



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 06:07 pm BST

PDB ID : 2OMB  
Title : Bence Jones KWR Protein- Immunoglobulin Light Chain Dimer, P3(1)21  
Crystal Form  
Authors : Makino, D.L.; Larson, S.B.; McPherson, A.  
Deposited on : 2007-01-21  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

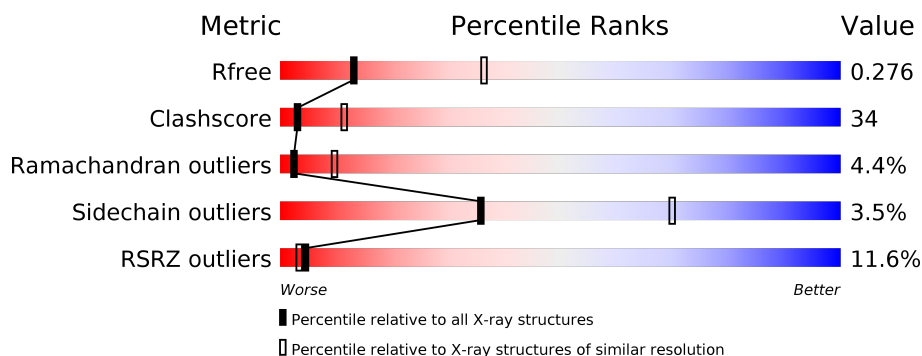
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	217	<div> <div>2%</div> <div> <div>52%</div> <div>44%</div> <div>.</div> </div> </div>
1	B	217	<div> <div>18%</div> <div> <div>39%</div> <div>57%</div> <div>.</div> </div> </div>
1	C	217	<div> <div>3%</div> <div> <div>56%</div> <div>41%</div> <div>.</div> </div> </div>
1	D	217	<div> <div>24%</div> <div> <div>44%</div> <div>49%</div> <div>7%</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IPH	A	2001	-	X	-	-
3	IPH	D	2002	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6459 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 Bence Jones KWR Protein - Immunoglobulin Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1596	991	267	333	5			
1	B	217	Total	C	N	O	S	0	0	0
			1596	991	267	333	5			
1	C	217	Total	C	N	O	S	0	0	0
			1596	991	267	333	5			
1	D	217	Total	C	N	O	S	0	0	0
			1596	991	267	333	5			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



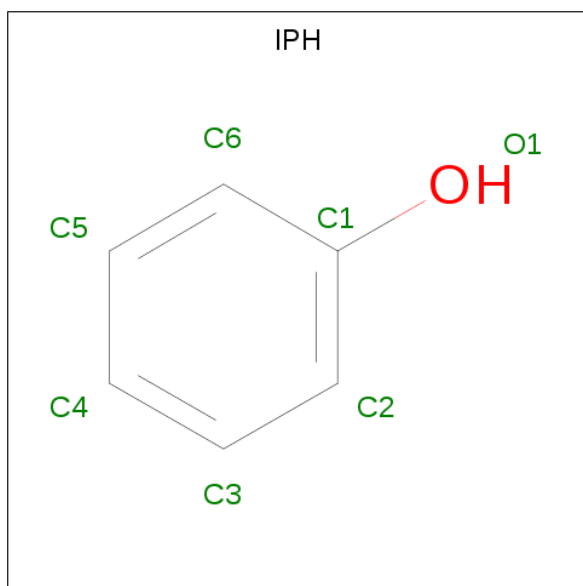
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is PHENOL (three-letter code: IPH) (formula: C<sub>6</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	6	1		
3	D	1	Total	C	O	0	0
			7	6	1		

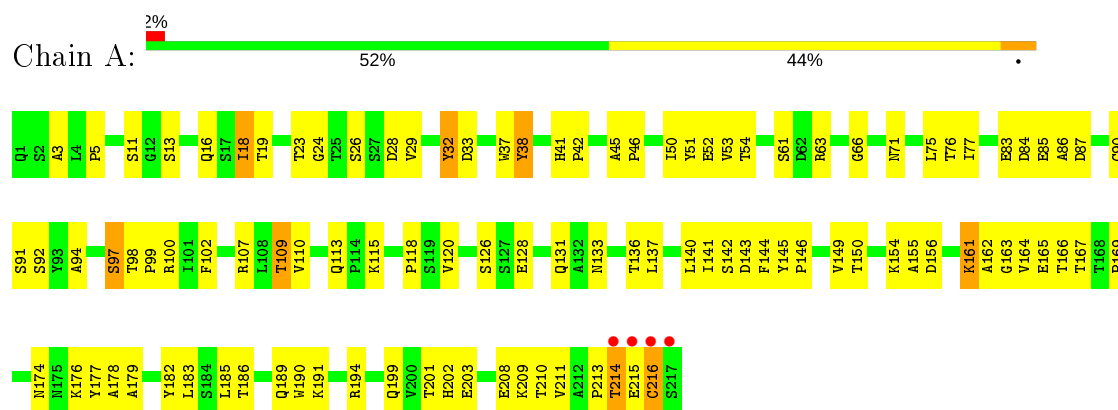
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	1	Total 1	O 1	0	0
4	C	3	Total 3	O 3	0	0
4	D	4	Total 4	O 4	0	0

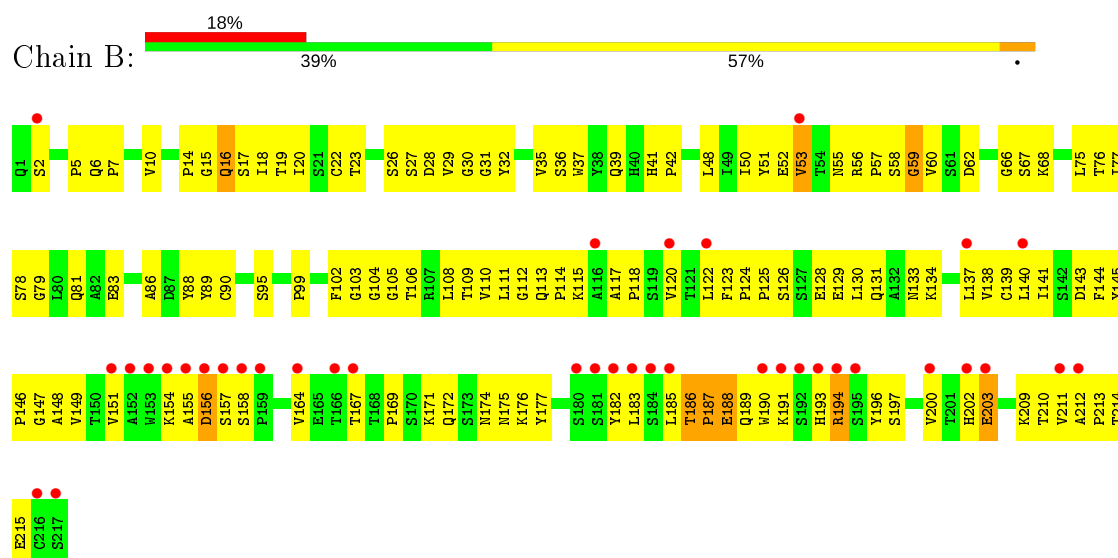
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

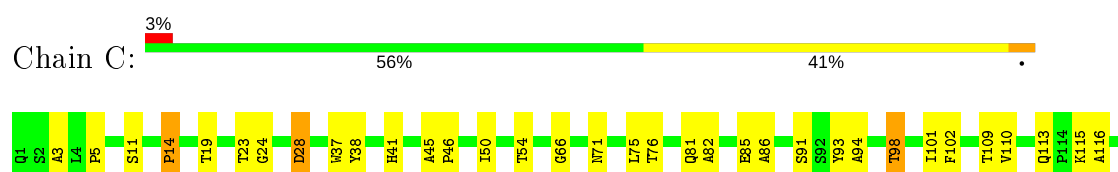
#### • Molecule 1: Bence Jones KWR Protein - Immunoglobulin Light Chain



#### • Molecule 1: Bence Jones KWR Protein - Immunoglobulin Light Chain

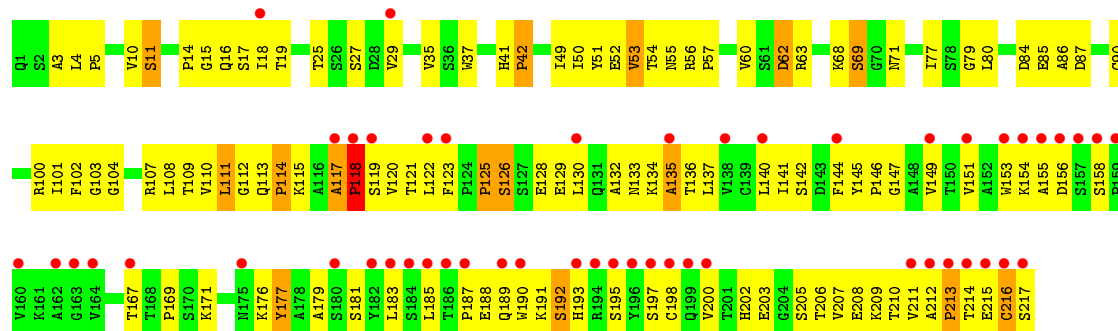
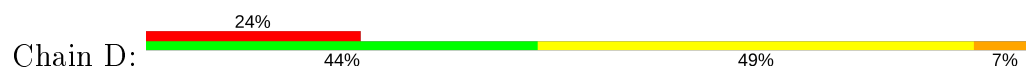


#### • Molecule 1: Bence Jones KWR Protein - Immunoglobulin Light Chain





● Molecule 1: Bence Jones KWR Protein - Immunoglobulin Light Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.52Å 153.52Å 93.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.90 76.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.5 (40.00-2.90) 91.5 (76.76-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.284 0.228 , 0.276	Depositor DCC
$R_{free}$ test set	1820 reflections (6.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 68.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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 61.55 % 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 1.2889e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPH, PCA, 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	0.43	0/1628	0.69	0/2224
1	B	0.36	0/1628	0.67	0/2224
1	C	0.41	0/1628	0.69	0/2224
1	D	0.36	0/1628	0.67	0/2224
All	All	0.39	0/6512	0.68	0/8896

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1529	87	0
1	B	1596	0	1529	142	0
1	C	1596	0	1529	94	0
1	D	1596	0	1529	125	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	7	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	6	0	0
4	A	8	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
All	All	6459	0	6128	426	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 34.

All (426) 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:D:169:PRO:HG3	1:D:179:ALA:HB2	1.43	0.99
1:C:124:PRO:HB3	1:C:211:VAL:HG11	1.49	0.92
1:D:195:SER:HA	1:D:212:ALA:HB2	1.51	0.92
1:B:19:THR:HG22	1:B:76:THR:HB	1.55	0.87
1:B:35:VAL:HG22	1:B:53:VAL:HA	1.57	0.86
1:D:120:VAL:HG13	1:D:140:LEU:O	1.77	0.83
1:B:10:VAL:HG23	1:B:108:LEU:HD13	1.57	0.83
1:A:161:LYS:H	1:A:161:LYS:HD3	1.43	0.83
1:B:197:SER:OG	1:B:210:THR:HG22	1.79	0.82
1:C:199:GLN:HG2	1:C:208:GLU:HG2	1.62	0.81
1:A:75:LEU:HD23	1:A:76:THR:N	1.95	0.81
1:B:112:GLY:C	1:B:114:PRO:HD3	2.01	0.81
1:A:161:LYS:HG2	1:A:162:ALA:H	1.45	0.80
1:C:126:SER:O	1:C:130:LEU:HB2	1.80	0.80
1:C:129:GLU:HG3	1:D:121:THR:HG21	1.64	0.80
1:D:208:GLU:HG2	1:D:209:LYS:H	1.46	0.79
1:A:186:THR:HG22	1:A:189:GLN:HG3	1.65	0.79
1:D:117:ALA:HB1	1:D:118:PRO:HD2	1.67	0.76
1:D:122:LEU:HG	1:D:211:VAL:HG21	1.68	0.75
1:B:190:TRP:NE1	1:B:213:PRO:HG3	2.01	0.75
1:D:188:GLU:OE2	1:D:192:SER:HB3	1.86	0.74
1:B:16:GLN:HE22	1:D:19:THR:H	1.34	0.73
1:B:185:LEU:HD23	1:B:190:TRP:HB2	1.70	0.73
1:D:117:ALA:HB1	1:D:118:PRO:CD	2.17	0.72
1:D:18:ILE:HD13	1:D:108:LEU:HD13	1.69	0.72
1:D:129:GLU:HG3	1:D:135:ALA:HA	1.70	0.72
1:B:113:GLN:N	1:B:114:PRO:HD3	2.05	0.72
1:A:54:THR:HG22	1:A:66:GLY:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:THR:HG22	1:B:76:THR:CB	2.19	0.71
1:B:118:PRO:HG2	1:B:202:HIS:HB2	1.71	0.71
1:B:167:THR:HG23	1:B:182:TYR:HE2	1.56	0.71
1:C:163:GLY:O	1:C:183:LEU:HD12	1.90	0.71
1:D:87:ASP:OD2	1:D:107:ARG:HG2	1.90	0.71
1:C:125:PRO:HG2	1:C:135:ALA:HB1	1.72	0.71
1:C:214:THR:HB	1:C:217:SER:HB2	1.73	0.71
1:D:18:ILE:HD13	1:D:108:LEU:CD1	2.20	0.71
1:A:126:SER:HB2	1:A:128:GLU:OE1	1.92	0.70
1:B:125:PRO:HD3	1:B:137:LEU:HD23	1.74	0.69
1:B:14:PRO:CG	1:B:112:GLY:HA2	2.23	0.69
1:B:188:GLU:HA	1:B:191:LYS:HD2	1.72	0.69
1:C:134:LYS:HZ3	1:C:187:PRO:HD3	1.57	0.69
1:D:126:SER:O	1:D:129:GLU:HB3	1.93	0.68
1:D:122:LEU:HD12	1:D:123:PHE:N	2.08	0.68
1:D:208:GLU:HG2	1:D:209:LYS:N	2.07	0.68
1:C:125:PRO:HB2	1:C:130:LEU:HD13	1.77	0.67
1:A:37:TRP:CZ3	1:A:90:CYS:HB3	2.30	0.67
1:C:124:PRO:HB3	1:C:211:VAL:CG1	2.23	0.67
1:B:167:THR:HG23	1:B:182:TYR:CE2	2.30	0.67
1:B:125:PRO:HD2	1:B:190:TRP:CZ2	2.29	0.66
1:A:190:TRP:HH2	1:A:211:VAL:HG12	1.58	0.66
1:B:53:VAL:HG11	1:B:68:LYS:HG2	1.78	0.66
1:A:156:ASP:OD1	1:A:194:ARG:HB2	1.96	0.66
1:A:41:HIS:CE1	1:A:86:ALA:HB2	2.31	0.66
1:C:134:LYS:NZ	1:C:134:LYS:HA	2.10	0.66
1:C:156:ASP:OD1	1:C:194:ARG:HB2	1.96	0.66
1:D:51:TYR:HD1	1:D:52:GLU:HG3	1.60	0.66
1:B:186:THR:HB	1:B:187:PRO:HD2	1.78	0.65
1:B:16:GLN:NE2	1:D:19:THR:H	1.93	0.65
1:B:164:VAL:HG22	1:B:183:LEU:HD13	1.78	0.64
1:B:143:ASP:O	1:B:176:LYS:HD3	1.98	0.64
1:A:51:TYR:CE2	1:B:99:PRO:HG2	2.32	0.64
1:B:186:THR:OG1	1:B:189:GLN:HB2	1.97	0.64
1:D:49:ILE:HA	1:D:60:VAL:HG21	1.78	0.64
1:A:150:THR:OG1	1:A:201:THR:HB	1.97	0.64
1:C:24:GLY:O	1:C:71:ASN:HB3	1.96	0.64
1:C:164:VAL:HG22	1:C:183:LEU:HD13	1.79	0.64
1:A:24:GLY:O	1:A:71:ASN:HB3	1.98	0.63
1:D:125:PRO:HD3	1:D:137:LEU:HG	1.80	0.63
1:D:215:GLU:HG2	1:D:216:CYS:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LYS:HG2	1:D:69:SER:N	2.14	0.63
1:D:122:LEU:HD12	1:D:123:PHE:H	1.62	0.63
1:C:172:GLN:HA	1:C:172:GLN:HE21	1.64	0.62
1:C:122:LEU:HD23	1:C:211:VAL:HG23	1.82	0.62
1:B:19:THR:HA	1:B:76:THR:HA	1.80	0.62
1:C:145:TYR:HA	1:C:146:PRO:C	2.19	0.62
1:A:75:LEU:C	1:A:75:LEU:HD23	2.20	0.62
1:B:144:PHE:HE1	1:B:147:GLY:HA2	1.65	0.62
1:C:134:LYS:HZ3	1:C:134:LYS:HA	1.64	0.61
1:C:113:GLN:HG3	1:C:145:TYR:CE2	2.35	0.61
1:D:68:LYS:HG2	1:D:69:SER:H	1.64	0.61
1:A:186:THR:HG22	1:A:189:GLN:CG	2.30	0.61
1:C:137:LEU:N	1:C:137:LEU:HD12	2.16	0.61
1:C:91:SER:HB3	1:C:102:PHE:CD1	2.36	0.60
1:A:155:ALA:O	1:A:156:ASP:HB2	1.99	0.60
1:C:156:ASP:HB3	1:C:194:ARG:HH21	1.67	0.60
1:C:45:ALA:HB2	1:D:104:GLY:HA2	1.84	0.60
1:D:197:SER:OG	1:D:210:THR:HG22	2.02	0.60
1:B:171:LYS:NZ	1:B:175:ASN:HA	2.16	0.60
1:B:90:CYS:O	1:B:103:GLY:N	2.33	0.60
1:C:172:GLN:NE2	1:C:172:GLN:HA	2.17	0.59
1:A:94:ALA:N	1:A:99:PRO:O	2.32	0.59
1:B:50:ILE:HD13	1:B:55:ASN:O	2.02	0.59
1:C:188:GLU:O	1:C:192:SER:HB2	2.02	0.59
1:B:18:ILE:HD11	1:B:77:ILE:HD12	1.84	0.59
1:B:126:SER:OG	1:B:129:GLU:HB2	2.02	0.59
1:B:17:SER:OG	1:B:78:SER:HA	2.03	0.59
1:D:130:LEU:HA	1:D:134:LYS:O	2.02	0.59
1:C:125:PRO:CG	1:C:135:ALA:HB1	2.32	0.59
1:C:174:ASN:HD21	1:C:176:LYS:HB2	1.67	0.59
1:B:51:TYR:O	1:B:55:ASN:HB2	2.03	0.59
1:D:129:GLU:O	1:D:132:ALA:HB3	2.02	0.59
1:D:169:PRO:HG3	1:D:179:ALA:CB	2.26	0.58
1:B:187:PRO:C	1:B:191:LYS:HE3	2.24	0.58
1:C:198:CYS:O	1:C:208:GLU:HA	2.04	0.58
1:C:98:THR:HG23	1:D:57:PRO:HG2	1.86	0.58
1:C:154:LYS:HA	1:C:160:VAL:HG23	1.86	0.58
1:D:111:LEU:HD12	1:D:111:LEU:O	2.03	0.58
1:D:100:ARG:HG2	1:D:102:PHE:CE2	2.38	0.57
1:D:10:VAL:O	1:D:108:LEU:HD12	2.05	0.57
1:B:14:PRO:HG2	1:B:112:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ALA:O	1:D:185:LEU:HB3	2.04	0.57
1:D:120:VAL:O	1:D:209:LYS:HE3	2.04	0.57
1:A:85:GLU:HG2	1:A:110:VAL:HG23	1.87	0.56
1:B:113:GLN:HA	1:B:145:TYR:HE2	1.70	0.56
1:B:149:VAL:HG22	1:B:202:HIS:ND1	2.20	0.56
1:B:37:TRP:HB2	1:B:50:ILE:HB	1.86	0.56
1:A:164:VAL:HG22	1:A:183:LEU:HD13	1.85	0.56
1:B:113:GLN:HA	1:B:145:TYR:CE2	2.41	0.56
1:C:116:ALA:O	1:C:144:PHE:HA	2.05	0.56
1:D:212:ALA:O	1:D:214:THR:HG22	2.05	0.56
1:B:154:LYS:HE3	1:B:157:SER:HA	1.87	0.56
1:D:141:ILE:HD11	1:D:151:VAL:HG21	1.86	0.56
1:A:186:THR:CG2	1:A:189:GLN:HG3	2.35	0.55
1:A:136:THR:O	1:B:123:PHE:HZ	1.89	0.55
1:C:153:TRP:CZ3	1:C:198:CYS:HB2	2.41	0.55
1:D:190:TRP:CH2	1:D:213:PRO:HA	2.40	0.55
1:C:131:GLN:C	1:C:133:ASN:H	2.07	0.55
1:C:210:THR:HG22	1:C:211:VAL:N	2.22	0.55
1:D:137:LEU:HD12	1:D:137:LEU:N	2.21	0.55
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.72	0.55
1:D:51:TYR:CD1	1:D:52:GLU:HG3	2.42	0.55
1:A:18:ILE:CD1	1:A:19:THR:H	2.19	0.55
1:B:48:LEU:O	1:B:57:PRO:HG2	2.07	0.55
1:B:39:GLN:NE2	1:B:88:TYR:OH	2.39	0.55
1:D:177:TYR:CD2	1:D:177:TYR:N	2.74	0.54
1:A:161:LYS:H	1:A:161:LYS:CD	2.16	0.54
1:A:164:VAL:HG12	1:A:165:GLU:N	2.22	0.54
1:B:174:ASN:O	1:B:175:ASN:HB2	2.07	0.54
1:C:41:HIS:CE1	1:C:86:ALA:HB2	2.43	0.54
1:D:185:LEU:HD23	1:D:190:TRP:HB2	1.88	0.54
1:D:206:THR:HG22	1:D:207:VAL:N	2.22	0.54
1:D:29:VAL:HG13	1:D:35:VAL:HG21	1.90	0.54
1:B:36:SER:O	1:B:90:CYS:HA	2.08	0.54
1:D:41:HIS:ND1	1:D:86:ALA:HB2	2.22	0.54
1:B:149:VAL:HG11	1:B:200:VAL:CG1	2.38	0.54
1:C:172:GLN:O	1:C:175:ASN:N	2.32	0.54
1:D:153:TRP:HE1	1:D:181:SER:HB3	1.72	0.54
1:D:11:SER:HA	1:D:109:THR:O	2.08	0.54
1:D:3:ALA:O	1:D:5:PRO:HD3	2.07	0.54
1:B:120:VAL:CG2	1:B:139:CYS:SG	2.96	0.53
1:B:118:PRO:HB3	1:B:141:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:SER:OG	1:D:129:GLU:HB2	2.08	0.53
1:D:187:PRO:O	1:D:191:LYS:HG3	2.08	0.53
1:B:120:VAL:HG13	1:B:209:LYS:HG3	1.89	0.53
1:B:131:GLN:C	1:B:133:ASN:H	2.12	0.53
1:C:126:SER:HB2	1:C:129:GLU:HB3	1.91	0.53
1:A:37:TRP:HB2	1:A:50:ILE:HB	1.91	0.53
1:D:145:TYR:CD1	1:D:146:PRO:HA	2.42	0.53
1:B:141:ILE:CD1	1:B:151:VAL:HG21	2.39	0.53
1:D:141:ILE:CD1	1:D:151:VAL:HG21	2.38	0.53
1:A:216:CYS:O	1:B:215:GLU:HG3	2.08	0.53
1:C:164:VAL:HG22	1:C:183:LEU:CD1	2.37	0.53
1:D:130:LEU:HD23	1:D:135:ALA:HB2	1.91	0.52
1:D:134:LYS:HG2	1:D:135:ALA:H	1.73	0.52
1:D:195:SER:HA	1:D:212:ALA:CB	2.34	0.52
1:D:50:ILE:HA	1:D:55:ASN:O	2.09	0.52
1:B:41:HIS:CD2	1:B:86:ALA:HB2	2.45	0.52
1:A:5:PRO:HD2	1:A:23:THR:O	2.10	0.52
1:D:169:PRO:CG	1:D:179:ALA:HB2	2.29	0.52
1:A:161:LYS:HG2	1:A:162:ALA:N	2.21	0.52
1:D:137:LEU:CD1	1:D:185:LEU:HD22	2.40	0.52
1:D:128:GLU:O	1:D:132:ALA:N	2.42	0.52
1:B:7:PRO:O	1:B:106:THR:HG23	2.10	0.52
1:C:191:LYS:H	1:C:191:LYS:HD2	1.75	0.52
1:A:178:ALA:O	1:A:179:ALA:HB2	2.10	0.51
1:B:188:GLU:HA	1:B:191:LYS:CD	2.39	0.51
1:B:36:SER:HA	1:B:50:ILE:O	2.11	0.51
1:C:188:GLU:HG2	1:C:189:GLN:N	2.25	0.51
1:D:18:ILE:HD11	1:D:77:ILE:HD12	1.91	0.51
1:C:133:ASN:O	1:C:134:LYS:HE2	2.10	0.51
1:B:141:ILE:HD11	1:B:151:VAL:HG21	1.92	0.51
1:B:37:TRP:HA	1:B:89:TYR:O	2.11	0.51
1:D:177:TYR:HD2	1:D:177:TYR:N	2.09	0.51
1:D:37:TRP:CZ3	1:D:90:CYS:HB3	2.45	0.51
1:B:186:THR:CB	1:B:187:PRO:HD2	2.39	0.51
1:C:174:ASN:ND2	1:C:176:LYS:HB2	2.26	0.51
1:A:118:PRO:HG3	1:A:144:PHE:HB3	1.92	0.50
1:A:45:ALA:HB2	1:B:104:GLY:HA2	1.93	0.50
1:B:185:LEU:HD23	1:B:190:TRP:CB	2.38	0.50
1:B:129:GLU:HG2	1:B:134:LYS:HB2	1.94	0.50
1:B:120:VAL:O	1:B:209:LYS:HE3	2.12	0.50
1:B:185:LEU:HD21	1:B:196:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:VAL:HG13	1:B:53:VAL:HG22	1.92	0.50
1:D:51:TYR:HE2	1:D:57:PRO:HG3	1.77	0.50
1:D:29:VAL:HG12	1:D:68:LYS:HG3	1.94	0.50
1:B:128:GLU:O	1:B:131:GLN:HG2	2.12	0.50
1:D:141:ILE:HG22	1:D:144:PHE:CE2	2.47	0.50
1:B:6:GLN:HB3	1:B:106:THR:OG1	2.13	0.49
1:C:134:LYS:NZ	1:C:187:PRO:HD3	2.26	0.49
1:A:164:VAL:O	1:A:165:GLU:HG2	2.11	0.49
1:A:210:THR:HG22	1:A:211:VAL:N	2.28	0.49
1:C:81:GLN:O	1:C:110:VAL:HG21	2.12	0.49
1:B:108:LEU:HD12	1:B:109:THR:N	2.27	0.49
1:D:144:PHE:HE1	1:D:147:GLY:HA2	1.78	0.49
1:A:28:ASP:OD2	1:A:29:VAL:HG23	2.12	0.49
1:B:193:HIS:HB2	1:B:196:TYR:CE2	2.47	0.49
1:D:136:THR:HG23	1:D:183:LEU:O	2.13	0.49
1:B:138:VAL:HG13	1:B:182:TYR:CE1	2.47	0.49
1:B:57:PRO:O	1:B:59:GLY:N	2.40	0.49
1:B:125:PRO:HD2	1:B:190:TRP:CH2	2.48	0.49
1:B:118:PRO:HA	1:B:144:PHE:HB3	1.93	0.49
1:C:142:SER:O	1:C:143:ASP:HB2	2.12	0.49
1:B:156:ASP:OD2	1:B:194:ARG:N	2.46	0.48
1:B:187:PRO:O	1:B:191:LYS:HG3	2.13	0.48
1:C:37:TRP:HB2	1:C:50:ILE:HB	1.96	0.48
1:B:10:VAL:HG23	1:B:108:LEU:CD1	2.37	0.48
1:B:144:PHE:CE1	1:B:147:GLY:HA2	2.46	0.48
1:C:139:CYS:HB2	1:C:153:TRP:CZ2	2.48	0.48
1:C:140:LEU:C	1:C:140:LEU:HD23	2.32	0.48
1:C:37:TRP:CD2	1:C:75:LEU:HB2	2.48	0.48
1:D:41:HIS:CE1	1:D:86:ALA:HB2	2.48	0.48
1:C:165:GLU:HB2	1:C:182:TYR:CZ	2.49	0.48
1:C:54:THR:HG22	1:C:66:GLY:O	2.13	0.48
1:C:216:CYS:HA	1:D:216:CYS:HB3	1.96	0.48
1:D:56:ARG:HG3	1:D:60:VAL:CG1	2.44	0.48
1:A:174:ASN:ND2	1:A:176:LYS:HB2	2.27	0.48
1:B:156:ASP:HB2	1:B:193:HIS:HB3	1.95	0.48
1:D:198:CYS:O	1:D:208:GLU:HG3	2.14	0.48
1:C:174:ASN:ND2	1:C:176:LYS:HD2	2.29	0.48
1:D:171:LYS:HA	1:D:176:LYS:O	2.13	0.48
1:D:155:ALA:O	1:D:156:ASP:HB2	2.13	0.48
1:B:18:ILE:HD12	1:B:18:ILE:C	2.34	0.48
1:D:114:PRO:HG2	1:D:115:LYS:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:O	1:A:209:LYS:HD3	2.14	0.48
1:D:154:LYS:HA	1:D:158:SER:O	2.13	0.48
1:D:130:LEU:C	1:D:132:ALA:H	2.16	0.47
1:C:177:TYR:CD2	1:C:177:TYR:N	2.82	0.47
1:D:155:ALA:O	1:D:158:SER:HB3	2.14	0.47
1:A:87:ASP:OD2	1:A:107:ARG:NE	2.47	0.47
1:D:122:LEU:HD11	1:D:137:LEU:HB3	1.95	0.47
1:C:172:GLN:OE1	1:D:167:THR:HG22	2.15	0.47
1:D:51:TYR:O	1:D:55:ASN:HB2	2.14	0.47
1:A:182:TYR:OH	1:B:172:GLN:NE2	2.42	0.47
1:A:28:ASP:OD2	1:A:29:VAL:N	2.45	0.47
1:B:35:VAL:CG2	1:B:53:VAL:HA	2.36	0.47
1:A:163:GLY:O	1:A:183:LEU:HD12	2.15	0.47
1:B:171:LYS:HZ2	1:B:175:ASN:HA	1.79	0.47
1:B:19:THR:HA	1:B:75:LEU:O	2.15	0.47
1:B:125:PRO:HD3	1:B:137:LEU:CD2	2.44	0.47
1:A:13:SER:O	1:A:16:GLN:HG3	2.15	0.47
1:A:33:ASP:O	1:A:52:GLU:HA	2.14	0.47
1:B:22:CYS:HB2	1:B:37:TRP:CH2	2.50	0.47
1:C:129:GLU:O	1:C:132:ALA:HB3	2.15	0.47
1:D:149:VAL:HG11	1:D:200:VAL:HG13	1.96	0.47
1:A:26:SER:N	1:A:71:ASN:ND2	2.63	0.47
1:D:129:GLU:CG	1:D:135:ALA:HA	2.43	0.47
1:A:115:LYS:HE3	1:A:203:GLU:HG3	1.97	0.46
1:B:167:THR:CG2	1:B:182:TYR:HE2	2.27	0.46
1:B:19:THR:HB	1:B:76:THR:HG22	1.97	0.46
1:B:19:THR:HG22	1:B:76:THR:CG2	2.44	0.46
1:B:83:GLU:CD	1:B:83:GLU:H	2.18	0.46
1:C:139:CYS:HB2	1:C:153:TRP:CH2	2.50	0.46
1:A:144:PHE:HZ	1:A:169:PRO:HB3	1.79	0.46
1:B:51:TYR:O	1:B:52:GLU:HB2	2.14	0.46
1:D:154:LYS:HB2	1:D:197:SER:HB2	1.96	0.46
1:B:37:TRP:HD1	1:B:50:ILE:HG21	1.81	0.46
1:C:141:ILE:HD11	1:C:151:VAL:HG21	1.97	0.46
1:A:137:LEU:CD1	1:A:185:LEU:HD12	2.45	0.46
1:C:196:TYR:O	1:C:210:THR:HG23	2.15	0.46
1:D:112:GLY:O	1:D:113:GLN:HB2	2.15	0.46
1:D:120:VAL:HG22	1:D:142:SER:H	1.81	0.46
1:A:120:VAL:HA	1:A:140:LEU:O	2.16	0.46
1:C:129:GLU:CG	1:D:121:THR:HG21	2.39	0.46
1:D:4:LEU:HB2	1:D:103:GLY:HA2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:CYS:O	1:D:217:SER:HB2	2.16	0.46
1:B:15:GLY:HA2	1:B:79:GLY:HA2	1.98	0.46
1:B:6:GLN:OE1	1:B:105:GLY:N	2.39	0.46
1:C:85:GLU:OE2	1:C:110:VAL:N	2.46	0.46
1:D:192:SER:O	1:D:193:HIS:C	2.53	0.46
1:C:125:PRO:CB	1:C:130:LEU:HD13	2.46	0.46
1:D:137:LEU:HD11	1:D:185:LEU:HD22	1.98	0.46
1:C:126:SER:O	1:C:130:LEU:N	2.49	0.45
1:C:82:ALA:O	1:C:85:GLU:HB2	2.15	0.45
1:B:148:ALA:HB1	1:D:203:GLU:HG2	1.96	0.45
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.83	0.45
1:B:156:ASP:C	1:B:158:SER:H	2.19	0.45
1:B:144:PHE:CE1	1:B:177:TYR:HB2	2.51	0.45
1:B:41:HIS:O	1:B:42:PRO:C	2.55	0.45
1:B:20:ILE:N	1:B:75:LEU:O	2.38	0.45
1:C:101:ILE:HG22	1:C:102:PHE:N	2.31	0.45
1:C:190:TRP:HB3	1:C:191:LYS:HD2	1.99	0.45
1:D:125:PRO:HB3	1:D:129:GLU:HG2	1.97	0.45
1:A:190:TRP:CH2	1:A:211:VAL:HG12	2.46	0.45
1:B:149:VAL:HG11	1:B:200:VAL:HG13	1.99	0.45
1:D:15:GLY:O	1:D:79:GLY:HA2	2.15	0.45
1:D:120:VAL:O	1:D:209:LYS:HG3	2.16	0.45
1:B:143:ASP:C	1:B:176:LYS:HD3	2.36	0.45
1:C:186:THR:OG1	1:C:189:GLN:HG3	2.17	0.45
1:B:18:ILE:HD12	1:B:18:ILE:O	2.17	0.45
1:C:154:LYS:HG3	1:C:158:SER:H	1.81	0.45
1:C:133:ASN:O	1:C:187:PRO:HG2	2.17	0.45
1:D:149:VAL:HG22	1:D:202:HIS:HA	1.99	0.45
1:A:199:GLN:HG2	1:A:208:GLU:HG2	1.99	0.45
1:A:145:TYR:HA	1:A:146:PRO:C	2.37	0.45
1:C:172:GLN:CA	1:C:172:GLN:HE21	2.25	0.45
1:B:118:PRO:HB3	1:B:141:ILE:CG2	2.47	0.45
1:A:216:CYS:HB2	1:B:215:GLU:HA	1.99	0.45
1:D:114:PRO:HB2	1:D:176:LYS:HD3	1.99	0.45
1:A:190:TRP:CZ2	1:A:213:PRO:HA	2.51	0.44
1:A:61:SER:OG	1:A:63:ARG:HG3	2.17	0.44
1:C:115:LYS:HE3	1:C:203:GLU:HG3	1.99	0.44
1:A:46:PRO:HG2	1:B:102:PHE:CB	2.48	0.44
1:B:32:TYR:OH	1:B:95:SER:HB3	2.17	0.44
1:A:32:TYR:N	1:A:32:TYR:CD2	2.84	0.44
1:B:131:GLN:C	1:B:133:ASN:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:HD13	1:A:19:THR:H	1.81	0.44
1:A:63:ARG:HH22	1:A:84:ASP:CG	2.20	0.44
1:B:164:VAL:HG22	1:B:183:LEU:CD1	2.45	0.44
1:C:94:ALA:HB3	1:C:98:THR:O	2.17	0.44
1:D:51:TYR:O	1:D:52:GLU:HB2	2.18	0.44
1:D:202:HIS:O	1:D:203:GLU:HB2	2.17	0.44
1:B:122:LEU:HD11	1:B:137:LEU:HB3	2.00	0.44
1:B:120:VAL:HG13	1:B:209:LYS:CG	2.47	0.44
1:C:131:GLN:C	1:C:133:ASN:N	2.71	0.44
1:A:144:PHE:CE1	1:A:177:TYR:HB2	2.53	0.43
1:B:113:GLN:N	1:B:114:PRO:CD	2.78	0.43
1:B:16:GLN:OE1	1:D:18:ILE:HA	2.18	0.43
1:C:194:ARG:O	1:C:195:SER:HB3	2.17	0.43
1:D:85:GLU:HG3	1:D:110:VAL:H	1.82	0.43
1:A:154:LYS:HD3	1:A:199:GLN:NE2	2.33	0.43
1:A:191:LYS:HE3	1:A:214:THR:HB	2.00	0.43
1:A:97:SER:HB2	1:A:98:THR:H	1.67	0.43
1:C:19:THR:HG22	1:C:76:THR:OG1	2.18	0.43
1:D:117:ALA:CB	1:D:118:PRO:CD	2.90	0.43
1:A:128:GLU:CD	1:A:128:GLU:H	2.22	0.43
1:A:11:SER:HA	1:A:109:THR:O	2.19	0.43
1:A:38:TYR:CD1	1:A:38:TYR:N	2.86	0.43
1:B:66:GLY:O	1:B:67:SER:HB3	2.17	0.43
1:C:5:PRO:HG2	1:C:23:THR:HG22	1.99	0.43
1:A:177:TYR:CD2	1:A:177:TYR:N	2.86	0.43
1:B:81:GLN:O	1:B:110:VAL:HG11	2.19	0.43
1:B:124:PRO:HB3	1:B:211:VAL:HG11	1.99	0.43
1:C:154:LYS:O	1:C:197:SER:N	2.50	0.43
1:A:137:LEU:HD12	1:A:137:LEU:N	2.34	0.43
1:B:120:VAL:HA	1:B:140:LEU:O	2.18	0.43
1:B:57:PRO:HB2	1:B:60:VAL:HG23	2.01	0.43
1:B:53:VAL:HG12	1:B:67:SER:HA	1.99	0.43
1:C:153:TRP:CH2	1:C:198:CYS:HB2	2.54	0.43
1:D:130:LEU:C	1:D:132:ALA:N	2.72	0.43
1:B:14:PRO:CD	1:B:112:GLY:HA2	2.48	0.43
1:B:130:LEU:O	1:B:133:ASN:HA	2.18	0.43
1:B:155:ALA:O	1:B:156:ASP:HB3	2.18	0.43
1:B:16:GLN:NE2	1:D:19:THR:O	2.52	0.43
1:D:120:VAL:O	1:D:120:VAL:HG12	2.19	0.43
1:D:206:THR:CG2	1:D:207:VAL:N	2.81	0.43
1:A:18:ILE:HD12	1:A:19:THR:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PRO:HG3	1:A:144:PHE:CB	2.48	0.42
1:A:142:SER:O	1:A:143:ASP:HB2	2.19	0.42
1:A:92:SER:O	1:A:100:ARG:HD2	2.19	0.42
1:B:126:SER:O	1:B:130:LEU:HG	2.19	0.42
1:B:5:PRO:HD2	1:B:23:THR:HB	2.00	0.42
1:A:136:THR:O	1:B:123:PHE:CZ	2.72	0.42
1:A:41:HIS:ND1	1:A:86:ALA:HB2	2.33	0.42
1:B:138:VAL:HG13	1:B:182:TYR:HE1	1.84	0.42
1:D:211:VAL:HG12	1:D:212:ALA:N	2.35	0.42
1:D:52:GLU:O	1:D:54:THR:N	2.49	0.42
1:A:163:GLY:C	1:A:183:LEU:HD12	2.39	0.42
1:B:120:VAL:HG23	1:B:139:CYS:SG	2.59	0.42
1:C:214:THR:CB	1:C:217:SER:HB2	2.45	0.42
1:A:166:THR:HG22	1:A:167:THR:N	2.34	0.42
1:A:141:ILE:N	1:A:141:ILE:HD12	2.35	0.42
1:C:11:SER:HA	1:C:109:THR:O	2.20	0.42
1:A:75:LEU:HD21	1:A:77:ILE:HG12	2.01	0.42
1:B:26:SER:HA	1:B:30:GLY:O	2.20	0.42
1:C:123:PHE:O	1:C:137:LEU:HB3	2.20	0.42
1:D:25:THR:HA	1:D:71:ASN:HB3	2.02	0.42
1:A:113:GLN:HG3	1:A:145:TYR:CE2	2.55	0.42
1:B:117:ALA:HA	1:B:118:PRO:HD3	1.80	0.42
1:B:186:THR:HB	1:B:187:PRO:CD	2.48	0.42
1:A:215:GLU:HG2	1:A:216:CYS:N	2.35	0.42
1:B:27:SER:O	1:B:32:TYR:HE2	2.02	0.42
1:D:188:GLU:O	1:D:190:TRP:N	2.52	0.42
1:A:164:VAL:CG1	1:A:165:GLU:N	2.83	0.41
1:A:98:THR:HA	1:A:99:PRO:HD3	1.77	0.41
1:D:122:LEU:HG	1:D:211:VAL:CG2	2.47	0.41
1:A:18:ILE:CD1	1:A:19:THR:N	2.82	0.41
1:B:16:GLN:HE22	1:D:19:THR:N	2.09	0.41
1:C:46:PRO:HG2	1:D:102:PHE:CG	2.55	0.41
1:A:133:ASN:CG	1:A:133:ASN:O	2.59	0.41
1:B:214:THR:OG1	1:B:215:GLU:N	2.53	0.41
1:D:18:ILE:CD1	1:D:108:LEU:HD13	2.43	0.41
1:A:91:SER:HB3	1:A:102:PHE:CD1	2.56	0.41
1:D:215:GLU:HG2	1:D:216:CYS:H	1.85	0.41
1:D:41:HIS:O	1:D:42:PRO:C	2.59	0.41
1:B:50:ILE:CD1	1:B:55:ASN:O	2.65	0.41
1:B:6:GLN:HE22	1:B:89:TYR:HA	1.86	0.41
1:C:75:LEU:HD12	1:C:76:THR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLY:C	1:B:114:PRO:CD	2.82	0.41
1:B:146:PRO:HD2	1:B:203:GLU:CD	2.41	0.41
1:D:192:SER:OG	1:D:193:HIS:N	2.50	0.41
1:B:10:VAL:O	1:B:108:LEU:HD12	2.21	0.41
1:B:56:ARG:HA	1:B:57:PRO:HD3	1.98	0.41
1:C:14:PRO:HG3	1:C:110:VAL:HG12	2.03	0.41
1:C:120:VAL:HA	1:C:140:LEU:O	2.21	0.41
1:C:191:LYS:HD2	1:C:191:LYS:N	2.34	0.41
1:D:101:ILE:H	1:D:101:ILE:HG12	1.64	0.41
1:B:53:VAL:CG1	1:B:68:LYS:HG2	2.47	0.41
1:D:130:LEU:CD2	1:D:135:ALA:HB2	2.50	0.41
1:D:63:ARG:HH22	1:D:84:ASP:CG	2.24	0.41
1:A:53:VAL:HG12	1:A:54:THR:HG23	2.02	0.41
1:B:155:ALA:O	1:B:156:ASP:CB	2.69	0.41
1:C:134:LYS:CE	1:C:134:LYS:HA	2.51	0.41
1:C:183:LEU:C	1:C:185:LEU:H	2.21	0.41
1:D:53:VAL:C	1:D:54:THR:CG2	2.89	0.41
1:B:118:PRO:CG	1:B:202:HIS:HB2	2.47	0.40
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.91	0.40
1:D:125:PRO:HB3	1:D:135:ALA:HA	2.03	0.40
1:A:131:GLN:C	1:A:133:ASN:H	2.25	0.40
1:C:38:TYR:N	1:C:38:TYR:CD1	2.89	0.40
1:C:91:SER:HB3	1:C:102:PHE:CE1	2.57	0.40
1:D:203:GLU:O	1:D:205:SER:N	2.48	0.40
1:A:149:VAL:HG12	1:A:202:HIS:HB2	2.02	0.40
1:C:133:ASN:O	1:C:134:LYS:HG2	2.21	0.40
1:C:28:ASP:HA	1:C:93:TYR:O	2.21	0.40
1:D:132:ALA:O	1:D:133:ASN:HB3	2.21	0.40
1:D:134:LYS:HA	1:D:187:PRO:HD3	2.03	0.40

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	215/217 (99%)	189 (88%)	23 (11%)	3 (1%)	11	36
1	B	215/217 (99%)	166 (77%)	35 (16%)	14 (6%)	1	3
1	C	215/217 (99%)	177 (82%)	34 (16%)	4 (2%)	8	28
1	D	215/217 (99%)	164 (76%)	34 (16%)	17 (8%)	1	2
All	All	860/868 (99%)	696 (81%)	126 (15%)	38 (4%)	2	10

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ALA
1	A	97	SER
1	A	214	THR
1	B	111	LEU
1	B	115	LYS
1	C	3	ALA
1	C	161	LYS
1	D	119	SER
1	D	126	SER
1	B	2	SER
1	B	187	PRO
1	C	194	ARG
1	D	53	VAL
1	D	118	PRO
1	D	189	GLN
1	B	58	SER
1	C	184	SER
1	D	114	PRO
1	D	125	PRO
1	D	192	SER
1	B	59	GLY
1	B	156	ASP
1	B	194	ARG
1	D	14	PRO
1	D	16	GLN
1	D	62	ASP
1	D	80	LEU
1	D	135	ALA
1	D	213	PRO
1	D	216	CYS
1	B	16	GLN
1	B	203	GLU
1	D	117	ALA

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Mol	Chain	Res	Type
1	B	29	VAL
1	D	42	PRO
1	B	31	GLY
1	B	169	PRO
1	B	53	VAL

### 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	179/179 (100%)	171 (96%)	8 (4%)	27	61
1	B	179/179 (100%)	175 (98%)	4 (2%)	52	81
1	C	179/179 (100%)	174 (97%)	5 (3%)	43	76
1	D	179/179 (100%)	171 (96%)	8 (4%)	27	61
All	All	716/716 (100%)	691 (96%)	25 (4%)	36	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	32	TYR
1	A	38	TYR
1	A	42	PRO
1	A	83	GLU
1	A	109	THR
1	A	161	LYS
1	A	216	CYS
1	B	28	ASP
1	B	62	ASP
1	B	186	THR
1	B	188	GLU
1	C	14	PRO
1	C	28	ASP
1	C	98	THR
1	C	134	LYS

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Mol	Chain	Res	Type
1	C	137	LEU
1	D	11	SER
1	D	17	SER
1	D	27	SER
1	D	62	ASP
1	D	69	SER
1	D	111	LEU
1	D	118	PRO
1	D	177	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	71	ASN
1	A	81	GLN
1	A	199	GLN
1	B	16	GLN
1	B	113	GLN
1	B	172	GLN
1	C	39	GLN
1	C	202	HIS
1	D	55	ASN
1	D	175	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
1	PCA	D	1	1	7,8,9	1.22	1 (14%)	9,10,12	1.10	0
1	PCA	C	1	1	7,8,9	1.30	1 (14%)	9,10,12	1.21	0
1	PCA	B	1	1	7,8,9	1.03	0	9,10,12	1.16	0
1	PCA	A	1	1	7,8,9	1.25	0	9,10,12	1.05	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
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CA-N	2.55	1.49	1.46
1	D	1	PCA	CA-N	2.13	1.49	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

11 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
2	SO4	A	1001	-	4,4,4	1.87	1 (25%)	6,6,6	0.99	0
2	SO4	A	1008	-	4,4,4	1.91	2 (50%)	6,6,6	0.88	0
3	IPH	A	2001	-	7,7,7	2.45	5 (71%)	8,8,8	1.86	2 (25%)
2	SO4	B	1003	-	4,4,4	1.82	1 (25%)	6,6,6	0.95	0
2	SO4	B	1002	-	4,4,4	1.87	2 (50%)	6,6,6	0.93	0
2	SO4	C	1006	-	4,4,4	1.93	2 (50%)	6,6,6	0.88	0
3	IPH	D	2002	-	7,7,7	2.73	6 (85%)	8,8,8	1.80	3 (37%)
2	SO4	C	1009	-	4,4,4	1.85	2 (50%)	6,6,6	0.88	0
2	SO4	A	1007	-	4,4,4	1.88	2 (50%)	6,6,6	0.87	0
2	SO4	D	1005	-	4,4,4	1.83	2 (50%)	6,6,6	0.89	0
2	SO4	D	1004	-	4,4,4	1.90	2 (50%)	6,6,6	0.92	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	IPH	D	2002	-	-	-	0/1/1/1
3	IPH	A	2001	-	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2002	IPH	C5-C6	3.91	1.47	1.38
3	A	2001	IPH	C5-C6	3.57	1.46	1.38
3	D	2002	IPH	C2-C1	3.31	1.45	1.38
2	D	1004	SO4	O1-S	3.17	1.63	1.46
3	D	2002	IPH	C3-C2	3.15	1.45	1.38
2	A	1001	SO4	O1-S	3.12	1.62	1.46
2	A	1008	SO4	O1-S	3.11	1.62	1.46
2	B	1002	SO4	O1-S	3.10	1.62	1.46
2	A	1007	SO4	O1-S	3.09	1.62	1.46
2	C	1006	SO4	O1-S	3.09	1.62	1.46
2	C	1009	SO4	O1-S	3.02	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1003	SO4	O1-S	3.01	1.62	1.46
2	D	1005	SO4	O1-S	3.00	1.62	1.46
3	A	2001	IPH	C3-C2	2.73	1.44	1.38
3	A	2001	IPH	C2-C1	2.68	1.44	1.38
3	D	2002	IPH	C6-C1	2.64	1.44	1.38
3	A	2001	IPH	C6-C1	2.61	1.43	1.38
2	C	1006	SO4	O3-S	-2.26	1.29	1.47
2	A	1008	SO4	O3-S	-2.18	1.30	1.47
3	A	2001	IPH	C4-C3	2.13	1.43	1.38
3	D	2002	IPH	C5-C4	2.09	1.43	1.38
2	C	1009	SO4	O3-S	-2.08	1.30	1.47
2	A	1007	SO4	O3-S	-2.08	1.30	1.47
2	D	1005	SO4	O3-S	-2.07	1.30	1.47
3	D	2002	IPH	C4-C3	2.07	1.43	1.38
2	B	1002	SO4	O3-S	-2.04	1.31	1.47
2	D	1004	SO4	O3-S	-2.04	1.31	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	IPH	C6-C1-C2	3.54	125.73	119.77
3	D	2002	IPH	C6-C1-C2	3.43	125.54	119.77
3	A	2001	IPH	C3-C2-C1	-2.64	115.58	119.31
3	D	2002	IPH	C3-C2-C1	-2.42	115.89	119.31
3	D	2002	IPH	C5-C6-C1	-2.11	116.33	119.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	216/217 (99%)	0.16	4 (1%) 66 65	26, 48, 79, 128	0
1	B	216/217 (99%)	0.91	38 (17%) 1 1	34, 72, 121, 127	0
1	C	216/217 (99%)	0.31	7 (3%) 47 43	28, 51, 122, 143	0
1	D	216/217 (99%)	0.96	51 (23%) 0 0	33, 74, 128, 146	0
All	All	864/868 (99%)	0.58	100 (11%) 4 3	26, 55, 122, 146	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	10.4
1	B	195	SER	9.7
1	C	217	SER	9.7
1	A	217	SER	8.1
1	C	215	GLU	8.0
1	B	164	VAL	7.7
1	D	211	VAL	6.9
1	D	199	GLN	6.6
1	B	166	THR	6.2
1	C	216	CYS	6.2
1	B	167	THR	5.5
1	D	138	VAL	5.3
1	D	186	THR	5.3
1	B	2	SER	5.2
1	D	196	TYR	5.2
1	D	135	ALA	5.1
1	D	214	THR	5.1
1	D	154	LYS	5.1
1	D	156	ASP	5.1
1	A	216	CYS	4.9
1	C	190	TRP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	217	SER	4.7
1	D	117	ALA	4.7
1	B	194	ARG	4.7
1	B	181	SER	4.6
1	D	164	VAL	4.5
1	B	216	CYS	4.5
1	B	183	LEU	4.4
1	B	155	ALA	4.4
1	B	191	LYS	4.4
1	D	195	SER	4.3
1	B	158	SER	4.2
1	B	137	LEU	4.2
1	B	212	ALA	4.1
1	D	185	LEU	4.1
1	D	193	HIS	4.1
1	B	184	SER	4.1
1	D	217	SER	4.0
1	D	189	GLN	4.0
1	D	184	SER	4.0
1	B	200	VAL	3.8
1	D	153	TRP	3.5
1	D	157	SER	3.5
1	D	182	TYR	3.5
1	C	185	LEU	3.4
1	B	211	VAL	3.4
1	B	190	TRP	3.4
1	D	122	LEU	3.3
1	D	197	SER	3.3
1	D	190	TRP	3.3
1	B	122	LEU	3.3
1	C	214	THR	3.3
1	B	182	TYR	3.3
1	A	214	THR	3.3
1	B	159	PRO	3.3
1	D	159	PRO	3.2
1	D	212	ALA	3.2
1	D	118	PRO	3.2
1	B	154	LYS	3.1
1	D	160	VAL	3.0
1	D	149	VAL	3.0
1	D	158	SER	3.0
1	D	216	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	175	ASN	3.0
1	C	123	PHE	2.9
1	B	157	SER	2.9
1	B	185	LEU	2.9
1	B	120	VAL	2.9
1	D	200	VAL	2.8
1	D	163	GLY	2.8
1	D	123	PHE	2.8
1	D	162	ALA	2.7
1	D	183	LEU	2.7
1	D	29	VAL	2.6
1	B	116	ALA	2.5
1	B	192	SER	2.5
1	B	151	VAL	2.4
1	D	144	PHE	2.4
1	A	215	GLU	2.4
1	D	167	THR	2.4
1	B	152	ALA	2.4
1	B	153	TRP	2.3
1	B	193	HIS	2.3
1	B	53	VAL	2.3
1	D	151	VAL	2.3
1	D	215	GLU	2.3
1	D	119	SER	2.3
1	D	187	PRO	2.2
1	D	130	LEU	2.2
1	D	180	SER	2.2
1	D	198	CYS	2.2
1	D	18	ILE	2.2
1	D	213	PRO	2.1
1	B	180	SER	2.1
1	B	202	HIS	2.1
1	D	140	LEU	2.1
1	D	194	ARG	2.1
1	B	156	ASP	2.1
1	B	203	GLU	2.0
1	B	140	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	D	1	8/9	0.81	0.30	87,91,93,93	0
1	PCA	A	1	8/9	0.84	0.24	77,79,80,80	0
1	PCA	B	1	8/9	0.86	0.31	81,83,84,84	0
1	PCA	C	1	8/9	0.88	0.23	76,79,80,81	0

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	1007	5/5	0.86	0.17	133,134,134,134	0
3	IPH	D	2002	7/7	0.92	0.22	43,45,48,50	0
3	IPH	A	2001	7/7	0.92	0.25	53,53,58,58	0
2	SO4	A	1008	5/5	0.94	0.24	106,107,108,108	0
2	SO4	B	1002	5/5	0.94	0.21	104,104,105,105	0
2	SO4	D	1004	5/5	0.94	0.16	93,94,94,95	0
2	SO4	B	1003	5/5	0.95	0.14	91,92,93,93	0
2	SO4	C	1009	5/5	0.95	0.21	97,97,98,99	0
2	SO4	D	1005	5/5	0.96	0.14	94,94,94,95	0
2	SO4	A	1001	5/5	0.96	0.20	74,75,76,76	0
2	SO4	C	1006	5/5	0.98	0.14	62,63,64,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.