



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:03 am GMT

PDB ID : 1OXK
Title : Complex between YPD1 and SLN1 response regulator domain in space group P3(2)
Authors : Xu, Q.; Porter, S.W.; West, A.H.
Deposited on : 2003-04-02
Resolution : 2.10 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 ⓘ 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

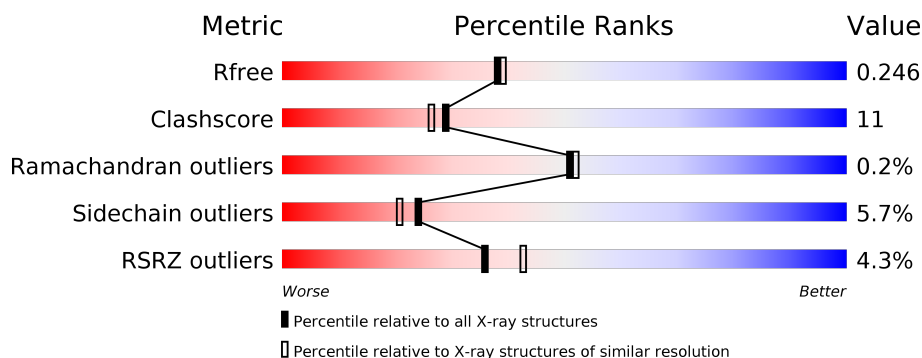
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 $\leq 5\%$. 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	166	<div> <div>2%</div> <div>75% 16% 6%</div> </div>
1	C	166	<div> <div>4%</div> <div>77% 14% 6%</div> </div>
1	E	166	<div> <div>2%</div> <div>77% 14% 6%</div> </div>
1	G	166	<div> <div>2%</div> <div>79% 13% 6%</div> </div>
1	I	166	<div> <div>2%</div> <div>75% 17% 6%</div> </div>
1	K	166	<div> <div>2%</div> <div>78% 13% 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	134	
2	D	134	
2	F	134	
2	H	134	
2	J	134	
2	L	134	

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
3	SO4	B	5003	-	-	X	-
3	SO4	C	5006	-	-	X	-
3	SO4	F	5009	-	-	X	-
3	SO4	H	5012	-	-	X	-
3	SO4	J	5015	-	-	X	-
3	SO4	L	5018	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13623 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 Ypd1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1256	794	211	247	4			
1	C	156	Total	C	N	O	S	0	0	0
			1255	794	211	246	4			
1	E	156	Total	C	N	O	S	0	0	0
			1255	794	211	246	4			
1	G	156	Total	C	N	O	S	0	0	0
			1255	794	211	246	4			
1	I	156	Total	C	N	O	S	0	0	0
			1255	794	211	246	4			
1	K	156	Total	C	N	O	S	0	0	0
			1255	794	211	246	4			

- Molecule 2 is a protein called SLN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			962	612	160	181	9			
2	D	128	Total	C	N	O	S	0	0	0
			965	612	160	184	9			
2	F	128	Total	C	N	O	S	0	0	0
			975	621	162	183	9			
2	H	128	Total	C	N	O	S	0	0	0
			974	620	162	183	9			
2	J	128	Total	C	N	O	S	0	0	0
			955	608	159	179	9			
2	L	128	Total	C	N	O	S	0	0	0
			964	613	160	182	9			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

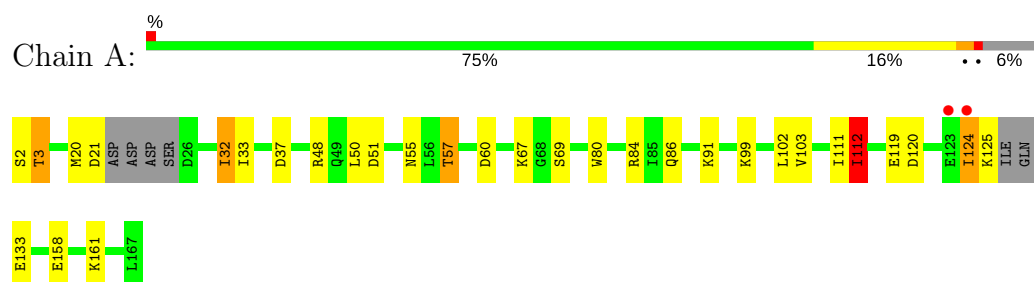
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	11	Total	O	0	0
			11	11		
4	C	16	Total	O	0	0
			16	16		
4	D	10	Total	O	0	0
			10	10		
4	E	18	Total	O	0	0
			18	18		
4	F	21	Total	O	0	0
			21	21		
4	G	27	Total	O	0	0
			27	27		
4	H	14	Total	O	0	0
			14	14		
4	I	26	Total	O	0	0
			26	26		
4	J	10	Total	O	0	0
			10	10		
4	K	22	Total	O	0	0
			22	22		
4	L	16	Total	O	0	0
			16	16		

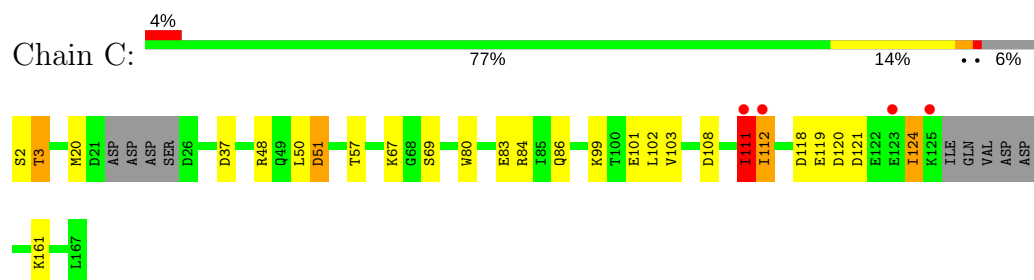
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

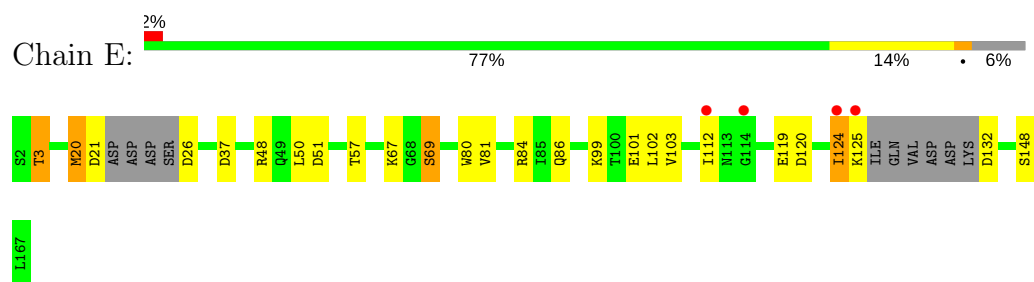
• Molecule 1: Ypd1p



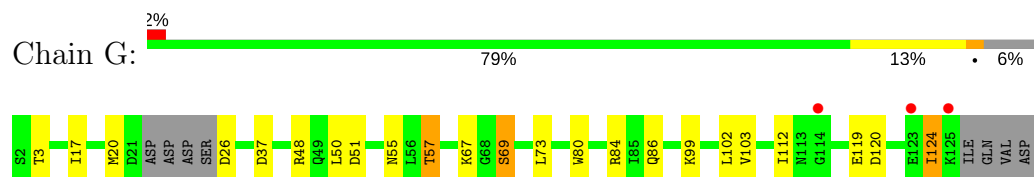
• Molecule 1: Ypd1p

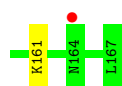


• Molecule 1: Ypd1p

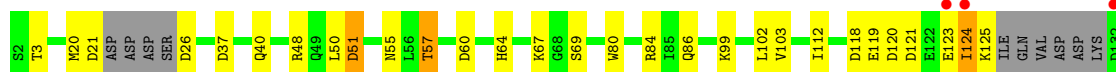
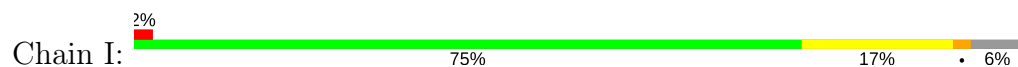


• Molecule 1: Ypd1p

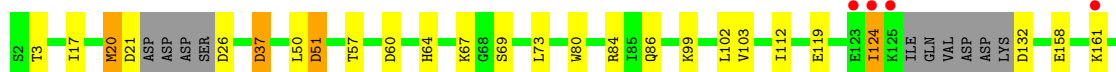
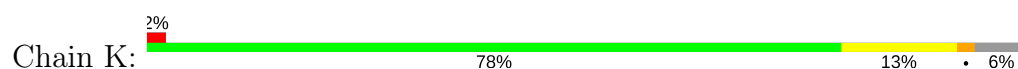




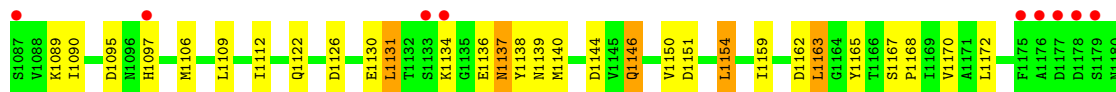
• Molecule 1: Ypd1p



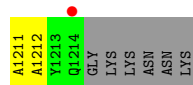
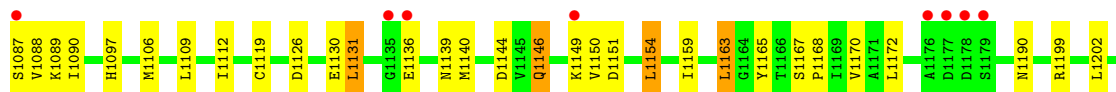
• Molecule 1: Ypd1p



• Molecule 2: SLN1

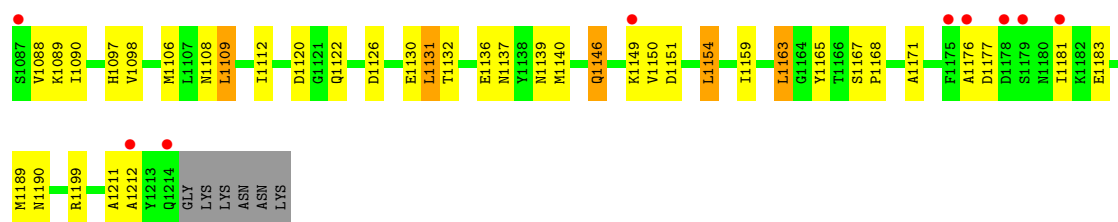


• Molecule 2: SLN1

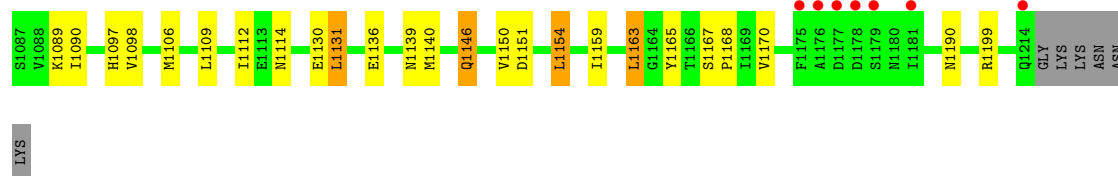
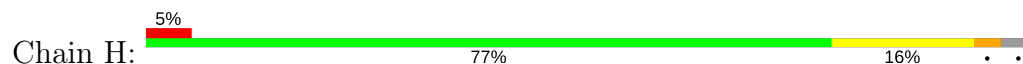


• Molecule 2: SLN1

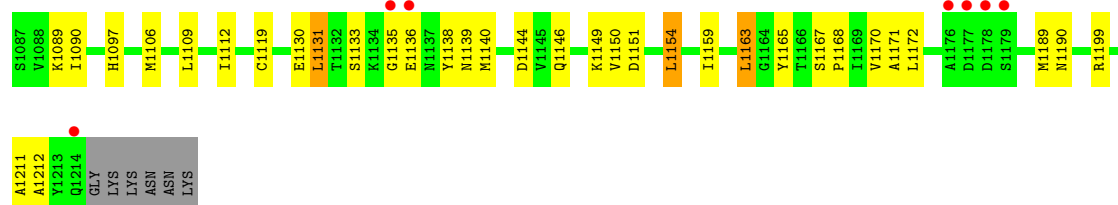




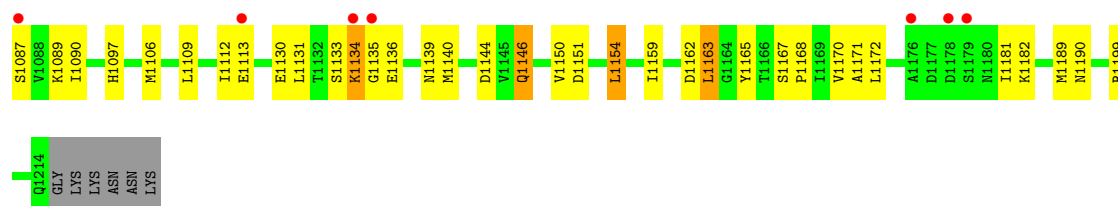
● Molecule 2: SLN1



● Molecule 2: SLN1



● Molecule 2: SLN1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	91.30Å 91.30Å 200.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.00-2.10) 95.6 (29.56-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.236 , 0.258 0.244 , 0.246	Depositor DCC
R_{free} test set	5259 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.310 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13623	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.27 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2745e-03.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	3.45	2/1271 (0.2%)	1.30	11/1710 (0.6%)
1	C	1.96	1/1270 (0.1%)	1.07	7/1709 (0.4%)
1	E	0.86	1/1270 (0.1%)	1.01	8/1709 (0.5%)
1	G	0.83	0/1270	0.90	3/1709 (0.2%)
1	I	0.86	0/1270	0.94	8/1709 (0.5%)
1	K	0.85	1/1270 (0.1%)	0.94	6/1709 (0.4%)
2	B	0.75	0/974	0.91	4/1315 (0.3%)
2	D	0.76	0/977	0.90	2/1319 (0.2%)
2	F	0.77	0/987	0.89	3/1330 (0.2%)
2	H	0.76	0/986	0.86	1/1328 (0.1%)
2	J	0.75	0/967	0.90	1/1306 (0.1%)
2	L	0.75	0/976	0.90	2/1316 (0.2%)
All	All	1.42	5/13488 (0.0%)	0.98	56/18169 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ILE	CG1-CD1	88.20	7.59	1.50
1	A	112	ILE	CG1-CD1	80.25	7.04	1.50
1	C	111	ILE	CG1-CD1	62.26	5.80	1.50
1	E	20	MET	SD-CE	-5.48	1.47	1.77
1	K	20	MET	SD-CE	-5.24	1.48	1.77

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ILE	CB-CG1-CD1	-31.17	26.61	113.90
1	C	111	ILE	CB-CG1-CD1	-18.81	61.22	113.90
1	E	124	ILE	C-N-CA	14.06	156.85	121.70
1	A	124	ILE	C-N-CA	13.71	155.96	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1151	ASP	CB-CG-OD2	10.15	127.44	118.30
2	J	1151	ASP	CB-CG-OD2	9.62	126.95	118.30
2	L	1151	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	112	ILE	CB-CG1-CD1	-8.92	88.92	113.90
2	D	1151	ASP	CB-CG-OD2	8.36	125.82	118.30
2	D	1126	ASP	CB-CG-OD2	8.29	125.77	118.30
2	H	1151	ASP	CB-CG-OD2	8.16	125.64	118.30
2	F	1151	ASP	CB-CG-OD2	8.06	125.55	118.30
1	I	51	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	60	ASP	CB-CG-OD1	7.27	124.85	118.30
1	G	124	ILE	C-N-CA	7.21	139.72	121.70
2	B	1126	ASP	CB-CG-OD2	6.99	124.59	118.30
1	K	124	ILE	C-N-CA	6.99	139.18	121.70
1	I	21	ASP	CB-CG-OD2	6.89	124.50	118.30
1	E	120	ASP	CB-CG-OD2	6.88	124.50	118.30
1	C	51	ASP	CB-CG-OD2	6.81	124.43	118.30
1	I	60	ASP	CB-CG-OD1	6.72	124.35	118.30
1	K	21	ASP	CB-CG-OD2	6.71	124.34	118.30
1	C	124	ILE	C-N-CA	6.68	138.41	121.70
1	I	124	ILE	C-N-CA	6.68	138.40	121.70
1	A	124	ILE	CA-C-N	6.46	131.42	117.20
1	E	132	ASP	CB-CG-OD2	6.46	124.11	118.30
1	E	124	ILE	O-C-N	-6.38	112.48	122.70
1	A	124	ILE	O-C-N	-6.38	112.49	122.70
1	C	37	ASP	CB-CG-OD2	6.36	124.02	118.30
1	E	124	ILE	CA-C-N	6.28	131.02	117.20
1	I	120	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	125	LYS	N-CA-CB	-5.99	99.83	110.60
1	A	120	ASP	CB-CG-OD2	5.98	123.68	118.30
2	L	1162	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	21	ASP	CB-CG-OD2	5.93	123.63	118.30
1	E	21	ASP	CB-CG-OD2	5.91	123.62	118.30
1	G	26	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	118	ASP	CB-CG-OD2	5.79	123.52	118.30
1	K	51	ASP	CB-CG-OD2	5.66	123.39	118.30
1	K	37	ASP	CB-CG-OD2	5.63	123.37	118.30
1	C	120	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	37	ASP	CB-CG-OD2	5.60	123.34	118.30
2	B	1095	ASP	CB-CG-OD2	5.59	123.33	118.30
1	I	37	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	125	LYS	N-CA-CB	-5.53	100.65	110.60
2	F	1126	ASP	CB-CG-OD2	5.50	123.25	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	60	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	108	ASP	CB-CG-OD2	5.38	123.14	118.30
1	I	118	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	124	ILE	N-CA-C	-5.21	96.94	111.00
1	E	124	ILE	N-CA-C	-5.18	97.01	111.00
1	G	120	ASP	CB-CG-OD2	5.15	122.93	118.30
2	B	1162	ASP	CB-CG-OD2	5.08	122.87	118.30
1	K	132	ASP	CB-CG-OD2	5.04	122.83	118.30
1	I	125	LYS	N-CA-C	-5.03	97.43	111.00
2	F	1120	ASP	CB-CG-OD1	5.01	122.81	118.30

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	1256	0	1250	34	0
1	C	1255	0	1248	35	0
1	E	1255	0	1247	24	0
1	G	1255	0	1248	26	0
1	I	1255	0	1248	28	0
1	K	1255	0	1248	23	0
2	B	962	0	950	35	0
2	D	965	0	950	33	0
2	F	975	0	978	39	0
2	H	974	0	976	26	0
2	J	955	0	934	31	0
2	L	964	0	952	32	0
3	A	10	0	0	1	0
3	B	5	0	0	3	0
3	C	15	0	0	2	0
3	E	10	0	0	0	0
3	F	5	0	0	3	0
3	G	10	0	0	0	0
3	H	5	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	10	0	0	1	0
3	J	5	0	0	3	0
3	K	10	0	0	1	0
3	L	5	0	0	3	0
4	A	16	0	0	0	0
4	B	11	0	0	3	0
4	C	16	0	0	0	0
4	D	10	0	0	3	0
4	E	18	0	0	1	1
4	F	21	0	0	1	0
4	G	27	0	0	1	0
4	H	14	0	0	0	0
4	I	26	0	0	3	0
4	J	10	0	0	1	1
4	K	22	0	0	1	0
4	L	16	0	0	1	0
All	All	13623	0	13229	289	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (289) 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:20:MET:HE1	2:B:1106:MET:HA	1.41	1.00
1:C:67:LYS:HZ3	1:C:86:GLN:NE2	1.59	0.99
1:I:20:MET:HE1	2:J:1106:MET:HA	1.43	0.99
1:I:40:GLN:HG2	4:I:5107:HOH:O	1.64	0.98
1:C:67:LYS:NZ	1:C:86:GLN:HE22	1.61	0.98
1:C:20:MET:HE1	2:D:1106:MET:HA	1.42	0.98
1:K:20:MET:HE1	2:L:1106:MET:HA	1.46	0.96
2:D:1131:LEU:HD22	2:D:1136:GLU:HB2	1.48	0.95
1:E:20:MET:HE3	2:F:1199:ARG:HD3	1.50	0.93
1:A:20:MET:HE3	2:B:1199:ARG:HD3	1.51	0.91
1:E:20:MET:HE1	2:F:1106:MET:HA	1.53	0.90
1:A:3:THR:HG23	4:D:5115:HOH:O	1.71	0.89
1:G:20:MET:HE3	2:H:1199:ARG:HD3	1.56	0.87
1:C:20:MET:HE1	2:D:1106:MET:CA	2.06	0.86
3:F:5009:SO4:O2	1:I:48:ARG:HD3	1.76	0.86
1:G:20:MET:HE1	2:H:1106:MET:HA	1.59	0.85
2:B:1131:LEU:HD22	2:B:1136:GLU:HB2	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASP:OD1	1:C:124:ILE:HG22	1.79	0.83
1:I:67:LYS:NZ	1:I:86:GLN:HE22	1.79	0.81
1:C:67:LYS:HZ3	1:C:86:GLN:HE22	0.83	0.81
1:E:20:MET:CE	2:F:1199:ARG:HD3	2.11	0.80
1:K:20:MET:HE1	2:L:1106:MET:CA	2.11	0.79
1:I:20:MET:HE3	2:J:1106:MET:CG	2.13	0.78
1:C:20:MET:HE3	2:D:1199:ARG:HD3	1.65	0.77
1:A:20:MET:CE	2:B:1199:ARG:HD3	2.15	0.77
2:D:1089:LYS:NZ	2:D:1136:GLU:OE2	2.17	0.77
1:C:20:MET:CE	2:D:1106:MET:HA	2.18	0.74
1:I:20:MET:CE	2:J:1106:MET:HA	2.16	0.74
1:I:51:ASP:OD1	1:I:124:ILE:HG22	1.87	0.74
1:C:101:GLU:OE1	2:F:1122:GLN:NE2	2.22	0.73
1:K:20:MET:CE	2:L:1106:MET:HG3	2.19	0.72
2:F:1089:LYS:H	2:F:1139:ASN:ND2	1.87	0.72
1:E:26:ASP:N	4:E:5192:HOH:O	2.22	0.71
1:I:20:MET:HE1	2:J:1106:MET:CA	2.19	0.71
1:I:20:MET:HE3	2:J:1106:MET:HG2	1.71	0.71
2:F:1177:ASP:O	2:F:1181:ILE:HG13	1.90	0.71
1:A:20:MET:HE1	2:B:1106:MET:CA	2.21	0.70
2:F:1131:LEU:HD22	2:F:1136:GLU:HB2	1.71	0.70
1:C:20:MET:CE	2:D:1106:MET:CG	2.70	0.70
1:I:26:ASP:N	4:I:5163:HOH:O	2.25	0.70
1:G:67:LYS:NZ	1:G:86:GLN:HE22	1.90	0.70
2:L:1089:LYS:H	2:L:1139:ASN:ND2	1.90	0.70
1:K:51:ASP:OD1	1:K:124:ILE:HG22	1.91	0.69
1:C:20:MET:CE	2:D:1106:MET:HG3	2.23	0.69
2:J:1089:LYS:H	2:J:1139:ASN:ND2	1.92	0.68
1:E:20:MET:HE3	2:F:1106:MET:HG2	1.76	0.67
1:K:20:MET:HE3	2:L:1199:ARG:HD3	1.75	0.67
1:I:20:MET:HE3	2:J:1199:ARG:HD3	1.76	0.67
1:C:20:MET:HE3	2:D:1106:MET:HG2	1.77	0.67
2:F:1097:HIS:CD2	3:F:5009:SO4:O4	2.48	0.66
1:C:48:ARG:HD3	3:L:5018:SO4:O2	1.95	0.66
1:A:20:MET:HE3	2:B:1106:MET:HG2	1.77	0.66
1:K:20:MET:HE1	2:L:1106:MET:HG3	1.77	0.66
1:G:20:MET:CE	2:H:1199:ARG:HD3	2.25	0.65
1:K:20:MET:CE	2:L:1106:MET:HA	2.25	0.65
1:K:20:MET:CE	2:L:1106:MET:CG	2.75	0.64
2:B:1089:LYS:H	2:B:1139:ASN:ND2	1.95	0.64
1:A:50:LEU:HB3	1:A:124:ILE:HG21	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LEU:HB3	1:E:124:ILE:HG21	1.78	0.64
2:L:1133:SER:C	2:L:1135:GLY:H	1.99	0.64
1:K:20:MET:HE1	2:L:1106:MET:CG	2.28	0.64
1:C:20:MET:HE1	2:D:1106:MET:CG	2.27	0.63
1:E:51:ASP:OD1	1:E:124:ILE:HG22	1.98	0.63
2:F:1168:PRO:HB3	2:F:1190:ASN:HD21	1.62	0.63
4:B:5175:HOH:O	1:G:48:ARG:HG3	1.98	0.63
1:K:67:LYS:NZ	1:K:86:GLN:HE22	1.97	0.63
1:C:67:LYS:NZ	1:C:86:GLN:NE2	2.33	0.63
2:D:1119:CYS:SG	4:D:5051:HOH:O	2.34	0.63
1:I:20:MET:HE3	2:J:1106:MET:HG3	1.81	0.62
1:I:67:LYS:HZ3	1:I:86:GLN:HE22	1.47	0.62
1:A:3:THR:CG2	4:D:5115:HOH:O	2.39	0.61
1:G:20:MET:HE3	2:H:1106:MET:HG2	1.81	0.61
2:H:1168:PRO:HB3	2:H:1190:ASN:HD21	1.64	0.61
1:G:67:LYS:HZ3	1:G:86:GLN:NE2	1.99	0.61
2:D:1089:LYS:H	2:D:1139:ASN:ND2	1.98	0.60
2:J:1133:SER:C	2:J:1135:GLY:H	2.02	0.60
1:A:48:ARG:HD3	3:H:5012:SO4:O2	2.01	0.60
2:H:1089:LYS:H	2:H:1139:ASN:ND2	2.00	0.60
1:G:50:LEU:HB3	1:G:124:ILE:HG21	1.83	0.60
1:C:50:LEU:HB3	1:C:124:ILE:HG21	1.84	0.60
1:K:99:LYS:O	1:K:103:VAL:HG13	2.02	0.60
2:D:1168:PRO:HB3	2:D:1190:ASN:HD21	1.66	0.59
1:C:20:MET:HE3	2:D:1106:MET:CG	2.33	0.59
1:I:20:MET:CE	2:J:1106:MET:HG3	2.33	0.59
1:C:20:MET:HE1	2:D:1106:MET:HG3	1.83	0.59
2:H:1131:LEU:HD22	2:H:1136:GLU:HB2	1.84	0.59
1:G:55:ASN:OD1	1:G:57:THR:HB	2.03	0.58
2:H:1165:TYR:CZ	2:H:1167:SER:HB2	2.38	0.58
1:I:50:LEU:HB3	1:I:124:ILE:HG21	1.86	0.58
2:F:1131:LEU:HD22	2:F:1136:GLU:CB	2.33	0.58
2:L:1097:HIS:CD2	3:L:5018:SO4:O4	2.56	0.58
1:E:20:MET:HE3	2:F:1106:MET:CG	2.34	0.57
2:H:1097:HIS:HD2	3:H:5012:SO4:O1	1.86	0.57
2:J:1168:PRO:HB3	2:J:1190:ASN:HD21	1.68	0.57
1:A:67:LYS:NZ	1:A:86:GLN:HE22	2.02	0.57
1:G:67:LYS:NZ	1:G:86:GLN:NE2	2.52	0.57
1:A:55:ASN:OD1	1:A:57:THR:HB	2.05	0.57
2:B:1106:MET:HG2	2:B:1199:ARG:HD3	1.86	0.57
1:A:51:ASP:OD2	1:G:37:ASP:OD1	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1168:PRO:HB3	2:B:1190:ASN:HD21	1.70	0.57
1:A:20:MET:HE3	2:B:1106:MET:CG	2.35	0.56
2:B:1137:ASN:HD22	2:B:1138:TYR:H	1.53	0.56
4:G:5122:HOH:O	2:L:1134:LYS:HE3	2.05	0.56
1:G:51:ASP:OD1	1:G:124:ILE:HG22	2.05	0.56
2:L:1097:HIS:HD2	3:L:5018:SO4:O4	1.87	0.56
1:A:20:MET:CE	2:B:1106:MET:CG	2.84	0.56
2:H:1146:GLN:NE2	2:H:1146:GLN:H	2.04	0.55
2:D:1106:MET:HG2	2:D:1199:ARG:HD3	1.89	0.55
1:C:20:MET:CE	2:D:1199:ARG:HD3	2.37	0.54
2:F:1097:HIS:HD2	3:F:5009:SO4:O4	1.90	0.54
2:L:1159:ILE:O	2:L:1163:LEU:HB2	2.07	0.54
2:L:1136:GLU:CB	4:L:5144:HOH:O	2.55	0.54
1:A:51:ASP:OD1	1:A:124:ILE:HG22	2.07	0.54
2:F:1146:GLN:NE2	2:F:1146:GLN:H	2.05	0.54
2:H:1150:VAL:HG13	2:H:1154:LEU:HD13	1.90	0.54
2:B:1097:HIS:CD2	3:B:5003:SO4:O4	2.61	0.54
1:G:99:LYS:O	1:G:103:VAL:HG13	2.08	0.54
2:L:1133:SER:C	2:L:1135:GLY:N	2.62	0.54
1:K:50:LEU:HB3	1:K:124:ILE:HG21	1.88	0.53
1:E:20:MET:CE	2:F:1199:ARG:CD	2.83	0.53
1:C:2:SER:N	2:F:1183:GLU:OE1	2.42	0.53
1:K:26:ASP:N	4:K:5126:HOH:O	2.40	0.53
1:E:20:MET:HE1	2:F:1106:MET:CA	2.35	0.53
2:J:1106:MET:HG2	2:J:1199:ARG:HD3	1.89	0.53
2:J:1165:TYR:CZ	2:J:1167:SER:HB2	2.43	0.53
1:A:99:LYS:O	1:A:103:VAL:HG13	2.09	0.53
2:L:1146:GLN:NE2	2:L:1146:GLN:H	2.06	0.53
1:G:20:MET:HE3	2:H:1106:MET:CG	2.38	0.52
1:I:20:MET:CE	2:J:1106:MET:CG	2.85	0.52
1:E:99:LYS:O	1:E:103:VAL:HG13	2.09	0.52
2:F:1106:MET:HG2	2:F:1199:ARG:HD3	1.91	0.52
2:D:1168:PRO:HA	2:D:1190:ASN:OD1	2.09	0.52
1:I:80:TRP:CZ2	1:I:84:ARG:HD2	2.45	0.52
2:L:1106:MET:HG2	2:L:1199:ARG:HD3	1.92	0.52
1:E:67:LYS:NZ	1:E:86:GLN:HE22	2.08	0.52
1:I:99:LYS:NZ	1:I:121:ASP:OD1	2.41	0.52
1:A:20:MET:HE3	2:B:1199:ARG:CD	2.34	0.52
1:G:20:MET:HE1	2:H:1106:MET:CA	2.35	0.52
1:C:101:GLU:HG2	2:F:1122:GLN:HE22	1.74	0.51
2:H:1106:MET:HG2	2:H:1199:ARG:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1150:VAL:HG13	2:D:1154:LEU:HD13	1.92	0.51
2:J:1119:CYS:SG	4:J:5069:HOH:O	2.44	0.51
1:A:20:MET:CE	2:B:1106:MET:HG3	2.40	0.51
1:C:20:MET:CE	2:D:1106:MET:HG2	2.38	0.51
2:D:1165:TYR:CZ	2:D:1167:SER:HB2	2.45	0.51
2:B:1097:HIS:HD2	3:B:5003:SO4:O4	1.94	0.51
2:D:1089:LYS:H	2:D:1139:ASN:HD22	1.58	0.51
2:J:1150:VAL:HG13	2:J:1154:LEU:HD13	1.93	0.51
2:L:1133:SER:O	2:L:1135:GLY:N	2.44	0.51
2:L:1165:TYR:CZ	2:L:1167:SER:HB2	2.46	0.50
2:D:1159:ILE:O	2:D:1163:LEU:HB2	2.11	0.50
1:K:20:MET:HE3	2:L:1106:MET:CG	2.40	0.50
2:H:1090:ILE:HD12	2:H:1112:ILE:HG21	1.93	0.50
2:B:1150:VAL:HG13	2:B:1154:LEU:HD13	1.94	0.50
1:G:20:MET:CE	2:H:1106:MET:CG	2.90	0.50
1:I:20:MET:CE	2:J:1199:ARG:HD3	2.41	0.50
2:J:1133:SER:C	2:J:1135:GLY:N	2.65	0.50
2:B:1112:ILE:HG23	4:B:5045:HOH:O	2.11	0.50
1:K:20:MET:CE	2:L:1199:ARG:HD3	2.40	0.50
1:A:20:MET:CE	2:B:1199:ARG:CD	2.89	0.50
1:E:20:MET:HE3	2:F:1199:ARG:CD	2.34	0.50
1:C:99:LYS:O	1:C:103:VAL:HG13	2.12	0.50
2:B:1090:ILE:HD12	2:B:1112:ILE:HG21	1.94	0.49
1:K:64:HIS:ND1	3:K:5016:SO4:O2	2.30	0.49
2:L:1168:PRO:HB3	2:L:1190:ASN:HD21	1.76	0.49
1:K:20:MET:HE3	2:L:1106:MET:HG2	1.94	0.49
1:A:32:ILE:CD1	1:A:33:ILE:HD13	0.97	0.49
2:B:1165:TYR:CZ	2:B:1167:SER:HB2	2.48	0.49
1:A:111:ILE:CD1	1:A:112:ILE:HD11	0.97	0.49
1:A:111:ILE:CD1	1:A:112:ILE:HD12	0.97	0.49
1:E:20:MET:CE	2:F:1106:MET:CG	2.90	0.49
1:E:48:ARG:HD3	3:J:5015:SO4:O2	2.13	0.49
1:I:67:LYS:NZ	1:I:86:GLN:NE2	2.57	0.49
1:A:111:ILE:HD11	1:A:112:ILE:CD1	0.97	0.48
1:A:32:ILE:CD1	1:A:33:ILE:HD12	0.97	0.48
1:I:123:GLU:C	4:I:5165:HOH:O	2.51	0.48
1:A:32:ILE:CD1	1:A:33:ILE:HD11	0.97	0.48
1:I:64:HIS:ND1	3:I:5013:SO4:O2	2.27	0.48
2:H:1097:HIS:CD2	3:H:5012:SO4:O1	2.66	0.48
1:A:32:ILE:HD12	1:A:33:ILE:CD1	0.97	0.48
1:A:32:ILE:HD13	1:A:33:ILE:CD1	0.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:CD1	1:C:112:ILE:HD12	0.97	0.48
3:C:5006:SO4:O4	2:D:1097:HIS:HD2	1.97	0.48
1:G:80:TRP:CZ2	1:G:84:ARG:HD2	2.48	0.48
2:J:1090:ILE:HD12	2:J:1112:ILE:HG21	1.94	0.48
1:A:111:ILE:HD13	1:A:112:ILE:CD1	0.97	0.48
2:F:1090:ILE:HD12	2:F:1112:ILE:HG21	1.95	0.48
2:J:1097:HIS:CD2	3:J:5015:SO4:O4	2.67	0.48
1:A:32:ILE:HD11	1:A:33:ILE:CD1	0.97	0.48
2:D:1090:ILE:HD12	2:D:1112:ILE:HG21	1.95	0.48
1:K:80:TRP:CZ2	1:K:84:ARG:HD2	2.48	0.48
1:C:51:ASP:OD2	1:K:37:ASP:OD1	2.31	0.48
1:G:20:MET:CE	2:H:1106:MET:HG3	2.44	0.48
2:L:1139:ASN:HD22	2:L:1139:ASN:H	1.62	0.47
2:L:1150:VAL:HG13	2:L:1154:LEU:HD13	1.95	0.47
2:F:1168:PRO:HA	2:F:1190:ASN:OD1	2.13	0.47
2:J:1131:LEU:HD22	2:J:1136:GLU:HB2	1.95	0.47
2:B:1144:ASP:HA	2:B:1172:LEU:HB2	1.95	0.47
2:F:1089:LYS:H	2:F:1139:ASN:HD22	1.59	0.47
1:I:55:ASN:OD1	1:I:57:THR:HB	2.13	0.47
2:J:1159:ILE:O	2:J:1163:LEU:HB2	2.15	0.47
2:F:1150:VAL:HG13	2:F:1154:LEU:HD13	1.96	0.47
1:C:99:LYS:NZ	1:C:121:ASP:OD1	2.48	0.47
2:B:1168:PRO:HA	2:B:1190:ASN:OD1	2.15	0.47
2:L:1090:ILE:HD12	2:L:1112:ILE:HG21	1.96	0.47
2:F:1165:TYR:CZ	2:F:1167:SER:HB2	2.50	0.46
2:H:1139:ASN:H	2:H:1139:ASN:HD22	1.63	0.46
1:K:67:LYS:HZ1	1:K:86:GLN:HE22	1.64	0.46
1:E:69:SER:OG	2:F:1098:VAL:HB	2.15	0.46
2:H:1140:MET:HE1	2:H:1170:VAL:HG21	1.97	0.46
2:B:1146:GLN:NE2	2:B:1146:GLN:H	2.13	0.46
2:B:1159:ILE:O	2:B:1163:LEU:HB2	2.15	0.46
1:A:20:MET:CE	2:B:1106:MET:HG2	2.45	0.46
1:E:158:GLU:O	1:E:161:LYS:HG2	2.15	0.46
1:A:158:GLU:O	1:A:161:LYS:HG2	2.15	0.46
2:F:1171:ALA:HB2	2:F:1189:MET:SD	2.56	0.46
2:H:1159:ILE:O	2:H:1163:LEU:HB2	2.15	0.46
2:F:1159:ILE:O	2:F:1163:LEU:HB2	2.16	0.45
1:C:101:GLU:HG2	2:F:1122:GLN:NE2	2.31	0.45
2:B:1196:PRO:HA	4:B:5058:HOH:O	2.16	0.45
2:F:1137:ASN:HA	4:F:5198:HOH:O	2.16	0.45
2:J:1168:PRO:HA	2:J:1190:ASN:OD1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1122:GLN:NE2	1:E:101:GLU:OE1	2.48	0.45
2:L:1171:ALA:HB2	2:L:1189:MET:SD	2.56	0.45
1:G:69:SER:OG	2:H:1098:VAL:HB	2.16	0.45
2:B:1154:LEU:HA	1:E:3:THR:HG21	1.99	0.45
2:D:1211:ALA:O	2:D:1212:ALA:HB3	2.16	0.45
1:G:20:MET:HE3	2:H:1199:ARG:CD	2.37	0.45
2:B:1140:MET:HE1	2:B:1170:VAL:HG21	1.99	0.45
1:E:20:MET:CE	2:F:1106:MET:HG3	2.47	0.45
2:J:1097:HIS:HD2	3:J:5015:SO4:O4	2.00	0.45
1:K:17:ILE:HD13	1:K:73:LEU:HD23	1.99	0.44
1:G:67:LYS:HZ1	1:G:86:GLN:HE22	1.64	0.44
2:J:1140:MET:HE1	2:J:1170:VAL:HG21	2.00	0.44
1:G:17:ILE:CD1	1:G:73:LEU:HD23	2.47	0.44
2:J:1171:ALA:HB2	2:J:1189:MET:SD	2.57	0.44
1:K:17:ILE:CD1	1:K:73:LEU:HD23	2.48	0.44
3:B:5003:SO4:O2	1:G:48:ARG:HD3	2.18	0.44
1:K:158:GLU:O	1:K:161:LYS:HG2	2.17	0.44
2:D:1140:MET:HE2	2:D:1140:MET:HB3	1.89	0.44
1:I:99:LYS:O	1:I:103:VAL:HG13	2.18	0.44
1:I:67:LYS:HZ2	1:I:86:GLN:HE22	1.58	0.43
2:F:1176:ALA:O	2:F:1181:ILE:HD11	2.18	0.43
1:E:37:ASP:OD1	1:I:51:ASP:OD2	2.36	0.43
2:H:1168:PRO:HA	2:H:1190:ASN:OD1	2.18	0.43
1:C:158:GLU:O	1:C:161:LYS:HG2	2.18	0.43
3:C:5006:SO4:O4	2:D:1097:HIS:CD2	2.71	0.43
1:G:17:ILE:HD13	1:G:73:LEU:HD23	2.01	0.43
2:J:1140:MET:HE2	2:J:1140:MET:HB3	1.90	0.43
1:E:81:VAL:HG11	1:E:148:SER:OG	2.18	0.43
2:H:1089:LYS:HD3	2:H:1114:ASN:ND2	2.33	0.43
1:I:67:LYS:HZ2	1:I:86:GLN:NE2	2.15	0.43
2:B:1139:ASN:HD22	2:B:1139:ASN:H	1.67	0.43
2:B:1211:ALA:O	2:B:1212:ALA:HB3	2.18	0.42
1:E:80:TRP:CZ2	1:E:84:ARG:HD2	2.54	0.42
2:J:1167:SER:HB3	2:J:1168:PRO:CD	2.50	0.42
2:J:1131:LEU:HD12	2:J:1138:TYR:CE2	2.54	0.42
2:B:1122:GLN:HE22	1:E:101:GLU:HG2	1.85	0.42
1:C:111:ILE:CD1	1:C:112:ILE:HD13	0.97	0.42
1:A:67:LYS:NZ	3:A:5001:SO4:O3	2.49	0.42
2:L:1140:MET:HE1	2:L:1170:VAL:HG21	2.01	0.42
1:G:20:MET:CE	2:H:1106:MET:HA	2.41	0.42
1:I:158:GLU:O	1:I:161:LYS:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1181:ILE:O	2:L:1182:LYS:C	2.57	0.42
2:D:1146:GLN:H	2:D:1146:GLN:NE2	2.18	0.41
2:D:1167:SER:HB3	2:D:1168:PRO:CD	2.51	0.41
2:F:1108:ASN:HA	2:F:1112:ILE:O	2.21	0.41
2:L:1144:ASP:HA	2:L:1172:LEU:HB2	2.02	0.41
1:C:111:ILE:HD12	1:C:112:ILE:CD1	0.97	0.41
2:F:1211:ALA:O	2:F:1212:ALA:HB3	2.20	0.41
1:A:80:TRP:CZ2	1:A:84:ARG:HD2	2.55	0.41
1:C:3:THR:HG21	2:F:1154:LEU:HA	2.03	0.41
1:C:111:ILE:CD1	1:C:112:ILE:HD11	0.97	0.41
2:D:1088:VAL:HA	2:D:1139:ASN:ND2	2.35	0.41
2:F:1088:VAL:HA	2:F:1139:ASN:ND2	2.36	0.41
1:A:91:LYS:NZ	1:A:133:GLU:OE2	2.47	0.41
1:C:111:ILE:HD11	1:C:112:ILE:CD1	0.97	0.41
1:C:80:TRP:CZ2	1:C:84:ARG:HD2	2.56	0.41
2:F:1140:MET:HE2	2:F:1140:MET:HB3	1.95	0.41
2:B:1134:LYS:O	2:B:1136:GLU:HG3	2.20	0.41
2:D:1140:MET:HE1	2:D:1170:VAL:HG21	2.03	0.41
2:D:1144:ASP:HA	2:D:1172:LEU:HB2	2.03	0.41
2:L:1168:PRO:HA	2:L:1190:ASN:OD1	2.21	0.41
2:F:1109:LEU:HA	2:F:1109:LEU:HD12	1.98	0.40
1:G:158:GLU:O	1:G:161:LYS:HG2	2.21	0.40
2:J:1144:ASP:HA	2:J:1172:LEU:HB2	2.04	0.40
1:C:67:LYS:CE	1:C:86:GLN:HE22	2.33	0.40
2:B:1131:LEU:HD13	2:B:1137:ASN:HA	2.04	0.40
2:J:1211:ALA:O	2:J:1212:ALA:HB3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:5201:HOH:O	4:J:5194:HOH:O[2_664]	2.15	0.05

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	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
1	C	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
1	E	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
1	G	150/166 (90%)	147 (98%)	3 (2%)	0	100	100
1	I	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
1	K	150/166 (90%)	146 (97%)	4 (3%)	0	100	100
2	B	126/134 (94%)	123 (98%)	3 (2%)	0	100	100
2	D	126/134 (94%)	124 (98%)	1 (1%)	1 (1%)	22	17
2	F	126/134 (94%)	123 (98%)	3 (2%)	0	100	100
2	H	126/134 (94%)	124 (98%)	2 (2%)	0	100	100
2	J	126/134 (94%)	123 (98%)	2 (2%)	1 (1%)	22	17
2	L	126/134 (94%)	124 (98%)	1 (1%)	1 (1%)	22	17
All	All	1656/1800 (92%)	1618 (98%)	35 (2%)	3 (0%)	51	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	1134	LYS
2	D	1149	LYS
2	J	1149	LYS

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	140/151 (93%)	133 (95%)	7 (5%)	28	26
1	C	139/151 (92%)	131 (94%)	8 (6%)	23	20
1	E	139/151 (92%)	133 (96%)	6 (4%)	33	32
1	G	139/151 (92%)	133 (96%)	6 (4%)	33	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	139/151 (92%)	133 (96%)	6 (4%)	33	32
1	K	139/151 (92%)	133 (96%)	6 (4%)	33	32
2	B	101/119 (85%)	94 (93%)	7 (7%)	18	14
2	D	102/119 (86%)	94 (92%)	8 (8%)	15	11
2	F	104/119 (87%)	96 (92%)	8 (8%)	15	11
2	H	104/119 (87%)	98 (94%)	6 (6%)	23	20
2	J	98/119 (82%)	92 (94%)	6 (6%)	22	18
2	L	101/119 (85%)	93 (92%)	8 (8%)	14	10
All	All	1445/1620 (89%)	1363 (94%)	82 (6%)	24	21

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	THR
1	A	57	THR
1	A	69	SER
1	A	102	LEU
1	A	112	ILE
1	A	119	GLU
2	B	1109	LEU
2	B	1130	GLU
2	B	1131	LEU
2	B	1137	ASN
2	B	1146	GLN
2	B	1154	LEU
2	B	1163	LEU
1	C	3	THR
1	C	57	THR
1	C	69	SER
1	C	83	GLU
1	C	102	LEU
1	C	111	ILE
1	C	112	ILE
1	C	119	GLU
2	D	1087	SER
2	D	1109	LEU
2	D	1130	GLU
2	D	1131	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	1146	GLN
2	D	1154	LEU
2	D	1163	LEU
2	D	1202	LEU
1	E	3	THR
1	E	57	THR
1	E	69	SER
1	E	102	LEU
1	E	112	ILE
1	E	119	GLU
2	F	1109	LEU
2	F	1130	GLU
2	F	1131	LEU
2	F	1132	THR
2	F	1146	GLN
2	F	1149	LYS
2	F	1154	LEU
2	F	1163	LEU
1	G	3	THR
1	G	57	THR
1	G	69	SER
1	G	102	LEU
1	G	112	ILE
1	G	119	GLU
2	H	1109	LEU
2	H	1130	GLU
2	H	1131	LEU
2	H	1146	GLN
2	H	1154	LEU
2	H	1163	LEU
1	I	3	THR
1	I	57	THR
1	I	69	SER
1	I	102	LEU
1	I	112	ILE
1	I	119	GLU
2	J	1109	LEU
2	J	1130	GLU
2	J	1131	LEU
2	J	1146	GLN
2	J	1154	LEU
2	J	1163	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	3	THR
1	K	57	THR
1	K	69	SER
1	K	102	LEU
1	K	112	ILE
1	K	119	GLU
2	L	1087	SER
2	L	1109	LEU
2	L	1113	GLU
2	L	1130	GLU
2	L	1131	LEU
2	L	1146	GLN
2	L	1154	LEU
2	L	1163	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	86	GLN
1	A	87	ASN
1	A	113	ASN
2	B	1097	HIS
2	B	1122	GLN
2	B	1137	ASN
2	B	1139	ASN
2	B	1146	GLN
1	C	45	GLN
1	C	86	GLN
1	C	87	ASN
1	C	113	ASN
2	D	1097	HIS
2	D	1122	GLN
2	D	1139	ASN
2	D	1146	GLN
1	E	86	GLN
1	E	87	ASN
1	E	113	ASN
2	F	1097	HIS
2	F	1122	GLN
2	F	1139	ASN
2	F	1146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	45	GLN
1	G	86	GLN
1	G	87	ASN
1	G	113	ASN
2	H	1097	HIS
2	H	1139	ASN
2	H	1146	GLN
1	I	45	GLN
1	I	86	GLN
1	I	113	ASN
2	J	1097	HIS
2	J	1139	ASN
2	J	1146	GLN
1	K	45	GLN
1	K	86	GLN
1	K	87	ASN
1	K	113	ASN
2	L	1097	HIS
2	L	1139	ASN
2	L	1146	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	SO4	A	5001	-	4,4,4	0.15	0	6,6,6	0.45	0
3	SO4	A	5002	-	4,4,4	0.08	0	6,6,6	0.65	0
3	SO4	B	5003	-	4,4,4	0.40	0	6,6,6	0.38	0
3	SO4	C	5004	-	4,4,4	0.31	0	6,6,6	0.41	0
3	SO4	C	5005	-	4,4,4	0.28	0	6,6,6	0.47	0
3	SO4	C	5006	-	4,4,4	0.39	0	6,6,6	0.95	0
3	SO4	E	5007	-	4,4,4	0.36	0	6,6,6	0.52	0
3	SO4	E	5008	-	4,4,4	0.26	0	6,6,6	0.91	0
3	SO4	F	5009	-	4,4,4	0.26	0	6,6,6	0.25	0
3	SO4	G	5010	-	4,4,4	0.25	0	6,6,6	0.60	0
3	SO4	G	5011	-	4,4,4	0.17	0	6,6,6	0.33	0
3	SO4	H	5012	-	4,4,4	0.31	0	6,6,6	0.47	0
3	SO4	I	5013	-	4,4,4	0.32	0	6,6,6	0.22	0
3	SO4	I	5014	-	4,4,4	0.20	0	6,6,6	0.42	0
3	SO4	J	5015	-	4,4,4	0.25	0	6,6,6	0.29	0
3	SO4	K	5016	-	4,4,4	0.30	0	6,6,6	0.35	0
3	SO4	K	5017	-	4,4,4	0.18	0	6,6,6	0.64	0
3	SO4	L	5018	-	4,4,4	0.26	0	6,6,6	0.35	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	SO4	A	5001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5002	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5003	-	-	0/0/0/0	0/0/0/0
3	SO4	C	5004	-	-	0/0/0/0	0/0/0/0
3	SO4	C	5005	-	-	0/0/0/0	0/0/0/0
3	SO4	C	5006	-	-	0/0/0/0	0/0/0/0
3	SO4	E	5007	-	-	0/0/0/0	0/0/0/0
3	SO4	E	5008	-	-	0/0/0/0	0/0/0/0
3	SO4	F	5009	-	-	0/0/0/0	0/0/0/0
3	SO4	G	5010	-	-	0/0/0/0	0/0/0/0
3	SO4	G	5011	-	-	0/0/0/0	0/0/0/0
3	SO4	H	5012	-	-	0/0/0/0	0/0/0/0
3	SO4	I	5013	-	-	0/0/0/0	0/0/0/0
3	SO4	I	5014	-	-	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	SO4	J	5015	-	-	0/0/0/0	0/0/0/0
3	SO4	K	5016	-	-	0/0/0/0	0/0/0/0
3	SO4	K	5017	-	-	0/0/0/0	0/0/0/0
3	SO4	L	5018	-	-	0/0/0/0	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.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5001	SO4	1	0
3	B	5003	SO4	3	0
3	C	5006	SO4	2	0
3	F	5009	SO4	3	0
3	H	5012	SO4	3	0
3	I	5013	SO4	1	0
3	J	5015	SO4	3	0
3	K	5016	SO4	1	0
3	L	5018	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	156/166 (93%)	0.03	2 (1%) 77 81	20, 26, 47, 64	0
1	C	156/166 (93%)	0.07	6 (3%) 41 48	20, 26, 47, 64	0
1	E	156/166 (93%)	0.04	4 (2%) 56 62	20, 26, 47, 64	0
1	G	156/166 (93%)	0.00	4 (2%) 56 62	20, 26, 47, 64	0
1	I	156/166 (93%)	0.09	4 (2%) 56 62	19, 26, 46, 64	0
1	K	156/166 (93%)	0.04	4 (2%) 56 62	20, 26, 47, 64	0
2	B	128/134 (95%)	0.39	11 (8%) 11 14	23, 31, 53, 63	0
2	D	128/134 (95%)	0.32	9 (7%) 17 22	23, 31, 52, 63	0
2	F	128/134 (95%)	0.34	9 (7%) 17 22	23, 31, 50, 63	0
2	H	128/134 (95%)	0.31	7 (5%) 26 32	23, 31, 52, 63	0
2	J	128/134 (95%)	0.30	7 (5%) 26 32	23, 31, 53, 63	0
2	L	128/134 (95%)	0.29	7 (5%) 26 32	23, 31, 52, 63	0
All	All	1704/1800 (94%)	0.17	74 (4%) 36 43	19, 29, 49, 64	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1176	ALA	10.3
2	B	1178	ASP	8.7
2	L	1176	ALA	6.7
2	J	1136	GLU	5.2
2	L	1135	GLY	5.2
2	B	1214	GLN	5.1
2	F	1176	ALA	5.0
2	H	1176	ALA	4.9
2	B	1175	PHE	4.9
2	H	1178	ASP	4.7
2	B	1176	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	1176	ALA	4.4
2	J	1135	GLY	4.2
2	H	1175	PHE	4.2
2	B	1179	SER	4.2
1	E	114	GLY	4.1
2	D	1178	ASP	4.0
2	H	1181	ILE	4.0
2	J	1178	ASP	3.9
2	F	1178	ASP	3.8
2	B	1087	SER	3.8
1	E	124	ILE	3.7
2	J	1214	GLN	3.6
2	L	1179	SER	3.6
2	F	1212	ALA	3.5
2	H	1179	SER	3.5
1	K	125	LYS	3.3
1	I	124	ILE	3.3
1	I	123	GLU	3.2
2	B	1181	ILE	3.1
2	F	1179	SER	3.1
2	D	1135	GLY	3.1
1	A	123	GLU	3.0
2	F	1175	PHE	2.9
1	C	125	LYS	2.9
2	D	1179	SER	2.9
2	F	1181	ILE	2.9
2	F	1214	GLN	2.8
1	I	133	GLU	2.8
2	F	1087	SER	2.8
1	A	124	ILE	2.8
1	G	123	GLU	2.7
2	B	1177	ASP	2.7
1	G	114	GLY	2.7
2	H	1177	ASP	2.7
2	J	1179	SER	2.6
2	D	1136	GLU	2.6
2	D	1087	SER	2.6
1	C	132	ASP	2.6
2	D	1149	LYS	2.5
2	D	1177	ASP	2.5
2	L	1178	ASP	2.5
1	K	161	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	125	LYS	2.5
2	H	1214	GLN	2.4
2	F	1149	LYS	2.4
1	I	132	ASP	2.4
2	B	1133	SER	2.3
2	J	1177	ASP	2.3
1	G	164	ASN	2.3
2	L	1087	SER	2.3
2	D	1214	GLN	2.2
2	L	1134	LYS	2.2
1	C	111	ILE	2.2
2	B	1097	HIS	2.2
1	C	123	GLU	2.2
1	C	112	ILE	2.2
1	K	123	GLU	2.1
2	L	1113	GLU	2.1
1	E	125	LYS	2.1
1	C	133	GLU	2.1
1	K	124	ILE	2.0
2	B	1134	LYS	2.0
1	E	112	ILE	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, 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
3	SO4	E	5008	5/5	0.96	0.13	0.20	31,35,39,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	C	5006	5/5	0.93	0.16	-0.02	35,38,39,41	0
3	SO4	G	5010	5/5	0.95	0.14	-0.15	36,42,44,45	0
3	SO4	E	5007	5/5	0.95	0.14	-0.16	47,50,51,52	0
3	SO4	L	5018	5/5	0.95	0.15	-0.20	31,32,35,36	0
3	SO4	A	5002	5/5	0.94	0.11	-0.31	39,44,46,46	0
3	SO4	C	5004	5/5	0.95	0.12	-0.33	36,38,40,40	0
3	SO4	C	5005	5/5	0.96	0.11	-0.80	39,40,42,46	0
3	SO4	A	5001	5/5	0.97	0.10	-0.82	36,39,41,42	0
3	SO4	J	5015	5/5	0.97	0.11	-0.93	39,39,42,43	0
3	SO4	H	5012	5/5	0.98	0.10	-0.96	32,34,37,37	0
3	SO4	K	5017	5/5	0.96	0.09	-1.04	34,37,41,44	0
3	SO4	I	5014	5/5	0.98	0.11	-1.05	36,37,40,40	0
3	SO4	I	5013	5/5	0.98	0.09	-1.06	31,31,33,33	0
3	SO4	B	5003	5/5	0.98	0.07	-1.24	30,33,36,36	0
3	SO4	F	5009	5/5	0.98	0.08	-1.33	31,33,35,37	0
3	SO4	K	5016	5/5	0.97	0.11	-1.34	37,39,43,44	0
3	SO4	G	5011	5/5	0.98	0.08	-1.65	39,42,43,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.