (96%)	17 (4%)	1 (0%)	51	76
1	F	466/471 (99%)	445 (96%)	20 (4%)	1 (0%)	51	76
1	G	465/471 (99%)	452 (97%)	12 (3%)	1 (0%)	51	76
1	H	464/471 (98%)	443 (96%)	19 (4%)	2 (0%)	38	63
2	J	2/6 (33%)	2 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
2	L	2/6 (33%)	2 (100%)	0	0	100	100
2	M	2/6 (33%)	2 (100%)	0	0	100	100
2	N	2/6 (33%)	2 (100%)	0	0	100	100
2	P	2/6 (33%)	2 (100%)	0	0	100	100
2	Q	2/6 (33%)	2 (100%)	0	0	100	100
2	R	2/6 (33%)	2 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3740/3816 (98%)	3587 (96%)	141 (4%)	12 (0%)	44 70

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	VAL
1	E	127	VAL
1	B	575	PRO
1	F	109	VAL
1	C	153	ASP

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	379/380 (100%)	366 (97%)	13 (3%)	42 69
1	B	378/380 (100%)	364 (96%)	14 (4%)	39 66
1	C	377/380 (99%)	368 (98%)	9 (2%)	54 80
1	D	377/380 (99%)	366 (97%)	11 (3%)	48 75
1	E	377/380 (99%)	365 (97%)	12 (3%)	44 72
1	F	378/380 (100%)	367 (97%)	11 (3%)	48 75
1	G	377/380 (99%)	368 (98%)	9 (2%)	54 80
1	H	376/380 (99%)	365 (97%)	11 (3%)	48 75
2	J	3/3 (100%)	3 (100%)	0	100 100
2	K	3/3 (100%)	3 (100%)	0	100 100
2	L	3/3 (100%)	3 (100%)	0	100 100
2	M	3/3 (100%)	3 (100%)	0	100 100
2	N	3/3 (100%)	3 (100%)	0	100 100
2	P	3/3 (100%)	3 (100%)	0	100 100
2	Q	3/3 (100%)	3 (100%)	0	100 100
2	R	3/3 (100%)	3 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3043/3064 (99%)	2953 (97%)	90 (3%)	46 74

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	275	PHE
1	E	268	ARG
1	H	275	PHE
1	D	291	TRP
1	D	469	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	243	ASN
1	E	243	ASN
1	H	243	ASN
1	D	358	GLN
1	E	120	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	AR7	J	805	2	10,10,11	0.41	0	8,11,13	0.59	0
2	AR7	K	805	2	10,10,11	0.38	0	8,11,13	0.58	0
2	AR7	L	805	2	10,10,11	0.48	0	8,11,13	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AR7	M	805	2	10,10,11	0.54	0	8,11,13	0.55	0
2	AR7	N	805	2	10,10,11	0.48	0	8,11,13	0.62	0
2	AR7	P	805	2	10,10,11	0.48	0	8,11,13	0.57	0
2	AR7	Q	805	2	10,10,11	0.53	0	8,11,13	0.51	0
2	AR7	R	805	2	10,10,11	0.64	0	8,11,13	0.57	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	AR7	J	805	2	-	0/9/9/11	0/0/0/0
2	AR7	K	805	2	-	0/9/9/11	0/0/0/0
2	AR7	L	805	2	-	0/9/9/11	0/0/0/0
2	AR7	M	805	2	-	0/9/9/11	0/0/0/0
2	AR7	N	805	2	-	0/9/9/11	0/0/0/0
2	AR7	P	805	2	-	0/9/9/11	0/0/0/0
2	AR7	Q	805	2	-	0/9/9/11	0/0/0/0
2	AR7	R	805	2	-	0/9/9/11	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	805	AR7	1	0
2	R	805	AR7	1	0

5.5 Carbohydrates

15 carbohydrates 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	$\# Z > 2$
4	NAG	A	951	1,4	14,14,15	0.55	0	15,19,21	0.86	1 (6%)
4	NAG	A	952	4	14,14,15	0.40	0	15,19,21	0.70	0
4	FUL	A	953	4	9,10,11	0.50	0	13,14,16	0.94	1 (7%)
4	BMA	A	954	4	11,11,12	0.36	0	13,15,17	1.43	2 (15%)
4	MAN	A	955	4	11,11,12	0.70	0	13,15,17	0.49	0
4	MAN	A	956	4	11,11,12	0.77	0	13,15,17	0.60	0
4	NAG	A	957	4	14,14,15	0.62	0	15,19,21	0.59	0
4	NAG	A	958	4	14,14,15	0.59	0	15,19,21	0.69	0
4	NAG	A	959	4	14,14,15	0.75	1 (7%)	15,19,21	0.57	0
4	GAL	A	960	4	11,11,12	0.59	0	13,15,17	0.40	0
4	GAL	A	961	4	11,11,12	0.48	0	13,15,17	0.52	0
7	NAG	G	951	1,7	14,14,15	0.74	0	15,19,21	0.92	1 (6%)
7	NAG	G	952	7	14,14,15	0.76	0	15,19,21	0.91	0
7	FUC	G	953	7	9,10,11	0.53	0	13,14,16	1.17	1 (7%)
7	BMA	G	954	7	11,11,12	0.81	0	13,15,17	0.76	1 (7%)

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
4	NAG	A	951	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	952	4	-	0/6/23/26	0/1/1/1
4	FUL	A	953	4	-	0/0/17/20	0/1/1/1
4	BMA	A	954	4	-	0/2/19/22	0/1/1/1
4	MAN	A	955	4	-	0/2/19/22	0/1/1/1
4	MAN	A	956	4	-	0/2/19/22	0/1/1/1
4	NAG	A	957	4	-	0/6/23/26	0/1/1/1
4	NAG	A	958	4	-	0/6/23/26	0/1/1/1
4	NAG	A	959	4	-	0/6/23/26	0/1/1/1
4	GAL	A	960	4	-	0/2/19/22	0/1/1/1
4	GAL	A	961	4	-	0/2/19/22	0/1/1/1
7	NAG	G	951	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	952	7	-	0/6/23/26	0/1/1/1
7	FUC	G	953	7	1/1/4/5	0/0/17/20	0/1/1/1
7	BMA	G	954	7	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	959	NAG	C1-C2	2.09	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	953	FUC	C1-C2-C3	-3.75	104.90	109.65
4	A	954	BMA	C6-C5-C4	-2.96	106.09	113.00
4	A	951	NAG	C2-N2-C7	-2.64	119.09	122.94
7	G	954	BMA	C2-C3-C4	-2.01	107.37	110.88
4	A	953	FUL	C1-C2-C3	2.06	112.26	109.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	953	FUC	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	951	NAG	1	0
4	A	952	NAG	1	0
4	A	955	MAN	2	0
4	A	958	NAG	2	0
7	G	952	NAG	2	0
7	G	954	BMA	2	0

5.6 Ligand geometry

Of 92 ligands modelled in this entry, 16 are monoatomic - leaving 76 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
6	SO4	A	4004	-	4,4,4	0.32	0	6,6,6	0.13	0
6	SO4	A	4005	-	4,4,4	0.38	0	6,6,6	0.07	0
6	SO4	A	4014	-	4,4,4	0.37	0	6,6,6	0.13	0
6	SO4	A	4025	-	4,4,4	0.33	0	6,6,6	0.11	0
6	SO4	A	4028	-	4,4,4	0.36	0	6,6,6	0.08	0
6	SO4	A	4054	-	4,4,4	0.37	0	6,6,6	0.11	0
6	SO4	A	4055	-	4,4,4	0.40	0	6,6,6	0.10	0
6	SO4	A	4061	-	4,4,4	0.35	0	6,6,6	0.15	0
6	SO4	A	4064	-	4,4,4	0.35	0	6,6,6	0.11	0
6	SO4	A	4066	-	4,4,4	0.37	0	6,6,6	0.08	0
6	SO4	A	4069	-	4,4,4	0.39	0	6,6,6	0.32	0
3	NAG	A	901	1	14,14,15	0.72	0	15,19,21	0.72	1 (6%)
6	SO4	B	4021	-	4,4,4	0.36	0	6,6,6	0.12	0
6	SO4	B	4022	-	4,4,4	0.34	0	6,6,6	0.21	0
6	SO4	B	4023	-	4,4,4	0.36	0	6,6,6	0.16	0
6	SO4	B	4026	-	4,4,4	0.33	0	6,6,6	0.17	0
6	SO4	B	4027	-	4,4,4	0.39	0	6,6,6	0.32	0
6	SO4	B	4050	-	4,4,4	0.33	0	6,6,6	0.10	0
3	NAG	B	901	1	14,14,15	0.65	0	15,19,21	0.74	1 (6%)
6	SO4	C	4007	-	4,4,4	0.34	0	6,6,6	0.05	0
6	SO4	C	4008	-	4,4,4	0.34	0	6,6,6	0.14	0
6	SO4	C	4010	-	4,4,4	0.38	0	6,6,6	0.08	0
6	SO4	C	4013	-	4,4,4	0.42	0	6,6,6	0.19	0
6	SO4	C	4058	-	4,4,4	0.37	0	6,6,6	0.09	0
6	SO4	C	4059	-	4,4,4	0.40	0	6,6,6	0.12	0
6	SO4	D	4011	-	4,4,4	0.39	0	6,6,6	0.06	0
6	SO4	D	4012	-	4,4,4	0.37	0	6,6,6	0.22	0
6	SO4	D	4015	-	4,4,4	0.37	0	6,6,6	0.08	0
6	SO4	D	4016	-	4,4,4	0.42	0	6,6,6	0.14	0
6	SO4	D	4018	-	4,4,4	0.34	0	6,6,6	0.18	0
6	SO4	D	4019	-	4,4,4	0.39	0	6,6,6	0.11	0
6	SO4	D	4020	-	4,4,4	0.38	0	6,6,6	0.11	0
6	SO4	D	4063	-	4,4,4	0.36	0	6,6,6	0.08	0
6	SO4	D	4065	-	4,4,4	0.36	0	6,6,6	0.07	0
6	SO4	E	4037	-	4,4,4	0.37	0	6,6,6	0.06	0
6	SO4	E	4038	-	4,4,4	0.31	0	6,6,6	0.10	0
6	SO4	E	4039	-	4,4,4	0.38	0	6,6,6	0.08	0
6	SO4	E	4040	-	4,4,4	0.37	0	6,6,6	0.11	0
6	SO4	E	4041	-	4,4,4	0.39	0	6,6,6	0.09	0
6	SO4	E	4046	-	4,4,4	0.35	0	6,6,6	0.11	0
6	SO4	E	4049	-	4,4,4	0.38	0	6,6,6	0.07	0
6	SO4	E	4060	-	4,4,4	0.35	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	E	4062	-	4,4,4	0.39	0	6,6,6	0.09	0
3	NAG	E	901	1	14,14,15	0.66	0	15,19,21	0.86	0
6	SO4	F	4002	-	4,4,4	0.35	0	6,6,6	0.10	0
6	SO4	F	4003	-	4,4,4	0.40	0	6,6,6	0.21	0
6	SO4	F	4036	-	4,4,4	0.36	0	6,6,6	0.11	0
6	SO4	F	4051	-	4,4,4	0.34	0	6,6,6	0.13	0
6	SO4	F	4056	-	4,4,4	0.36	0	6,6,6	0.12	0
6	SO4	F	4057	-	4,4,4	0.38	0	6,6,6	0.12	0
6	SO4	F	4067	-	4,4,4	0.38	0	6,6,6	0.06	0
6	SO4	F	4068	-	4,4,4	0.33	0	6,6,6	0.09	0
6	SO4	F	4070	-	4,4,4	0.42	0	6,6,6	0.30	0
3	NAG	F	901	1	14,14,15	0.58	0	15,19,21	0.70	0
3	NAG	F	951	1	14,14,15	0.64	0	15,19,21	0.80	0
6	SO4	G	4029	-	4,4,4	0.33	0	6,6,6	0.21	0
6	SO4	G	4030	-	4,4,4	0.34	0	6,6,6	0.15	0
6	SO4	G	4031	-	4,4,4	0.38	0	6,6,6	0.08	0
6	SO4	G	4032	-	4,4,4	0.39	0	6,6,6	0.13	0
6	SO4	G	4034	-	4,4,4	0.40	0	6,6,6	0.07	0
6	SO4	G	4035	-	4,4,4	0.38	0	6,6,6	0.20	0
6	SO4	H	4042	-	4,4,4	0.38	0	6,6,6	0.10	0
6	SO4	H	4043	-	4,4,4	0.35	0	6,6,6	0.06	0
6	SO4	H	4044	-	4,4,4	0.36	0	6,6,6	0.07	0
6	SO4	H	4045	-	4,4,4	0.36	0	6,6,6	0.15	0
6	SO4	H	4047	-	4,4,4	0.36	0	6,6,6	0.08	0
6	SO4	H	4048	-	4,4,4	0.35	0	6,6,6	0.12	0
3	NAG	H	901	1	14,14,15	0.66	0	15,19,21	1.01	1 (6%)
6	SO4	J	4001	-	4,4,4	0.35	0	6,6,6	0.12	0
6	SO4	K	4024	-	4,4,4	0.38	0	6,6,6	0.11	0
6	SO4	L	4009	-	4,4,4	0.37	0	6,6,6	0.15	0
6	SO4	M	4017	-	4,4,4	0.38	0	6,6,6	0.09	0
6	SO4	N	4006	-	4,4,4	0.36	0	6,6,6	0.14	0
6	SO4	P	4052	-	4,4,4	0.38	0	6,6,6	0.08	0
6	SO4	Q	4033	-	4,4,4	0.33	0	6,6,6	0.15	0
6	SO4	R	4053	-	4,4,4	0.37	0	6,6,6	0.08	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
6	SO4	A	4004	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	4005	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4014	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4025	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4028	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4054	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4055	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4061	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4064	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4066	-	-	0/0/0/0	0/0/0/0
6	SO4	A	4069	-	-	0/0/0/0	0/0/0/0
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
6	SO4	B	4021	-	-	0/0/0/0	0/0/0/0
6	SO4	B	4022	-	-	0/0/0/0	0/0/0/0
6	SO4	B	4023	-	-	0/0/0/0	0/0/0/0
6	SO4	B	4026	-	-	0/0/0/0	0/0/0/0
6	SO4	B	4027	-	-	0/0/0/0	0/0/0/0
6	SO4	B	4050	-	-	0/0/0/0	0/0/0/0
3	NAG	B	901	1	-	0/6/23/26	0/1/1/1
6	SO4	C	4007	-	-	0/0/0/0	0/0/0/0
6	SO4	C	4008	-	-	0/0/0/0	0/0/0/0
6	SO4	C	4010	-	-	0/0/0/0	0/0/0/0
6	SO4	C	4013	-	-	0/0/0/0	0/0/0/0
6	SO4	C	4058	-	-	0/0/0/0	0/0/0/0
6	SO4	C	4059	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4011	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4012	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4015	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4016	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4018	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4019	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4020	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4063	-	-	0/0/0/0	0/0/0/0
6	SO4	D	4065	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4037	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4038	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4039	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4040	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4041	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4046	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4049	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4060	-	-	0/0/0/0	0/0/0/0
6	SO4	E	4062	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	901	1	-	0/6/23/26	0/1/1/1
6	SO4	F	4002	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4003	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4036	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4051	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4056	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4057	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4067	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4068	-	-	0/0/0/0	0/0/0/0
6	SO4	F	4070	-	-	0/0/0/0	0/0/0/0
3	NAG	F	901	1	-	0/6/23/26	0/1/1/1
3	NAG	F	951	1	-	1/6/23/26	0/1/1/1
6	SO4	G	4029	-	-	0/0/0/0	0/0/0/0
6	SO4	G	4030	-	-	0/0/0/0	0/0/0/0
6	SO4	G	4031	-	-	0/0/0/0	0/0/0/0
6	SO4	G	4032	-	-	0/0/0/0	0/0/0/0
6	SO4	G	4034	-	-	0/0/0/0	0/0/0/0
6	SO4	G	4035	-	-	0/0/0/0	0/0/0/0
6	SO4	H	4042	-	-	0/0/0/0	0/0/0/0
6	SO4	H	4043	-	-	0/0/0/0	0/0/0/0
6	SO4	H	4044	-	-	0/0/0/0	0/0/0/0
6	SO4	H	4045	-	-	0/0/0/0	0/0/0/0
6	SO4	H	4047	-	-	0/0/0/0	0/0/0/0
6	SO4	H	4048	-	-	0/0/0/0	0/0/0/0
3	NAG	H	901	1	-	0/6/23/26	0/1/1/1
6	SO4	J	4001	-	-	0/0/0/0	0/0/0/0
6	SO4	K	4024	-	-	0/0/0/0	0/0/0/0
6	SO4	L	4009	-	-	0/0/0/0	0/0/0/0
6	SO4	M	4017	-	-	0/0/0/0	0/0/0/0
6	SO4	N	4006	-	-	0/0/0/0	0/0/0/0
6	SO4	P	4052	-	-	0/0/0/0	0/0/0/0
6	SO4	Q	4033	-	-	0/0/0/0	0/0/0/0
6	SO4	R	4053	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	901	NAG	C2-N2-C7	-2.46	119.35	122.94
3	A	901	NAG	C2-N2-C7	-2.11	119.87	122.94
3	B	901	NAG	C2-N2-C7	-2.05	119.95	122.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	951	NAG	O7-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4069	SO4	1	0
6	B	4027	SO4	1	0
3	B	901	NAG	1	0
6	D	4012	SO4	1	0
6	E	4060	SO4	1	0
6	E	4062	SO4	1	0
6	F	4070	SO4	1	0
3	F	951	NAG	1	0
6	G	4029	SO4	1	0
6	L	4009	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 [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	470/471 (99%)	-0.80	1 (0%) 94 95	8, 18, 31, 52	17 (3%)
1	B	468/471 (99%)	-0.75	2 (0%) 92 91	8, 18, 33, 52	13 (2%)
1	C	467/471 (99%)	-0.80	4 (0%) 84 81	8, 18, 32, 49	22 (4%)
1	D	467/471 (99%)	-0.66	7 (1%) 74 69	9, 21, 37, 61	20 (4%)
1	E	467/471 (99%)	-0.78	2 (0%) 92 91	7, 19, 33, 52	18 (3%)
1	F	468/471 (99%)	-0.81	1 (0%) 94 95	7, 18, 31, 47	15 (3%)
1	G	467/471 (99%)	-0.82	0 100 100	8, 17, 28, 42	17 (3%)
1	H	466/471 (98%)	-0.74	3 (0%) 89 88	8, 20, 36, 55	19 (4%)
2	J	3/6 (50%)	-1.37	0 100 100	11, 11, 15, 17	0
2	K	3/6 (50%)	-0.98	0 100 100	14, 14, 18, 18	0
2	L	3/6 (50%)	-1.49	0 100 100	12, 12, 16, 17	0
2	M	3/6 (50%)	-0.83	0 100 100	15, 15, 19, 20	0
2	N	3/6 (50%)	-1.45	0 100 100	11, 11, 14, 16	0
2	P	3/6 (50%)	-1.40	0 100 100	11, 11, 16, 19	0
2	Q	3/6 (50%)	-1.23	0 100 100	11, 11, 18, 18	0
2	R	3/6 (50%)	-0.90	0 100 100	14, 14, 19, 20	0
All	All	3764/3816 (98%)	-0.77	20 (0%) 90 89	7, 19, 33, 61	141 (3%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	109	VAL	4.8
1	D	127	VAL	4.7
1	D	129	GLN	3.4
1	D	109	VAL	3.3
1	C	575	PRO	3.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	AR7	L	805	11/12	0.98	0.09	-	13,14,15,15	0
2	AR7	N	805	11/12	0.97	0.11	-	9,11,15,16	0
2	AR7	R	805	11/12	0.95	0.12	-	15,15,17,18	0
2	AR7	K	805	11/12	0.96	0.11	-	9,12,16,16	0
2	AR7	M	805	11/12	0.95	0.12	-	15,16,17,18	0
2	AR7	P	805	11/12	0.97	0.11	-	11,14,16,17	0
2	AR7	Q	805	11/12	0.98	0.10	-	13,13,15,15	0
2	AR7	J	805	11/12	0.97	0.09	-	13,14,15,16	0

6.3 Carbohydrates [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	951	14/15	0.91	0.18	1.37	33,35,44,44	0
4	FUL	A	953	10/11	0.94	0.11	-	25,28,29,30	0
4	NAG	A	957	14/15	0.84	0.29	-	57,59,61,63	0
4	NAG	A	952	14/15	0.92	0.18	-	41,43,46,49	0
4	MAN	A	955	11/12	0.91	0.16	-	51,52,54,56	0
7	NAG	G	952	14/15	0.89	0.30	-	39,46,48,51	0
4	NAG	A	959	14/15	0.81	0.34	-	62,64,64,65	1
4	BMA	A	954	11/12	0.90	0.24	-	51,53,57,58	0
4	GAL	A	960	11/12	0.87	0.41	-	64,64,65,65	3
7	BMA	G	954	11/12	0.66	0.39	-	54,56,57,57	0
7	FUC	G	953	10/11	0.94	0.20	-	38,39,40,41	0
7	NAG	G	951	14/15	0.94	0.17	-	30,32,37,39	0
4	MAN	A	956	11/12	0.76	0.40	-	59,62,63,63	0
4	GAL	A	961	11/12	0.90	0.41	-	59,60,61,62	0
4	NAG	A	958	14/15	0.86	0.30	-	44,51,53,56	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	A	4014	5/5	0.92	0.20	6.74	82,82,82,82	0
6	SO4	E	4060	5/5	0.95	0.27	6.16	72,72,74,74	0
6	SO4	E	4039	5/5	0.86	0.21	5.81	83,83,84,84	0
6	SO4	D	4012	5/5	0.86	0.22	4.56	73,74,75,75	0
6	SO4	A	4069	5/5	0.91	0.19	4.10	65,65,67,67	0
6	SO4	D	4015	5/5	0.99	0.15	3.69	41,42,43,43	0
6	SO4	C	4013	5/5	0.82	0.23	3.51	63,63,65,66	0
6	SO4	G	4032	5/5	0.97	0.17	3.38	48,48,50,50	0
6	SO4	A	4064	5/5	0.88	0.23	3.27	91,91,91,92	0
6	SO4	B	4027	5/5	0.86	0.19	2.80	62,63,64,65	0
6	SO4	F	4070	5/5	0.87	0.20	2.59	61,61,63,63	0
6	SO4	G	4030	5/5	0.89	0.17	2.39	53,54,55,56	0
6	SO4	A	4004	5/5	0.97	0.14	2.17	49,49,49,49	0
6	SO4	C	4059	5/5	0.91	0.20	1.82	64,64,65,66	0
6	SO4	H	4048	5/5	0.92	0.18	1.71	90,90,90,90	0
6	SO4	C	4008	5/5	0.95	0.15	1.53	58,58,58,59	0
6	SO4	G	4029	5/5	0.94	0.16	1.38	67,68,68,68	0
6	SO4	D	4018	5/5	0.97	0.13	0.68	61,61,62,62	0
6	SO4	A	4028	5/5	0.95	0.17	0.54	66,66,67,67	0
6	SO4	H	4043	5/5	0.98	0.11	0.07	55,55,56,56	0
6	SO4	F	4036	5/5	0.98	0.12	-0.03	47,47,47,47	0
5	CA	B	3003	1/1	0.97	0.07	-1.75	18,18,18,18	0
6	SO4	F	4003	5/5	0.97	0.09	-1.78	40,41,42,42	0
5	CA	E	3009	1/1	0.99	0.07	-1.80	21,21,21,21	0
5	CA	C	3005	1/1	0.99	0.06	-2.02	21,21,21,21	0
5	CA	H	3016	1/1	0.99	0.04	-2.46	16,16,16,16	0
5	CA	G	3013	1/1	0.99	0.05	-2.48	19,19,19,19	0
5	CA	E	3010	1/1	0.99	0.04	-2.51	9,9,9,9	0
5	CA	D	3008	1/1	0.99	0.04	-2.86	16,16,16,16	0
5	CA	A	3001	1/1	0.99	0.03	-2.94	17,17,17,17	0
5	CA	D	3007	1/1	0.97	0.04	-2.96	29,29,29,29	0
5	CA	F	3011	1/1	0.99	0.03	-3.42	19,19,19,19	0
5	CA	H	3015	1/1	0.97	0.03	-3.48	35,35,35,35	0
5	CA	B	3004	1/1	0.99	0.03	-3.59	11,11,11,11	0
5	CA	G	3014	1/1	0.98	0.04	-3.78	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	C	3006	1/1	0.99	0.04	-4.00	10,10,10,10	0
5	CA	A	3002	1/1	1.00	0.01	-4.10	7,7,7,7	0
5	CA	F	3012	1/1	0.99	0.04	-4.95	12,12,12,12	0
6	SO4	D	4011	5/5	0.97	0.29	-	67,68,68,69	0
6	SO4	A	4061	5/5	0.94	0.25	-	64,65,65,65	0
6	SO4	D	4019	5/5	0.93	0.23	-	76,77,78,78	0
6	SO4	H	4047	5/5	0.88	0.34	-	87,87,88,88	0
6	SO4	A	4054	5/5	0.91	0.23	-	80,80,80,80	0
6	SO4	N	4006	5/5	0.99	0.09	-	36,36,38,38	0
6	SO4	B	4021	5/5	0.88	0.19	-	85,85,86,86	0
6	SO4	B	4022	5/5	0.97	0.09	-	45,47,48,48	0
6	SO4	P	4052	5/5	0.96	0.16	-	66,66,66,66	0
6	SO4	J	4001	5/5	0.98	0.17	-	41,42,43,44	0
6	SO4	D	4016	5/5	0.80	0.32	-	90,90,90,91	0
6	SO4	D	4020	5/5	0.91	0.26	-	82,82,83,83	0
6	SO4	D	4063	5/5	0.91	0.32	-	91,91,91,91	0
6	SO4	E	4041	5/5	0.94	0.22	-	63,63,64,64	0
3	NAG	B	901	14/15	0.73	0.41	-	53,58,60,60	0
6	SO4	H	4045	5/5	0.96	0.17	-	71,71,72,72	0
3	NAG	F	901	14/15	0.78	0.37	-	54,59,61,62	0
6	SO4	A	4005	5/5	0.93	0.27	-	84,84,85,85	0
6	SO4	A	4055	5/5	0.94	0.28	-	72,72,73,73	0
6	SO4	E	4049	5/5	0.94	0.27	-	77,78,78,78	0
6	SO4	C	4007	5/5	0.95	0.24	-	72,72,73,73	0
6	SO4	E	4038	5/5	0.98	0.14	-	51,51,52,52	0
6	SO4	F	4068	5/5	0.94	0.28	-	75,76,77,77	0
6	SO4	A	4025	5/5	0.98	0.17	-	41,41,42,43	0
3	NAG	E	901	14/15	0.63	0.39	-	52,55,58,59	3
3	NAG	A	901	14/15	0.82	0.34	-	45,50,52,52	0
6	SO4	E	4037	5/5	0.96	0.18	-	58,59,60,60	0
6	SO4	C	4010	5/5	0.87	0.26	-	89,89,90,90	0
6	SO4	H	4044	5/5	0.96	0.24	-	71,72,72,72	0
6	SO4	H	4042	5/5	0.94	0.24	-	58,59,60,60	0
6	SO4	B	4023	5/5	0.93	0.20	-	63,64,64,64	0
3	NAG	F	951	14/15	0.75	0.43	-	55,58,59,59	0
6	SO4	L	4009	5/5	0.99	0.10	-	33,33,34,34	0
6	SO4	G	4034	5/5	0.90	0.20	-	77,77,78,78	0
6	SO4	B	4026	5/5	0.95	0.16	-	52,52,53,54	0
6	SO4	D	4065	5/5	0.84	0.26	-	86,86,87,87	0
6	SO4	F	4056	5/5	0.89	0.24	-	100,100,100,100	0
6	SO4	E	4062	5/5	0.90	0.36	-	89,90,90,90	0
6	SO4	G	4031	5/5	0.94	0.24	-	74,74,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	SO4	C	4058	5/5	0.92	0.21	-	80,80,81,81	0
6	SO4	F	4002	5/5	0.95	0.22	-	61,62,62,63	0
6	SO4	E	4046	5/5	0.97	0.17	-	63,63,64,64	0
6	SO4	G	4035	5/5	0.93	0.24	-	58,58,59,59	0
3	NAG	H	901	14/15	0.63	0.43	-	58,64,66,66	0
6	SO4	A	4066	5/5	0.93	0.24	-	94,94,95,95	0
6	SO4	K	4024	5/5	0.97	0.17	-	61,61,62,62	0
6	SO4	E	4040	5/5	0.87	0.27	-	85,85,86,86	0
6	SO4	F	4067	5/5	0.94	0.36	-	95,95,96,96	0
6	SO4	M	4017	5/5	0.92	0.20	-	82,82,83,83	0
6	SO4	F	4057	5/5	0.84	0.37	-	89,90,90,91	0
6	SO4	B	4050	5/5	0.94	0.23	-	71,71,72,72	0
6	SO4	Q	4033	5/5	0.98	0.16	-	46,47,47,48	0
6	SO4	F	4051	5/5	0.92	0.24	-	76,76,77,77	0
6	SO4	R	4053	5/5	0.93	0.27	-	81,81,81,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.