Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:59 AM EDT

PDB ID	:	1D9E
Title	:	STRUCTURE OF E. COLI KDO8P SYNTHASE
Authors	:	Radaev, S.; Dastidar, P.; Patel, M.; Woodard, R.W.; Gatti, D.L.
Deposited on	:	1999-10-27
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

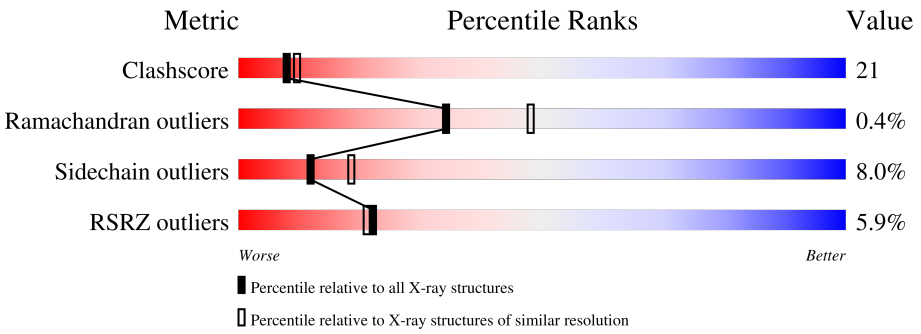
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	284	4%, 65%, 24%, •, 6%
1	B	284	4%, 68%, 20%, 6%, 6%
1	C	284	4%, 65%, 24%, 5%, 6%
1	D	284	10%, 49%, 39%, 5%, 7%

2 Entry composition (i)

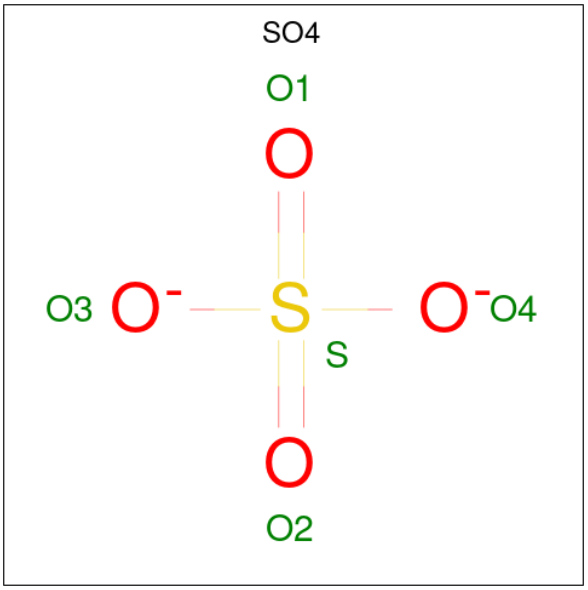
There are 3 unique types of molecules in this entry. The entry contains 8618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEOXY-D-MANNO-OCTULOSONATE 8-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2040	1305	344	379	12	0	0	0
1	B	266	2040	1305	344	379	12	0	0	0
1	C	266	2040	1305	344	379	12	0	0	0
1	D	264	2024	1295	342	375	12	0	0	0

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



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

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

- Molecule 3 is water.

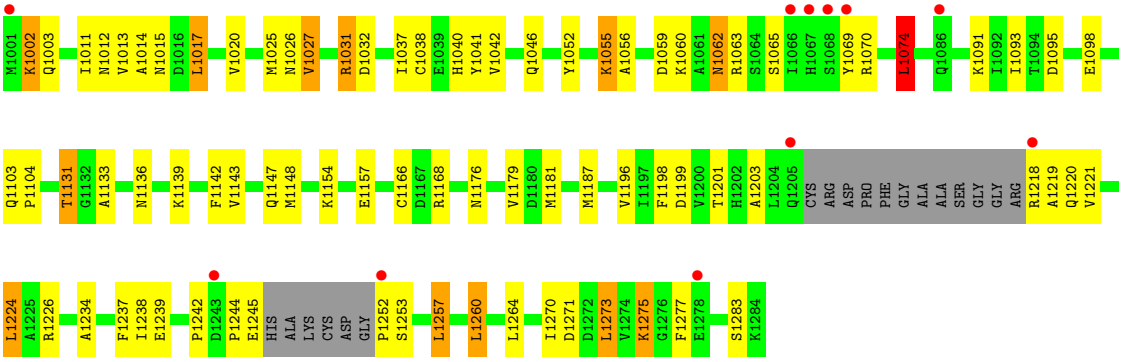
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	143	143	143	0	0
			Total	O		
3	B	122	122	122	0	0
			Total	O		
3	C	119	119	119	0	0
			Total	O		
3	D	40	40	40	0	0

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 in the model, are shown in grey.

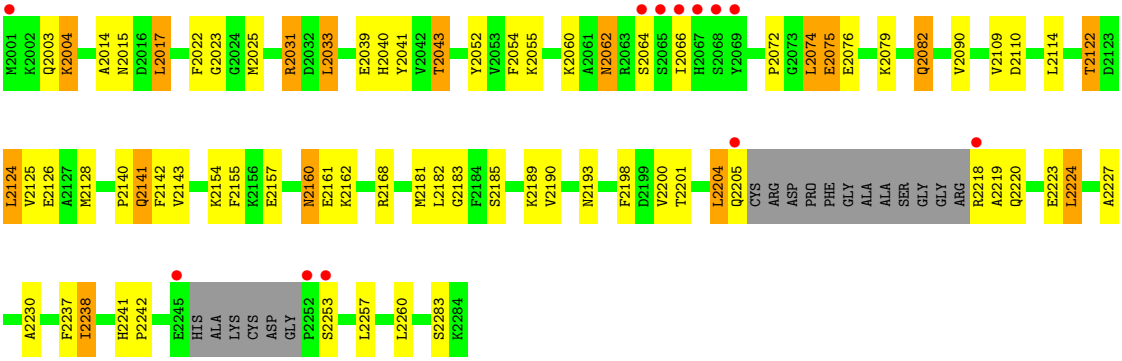
• Molecule 1: 3-DEOXY-D-MANNO-OCTULOSONATE 8-PHOSPHATE SYNTHASE

Chain A:



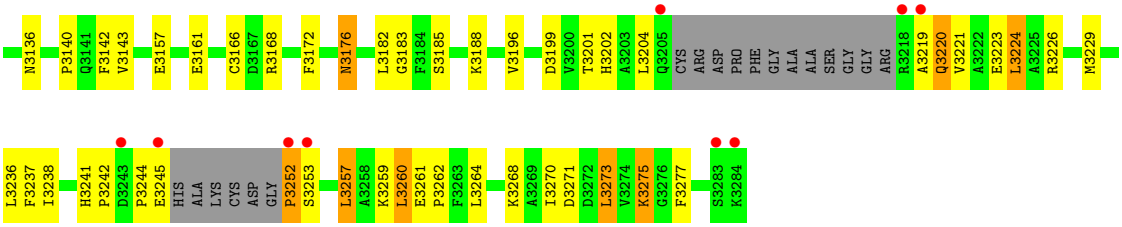
• Molecule 1: 3-DEOXY-D-MANNO-OCTULOSONATE 8-PHOSPHATE SYNTHASE

Chain B:



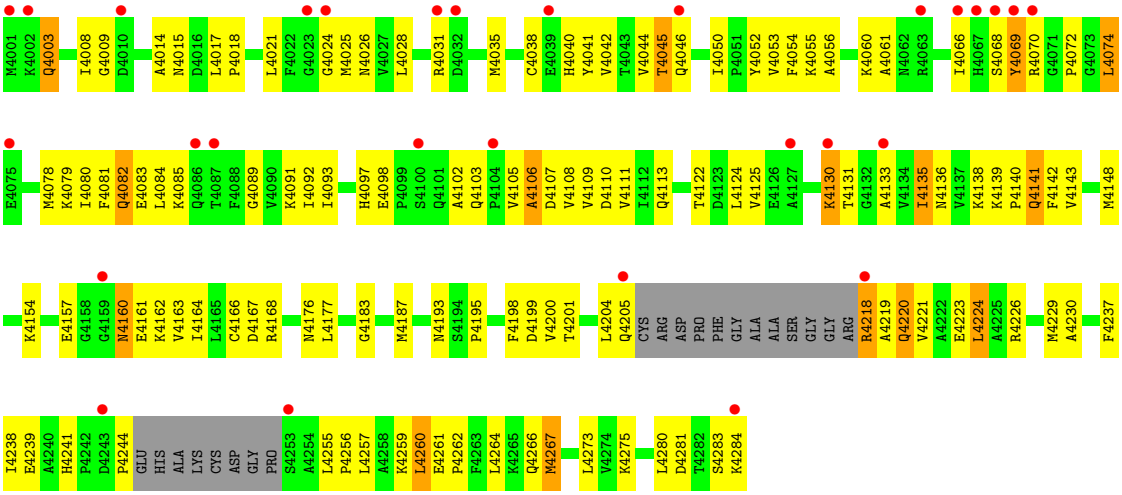
• Molecule 1: 3-DEOXY-D-MANNO-OCTULOSONATE 8-PHOSPHATE SYNTHASE

Chain C:



- Molecule 1: 3-DEOXY-D-MANNO-OCTULOSONATE 8-PHOSPHATE SYNTHASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	228.62Å 228.62Å 228.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.86 – 2.40 22.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (22.86-2.40) 99.3 (22.86-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.239 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.046 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8618	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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 (i)

5.1 Standard geometry (i)

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	0.56	0/2075	0.75	2/2796 (0.1%)
1	B	0.55	0/2075	0.74	1/2796 (0.0%)
1	C	0.57	0/2075	0.75	1/2796 (0.0%)
1	D	0.48	0/2058	0.72	0/2773
All	All	0.54	0/8283	0.74	4/11161 (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	C	3074	LEU	CA-CB-CG	7.78	133.18	115.30
1	A	1074	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	1095	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	2090	VAL	CB-CA-C	-5.22	101.48	111.40

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	2040	0	2081	65	0
1	B	2040	0	2081	83	0
1	C	2040	0	2081	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2024	0	2067	151	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	1	0
2	D	10	0	0	1	0
3	A	143	0	0	1	0
3	B	122	0	0	5	0
3	C	119	0	0	5	0
3	D	40	0	0	5	0
All	All	8618	0	8310	354	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 21.

All (354) 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:B:2141:GLN:H	1:B:2141:GLN:NE2	1.40	1.19
1:B:2141:GLN:HE21	1:B:2141:GLN:N	1.46	1.09
1:D:4045:THR:HG21	1:D:4052:TYR:HB2	1.41	1.02
1:A:1218:ARG:HH11	1:A:1253:SER:HB3	1.24	1.01
1:B:2114:LEU:HD13	1:B:2128:MET:HE1	1.43	1.00
1:D:4003:GLN:HE21	1:D:4015:ASN:HD22	1.04	1.00
1:D:4028:LEU:HB2	1:D:4072:PRO:HG2	1.45	0.96
1:C:3002:LYS:H	1:C:3002:LYS:HD3	1.30	0.94
1:C:3078:MET:HE3	1:C:3108:VAL:HB	1.48	0.93
1:D:4078:MET:HE1	1:D:4105:VAL:HA	1.51	0.92
1:D:4141:GLN:H	1:D:4141:GLN:NE2	1.68	0.92
1:A:1201:THR:HG21	1:A:1239:GLU:H	1.35	0.91
1:D:4168:ARG:HH22	1:D:4205:GLN:NE2	1.70	0.89
1:D:4141:GLN:HE21	1:D:4141:GLN:N	1.70	0.89
1:B:2185:SER:O	1:B:2189:LYS:HD3	1.73	0.87
1:D:4025:MET:HE2	1:D:4054:PHE:HZ	1.41	0.86
1:D:4003:GLN:NE2	1:D:4015:ASN:HD22	1.74	0.85
1:D:4160:ASN:ND2	1:D:4162:LYS:H	1.73	0.85
1:C:3002:LYS:HD3	1:C:3002:LYS:N	1.93	0.83
1:D:4131:THR:HG22	1:D:4133:ALA:H	1.44	0.82
1:D:4082:GLN:HA	1:D:4082:GLN:HE21	1.40	0.82
1:B:2223:GLU:HG3	3:B:24:HOH:O	1.78	0.82
1:D:4082:GLN:HA	1:D:4082:GLN:NE2	1.94	0.81
1:A:1015:ASN:HD21	1:A:1196:VAL:H	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3204:LEU:HD11	1:C:3221:VAL:HG22	1.62	0.80
1:B:2124:LEU:HD22	1:B:2128:MET:HE3	1.61	0.80
1:D:4078:MET:CE	1:D:4105:VAL:HA	2.12	0.80
1:B:2204:LEU:HD22	1:B:2220:GLN:HE21	1.46	0.79
1:B:2014:ALA:HB3	1:B:2017:LEU:HD22	1.64	0.79
1:D:4103:GLN:HG2	1:D:4130:LYS:HE2	1.65	0.79
1:C:3220:GLN:HG3	1:C:3223:GLU:CD	2.03	0.78
1:C:3229:MET:HE1	1:C:3236:LEU:HD13	1.66	0.78
1:A:1014:ALA:HB3	1:A:1017:LEU:HD22	1.65	0.77
1:D:4168:ARG:HH22	1:D:4205:GLN:HE22	1.33	0.77
1:D:4160:ASN:C	1:D:4160:ASN:HD22	1.88	0.77
1:A:1218:ARG:NH1	1:A:1253:SER:HB3	2.00	0.77
1:A:1131:THR:CG2	1:A:1133:ALA:H	1.98	0.76
1:C:3078:MET:HE1	1:C:3105:VAL:HA	1.68	0.76
1:D:4078:MET:CE	1:D:4108:VAL:HB	2.16	0.75
1:C:3015:ASN:HD21	1:C:3196:VAL:H	1.31	0.75
1:A:1055:LYS:HB2	1:A:1093:ILE:HG23	1.67	0.75
1:B:2122:THR:HG22	1:B:2154:LYS:NZ	2.02	0.74
1:C:3229:MET:CE	1:C:3236:LEU:HD13	2.17	0.74
1:D:4074:LEU:O	1:D:4078:MET:HG2	1.87	0.74
1:B:2168:ARG:HG3	1:B:2168:ARG:HH11	1.49	0.74
1:C:3002:LYS:H	1:C:3002:LYS:CD	1.93	0.74
1:B:2003:GLN:NE2	1:B:2015:ASN:HD22	1.86	0.73
1:D:4081:PHE:O	1:D:4085:LYS:HG3	1.87	0.73
1:B:2160:ASN:ND2	1:B:2162:LYS:H	1.86	0.73
1:D:4160:ASN:HD22	1:D:4161:GLU:N	1.85	0.73
1:C:3220:GLN:OE1	1:C:3223:GLU:HG2	1.89	0.72
1:D:4078:MET:HE3	1:D:4108:VAL:HB	1.70	0.72
1:C:3204:LEU:HD12	1:C:3253:SER:OG	1.88	0.72
1:B:2114:LEU:HD13	1:B:2128:MET:CE	2.20	0.72
1:D:4218:ARG:HG2	1:D:4220:GLN:OE1	1.90	0.71
1:B:2140:PRO:HB2	1:B:2143:VAL:HG13	1.72	0.71
1:B:2160:ASN:HD22	1:B:2162:LYS:H	1.39	0.71
1:C:3060:LYS:HE2	1:C:3060:LYS:HA	1.73	0.70
1:D:4082:GLN:HE21	1:D:4082:GLN:CA	2.02	0.70
1:D:4014:ALA:HB3	1:D:4017:LEU:HD22	1.72	0.70
1:D:4055:LYS:C	1:D:4055:LYS:HD3	2.12	0.70
1:D:4003:GLN:HE21	1:D:4015:ASN:ND2	1.85	0.70
1:D:4038:CYS:O	1:D:4042:VAL:HG23	1.92	0.69
1:D:4183:GLY:HA3	3:D:133:HOH:O	1.91	0.68
1:D:4267:MET:HE3	1:D:4267:MET:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2124:LEU:HD22	1:B:2128:MET:CE	2.23	0.68
1:D:4054:PHE:HB3	1:D:4092:ILE:HD13	1.74	0.68
1:D:4198:PHE:CE2	1:D:4200:VAL:HG22	2.28	0.68
1:D:4241:HIS:O	1:D:4244:PRO:HD3	1.93	0.68
1:C:3078:MET:CE	1:C:3105:VAL:HA	2.25	0.67
1:B:2075:GLU:CD	1:B:2075:GLU:H	1.97	0.67
1:C:3261:GLU:HB3	1:C:3262:PRO:HD3	1.76	0.66
1:A:1038:CYS:O	1:A:1042:VAL:HG23	1.95	0.66
1:C:3201:THR:HG23	1:C:3238:ILE:HG13	1.78	0.65
1:D:4042:VAL:O	1:D:4046:GLN:HB2	1.97	0.65
1:A:1199:ASP:HA	1:A:1237:PHE:HB3	1.77	0.65
1:C:3031:ARG:O	1:C:3035:MET:HG2	1.96	0.65
1:B:2205:GLN:HB2	1:B:2220:GLN:HE22	1.62	0.65
1:C:3078:MET:CE	1:C:3108:VAL:HB	2.24	0.64
1:A:1040:HIS:ND1	1:A:1257:LEU:HD22	2.12	0.64
1:B:2204:LEU:HD22	1:B:2220:GLN:NE2	2.11	0.64
1:B:2204:LEU:HD21	1:B:2220:GLN:HG3	1.79	0.64
1:B:2223:GLU:OE1	3:B:511:HOH:O	2.15	0.64
1:D:4003:GLN:CG	1:D:4015:ASN:HB2	2.27	0.64
1:A:1131:THR:HG23	1:A:1133:ALA:H	1.61	0.64
1:A:1025:MET:O	1:A:1055:LYS:HE3	1.98	0.64
1:D:4135:ILE:HD13	1:D:4136:ASN:N	2.13	0.64
1:B:2218:ARG:HB3	1:B:2220:GLN:HG2	1.80	0.63
1:D:4176:ASN:HD22	1:D:4177:LEU:H	1.45	0.63
1:C:3055:LYS:C	1:C:3055:LYS:HD3	2.19	0.63
1:A:1136:ASN:HD21	1:A:1166:CYS:HB2	1.64	0.62
1:D:4097:HIS:O	1:D:4098:GLU:HG3	1.99	0.62
1:A:1181:MET:HE3	1:B:2181:MET:HG3	1.80	0.62
1:D:4008:ILE:O	1:D:4091:LYS:NZ	2.29	0.62
1:D:4141:GLN:H	1:D:4141:GLN:HE21	0.84	0.62
1:A:1219:ALA:HB2	1:B:2283:SER:OG	1.99	0.62
1:D:4045:THR:HG22	1:D:4050:ILE:HB	1.82	0.62
1:B:2072:PRO:HB2	1:B:2076:GLU:HB3	1.81	0.61
1:D:4109:VAL:HG12	1:D:4110:ASP:N	2.16	0.60
1:D:4122:THR:HG22	1:D:4154:LYS:NZ	2.16	0.60
1:D:4218:ARG:O	1:D:4221:VAL:HG23	2.01	0.60
1:A:1220:GLN:NE2	1:B:2182:LEU:HD22	2.17	0.60
1:D:4015:ASN:O	1:D:4275:LYS:HE2	2.01	0.60
1:A:1042:VAL:O	1:A:1046:GLN:HB2	2.01	0.60
1:D:4168:ARG:NH2	1:D:4205:GLN:NE2	2.48	0.60
1:D:4055:LYS:HB2	1:D:4093:ILE:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:THR:HG22	1:A:1133:ALA:H	1.66	0.59
1:D:4168:ARG:HD2	2:D:4999:SO4:O4	2.03	0.59
1:A:1062:ASN:H	1:A:1062:ASN:HD22	1.48	0.59
1:C:3042:VAL:O	1:C:3046:GLN:HB2	2.02	0.59
1:D:4176:ASN:ND2	1:D:4177:LEU:H	2.02	0.58
1:D:4160:ASN:HD21	1:D:4162:LYS:H	1.50	0.58
1:D:4054:PHE:O	1:D:4093:ILE:HG22	2.04	0.58
1:B:2122:THR:HB	1:B:2154:LYS:HE3	1.86	0.58
1:C:3055:LYS:HD3	1:C:3056:ALA:N	2.20	0.57
1:D:4135:ILE:CG2	1:D:4163:VAL:HG22	2.33	0.57
1:D:4055:LYS:HD3	1:D:4056:ALA:N	2.19	0.57
1:D:4102:ALA:HB3	3:D:119:HOH:O	2.05	0.57
1:D:4140:PRO:HD2	1:D:4143:VAL:CG2	2.35	0.57
1:C:3220:GLN:HG3	1:C:3223:GLU:OE2	2.05	0.57
1:D:4135:ILE:HD13	1:D:4135:ILE:C	2.25	0.57
1:B:2060:LYS:HE2	1:B:2060:LYS:HA	1.87	0.56
1:B:2241:HIS:ND1	1:B:2242:PRO:HD2	2.19	0.56
1:A:1201:THR:CG2	1:A:1238:ILE:HG13	2.35	0.56
1:A:1031:ARG:HD3	1:A:1032:ASP:N	2.20	0.56
1:A:1218:ARG:O	1:A:1221:VAL:HG23	2.06	0.56
1:D:4044:VAL:HG13	1:D:4261:GLU:HG3	1.88	0.56
1:D:4078:MET:HE2	1:D:4108:VAL:HB	1.87	0.56
1:B:2190:VAL:HG22	1:B:2190:VAL:O	2.06	0.56
1:C:3136:ASN:HD21	1:C:3166:CYS:HB2	1.71	0.56
1:B:2039:GLU:O	1:B:2043:THR:HG23	2.05	0.56
1:C:3092:ILE:HG22	1:C:3109:VAL:HG22	1.86	0.56
1:D:4140:PRO:HD2	1:D:4143:VAL:HG21	1.87	0.55
1:D:4045:THR:HG22	1:D:4050:ILE:O	2.07	0.55
1:D:4003:GLN:NE2	1:D:4193:ASN:HB3	2.20	0.55
1:A:1063:ARG:NH1	1:A:1069:TYR:O	2.35	0.55
1:D:4160:ASN:ND2	1:D:4160:ASN:C	2.60	0.55
1:D:4009:GLY:HA3	1:D:4091:LYS:NZ	2.20	0.55
1:D:4109:VAL:CG1	1:D:4110:ASP:N	2.70	0.55
1:D:4226:ARG:HA	1:D:4267:MET:HE1	1.88	0.55
1:A:1055:LYS:HD2	1:A:1056:ALA:N	2.22	0.54
1:C:3048:LEU:O	1:C:3268:LYS:HE3	2.07	0.54
1:B:2025:MET:HE3	1:B:2033:LEU:HD13	1.89	0.54
1:C:3031:ARG:HD3	1:C:3083:GLU:OE2	2.07	0.54
1:B:2055:LYS:C	1:B:2055:LYS:HD3	2.27	0.54
1:C:3219:ALA:CB	1:D:4283:SER:HB3	2.38	0.54
1:A:1025:MET:HE3	1:A:1037:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3140:PRO:HB2	1:C:3143:VAL:HG23	1.90	0.53
1:D:4130:LYS:HD2	1:D:4131:THR:N	2.23	0.53
1:B:2168:ARG:HG3	1:B:2168:ARG:NH1	2.22	0.53
1:D:4102:ALA:O	1:D:4106:ALA:HB2	2.08	0.53
1:D:4160:ASN:HD22	1:D:4162:LYS:H	1.52	0.53
1:D:4031:ARG:HD3	1:D:4083:GLU:OE2	2.08	0.53
1:D:4176:ASN:ND2	1:D:4177:LEU:N	2.56	0.53
1:D:4052:TYR:CD1	1:D:4053:VAL:N	2.76	0.52
1:D:4201:THR:HG21	1:D:4239:GLU:HB2	1.90	0.52
1:A:1060:LYS:HE2	1:A:1060:LYS:HA	1.92	0.52
1:A:1062:ASN:HD22	1:A:1062:ASN:N	2.05	0.52
1:B:2031:ARG:HG2	3:B:287:HOH:O	2.09	0.52
1:B:2122:THR:HG22	1:B:2154:LYS:HZ1	1.74	0.52
1:D:4260:LEU:O	1:D:4260:LEU:HD23	2.10	0.52
1:A:1226:ARG:HD2	1:B:2230:ALA:O	2.09	0.52
1:D:4140:PRO:HB2	1:D:4143:VAL:HG13	1.92	0.52
1:A:1002:LYS:HG3	1:A:1003:GLN:O	2.10	0.52
1:A:1226:ARG:HG2	1:A:1270:ILE:CD1	2.40	0.52
1:D:4167:ASP:HB2	1:D:4187:MET:CE	2.40	0.52
1:D:4261:GLU:HB2	3:D:66:HOH:O	2.10	0.52
1:A:1027:VAL:HG22	1:A:1060:LYS:HD2	1.91	0.51
1:B:2039:GLU:OE1	1:B:2043:THR:HG21	2.10	0.51
1:C:3260:LEU:HD22	1:C:3264:LEU:HG	1.92	0.51
1:A:1143:VAL:CG1	1:A:1147:GLN:HB2	2.40	0.51
1:A:1154:LYS:HD2	1:C:3064:SER:O	2.09	0.51
1:B:2168:ARG:HG3	1:B:2168:ARG:O	2.11	0.51
1:D:4260:LEU:HD23	1:D:4264:LEU:HG	1.93	0.51
1:C:3022:PHE:O	1:C:3237:PHE:HA	2.11	0.51
1:D:4009:GLY:HA3	1:D:4091:LYS:HZ1	1.76	0.51
1:B:2142:PHE:CD2	1:D:4142:PHE:CD2	2.99	0.51
1:D:4074:LEU:O	1:D:4074:LEU:HD13	2.10	0.51
1:D:4113:GLN:HB3	1:D:4136:ASN:HB3	1.92	0.51
1:D:4199:ASP:HA	1:D:4237:PHE:HB3	1.93	0.50
1:A:1059:ASP:HA	1:A:1070:ARG:O	2.11	0.50
1:A:1198:PHE:HZ	1:A:1224:LEU:HD13	1.76	0.50
1:B:2066:ILE:HG13	1:D:4154:LYS:HG3	1.92	0.50
1:D:4093:ILE:HA	1:D:4111:VAL:O	2.12	0.50
1:A:1031:ARG:HD3	1:A:1031:ARG:C	2.32	0.50
1:D:4092:ILE:HG22	1:D:4093:ILE:N	2.27	0.50
1:A:1026:ASN:OD1	1:A:1060:LYS:HD2	2.11	0.50
1:A:1011:ILE:HG22	1:A:1012:ASN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2125:VAL:HG13	1:B:2155:PHE:CE1	2.47	0.49
1:C:3273:LEU:HD12	1:D:4273:LEU:HD22	1.94	0.49
1:D:4028:LEU:O	1:D:4072:PRO:HG3	2.12	0.49
1:D:4204:LEU:CD1	1:D:4221:VAL:HG22	2.41	0.49
1:C:3273:LEU:CD2	1:C:3277:PHE:CE1	2.95	0.49
1:D:4267:MET:HA	1:D:4267:MET:CE	2.40	0.49
1:D:4259:LYS:O	1:D:4262:PRO:HD2	2.13	0.49
1:D:4040:HIS:O	1:D:4044:VAL:HG23	2.13	0.49
1:D:4003:GLN:HG2	1:D:4015:ASN:HB2	1.94	0.49
1:B:2154:LYS:HG3	1:D:4066:ILE:HD12	1.94	0.49
1:B:2218:ARG:CB	1:B:2220:GLN:HG2	2.43	0.49
1:C:3188:LYS:HE2	3:C:353:HOH:O	2.11	0.49
1:C:3273:LEU:HD22	1:C:3277:PHE:CZ	2.48	0.49
1:A:1142:PHE:CD1	1:C:3142:PHE:CD2	3.01	0.48
1:C:3015:ASN:HD21	1:C:3196:VAL:N	2.05	0.48
1:D:4074:LEU:HD21	1:D:4105:VAL:HG23	1.95	0.48
1:C:3015:ASN:ND2	1:C:3196:VAL:H	2.07	0.48
1:A:1015:ASN:ND2	1:A:1196:VAL:H	2.05	0.48
1:C:3219:ALA:HB1	1:D:4283:SER:HB3	1.96	0.48
1:C:3074:LEU:O	1:C:3078:MET:HG2	2.13	0.48
1:B:2074:LEU:HD13	1:B:2074:LEU:C	2.34	0.48
1:B:2124:LEU:HD22	1:B:2128:MET:HG3	1.96	0.48
1:B:2200:VAL:HG12	1:B:2238:ILE:HG22	1.94	0.48
1:A:1065:SER:HB2	1:C:3157:GLU:OE2	2.13	0.48
1:D:4260:LEU:CD2	1:D:4264:LEU:HG	2.43	0.47
1:B:2003:GLN:HE21	1:B:2015:ASN:HD22	1.61	0.47
1:B:2198:PHE:HZ	1:B:2224:LEU:HD13	1.80	0.47
1:A:1148:MET:HG3	1:A:1187:MET:HE3	1.97	0.47
1:D:4199:ASP:OD1	1:D:4199:ASP:C	2.53	0.47
1:B:2004:LYS:HB2	1:B:2193:ASN:O	2.15	0.46
1:A:1041:TYR:HB3	1:A:1052:TYR:CZ	2.51	0.46
1:B:2062:ASN:N	1:B:2062:ASN:HD22	2.12	0.46
1:D:4041:TYR:HB3	1:D:4052:TYR:CZ	2.51	0.46
1:D:4125:VAL:HG11	1:D:4154:LYS:HG2	1.98	0.46
1:A:1148:MET:HG3	1:A:1187:MET:CE	2.45	0.46
1:B:2025:MET:CE	1:B:2033:LEU:HD13	2.45	0.46
1:B:2141:GLN:NE2	1:B:2141:GLN:N	2.26	0.46
1:D:4078:MET:HE1	1:D:4105:VAL:CA	2.34	0.46
1:C:3259:LYS:NZ	1:D:4281:ASP:O	2.46	0.46
1:A:1062:ASN:N	1:A:1062:ASN:ND2	2.63	0.46
1:B:2218:ARG:C	1:B:2220:GLN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:LYS:HE2	3:A:68:HOH:O	2.15	0.45
1:B:2022:PHE:O	1:B:2237:PHE:HA	2.16	0.45
1:B:2154:LYS:HG3	1:D:4066:ILE:CD1	2.46	0.45
1:C:3011:ILE:HD12	1:C:3091:LYS:HD2	1.97	0.45
1:D:4092:ILE:CG2	1:D:4093:ILE:N	2.79	0.45
1:D:4031:ARG:HD3	1:D:4083:GLU:CD	2.37	0.45
1:D:4041:TYR:O	1:D:4045:THR:OG1	2.33	0.45
1:B:2201:THR:HB	1:B:2253:SER:O	2.16	0.45
1:C:3182:LEU:HD22	1:D:4220:GLN:HB3	1.99	0.45
1:D:4080:ILE:O	1:D:4084:LEU:HG	2.16	0.45
1:A:1015:ASN:HD21	1:A:1196:VAL:N	2.05	0.45
1:D:4226:ARG:HD3	1:D:4266:GLN:OE1	2.17	0.45
1:B:2204:LEU:CD2	1:B:2220:GLN:HE21	2.23	0.45
1:D:4136:ASN:HD21	1:D:4166:CYS:HB2	1.82	0.45
1:A:1074:LEU:CD1	1:A:1074:LEU:C	2.86	0.45
1:A:1260:LEU:HD22	1:A:1264:LEU:HG	1.98	0.45
1:C:3040:HIS:ND1	1:C:3257:LEU:HD22	2.31	0.45
1:D:4218:ARG:N	1:D:4221:VAL:HG23	2.32	0.45
1:B:2122:THR:HG23	1:D:4061:ALA:O	2.17	0.45
1:B:2241:HIS:CE1	1:B:2242:PRO:HD2	2.52	0.45
1:C:3244:PRO:O	1:C:3245:GLU:HB2	2.17	0.45
1:D:4167:ASP:HB2	1:D:4187:MET:HE3	1.98	0.45
1:C:3201:THR:CG2	1:C:3238:ILE:HG13	2.47	0.44
1:D:4021:LEU:HD11	1:D:4238:ILE:HG22	1.99	0.44
1:D:4176:ASN:HD22	1:D:4177:LEU:N	2.09	0.44
1:A:1271:ASP:O	1:A:1275:LYS:HB2	2.17	0.44
1:A:1103:GLN:HB3	1:A:1104:PRO:HD3	1.99	0.44
1:D:4229:MET:HG3	1:D:4267:MET:HE3	1.99	0.44
1:A:1013:VAL:HG22	1:A:1020:VAL:HG21	1.97	0.44
1:B:2041:TYR:HB3	1:B:2052:TYR:CZ	2.52	0.44
1:D:4070:ARG:HD3	3:D:415:HOH:O	2.17	0.44
1:D:4255:LEU:HD12	1:D:4256:PRO:HD2	1.98	0.44
1:B:2039:GLU:OE1	1:B:2043:THR:CG2	2.66	0.44
1:C:3085:LYS:HD2	1:C:3090:VAL:O	2.18	0.44
1:D:4085:LYS:O	1:D:4089:GLY:HA2	2.18	0.44
1:D:4135:ILE:HD13	1:D:4136:ASN:C	2.38	0.44
1:C:3226:ARG:HG2	1:C:3270:ILE:CD1	2.48	0.44
1:D:4135:ILE:HG21	1:D:4163:VAL:HG22	1.99	0.44
1:D:4226:ARG:HA	1:D:4267:MET:CE	2.47	0.44
1:B:2124:LEU:HD13	1:B:2128:MET:HE2	1.99	0.44
1:B:2183:GLY:HA3	3:B:73:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2062:ASN:HD22	1:B:2062:ASN:H	1.66	0.44
1:C:3204:LEU:HD23	1:C:3204:LEU:HA	1.85	0.44
1:C:3202:HIS:CD2	1:C:3252:PRO:HD2	2.52	0.43
1:D:4025:MET:HE2	1:D:4054:PHE:CZ	2.33	0.43
1:D:4079:LYS:O	1:D:4083:GLU:HG2	2.18	0.43
1:B:2074:LEU:C	1:B:2074:LEU:CD1	2.86	0.43
1:C:3014:ALA:HB3	1:C:3017:LEU:HD22	1.99	0.43
1:C:3031:ARG:HD2	3:C:346:HOH:O	2.17	0.43
1:C:3260:LEU:HD22	1:C:3264:LEU:CD1	2.48	0.43
1:D:4052:TYR:CG	1:D:4053:VAL:N	2.86	0.43
1:B:2079:LYS:HA	1:B:2082:GLN:HG3	2.00	0.43
1:D:4003:GLN:HG3	1:D:4015:ASN:HB2	2.00	0.43
1:A:1037:ILE:HD11	1:A:1242:PRO:HD3	1.99	0.43
1:A:1074:LEU:C	1:A:1074:LEU:HD12	2.39	0.43
1:B:2064:SER:O	1:D:4154:LYS:HD3	2.18	0.43
1:C:3026:ASN:HD21	1:C:3060:LYS:NZ	2.16	0.43
1:C:3062:ASN:H	1:C:3062:ASN:HD22	1.66	0.43
1:C:3271:ASP:O	1:C:3275:LYS:HB2	2.18	0.43
1:C:3092:ILE:CG2	1:C:3109:VAL:HG22	2.49	0.43
1:D:4164:ILE:HG12	1:D:4195:PRO:HG2	2.01	0.43
1:B:2109:VAL:CG1	1:B:2110:ASP:N	2.82	0.43
1:A:1198:PHE:CZ	1:A:1224:LEU:HD13	2.54	0.43
1:C:3229:MET:HE3	1:C:3236:LEU:HD13	2.00	0.43
1:B:2122:THR:CB	1:B:2154:LYS:HE3	2.47	0.43
1:A:1176:ASN:HD22	1:A:1176:ASN:HA	1.68	0.43
1:A:1283:SER:HB3	1:B:2219:ALA:HB2	2.01	0.43
1:C:3226:ARG:NH1	1:D:4230:ALA:O	2.51	0.43
1:D:4113:GLN:CB	1:D:4136:ASN:HB3	2.48	0.43
1:B:2062:ASN:N	1:B:2062:ASN:ND2	2.67	0.43
1:C:3185:SER:OG	1:D:4223:GLU:OE2	2.36	0.43
1:D:4031:ARG:O	1:D:4035:MET:HB2	2.19	0.43
1:C:3241:HIS:ND1	1:C:3242:PRO:HD2	2.34	0.42
1:C:3241:HIS:CE1	1:C:3242:PRO:HD2	2.54	0.42
1:D:4068:SER:O	1:D:4069:TYR:C	2.57	0.42
1:D:4113:GLN:NE2	1:D:4138:LYS:HD2	2.34	0.42
1:B:2003:GLN:NE2	1:B:2015:ASN:HB2	2.33	0.42
1:C:3067:HIS:HB2	3:C:403:HOH:O	2.18	0.42
1:A:1055:LYS:HB2	1:A:1093:ILE:CG2	2.44	0.42
1:B:2154:LYS:O	1:B:2157:GLU:HG2	2.19	0.42
1:C:3041:TYR:HB3	1:C:3052:TYR:CZ	2.54	0.42
1:D:4280:LEU:HB3	3:D:188:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4055:LYS:CB	1:D:4093:ILE:HG23	2.49	0.42
1:C:3172:PHE:O	1:C:3176:ASN:HB3	2.19	0.42
1:D:4017:LEU:O	1:D:4018:PRO:C	2.57	0.42
1:A:1015:ASN:ND2	1:A:1234:ALA:HB2	2.35	0.42
1:B:2124:LEU:HD13	1:B:2128:MET:CE	2.49	0.42
1:D:4106:ALA:HB1	1:D:4131:THR:HG23	2.01	0.42
1:A:1011:ILE:HG13	1:A:1091:LYS:HE2	2.00	0.42
1:D:4014:ALA:CB	1:D:4017:LEU:HD22	2.47	0.42
1:C:3062:ASN:HD22	1:C:3062:ASN:N	2.17	0.42
1:A:1179:VAL:CG2	1:A:1203:ALA:HB1	2.49	0.42
1:B:2023:GLY:O	1:B:2054:PHE:HA	2.20	0.42
1:D:4139:LYS:HA	1:D:4148:MET:HE1	2.01	0.42
1:B:2122:THR:HG22	1:B:2154:LYS:HZ2	1.81	0.41
1:C:3257:LEU:O	1:C:3260:LEU:HB2	2.19	0.41
1:A:1154:LYS:O	1:A:1157:GLU:HB2	2.20	0.41
1:C:3063:ARG:HB3	2:C:3777:SO4:O1	2.20	0.41
1:A:1273:LEU:HD22	1:A:1277:PHE:CE1	2.55	0.41
1:B:2181:MET:HE3	1:B:2227:ALA:HB3	2.02	0.41
1:D:4025:MET:CE	1:D:4054:PHE:HZ	2.21	0.41
1:D:4201:THR:OG1	1:D:4238:ILE:HA	2.20	0.41
1:D:4260:LEU:O	1:D:4260:LEU:CD2	2.68	0.41
1:C:3183:GLY:HA3	3:C:150:HOH:O	2.20	0.41
1:C:3199:ASP:HA	1:C:3237:PHE:HB3	2.01	0.41
1:B:2141:GLN:H	1:B:2141:GLN:HE21	0.62	0.41
1:A:1015:ASN:HD22	1:A:1234:ALA:HB2	1.84	0.41
1:D:4154:LYS:O	1:D:4157:GLU:HG2	2.20	0.41
1:C:3062:ASN:N	1:C:3062:ASN:ND2	2.69	0.41
1:D:4218:ARG:O	1:D:4220:GLN:N	2.54	0.41
1:C:3004:LYS:NZ	1:C:3161:GLU:HB3	2.36	0.41
1:C:3253:SER:HA	3:C:296:HOH:O	2.20	0.41
1:A:1014:ALA:CB	1:A:1017:LEU:HD22	2.45	0.41
1:D:4224:LEU:HD23	1:D:4224:LEU:HA	1.92	0.41
1:B:2126:GLU:HG3	1:D:4066:ILE:HG12	2.03	0.41
1:B:2218:ARG:HD3	1:B:2218:ARG:HA	1.75	0.41
1:C:3031:ARG:HD3	1:C:3083:GLU:CD	2.41	0.41
1:D:4024:GLY:HA3	1:D:4055:LYS:O	2.21	0.41
1:C:3081:PHE:O	1:C:3085:LYS:HG2	2.20	0.40
1:D:4025:MET:HE3	1:D:4056:ALA:CB	2.52	0.40
1:D:4131:THR:HG22	1:D:4133:ALA:N	2.25	0.40
1:B:2040:HIS:HD2	3:B:148:HOH:O	2.04	0.40
1:C:3224:LEU:HD23	1:C:3224:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2004:LYS:NZ	1:B:2161:GLU:O	2.41	0.40
1:D:4025:MET:HE3	1:D:4056:ALA:HB2	2.04	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	260/284 (92%)	253 (97%)	6 (2%)	1 (0%)	34	48
1	B	260/284 (92%)	247 (95%)	13 (5%)	0	100	100
1	C	260/284 (92%)	251 (96%)	9 (4%)	0	100	100
1	D	258/284 (91%)	241 (93%)	14 (5%)	3 (1%)	13	19
All	All	1038/1136 (91%)	992 (96%)	42 (4%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4219	ALA
1	D	4069	TYR
1	D	4106	ALA
1	A	1244	PRO

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	222/233 (95%)	205 (92%)	17 (8%)	13	20
1	B	222/233 (95%)	204 (92%)	18 (8%)	11	18
1	C	222/233 (95%)	205 (92%)	17 (8%)	13	20
1	D	220/233 (94%)	201 (91%)	19 (9%)	10	16
All	All	886/932 (95%)	815 (92%)	71 (8%)	12	18

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	LYS
1	A	1017	LEU
1	A	1027	VAL
1	A	1031	ARG
1	A	1055	LYS
1	A	1062	ASN
1	A	1074	LEU
1	A	1098	GLU
1	A	1131	THR
1	A	1168	ARG
1	A	1224	LEU
1	A	1245	GLU
1	A	1252	PRO
1	A	1257	LEU
1	A	1260	LEU
1	A	1273	LEU
1	A	1275	LYS
1	B	2004	LYS
1	B	2017	LEU
1	B	2031	ARG
1	B	2033	LEU
1	B	2043	THR
1	B	2062	ASN
1	B	2074	LEU
1	B	2075	GLU
1	B	2082	GLN
1	B	2122	THR
1	B	2124	LEU
1	B	2141	GLN
1	B	2160	ASN
1	B	2204	LEU
1	B	2224	LEU
1	B	2238	ILE

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Mol	Chain	Res	Type
1	B	2257	LEU
1	B	2260	LEU
1	C	3002	LYS
1	C	3017	LEU
1	C	3031	ARG
1	C	3046	GLN
1	C	3062	ASN
1	C	3065	SER
1	C	3074	LEU
1	C	3109	VAL
1	C	3168	ARG
1	C	3176	ASN
1	C	3220	GLN
1	C	3224	LEU
1	C	3252	PRO
1	C	3257	LEU
1	C	3260	LEU
1	C	3273	LEU
1	C	3275	LYS
1	D	4003	GLN
1	D	4026	ASN
1	D	4045	THR
1	D	4060	LYS
1	D	4074	LEU
1	D	4082	GLN
1	D	4107	ASP
1	D	4124	LEU
1	D	4130	LYS
1	D	4135	ILE
1	D	4141	GLN
1	D	4160	ASN
1	D	4218	ARG
1	D	4220	GLN
1	D	4224	LEU
1	D	4257	LEU
1	D	4260	LEU
1	D	4267	MET
1	D	4284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1012	ASN
1	A	1015	ASN
1	A	1062	ASN
1	A	1097	HIS
1	A	1113	GLN
1	A	1136	ASN
1	A	1176	ASN
1	B	2003	GLN
1	B	2040	HIS
1	B	2062	ASN
1	B	2103	GLN
1	B	2136	ASN
1	B	2141	GLN
1	B	2160	ASN
1	B	2220	GLN
1	C	3015	ASN
1	C	3026	ASN
1	C	3062	ASN
1	C	3082	GLN
1	C	3086	GLN
1	C	3113	GLN
1	C	3136	ASN
1	C	3150	ASN
1	C	3171	ASN
1	C	3176	ASN
1	D	4003	GLN
1	D	4026	ASN
1	D	4082	GLN
1	D	4136	ASN
1	D	4141	GLN
1	D	4160	ASN
1	D	4176	ASN
1	D	4205	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	1999	-	4,4,4	0.48	0	6,6,6	0.40	0
2	SO4	C	3999	-	4,4,4	0.34	0	6,6,6	0.24	0
2	SO4	B	2888	-	4,4,4	0.34	0	6,6,6	0.21	0
2	SO4	A	1777	-	4,4,4	0.37	0	6,6,6	0.20	0
2	SO4	C	3777	-	4,4,4	0.34	0	6,6,6	0.19	0
2	SO4	D	4999	-	4,4,4	0.46	0	6,6,6	0.28	0
2	SO4	B	2999	-	4,4,4	0.41	0	6,6,6	0.26	0
2	SO4	D	4777	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	B	2777	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	C	3888	-	4,4,4	0.36	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3777	SO4	1	0
2	D	4999	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	266/284 (93%)	-0.32	11 (4%)	37	36	25, 36, 66, 89	0
1	B	266/284 (93%)	-0.17	12 (4%)	33	31	26, 40, 75, 93	0
1	C	266/284 (93%)	-0.27	11 (4%)	37	36	24, 38, 73, 95	0
1	D	264/284 (92%)	0.41	29 (10%)	5	5	31, 64, 90, 95	0
All	All	1062/1136 (93%)	-0.09	63 (5%)	22	21	24, 42, 84, 95	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4067	HIS	5.6
1	A	1067	HIS	5.1
1	B	2205	GLN	5.0
1	C	3218	ARG	4.6
1	C	3252	PRO	4.6
1	B	2067	HIS	4.5
1	D	4068	SER	4.4
1	B	2066	ILE	4.4
1	D	4069	TYR	4.2
1	D	4066	ILE	4.1
1	B	2245	GLU	4.1
1	D	4218	ARG	3.8
1	D	4205	GLN	3.7
1	A	1066	ILE	3.6
1	D	4002	LYS	3.5
1	B	2064	SER	3.4
1	D	4001	MET	3.4
1	B	2068	SER	3.4
1	D	4075	GLU	3.3
1	C	3284	LYS	3.3
1	B	2252	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	4086	GLN	3.2
1	C	3205	GLN	3.1
1	C	3245	GLU	2.9
1	C	3001	MET	2.8
1	C	3283	SER	2.8
1	D	4032	ASP	2.7
1	B	2001	MET	2.7
1	B	2218	ARG	2.6
1	B	2253	SER	2.6
1	C	3219	ALA	2.6
1	D	4087	THR	2.6
1	C	3253	SER	2.6
1	D	4063	ARG	2.6
1	D	4243	ASP	2.6
1	B	2069	TYR	2.6
1	A	1252	PRO	2.6
1	A	1001	MET	2.5
1	A	1069	TYR	2.5
1	A	1068	SER	2.4
1	D	4046	GLN	2.4
1	A	1218	ARG	2.4
1	D	4031	ARG	2.3
1	D	4127	ALA	2.3
1	D	4070	ARG	2.3
1	A	1243	ASP	2.3
1	C	3067	HIS	2.3
1	D	4039	GLU	2.3
1	D	4133	ALA	2.3
1	D	4104	PRO	2.2
1	D	4284	LYS	2.2
1	C	3243	ASP	2.2
1	D	4010	ASP	2.2
1	D	4159	GLY	2.2
1	A	1086	GLN	2.2
1	A	1205	GLN	2.2
1	D	4100	SER	2.2
1	A	1278	GLU	2.2
1	B	2065	SER	2.2
1	D	4023	GLY	2.1
1	D	4024	GLY	2.1
1	D	4130	LYS	2.1
1	D	4253	SER	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 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, 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	B-factors(Å^2)	Q<0.9
2	SO4	D	4777	5/5	0.80	0.36	88,90,91,91	5
2	SO4	A	1777	5/5	0.87	0.15	47,56,59,61	5
2	SO4	C	3777	5/5	0.89	0.19	44,53,57,57	5
2	SO4	B	2777	5/5	0.92	0.22	69,70,72,73	5
2	SO4	B	2888	5/5	0.97	0.14	53,59,66,71	0
2	SO4	D	4999	5/5	0.97	0.10	59,63,67,70	0
2	SO4	C	3888	5/5	0.97	0.11	57,59,62,63	5
2	SO4	B	2999	5/5	0.98	0.09	53,56,58,60	0
2	SO4	A	1999	5/5	0.99	0.09	27,28,34,35	0
2	SO4	C	3999	5/5	0.99	0.10	27,32,37,39	0

6.5 Other polymers (i)

There are no such residues in this entry.