Full wwPDB X-ray Structure Validation Report (i)

Jan 25, 2017 – 06:07 PM EST

PDB ID	:	3PKJ
Title	:	Human SIRT6 crystal structure in complex with 2'-N-Acetyl ADP ribose
Authors	:	Pan, P.W.; Dong, A.; Qiu, W.; Loppnau, P.; Wang, J.; Ravichandran, M.; Walker, J.R.; Bountra, C.; Weigelt, J.; Arrowsmith, C.H.; Min, J.; Edwards, A.M.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-11-11
Resolution	:	2.12 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

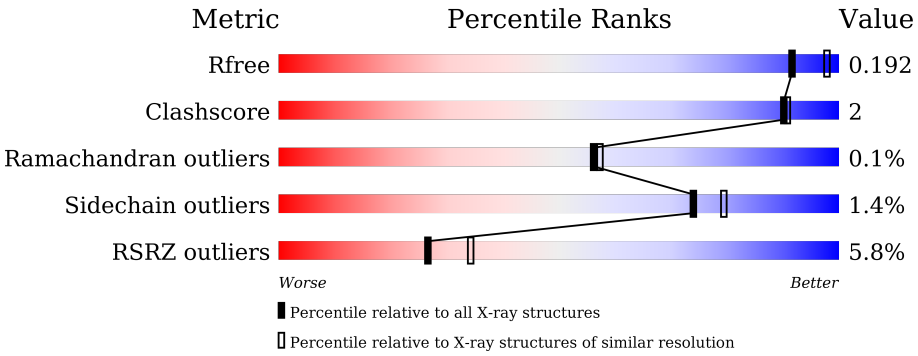
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	91344	4587 (2.14-2.10)
Clashscore	102246	5132 (2.14-2.10)
Ramachandran outliers	100387	5080 (2.14-2.10)
Sidechain outliers	100360	5081 (2.14-2.10)
RSRZ outliers	91569	4597 (2.14-2.10)

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 <=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	355	3% 76% • 22%
1	B	355	4% 73% 6% 21%
1	C	355	6% 72% 5% 22%
1	D	355	6% 71% 6% 22%
1	E	355	5% 73% 6% 22%
1	F	355	4% 73% 5% 22%

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
5	UNX	C	363	-	-	-	X
5	UNX	E	357	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13208 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.

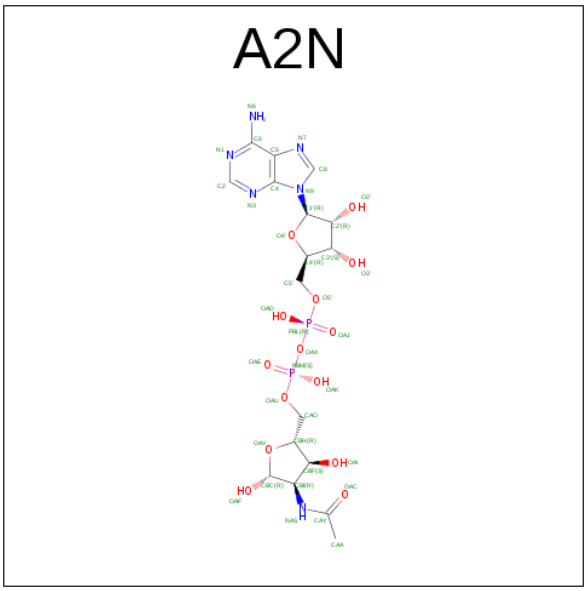
- Molecule 1 is a protein called NAD-dependent deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2050	1293	364	382	11			
1	B	280	Total	C	N	O	S	0	0	0
			2091	1314	371	395	11			
1	C	276	Total	C	N	O	S	0	0	0
			2083	1307	377	388	11			
1	D	276	Total	C	N	O	S	0	0	0
			2067	1307	371	379	10			
1	E	278	Total	C	N	O	S	0	0	0
			2049	1295	358	385	11			
1	F	277	Total	C	N	O	S	0	1	0
			2038	1281	367	379	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
A	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
B	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
B	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
C	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
C	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
D	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
D	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
E	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
E	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7
F	-1	GLY	-	EXPRESSION TAG	UNP Q8N6T7
F	265	GLU	LYS	ENGINEERED MUTATION	UNP Q8N6T7

- Molecule 2 is [(2R,3S,4R,5R)-4-(ACETYLAMINO)-3,5-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (three-letter code: A2N) (formula: $C_{17}H_{26}N_6O_{14}P_2$).

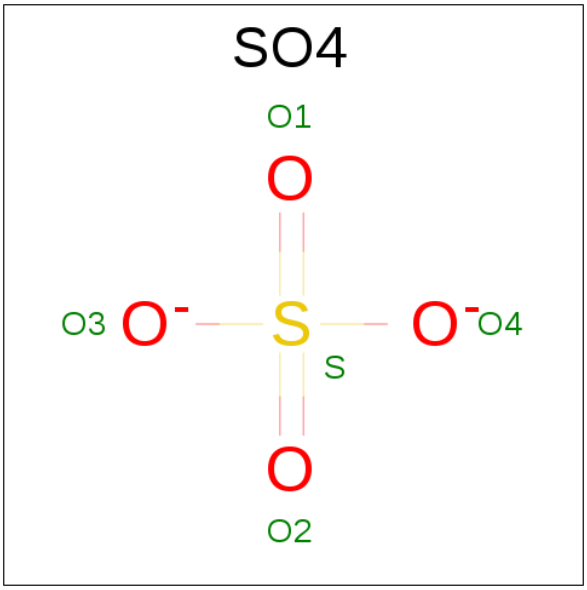


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
2	B	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
2	C	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
2	D	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
2	E	1	Total	C	N	O	P	0	0
			39	17	6	14	2		
2	F	1	Total	C	N	O	P	0	0
			39	17	6	14	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total X 3 3	0	0
5	E	4	Total X 4 4	0	0
5	B	5	Total X 5 5	0	0
5	C	12	Total X 12 12	0	0
5	A	3	Total X 3 3	0	0
5	F	8	Total X 8 8	0	0

- Molecule 6 is water.

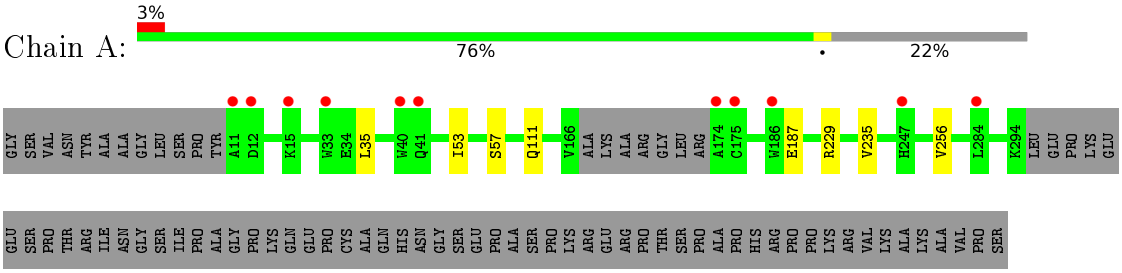
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	90	Total O 91 91	0	1
6	B	86	Total O 88 88	0	2
6	C	70	Total O 71 71	0	1
6	D	93	Total O 93 93	0	0
6	E	78	Total O 80 80	0	2
6	F	69	Total O 72 72	0	3

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 errors 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.

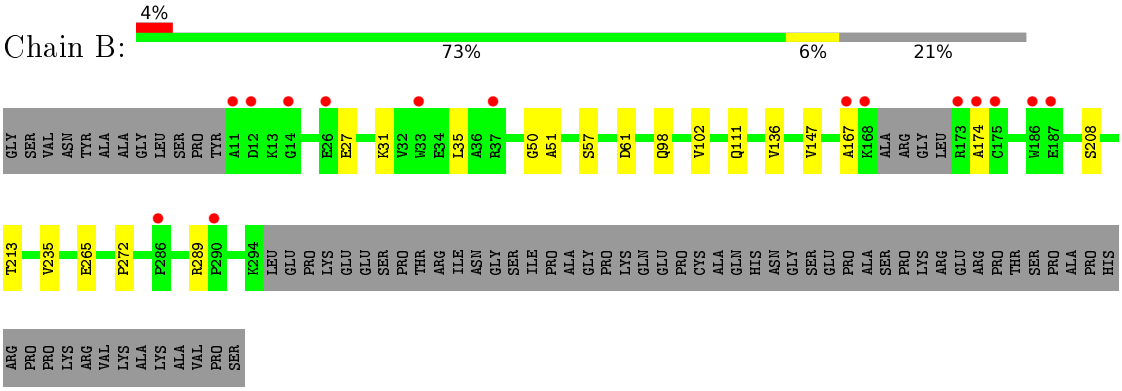
- Molecule 1: NAD-dependent deacetylase sirtuin-6

Chain A:



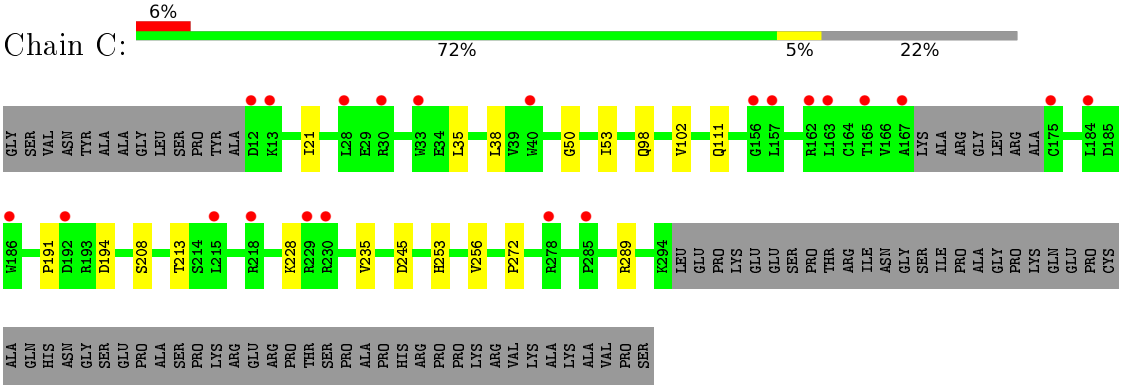
- Molecule 1: NAD-dependent deacetylase sirtuin-6

Chain B:

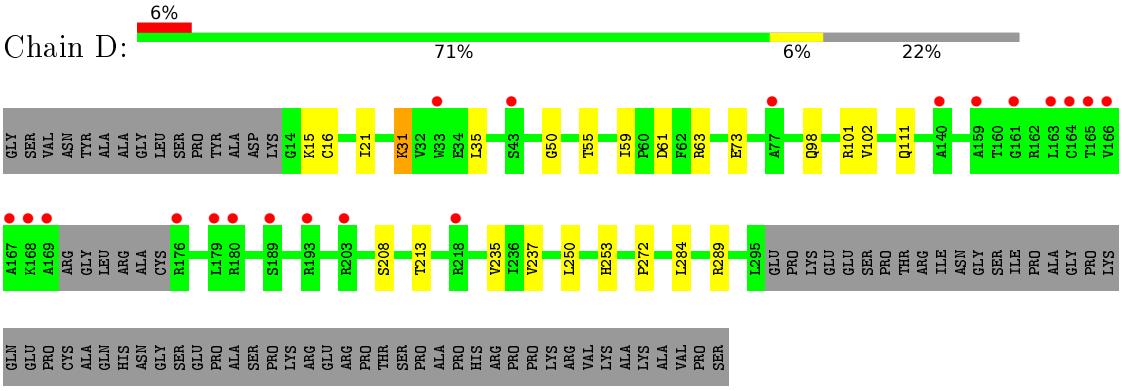


- Molecule 1: NAD-dependent deacetylase sirtuin-6

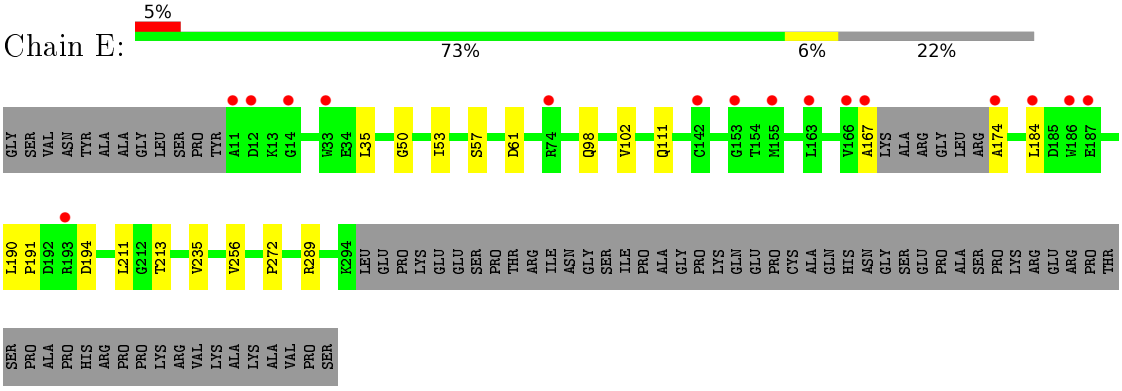
Chain C:



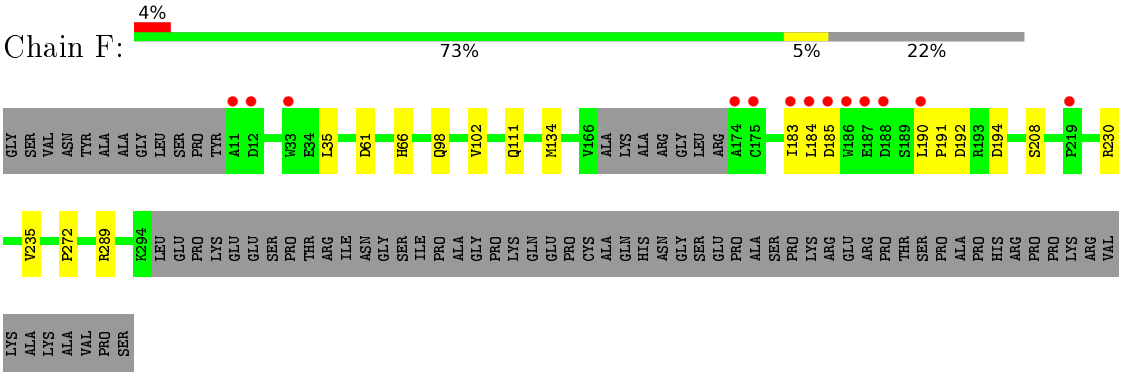
- Molecule 1: NAD-dependent deacetylase sirtuin-6



- Molecule 1: NAD-dependent deacetylase sirtuin-6



- Molecule 1: NAD-dependent deacetylase sirtuin-6



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.04Å 135.78Å 89.11Å 90.00° 120.02° 90.00°	Depositor
Resolution (Å)	20.50 – 2.12 20.50 – 2.12	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.50-2.12) 96.1 (20.50-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.11Å)	Xtriage
Refinement program	BUSTER 2.8.0, COOT 0.6	Depositor
R, R_{free}	0.234 , 0.265 0.187 , 0.192	Depositor DCC
R_{free} test set	4924 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 21.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.247 for l,k,-h-l 0.247 for -h-l,k,h 0.166 for h,-k,-h-l 0.164 for l,-k,h 0.145 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13208	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UNX, ZN, SO4, A2N

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	0.50	0/2097	0.55	0/2865
1	B	0.49	0/2138	0.56	0/2917
1	C	0.50	0/2130	0.55	0/2902
1	D	0.51	0/2114	0.57	0/2884
1	E	0.49	0/2096	0.56	0/2863
1	F	0.50	0/2085	0.56	0/2843
All	All	0.50	0/12660	0.56	0/17274

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

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	2050	0	1952	3	0
1	B	2091	0	1989	9	0
1	C	2083	0	2002	9	0
1	D	2067	0	2002	13	0
1	E	2049	0	1941	11	0
1	F	2038	0	1895	9	0
2	A	39	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	24	2	0
2	C	39	0	24	1	0
2	D	39	0	24	2	0
2	E	39	0	24	3	0
2	F	39	0	24	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	B	15	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	15	0	0	0	0
4	F	15	0	0	0	0
5	A	3	0	0	0	0
5	B	5	0	0	0	0
5	C	12	0	0	0	0
5	D	3	0	0	0	0
5	E	4	0	0	0	0
5	F	8	0	0	0	0
6	A	91	0	0	0	0
6	B	88	0	0	0	0
6	C	71	0	0	0	0
6	D	93	0	0	1	0
6	E	80	0	0	0	0
6	F	72	0	0	0	0
All	All	13208	0	11925	57	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 2.

All (57) 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:F:134:MET:HA	1:F:183:ILE:HD11	1.83	0.60
1:F:184:LEU:HD21	1:F:190:LEU:HA	1.85	0.59
1:F:184:LEU:HD11	1:F:191:PRO:HD3	1.86	0.56
1:F:35:LEU:HD13	1:F:235:VAL:HG11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD13	1:D:235:VAL:HG11	1.89	0.54
1:E:35:LEU:HD13	1:E:235:VAL:HG11	1.89	0.54
1:C:245:ASP:HB3	1:D:73:GLU:HG3	1.90	0.53
1:A:35:LEU:HD13	1:A:235:VAL:HG11	1.91	0.53
1:E:102:VAL:HB	1:E:289:ARG:HB3	1.94	0.50
1:E:191:PRO:HG2	1:E:194:ASP:HB2	1.93	0.49
1:C:35:LEU:HD13	1:C:235:VAL:HG11	1.94	0.49
1:F:102:VAL:HB	1:F:289:ARG:HB3	1.94	0.49
1:E:50:GLY:HA3	1:E:213:THR:HB	1.95	0.48
1:B:102:VAL:HB	1:B:289:ARG:HB3	1.94	0.48
2:B:1000:A2N:HBI	2:B:1000:A2N:HAA	1.66	0.48
1:C:102:VAL:HB	1:C:289:ARG:HB3	1.95	0.47
1:A:53:ILE:HG22	1:A:256:VAL:HG21	1.95	0.47
1:B:51:ALA:HB1	1:B:61:ASP:HA	1.97	0.47
2:E:1000:A2N:HBI	2:E:1000:A2N:HAA	1.66	0.47
1:D:102:VAL:HB	1:D:289:ARG:HB3	1.95	0.46
1:E:167:ALA:HA	1:E:174:ALA:HA	1.97	0.46
1:B:27:GLU:HG2	1:B:31:LYS:HE3	1.98	0.46
1:D:31:LYS:HG3	1:D:250:LEU:HD11	1.98	0.45
1:D:101:ARG:HH12	1:D:284:LEU:HD12	1.82	0.45
1:B:167:ALA:HA	1:B:174:ALA:HA	1.98	0.45
1:B:98:GLN:HB2	1:B:272:PRO:HD3	1.99	0.44
2:A:1000:A2N:HBI	2:A:1000:A2N:HAA	1.67	0.44
1:B:50:GLY:HA3	1:B:213:THR:HB	2.00	0.44
1:D:16:CYS:SG	1:D:63:ARG:HG2	2.57	0.44
1:E:184:LEU:HD11	1:E:190:LEU:HA	1.99	0.44
1:E:98:GLN:HB2	1:E:272:PRO:HD3	2.00	0.43
1:F:98:GLN:HB2	1:F:272:PRO:HD3	2.00	0.43
1:B:136:VAL:HG22	1:B:147:VAL:HG22	2.01	0.43
1:E:211:LEU:HB3	1:E:256:VAL:HG21	2.01	0.43
1:D:237:VAL:CG1	6:D:417:HOH:O	2.66	0.42
1:C:50:GLY:HA3	1:C:213:THR:HB	2.02	0.42
2:F:1000:A2N:HBI	2:F:1000:A2N:HAA	1.66	0.42
1:C:111:GLN:OE1	2:C:1000:A2N:HAO	2.20	0.42
1:D:21:ILE:HB	1:D:253:HIS:CD2	2.55	0.42
1:D:55:THR:HA	1:D:59:ILE:O	2.20	0.42
1:D:61:ASP:OD1	2:D:1000:A2N:H8	2.20	0.42
1:F:191:PRO:HG2	1:F:194:ASP:HB2	2.01	0.42
1:E:61:ASP:OD1	2:E:1000:A2N:H8	2.20	0.41
1:F:111:GLN:OE1	2:F:1000:A2N:HAO	2.20	0.41
1:C:53:ILE:HA	1:C:256:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLN:HB2	1:C:272:PRO:HD3	2.01	0.41
1:E:53:ILE:HG22	1:E:256:VAL:HG11	2.02	0.41
1:B:35:LEU:HD13	1:B:235:VAL:HG11	2.02	0.41
1:C:21:ILE:HB	1:C:253:HIS:CD2	2.56	0.41
1:D:111:GLN:OE1	2:D:1000:A2N:HAO	2.21	0.41
1:A:111:GLN:OE1	2:A:1000:A2N:HAO	2.21	0.41
1:D:98:GLN:HB2	1:D:272:PRO:HD3	2.02	0.41
1:B:111:GLN:OE1	2:B:1000:A2N:HAO	2.21	0.40
1:C:191:PRO:HG2	1:C:194:ASP:HB2	2.04	0.40
1:F:61:ASP:OD1	2:F:1000:A2N:H8	2.21	0.40
1:E:111:GLN:OE1	2:E:1000:A2N:HAO	2.21	0.40
1:D:50:GLY:HA3	1:D:213:THR:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/355 (77%)	271 (99%)	2 (1%)	0	100	100
1	B	276/355 (78%)	274 (99%)	2 (1%)	0	100	100
1	C	272/355 (77%)	270 (99%)	2 (1%)	0	100	100
1	D	272/355 (77%)	270 (99%)	2 (1%)	0	100	100
1	E	274/355 (77%)	270 (98%)	4 (2%)	0	100	100
1	F	274/355 (77%)	270 (98%)	3 (1%)	1 (0%)	39	36
All	All	1641/2130 (77%)	1625 (99%)	15 (1%)	1 (0%)	56	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	192	ASP

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	208/297 (70%)	205 (99%)	3 (1%)	74	79
1	B	213/297 (72%)	210 (99%)	3 (1%)	74	79
1	C	215/297 (72%)	212 (99%)	3 (1%)	74	79
1	D	212/297 (71%)	209 (99%)	3 (1%)	74	79
1	E	205/297 (69%)	204 (100%)	1 (0%)	92	95
1	F	196/297 (66%)	192 (98%)	4 (2%)	63	67
All	All	1249/1782 (70%)	1232 (99%)	17 (1%)	74	79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	187	GLU
1	A	229	ARG
1	B	57	SER
1	B	208	SER
1	B	265	GLU
1	C	38	LEU
1	C	208	SER
1	C	228	LYS
1	D	15	LYS
1	D	31	LYS
1	D	208	SER
1	E	57	SER
1	F	66	HIS
1	F	185	ASP
1	F	208	SER
1	F	230	ARG

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 35 are unknown and 6 are monoatomic - leaving 18 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	$\#\|Z\|>2$
2	A2N	A	1000	-	37,42,42	1.01	2 (5%)	38,64,64	1.91	3 (7%)
4	SO4	A	1008	-	4,4,4	0.21	0	6,6,6	0.07	0
2	A2N	B	1000	-	37,42,42	1.03	2 (5%)	38,64,64	1.89	2 (5%)
4	SO4	B	1005	-	4,4,4	0.26	0	6,6,6	0.11	0
4	SO4	B	1006	-	4,4,4	0.20	0	6,6,6	0.08	0
4	SO4	B	1011	-	4,4,4	0.36	0	6,6,6	0.11	0
2	A2N	C	1000	-	37,42,42	0.93	2 (5%)	38,64,64	1.97	3 (7%)
4	SO4	C	1003	-	4,4,4	0.40	0	6,6,6	0.12	0
2	A2N	D	1000	-	37,42,42	0.98	2 (5%)	38,64,64	1.97	4 (10%)
4	SO4	D	355	-	4,4,4	0.29	0	6,6,6	0.09	0
2	A2N	E	1000	-	37,42,42	0.98	2 (5%)	38,64,64	1.82	2 (5%)
4	SO4	E	1002	-	4,4,4	0.56	0	6,6,6	0.12	0
4	SO4	E	1007	-	4,4,4	0.22	0	6,6,6	0.05	0
4	SO4	E	1010	-	4,4,4	0.24	0	6,6,6	0.09	0
2	A2N	F	1000	-	37,42,42	1.14	2 (5%)	38,64,64	1.82	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	F	1001	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	F	1004	-	4,4,4	0.09	0	6,6,6	0.09	0
4	SO4	F	1009	-	4,4,4	0.87	0	6,6,6	0.10	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	A2N	A	1000	-	-	0/22/58/58	0/4/4/4
4	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
2	A2N	B	1000	-	-	0/22/58/58	0/4/4/4
4	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1011	-	-	0/0/0/0	0/0/0/0
2	A2N	C	1000	-	-	0/22/58/58	0/4/4/4
4	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
2	A2N	D	1000	-	-	0/22/58/58	0/4/4/4
4	SO4	D	355	-	-	0/0/0/0	0/0/0/0
2	A2N	E	1000	-	-	0/22/58/58	0/4/4/4
4	SO4	E	1002	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1010	-	-	0/0/0/0	0/0/0/0
2	A2N	F	1000	-	-	0/22/58/58	0/4/4/4
4	SO4	F	1001	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	F	1009	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1000	A2N	PBL-OAJ	2.04	1.58	1.51
2	A	1000	A2N	PBL-OAJ	2.04	1.58	1.51
2	C	1000	A2N	PBL-OAJ	2.28	1.59	1.51
2	B	1000	A2N	PBL-OAJ	2.38	1.59	1.51
2	E	1000	A2N	PBL-OAJ	2.66	1.61	1.51
2	E	1000	A2N	OAV-CBC	2.67	1.45	1.42
2	F	1000	A2N	PBL-OAJ	2.72	1.61	1.51
2	D	1000	A2N	OAV-CBC	2.98	1.46	1.42
2	B	1000	A2N	OAV-CBC	2.99	1.46	1.42
2	A	1000	A2N	OAV-CBC	3.05	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1000	A2N	OAV-CBC	3.06	1.46	1.42
2	F	1000	A2N	OAV-CBC	3.28	1.46	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1000	A2N	N3-C2-N1	-9.80	121.18	128.87
2	C	1000	A2N	N3-C2-N1	-9.72	121.24	128.87
2	B	1000	A2N	N3-C2-N1	-9.65	121.29	128.87
2	A	1000	A2N	N3-C2-N1	-9.56	121.36	128.87
2	F	1000	A2N	N3-C2-N1	-9.25	121.61	128.87
2	E	1000	A2N	N3-C2-N1	-9.09	121.73	128.87
2	A	1000	A2N	C4'-O4'-C1'	-3.47	105.97	109.64
2	B	1000	A2N	C4'-O4'-C1'	-3.21	106.24	109.64
2	E	1000	A2N	C4'-O4'-C1'	-3.20	106.25	109.64
2	D	1000	A2N	C4'-O4'-C1'	-2.98	106.48	109.64
2	C	1000	A2N	C4'-O4'-C1'	-2.90	106.57	109.64
2	F	1000	A2N	C4'-O4'-C1'	-2.67	106.82	109.64
2	F	1000	A2N	C1'-N9-C4	-2.25	124.29	126.81
2	D	1000	A2N	C1'-N9-C4	-2.23	124.32	126.81
2	A	1000	A2N	C1'-N9-C4	-2.05	124.52	126.81
2	D	1000	A2N	OAC-CAY-NAS	2.36	126.66	121.84
2	C	1000	A2N	OAC-CAY-NAS	2.47	126.89	121.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	A2N	2	0
2	B	1000	A2N	2	0
2	C	1000	A2N	1	0
2	D	1000	A2N	2	0
2	E	1000	A2N	3	0
2	F	1000	A2N	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	277/355 (78%)	0.53	11 (3%)	42	51	17, 31, 50, 77	0
1	B	280/355 (78%)	0.61	15 (5%)	29	37	18, 33, 55, 90	0
1	C	276/355 (77%)	0.61	22 (7%)	15	20	18, 33, 53, 82	0
1	D	276/355 (77%)	0.60	20 (7%)	18	25	19, 33, 54, 77	0
1	E	278/355 (78%)	0.58	16 (5%)	26	34	22, 36, 57, 81	0
1	F	277/355 (78%)	0.60	13 (4%)	35	44	20, 35, 58, 75	0
All	All	1664/2130 (78%)	0.59	97 (5%)	26	34	17, 33, 55, 90	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	ARG	10.3
1	E	11	ALA	9.7
1	A	11	ALA	9.0
1	F	186	TRP	7.9
1	D	169	ALA	7.0
1	A	174	ALA	6.6
1	F	174	ALA	6.1
1	A	12	ASP	6.0
1	C	33	TRP	5.9
1	D	33	TRP	5.5
1	F	190	LEU	5.3
1	B	167	ALA	5.3
1	B	168	LYS	5.2
1	B	174	ALA	5.0
1	F	33	TRP	5.0
1	D	167	ALA	4.7
1	C	184	LEU	4.6
1	E	12	ASP	4.6
1	A	186	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	11	ALA	4.4
1	D	163	LEU	4.3
1	B	11	ALA	4.0
1	C	186	TRP	4.0
1	D	179	LEU	3.9
1	C	163	LEU	3.9
1	B	187	GLU	3.9
1	E	186	TRP	3.8
1	F	12	ASP	3.7
1	B	186	TRP	3.4
1	B	33	TRP	3.4
1	C	192	ASP	3.3
1	D	189	SER	3.3
1	E	33	TRP	3.3
1	B	12	ASP	3.2
1	D	168	LYS	3.2
1	C	156	GLY	3.1
1	F	185	ASP	3.1
1	F	175	CYS	3.1
1	C	167	ALA	3.0
1	D	180	ARG	2.9
1	E	167	ALA	2.9
1	B	37	ARG	2.9
1	A	247	HIS	2.9
1	E	187	GLU	2.8
1	F	184	LEU	2.8
1	D	140	ALA	2.8
1	E	193	ARG	2.8
1	B	286	PRO	2.8
1	D	77	ALA	2.7
1	D	193	ARG	2.7
1	D	159	ALA	2.6
1	D	218	ARG	2.6
1	D	166	VAL	2.6
1	A	41	GLN	2.6
1	C	215	LEU	2.6
1	D	164	CYS	2.6
1	A	33	TRP	2.5
1	C	157	LEU	2.5
1	E	74	ARG	2.5
1	F	187	GLU	2.5
1	B	14	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	203	ARG	2.5
1	A	284	LEU	2.4
1	C	229	ARG	2.4
1	F	188	ASP	2.4
1	C	12	ASP	2.4
1	C	28	LEU	2.4
1	C	162	ARG	2.4
1	E	163	LEU	2.4
1	E	153	GLY	2.3
1	C	13	LYS	2.3
1	A	175	CYS	2.3
1	E	166	VAL	2.3
1	D	43	SER	2.3
1	E	174	ALA	2.3
1	A	15	LYS	2.3
1	D	161	GLY	2.3
1	E	184	LEU	2.3
1	E	155	MET	2.2
1	B	26	GLU	2.2
1	C	285	PRO	2.2
1	A	40	TRP	2.2
1	C	278	ARG	2.2
1	B	175	CYS	2.1
1	C	218	ARG	2.1
1	E	142	CYS	2.1
1	C	165	THR	2.1
1	C	30	ARG	2.1
1	B	290	PRO	2.1
1	F	219	PRO	2.1
1	D	176	ARG	2.0
1	F	183	ILE	2.0
1	D	165	THR	2.0
1	C	175	CYS	2.0
1	C	230	ARG	2.0
1	C	40	TRP	2.0
1	E	14	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 (i)

There are no carbohydrates 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. 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, 95^{th} 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
5	UNX	C	363	1/1	0.75	0.60	12.73	30,30,30,30	0
5	UNX	E	357	1/1	0.87	0.29	7.60	30,30,30,30	0
5	UNX	C	358	1/1	0.67	0.26	1.74	30,30,30,30	0
4	SO4	F	1004	5/5	0.82	0.21	1.32	63,68,68,69	0
4	SO4	E	1002	5/5	0.95	0.16	1.03	43,47,48,48	0
2	A2N	B	1000	39/39	0.93	0.16	0.56	21,32,99,138	0
4	SO4	B	1005	5/5	0.91	0.20	0.35	52,57,57,58	0
5	UNX	F	360	1/1	0.79	0.21	0.19	30,30,30,30	0
2	A2N	E	1000	39/39	0.93	0.16	0.11	11,37,105,157	0
4	SO4	F	1009	5/5	0.95	0.14	0.02	39,43,44,45	0
2	A2N	A	1000	39/39	0.94	0.15	0.02	11,28,101,119	0
4	SO4	E	1007	5/5	0.92	0.17	-0.05	60,65,65,66	0
2	A2N	D	1000	39/39	0.97	0.14	-0.06	10,25,109,164	0
2	A2N	F	1000	39/39	0.94	0.15	-0.11	8,34,117,144	0
4	SO4	D	355	5/5	0.98	0.13	-0.18	35,39,41,41	0
2	A2N	C	1000	39/39	0.94	0.14	-0.34	14,26,112,149	0
4	SO4	B	1006	5/5	0.90	0.16	-0.78	51,56,56,57	0
3	ZN	B	354	1/1	0.85	0.13	-0.94	59,59,59,59	0
5	UNX	E	356	1/1	0.91	0.14	-0.95	30,30,30,30	0
3	ZN	C	354	1/1	0.98	0.12	-1.69	49,49,49,49	0
3	ZN	A	354	1/1	0.95	0.08	-2.19	47,47,47,47	0
3	ZN	F	354	1/1	0.99	0.03	-2.77	40,40,40,40	0
3	ZN	E	354	1/1	0.93	0.09	-2.86	57,57,57,57	0
3	ZN	D	354	1/1	0.97	0.04	-3.19	46,46,46,46	0
5	UNX	B	357	1/1	0.55	0.21	-	30,30,30,30	0
5	UNX	A	357	1/1	0.92	0.27	-	30,30,30,30	0
5	UNX	C	362	1/1	0.83	0.41	-	30,30,30,30	0
5	UNX	F	356	1/1	0.62	0.27	-	30,30,30,30	0
5	UNX	C	359	1/1	0.60	0.55	-	30,30,30,30	0
5	UNX	F	361	1/1	0.78	0.32	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	UNX	B	358	1/1	0.70	0.89	-	30,30,30,30	0
5	UNX	C	365	1/1	0.76	0.42	-	30,30,30,30	0
5	UNX	E	355	1/1	0.89	0.20	-	30,30,30,30	0
5	UNX	F	359	1/1	0.65	0.27	-	30,30,30,30	0
5	UNX	D	357	1/1	0.53	0.55	-	30,30,30,30	0
5	UNX	C	361	1/1	0.79	0.18	-	30,30,30,30	0
5	UNX	F	355	1/1	0.31	0.25	-	30,30,30,30	0
5	UNX	E	358	1/1	0.63	0.51	-	30,30,30,30	0
4	SO4	A	1008	5/5	0.85	0.15	-	48,52,53,54	0
4	SO4	B	1011	5/5	0.91	0.17	-	61,66,66,67	0
5	UNX	F	358	1/1	0.89	0.45	-	30,30,30,30	0
5	UNX	C	357	1/1	0.83	0.68	-	30,30,30,30	0
5	UNX	D	358	1/1	0.56	0.22	-	30,30,30,30	0
5	UNX	F	362	1/1	0.68	0.21	-	30,30,30,30	0
5	UNX	B	356	1/1	0.86	0.29	-	30,30,30,30	0
5	UNX	D	356	1/1	0.53	0.59	-	30,30,30,30	0
5	UNX	F	357	1/1	0.57	0.31	-	30,30,30,30	0
5	UNX	C	355	1/1	0.88	0.10	-	30,30,30,30	0
4	SO4	E	1010	5/5	0.81	0.45	-	64,68,69,70	0
5	UNX	C	364	1/1	0.72	0.20	-	30,30,30,30	0
5	UNX	B	359	1/1	0.77	0.55	-	30,30,30,30	0
5	UNX	C	356	1/1	0.33	0.35	-	30,30,30,30	0
5	UNX	A	356	1/1	0.83	0.48	-	30,30,30,30	0
5	UNX	A	355	1/1	0.63	0.46	-	30,30,30,30	0
4	SO4	F	1001	5/5	0.57	0.68	-	75,80,81,81	0
5	UNX	C	360	1/1	0.82	0.30	-	30,30,30,30	0
4	SO4	C	1003	5/5	0.91	0.15	-	57,61,61,62	0
5	UNX	C	366	1/1	0.57	0.33	-	30,30,30,30	0
5	UNX	B	355	1/1	0.81	0.58	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.