Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 09:57 AM EDT

PDB ID	:	1S57
Title	:	crystal structure of nucleoside diphosphate kinase 2 from Arabidopsis
Authors	:	Im, Y.J.; Kim, J.-I.; Shen, Y.; Na, Y.; Han, Y.-J.; Kim, S.-H.; Song, P.-S.; Eom, S.H.
Deposited on	:	2004-01-20
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

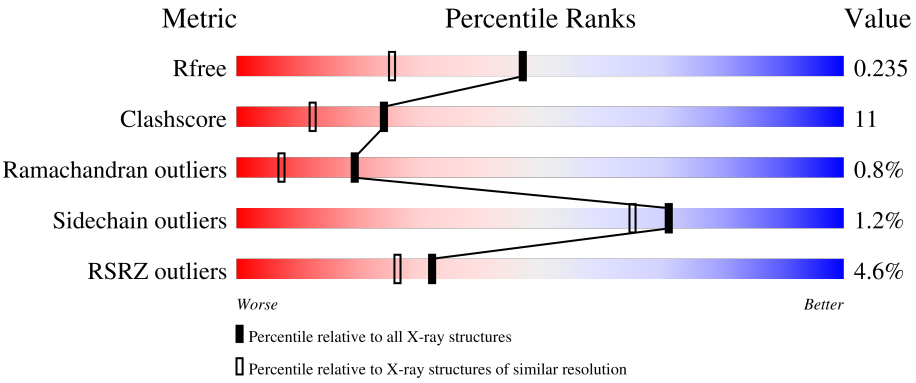
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	153	10% 77% 22%
1	B	153	2% 73% 24%
1	C	153	7% 71% 25%
1	D	153	% 75% 24%
1	E	153	7% 79% 17%

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Mol	Chain	Length	Quality of chain
1	F	153	

2 Entry composition (i)

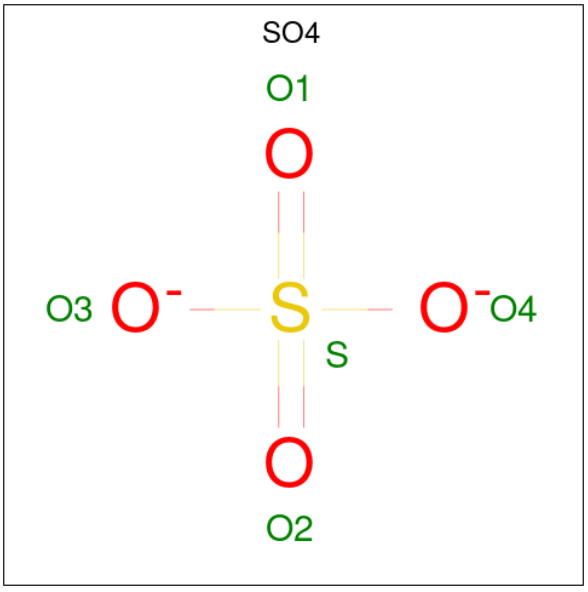
There are 4 unique types of molecules in this entry. The entry contains 7820 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoside diphosphate kinase II.

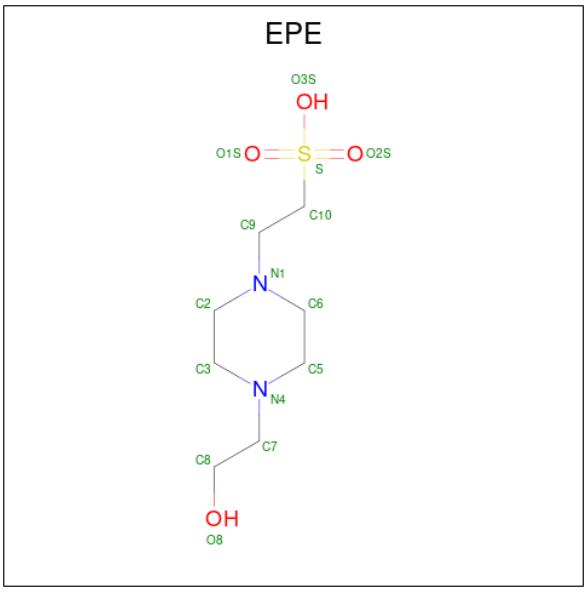
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1198	765	202	224	7			
1	B	149	Total	C	N	O	S	0	0	0
			1167	748	198	215	6			
1	C	149	Total	C	N	O	S	0	0	0
			1167	748	198	215	6			
1	D	153	Total	C	N	O	S	0	0	0
			1198	765	202	224	7			
1	E	149	Total	C	N	O	S	0	0	0
			1167	748	198	215	6			
1	F	153	Total	C	N	O	S	0	0	0
			1198	765	202	224	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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		
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	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	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		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is water.

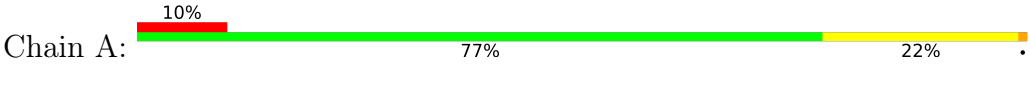
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	88	Total	O	0	0
			88	88		
4	C	70	Total	O	0	0
			70	70		
4	D	127	Total	O	0	0
			127	127		
4	E	70	Total	O	0	0
			70	70		
4	F	107	Total	O	0	0
			107	107		

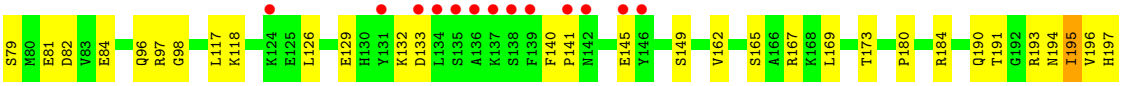
3 Residue-property plots (i)

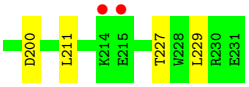
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nucleoside diphosphate kinase II

Chain A:

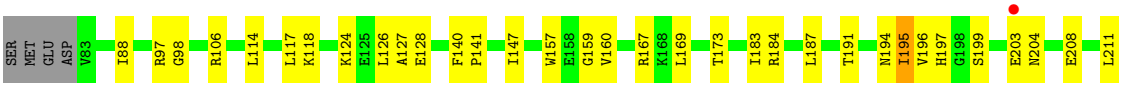






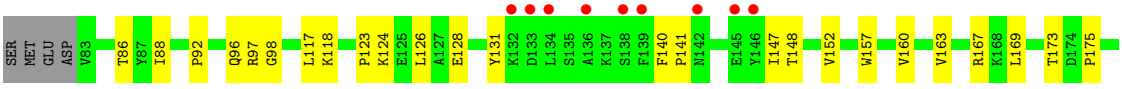
• Molecule 1: Nucleoside diphosphate kinase II

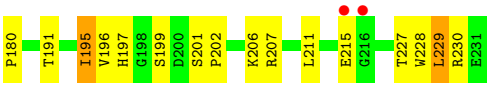
Chain B:



• Molecule 1: Nucleoside diphosphate kinase II

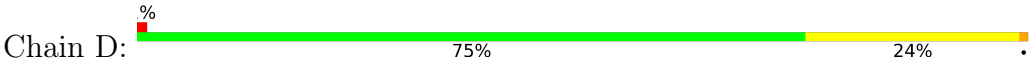
Chain C:

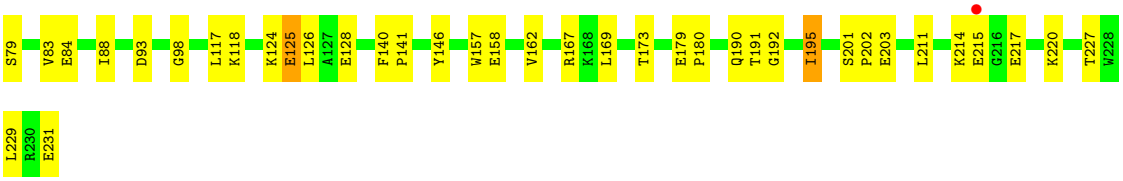




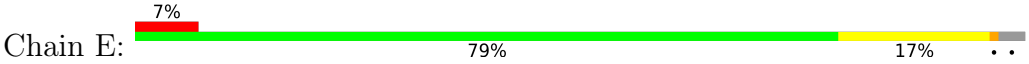
• Molecule 1: Nucleoside diphosphate kinase II

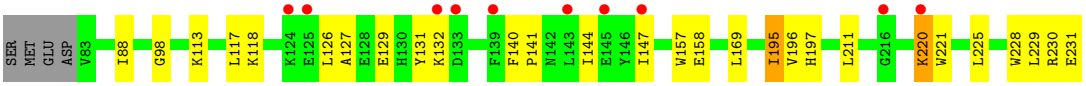
Chain D:



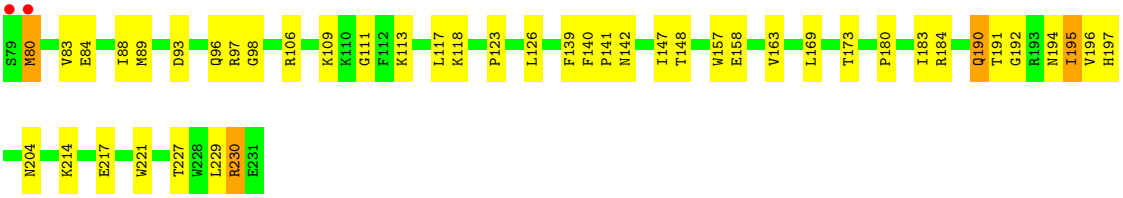


• Molecule 1: Nucleoside diphosphate kinase II





• Molecule 1: Nucleoside diphosphate kinase II



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.39Å 108.86Å 119.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 1.80 45.24 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.24-1.80) 99.8 (45.24-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.241 0.205 , 0.235	Depositor DCC
R_{free} test set	4284 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7820	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: EPE, 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	0.29	0/1223	0.58	1/1647 (0.1%)
1	B	0.29	0/1192	0.61	1/1606 (0.1%)
1	C	0.28	0/1192	0.58	0/1606
1	D	0.30	0/1223	0.60	1/1647 (0.1%)
1	E	0.28	0/1192	0.59	1/1606 (0.1%)
1	F	0.31	0/1223	0.63	0/1647
All	All	0.29	0/7245	0.60	4/9759 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ILE	N-CA-C	5.55	125.97	111.00
1	E	195	ILE	N-CA-C	5.40	125.58	111.00
1	B	195	ILE	N-CA-C	5.37	125.50	111.00
1	D	195	ILE	N-CA-C	5.05	124.64	111.00

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	1198	0	1202	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1167	0	1178	31	0
1	C	1167	0	1178	31	0
1	D	1198	0	1202	27	0
1	E	1167	0	1178	26	0
1	F	1198	0	1202	43	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	1	0
2	E	15	0	0	0	0
2	F	15	0	0	0	0
3	A	15	0	17	2	0
3	B	15	0	17	1	0
3	C	30	0	34	4	0
3	D	15	0	17	2	0
3	F	15	0	17	4	0
4	A	83	0	0	3	0
4	B	88	0	0	2	0
4	C	70	0	0	2	0
4	D	127	0	0	4	0
4	E	70	0	0	2	0
4	F	107	0	0	2	0
All	All	7820	0	7242	160	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 11.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:GLU:HG3	1:F:190:GLN:HE22	1.25	1.00
1:E:127:ALA:HB1	1:E:147:ILE:HD11	1.43	1.00
1:A:167:ARG:HD2	1:A:200:ASP:HA	1.46	0.97
1:F:97:ARG:HH11	1:F:195:ILE:HD11	1.37	0.88
1:F:184:ARG:HD2	1:F:194:ASN:HB2	1.58	0.86
1:C:229:LEU:HD13	3:C:1103:EPE:H61	1.60	0.84
3:A:1101:EPE:H81	1:D:98:GLY:HA3	1.59	0.84
1:B:98:GLY:HA3	3:F:1106:EPE:H81	1.60	0.81
3:C:1103:EPE:H81	1:E:98:GLY:HA3	1.65	0.78
1:F:80:MET:H	1:F:80:MET:HE2	1.50	0.77
1:A:184:ARG:HD2	1:A:194:ASN:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1102:EPE:H81	1:F:98:GLY:HA3	1.70	0.73
1:F:229:LEU:HD12	3:F:1106:EPE:H101	1.70	0.73
1:C:98:GLY:HA3	3:C:1105:EPE:H81	1.70	0.72
1:B:160:VAL:HG13	4:C:1126:HOH:O	1.90	0.71
1:F:93:ASP:OD2	1:F:195:ILE:HD13	1.91	0.71
1:B:97:ARG:HD2	4:B:1186:HOH:O	1.91	0.70
1:B:184:ARG:HD2	1:B:194:ASN:HB2	1.74	0.69
1:F:184:ARG:CD	1:F:194:ASN:HB2	2.22	0.69
1:E:127:ALA:CB	1:E:147:ILE:HD11	2.22	0.69
1:A:98:GLY:HA3	3:D:1104:EPE:H81	1.76	0.67
1:D:79:SER:HA	4:D:1149:HOH:O	1.93	0.67
1:A:126:LEU:HD11	1:A:211:LEU:HG	1.78	0.65
1:F:97:ARG:NH1	1:F:195:ILE:HD11	2.11	0.65
1:A:97:ARG:HD2	4:A:1133:HOH:O	1.96	0.64
1:D:83:VAL:HG12	1:D:158:GLU:HG2	1.80	0.64
1:B:140:PHE:HB3	1:B:141:PRO:HD3	1.81	0.62
1:A:79:SER:HB3	4:A:1172:HOH:O	1.98	0.62
1:E:131:TYR:HE2	1:E:147:ILE:HD13	1.63	0.62
1:A:140:PHE:HB3	1:A:141:PRO:HD3	1.83	0.61
1:E:126:LEU:HD11	1:E:211:LEU:HG	1.83	0.60
1:B:220:LYS:HE3	4:B:1156:HOH:O	2.02	0.59
1:F:148:THR:HG22	1:F:148:THR:O	2.02	0.59
1:E:231:GLU:HG3	1:F:190:GLN:NE2	2.07	0.59
1:A:79:SER:OG	1:A:81:GLU:HG3	2.03	0.58
1:D:201:SER:OG	1:D:203:GLU:HG2	2.04	0.58
1:C:140:PHE:N	1:C:141:PRO:HD2	2.19	0.58
1:F:84:GLU:HG2	1:F:163:VAL:HG23	1.86	0.57
1:F:139:PHE:HA	1:F:142:ASN:HD22	1.70	0.56
1:B:124:LYS:O	1:B:128:GLU:HG3	2.06	0.56
1:C:196:VAL:HG22	1:C:197:HIS:N	2.20	0.56
1:D:83:VAL:CG1	1:D:158:GLU:HG2	2.34	0.56
1:D:202:PRO:HG2	1:D:203:GLU:OE2	2.05	0.56
1:B:126:LEU:HD11	1:B:211:LEU:HG	1.88	0.56
1:A:180:PRO:HG3	1:C:169:LEU:HD23	1.87	0.56
1:B:159:GLY:HA2	1:B:230:ARG:NH2	2.21	0.55
1:A:190:GLN:NE2	1:C:230:ARG:HG3	2.22	0.55
1:B:160:VAL:HG12	1:B:230:ARG:NE	2.21	0.55
1:E:230:ARG:HD2	4:E:1055:HOH:O	2.05	0.55
1:C:88:ILE:HD12	1:C:157:TRP:CD1	2.41	0.55
1:C:124:LYS:O	1:C:128:GLU:HG3	2.06	0.54
1:D:84:GLU:HG3	1:D:162:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:ILE:HD12	1:F:157:TRP:CD1	2.43	0.54
1:B:118:LYS:HA	1:F:117:LEU:O	2.07	0.54
1:C:131:TYR:HE2	1:C:147:ILE:HG13	1.73	0.53
1:D:229:LEU:HD22	3:D:1104:EPE:H101	1.90	0.53
1:F:80:MET:H	1:F:80:MET:CE	2.18	0.53
1:D:214:LYS:HB2	1:D:217:GLU:HG3	1.91	0.53
1:B:204:ASN:O	1:B:208:GLU:HG3	2.08	0.53
1:E:131:TYR:CE2	1:E:147:ILE:HD13	2.43	0.53
1:F:148:THR:HG23	4:F:1165:HOH:O	2.09	0.53
1:D:167:ARG:HD2	2:D:1010:SO4:O1	2.08	0.52
1:A:184:ARG:CD	1:A:194:ASN:HB2	2.38	0.52
1:B:167:ARG:HD3	1:B:199:SER:O	2.10	0.52
1:D:227:THR:HG22	1:D:227:THR:O	2.10	0.52
1:D:227:THR:HG22	4:D:1191:HOH:O	2.08	0.52
1:F:196:VAL:HG22	1:F:197:HIS:N	2.24	0.52
1:A:84:GLU:HG3	1:A:162:VAL:HG12	1.90	0.52
1:C:148:THR:HG22	1:C:148:THR:O	2.09	0.51
1:F:123:PRO:HG2	1:F:126:LEU:HB2	1.90	0.51
1:D:190:GLN:NE2	1:D:192:GLY:H	2.07	0.51
1:E:231:GLU:H	1:F:190:GLN:NE2	2.08	0.51
1:D:88:ILE:HD12	1:D:157:TRP:CD1	2.46	0.51
1:A:193:ARG:NH2	1:C:227:THR:O	2.44	0.51
1:F:111:GLY:O	1:F:229:LEU:HD13	2.10	0.51
1:B:117:LEU:O	1:F:118:LYS:HA	2.11	0.50
1:B:127:ALA:HB1	1:B:147:ILE:HG21	1.93	0.50
1:C:207:ARG:O	1:C:211:LEU:HD13	2.11	0.50
1:A:96:GLN:HG3	1:C:228:TRP:CE2	2.47	0.50
1:E:88:ILE:HD12	1:E:157:TRP:CD1	2.47	0.50
1:F:230:ARG:HH11	1:F:230:ARG:HB2	1.77	0.50
1:F:229:LEU:HD12	3:F:1106:EPE:H61	1.92	0.50
1:D:140:PHE:HB3	1:D:141:PRO:HD3	1.93	0.49
1:B:173:THR:HG22	1:B:191:THR:HG23	1.94	0.49
1:D:126:LEU:HD11	1:D:211:LEU:HG	1.94	0.49
1:D:179:GLU:HG3	1:D:180:PRO:HD2	1.95	0.49
1:D:125:GLU:CD	1:D:125:GLU:H	2.15	0.49
3:A:1101:EPE:H81	1:D:98:GLY:CA	2.38	0.49
1:E:169:LEU:HD23	1:F:180:PRO:HG3	1.95	0.49
1:B:203:GLU:HG3	1:B:204:ASN:N	2.28	0.48
1:E:140:PHE:N	1:E:141:PRO:HD2	2.28	0.48
1:D:79:SER:N	1:D:231:GLU:O	2.46	0.48
1:E:228:TRP:CE2	1:F:96:GLN:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1205:HOH:O	1:F:109:LYS:HD2	2.13	0.48
1:A:118:LYS:HA	1:D:117:LEU:O	2.13	0.48
1:F:111:GLY:O	1:F:229:LEU:CD1	2.62	0.48
1:C:229:LEU:CD1	3:C:1103:EPE:H61	2.39	0.47
1:D:169:LEU:HD22	4:E:1041:HOH:O	2.13	0.47
1:B:225:LEU:HD11	1:E:225:LEU:HD11	1.96	0.47
1:C:167:ARG:HD3	1:C:199:SER:O	2.14	0.47
1:A:117:LEU:O	1:D:118:LYS:HA	2.15	0.47
1:E:113:LYS:HG3	1:E:221:TRP:CZ2	2.50	0.47
1:C:117:LEU:O	1:E:118:LYS:HA	2.15	0.47
1:E:196:VAL:HG22	1:E:197:HIS:N	2.30	0.46
1:A:196:VAL:HG22	1:A:197:HIS:N	2.29	0.46
1:B:98:GLY:CA	3:F:1106:EPE:H81	2.38	0.46
1:C:227:THR:HG22	4:C:1155:HOH:O	2.15	0.46
1:F:230:ARG:HB2	1:F:230:ARG:NH1	2.31	0.46
1:C:123:PRO:HG2	1:C:126:LEU:HB3	1.98	0.46
1:E:140:PHE:O	1:E:144:ILE:HG12	2.16	0.45
1:B:228:TRP:CE2	1:C:96:GLN:HG3	2.51	0.45
1:F:83:VAL:CG1	1:F:158:GLU:HG2	2.46	0.45
1:A:229:LEU:HD21	1:B:97:ARG:HD3	1.97	0.45
1:D:173:THR:HG22	1:D:191:THR:HG23	1.97	0.45
1:F:173:THR:HG22	1:F:191:THR:HG23	1.98	0.45
1:F:227:THR:HG23	4:F:1166:HOH:O	2.15	0.45
1:C:206:LYS:NZ	1:C:206:LYS:HB3	2.31	0.45
4:D:1151:HOH:O	1:F:169:LEU:HD22	2.16	0.45
1:F:140:PHE:HB3	1:F:141:PRO:HD3	1.98	0.45
1:F:148:THR:O	1:F:148:THR:CG2	2.65	0.45
1:C:86:THR:HB	1:C:163:VAL:HG22	2.00	0.44
1:F:106:ARG:HD2	1:F:183:ILE:HG12	1.98	0.44
1:C:92:PRO:HD3	1:C:152:VAL:HG12	1.99	0.44
1:D:93:ASP:OD1	1:D:146:TYR:OH	2.36	0.44
1:E:129:GLU:O	1:E:132:LYS:HB2	2.17	0.44
1:B:184:ARG:CD	1:B:194:ASN:HB2	2.47	0.44
1:A:173:THR:HG22	1:A:191:THR:HG23	1.99	0.43
1:B:97:ARG:NH1	1:B:187:LEU:O	2.41	0.43
1:E:229:LEU:HD21	1:F:97:ARG:HD3	2.00	0.43
1:C:201:SER:HB2	1:C:202:PRO:HD2	2.01	0.43
1:B:88:ILE:HD12	1:B:157:TRP:CD1	2.54	0.43
1:F:214:LYS:HB2	1:F:217:GLU:HG3	2.00	0.42
1:A:165:SER:O	1:A:169:LEU:HD13	2.20	0.42
1:F:89:MET:O	1:F:196:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ARG:HG2	1:E:230:ARG:HH11	1.84	0.42
1:A:145:GLU:O	1:A:149:SER:HB3	2.19	0.42
1:B:169:LEU:HD23	1:C:180:PRO:HG3	2.02	0.42
1:F:113:LYS:HG3	1:F:221:TRP:CZ2	2.55	0.42
1:E:231:GLU:CG	1:F:192:GLY:HA3	2.50	0.42
1:A:227:THR:HG22	4:A:1147:HOH:O	2.19	0.41
1:B:196:VAL:HG22	1:B:197:HIS:N	2.35	0.41
1:C:97:ARG:NH1	1:C:195:ILE:HD11	2.35	0.41
1:C:118:LYS:HA	1:E:117:LEU:O	2.20	0.41
1:F:204:ASN:HD22	1:F:204:ASN:HA	1.66	0.41
1:A:129:GLU:OE2	1:A:132:LYS:HE3	2.21	0.41
1:A:132:LYS:HG3	1:A:133:ASP:N	2.36	0.41
1:F:196:VAL:CG2	1:F:197:HIS:N	2.84	0.41
1:C:160:VAL:HG13	1:C:160:VAL:O	2.21	0.41
1:C:196:VAL:CG2	1:C:197:HIS:N	2.83	0.41
1:B:106:ARG:HD2	1:B:183:ILE:HG12	2.02	0.41
1:B:229:LEU:HD21	1:C:97:ARG:HD3	2.02	0.41
1:E:158:GLU:OE2	1:E:220:LYS:HE3	2.21	0.41
1:E:220:LYS:NZ	1:E:220:LYS:HB2	2.35	0.41
1:B:184:ARG:HD3	1:B:194:ASN:O	2.20	0.41
1:C:173:THR:HG22	1:C:191:THR:HG23	2.02	0.41
1:D:220:LYS:HB3	1:D:220:LYS:NZ	2.36	0.41
1:C:173:THR:O	1:C:175:PRO:HD3	2.20	0.41
1:D:124:LYS:O	1:D:128:GLU:HG3	2.21	0.40
1:B:114:LEU:HD13	1:B:157:TRP:CZ2	2.56	0.40
1:B:159:GLY:HA2	1:B:230:ARG:HH21	1.86	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	151/153 (99%)	147 (97%)	3 (2%)	1 (1%)	22 10
1	B	147/153 (96%)	142 (97%)	4 (3%)	1 (1%)	22 10
1	C	147/153 (96%)	142 (97%)	3 (2%)	2 (1%)	11 3
1	D	151/153 (99%)	147 (97%)	3 (2%)	1 (1%)	22 10
1	E	147/153 (96%)	142 (97%)	4 (3%)	1 (1%)	22 10
1	F	151/153 (99%)	149 (99%)	1 (1%)	1 (1%)	22 10
All	All	894/918 (97%)	869 (97%)	18 (2%)	7 (1%)	19 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ILE
1	B	195	ILE
1	C	195	ILE
1	C	215	GLU
1	E	195	ILE
1	F	195	ILE
1	D	195	ILE

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	128/128 (100%)	127 (99%)	1 (1%)	81 78
1	B	124/128 (97%)	124 (100%)	0	100 100
1	C	124/128 (97%)	123 (99%)	1 (1%)	81 78
1	D	128/128 (100%)	126 (98%)	2 (2%)	62 54
1	E	124/128 (97%)	123 (99%)	1 (1%)	81 78
1	F	128/128 (100%)	124 (97%)	4 (3%)	40 25
All	All	756/768 (98%)	747 (99%)	9 (1%)	71 65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	C	229	LEU
1	D	125	GLU
1	D	215	GLU
1	E	220	LYS
1	F	80	MET
1	F	147	ILE
1	F	190	GLN
1	F	230	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	177	GLN
1	B	121	GLN
1	B	142	ASN
1	B	204	ASN
1	E	121	GLN
1	E	142	ASN
1	F	142	ASN
1	F	190	GLN
1	F	204	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	D	1012	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	F	1016	-	4,4,4	0.27	0	6,6,6	0.05	0
2	SO4	D	1011	-	4,4,4	0.25	0	6,6,6	0.04	0
2	SO4	C	1007	-	4,4,4	0.25	0	6,6,6	0.05	0
3	EPE	D	1104	-	15,15,15	1.87	6 (40%)	18,20,20	1.39	2 (11%)
3	EPE	C	1105	-	15,15,15	1.84	4 (26%)	18,20,20	1.37	3 (16%)
2	SO4	F	1018	-	4,4,4	0.27	0	6,6,6	0.06	0
3	EPE	B	1102	-	15,15,15	1.76	4 (26%)	18,20,20	1.35	2 (11%)
2	SO4	E	1014	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	B	1006	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	A	1002	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	E	1013	-	4,4,4	0.26	0	6,6,6	0.04	0
2	SO4	A	1003	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	B	1004	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	F	1017	-	4,4,4	0.25	0	6,6,6	0.05	0
2	SO4	C	1009	-	4,4,4	0.26	0	6,6,6	0.05	0
3	EPE	A	1101	-	15,15,15	1.83	5 (33%)	18,20,20	1.40	3 (16%)
3	EPE	F	1106	-	15,15,15	1.76	5 (33%)	18,20,20	1.34	2 (11%)
2	SO4	C	1008	-	4,4,4	0.27	0	6,6,6	0.05	0
2	SO4	D	1010	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	B	1005	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	E	1015	-	4,4,4	0.26	0	6,6,6	0.05	0
2	SO4	A	1001	-	4,4,4	0.25	0	6,6,6	0.05	0
3	EPE	C	1103	-	15,15,15	1.88	6 (40%)	18,20,20	1.35	2 (11%)

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	EPE	C	1105	-	-	2/9/19/19	0/1/1/1
3	EPE	B	1102	-	-	3/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	1101	-	-	2/9/19/19	0/1/1/1
3	EPE	F	1106	-	-	3/9/19/19	0/1/1/1
3	EPE	D	1104	-	-	3/9/19/19	0/1/1/1
3	EPE	C	1103	-	-	1/9/19/19	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1105	EPE	C6-N1	3.81	1.57	1.46
3	D	1104	EPE	C6-N1	3.58	1.56	1.46
3	A	1101	EPE	C6-N1	3.57	1.56	1.46
3	C	1103	EPE	C6-N1	3.55	1.56	1.46
3	B	1102	EPE	C6-N1	3.53	1.56	1.46
3	C	1103	EPE	C2-N1	3.43	1.56	1.46
3	F	1106	EPE	C6-N1	3.42	1.56	1.46
3	C	1105	EPE	C2-N1	3.41	1.56	1.46
3	B	1102	EPE	C2-N1	3.34	1.56	1.46
3	D	1104	EPE	C2-N1	3.34	1.56	1.46
3	A	1101	EPE	C2-N1	3.33	1.56	1.46
3	F	1106	EPE	C2-N1	3.25	1.55	1.46
3	D	1104	EPE	C9-N1	2.94	1.54	1.47
3	C	1103	EPE	C9-N1	2.90	1.54	1.47
3	F	1106	EPE	C9-N1	2.77	1.53	1.47
3	A	1101	EPE	C9-N1	2.73	1.53	1.47
3	C	1105	EPE	C9-N1	2.71	1.53	1.47
3	B	1102	EPE	C9-N1	2.49	1.53	1.47
3	D	1104	EPE	C3-N4	2.47	1.53	1.46
3	A	1101	EPE	C3-N4	2.41	1.53	1.46
3	C	1103	EPE	C3-N4	2.41	1.53	1.46
3	B	1102	EPE	C3-N4	2.29	1.53	1.46
3	F	1106	EPE	C3-N4	2.29	1.53	1.46
3	C	1105	EPE	C3-N4	2.23	1.53	1.46
3	D	1104	EPE	C9-C10	2.20	1.58	1.52
3	C	1103	EPE	C9-C10	2.12	1.58	1.52
3	F	1106	EPE	C9-C10	2.11	1.58	1.52
3	A	1101	EPE	C7-N4	2.08	1.52	1.47
3	D	1104	EPE	C7-N4	2.07	1.52	1.47
3	C	1103	EPE	C7-N4	2.05	1.52	1.47

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1106	EPE	C7-N4-C5	-3.35	102.67	111.23
3	D	1104	EPE	C7-N4-C5	-3.20	103.05	111.23
3	A	1101	EPE	C7-N4-C5	-3.17	103.13	111.23
3	B	1102	EPE	C7-N4-C5	-3.14	103.22	111.23
3	C	1103	EPE	C7-N4-C5	-3.08	103.36	111.23
3	C	1105	EPE	C7-N4-C5	-3.08	103.36	111.23
3	F	1106	EPE	C3-C2-N1	-2.86	104.77	110.64
3	B	1102	EPE	C3-C2-N1	-2.85	104.79	110.64
3	A	1101	EPE	C3-C2-N1	-2.81	104.87	110.64
3	D	1104	EPE	C3-C2-N1	-2.79	104.91	110.64
3	C	1103	EPE	C3-C2-N1	-2.77	104.96	110.64
3	C	1105	EPE	C3-C2-N1	-2.72	105.06	110.64
3	C	1105	EPE	O1S-S-C10	-2.33	104.11	106.92
3	A	1101	EPE	O1S-S-C10	-2.20	104.26	106.92

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	EPE	N4-C7-C8-O8
3	B	1102	EPE	N4-C7-C8-O8
3	C	1103	EPE	N4-C7-C8-O8
3	C	1105	EPE	N4-C7-C8-O8
3	D	1104	EPE	N4-C7-C8-O8
3	F	1106	EPE	N4-C7-C8-O8
3	C	1105	EPE	S-C10-C9-N1
3	B	1102	EPE	S-C10-C9-N1
3	D	1104	EPE	C8-C7-N4-C3
3	D	1104	EPE	C8-C7-N4-C5
3	A	1101	EPE	C8-C7-N4-C5
3	B	1102	EPE	C8-C7-N4-C5
3	F	1106	EPE	C8-C7-N4-C5
3	F	1106	EPE	C8-C7-N4-C3

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1104	EPE	2	0
3	C	1105	EPE	1	0
3	B	1102	EPE	1	0
3	A	1101	EPE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1106	EPE	4	0
2	D	1010	SO4	1	0
3	C	1103	EPE	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, 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	153/153 (100%)	0.45	15 (9%) 7 5	12, 18, 52, 62	0
1	B	149/153 (97%)	0.14	3 (2%) 65 61	10, 18, 27, 40	0
1	C	149/153 (97%)	0.46	11 (7%) 14 11	14, 20, 52, 57	0
1	D	153/153 (100%)	0.01	1 (0%) 87 86	10, 15, 25, 44	0
1	E	149/153 (97%)	0.32	10 (6%) 17 14	11, 20, 40, 51	0
1	F	153/153 (100%)	0.10	2 (1%) 77 74	10, 16, 27, 50	0
All	All	906/918 (98%)	0.25	42 (4%) 32 26	10, 18, 41, 62	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	GLU	6.8
1	F	79	SER	5.9
1	F	80	MET	5.6
1	A	134	LEU	5.4
1	A	139	PHE	5.1
1	C	215	GLU	5.0
1	D	215	GLU	5.0
1	A	135	SER	4.9
1	E	133	ASP	4.6
1	C	133	ASP	4.6
1	A	136	ALA	4.2
1	A	133	ASP	3.9
1	A	138	SER	3.8
1	E	132	LYS	3.5
1	A	142	ASN	3.2
1	C	138	SER	3.2
1	B	203	GLU	3.1
1	C	139	PHE	3.1
1	E	139	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLU	3.1
1	A	131	TYR	2.9
1	C	216	GLY	2.8
1	A	137	LYS	2.8
1	E	125	GLU	2.8
1	E	124	LYS	2.7
1	A	146	TYR	2.7
1	E	220	LYS	2.6
1	E	147	ILE	2.6
1	B	230	ARG	2.6
1	E	143	LEU	2.6
1	A	124	LYS	2.5
1	A	145	GLU	2.5
1	C	146	TYR	2.4
1	C	142	ASN	2.4
1	E	145	GLU	2.4
1	A	141	PRO	2.4
1	C	132	LYS	2.3
1	C	145	GLU	2.3
1	E	216	GLY	2.1
1	C	136	ALA	2.1
1	C	134	LEU	2.1
1	A	214	LYS	2.1

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 monosaccharides 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^{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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1004	5/5	0.62	0.30	89,89,89,90	0
2	SO4	B	1005	5/5	0.75	0.24	76,77,77,77	0
2	SO4	C	1008	5/5	0.77	0.20	70,70,70,70	0
2	SO4	E	1015	5/5	0.80	0.27	83,83,83,84	0
2	SO4	F	1017	5/5	0.83	0.29	78,78,78,79	0
2	SO4	E	1014	5/5	0.85	0.20	60,60,61,61	0
2	SO4	D	1011	5/5	0.86	0.15	59,60,60,60	0
2	SO4	A	1002	5/5	0.86	0.27	77,77,78,78	0
2	SO4	C	1009	5/5	0.88	0.22	57,57,57,58	0
2	SO4	A	1003	5/5	0.90	0.17	54,54,55,55	0
2	SO4	B	1006	5/5	0.91	0.41	73,73,74,74	0
2	SO4	F	1018	5/5	0.92	0.20	43,45,45,45	0
2	SO4	E	1013	5/5	0.93	0.26	70,71,71,71	0
2	SO4	F	1016	5/5	0.94	0.25	53,53,54,54	0
3	EPE	D	1104	15/15	0.94	0.14	21,22,30,30	0
2	SO4	A	1001	5/5	0.95	0.20	61,61,62,62	0
3	EPE	B	1102	15/15	0.95	0.10	16,18,22,24	0
3	EPE	C	1105	15/15	0.95	0.10	15,17,24,24	0
2	SO4	C	1007	5/5	0.95	0.21	46,47,48,48	0
3	EPE	C	1103	15/15	0.96	0.11	20,21,23,23	0
3	EPE	A	1101	15/15	0.96	0.10	13,15,17,21	0
2	SO4	D	1010	5/5	0.96	0.20	48,49,50,50	0
3	EPE	F	1106	15/15	0.96	0.13	12,14,18,18	0
2	SO4	D	1012	5/5	0.97	0.18	37,38,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.