



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:21 PM GMT

PDB ID : 1JUM  
Title : Crystal structure of the multidrug binding transcriptional repressor QacR bound to the natural drug berberine  
Authors : Schumacher, M.A.; Miller, M.C.; Grkovic, S.; Brown, M.H.; Skurray, R.A.; Brennan, R.G.  
Deposited on : 2001-08-24  
Resolution : 2.98 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

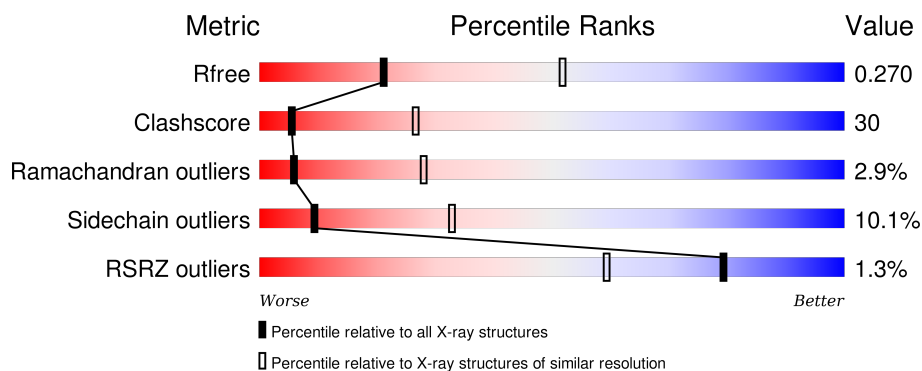
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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. 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	194	<div> <div>50%</div> <div>38%</div> <div>8%</div> <div>.</div> </div>
1	B	194	<div> <div>5%</div> <div>37%</div> <div>48%</div> <div>10%</div> <div>..</div> </div>
1	D	194	<div> <div>48%</div> <div>41%</div> <div>6%</div> <div>.</div> </div>
1	E	194	<div> <div>%</div> <div>42%</div> <div>48%</div> <div>6%</div> <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
2	SO4	A	799	-	-	-	X
2	SO4	A	802	-	-	-	X
2	SO4	B	199	-	-	-	X
2	SO4	D	1000	-	-	-	X
2	SO4	D	999	-	-	-	X
2	SO4	E	399	-	-	-	X
2	SO4	E	639	-	-	-	X
2	SO4	E	901	-	-	-	X
3	BER	A	803	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6330 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 HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	D	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	A	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	E	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			

There are 32 discrepancies between the modelled and reference sequences:

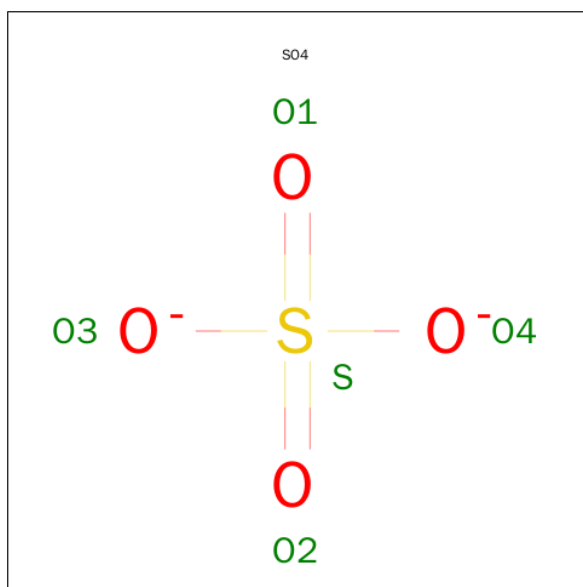
Chain	Residue	Modelled	Actual	Comment	Reference
B	72	ALA	CYS	ENGINEERED	UNP P0A0N4
B	141	SER	CYS	ENGINEERED	UNP P0A0N4
B	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	72	ALA	CYS	ENGINEERED	UNP P0A0N4
D	141	SER	CYS	ENGINEERED	UNP P0A0N4
D	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	72	ALA	CYS	ENGINEERED	UNP P0A0N4
A	141	SER	CYS	ENGINEERED	UNP P0A0N4
A	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	190	HIS	-	EXPRESSION TAG	UNP P0A0N4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	72	ALA	CYS	ENGINEERED	UNP P0A0N4
E	141	SER	CYS	ENGINEERED	UNP P0A0N4
E	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	194	HIS	-	EXPRESSION TAG	UNP P0A0N4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



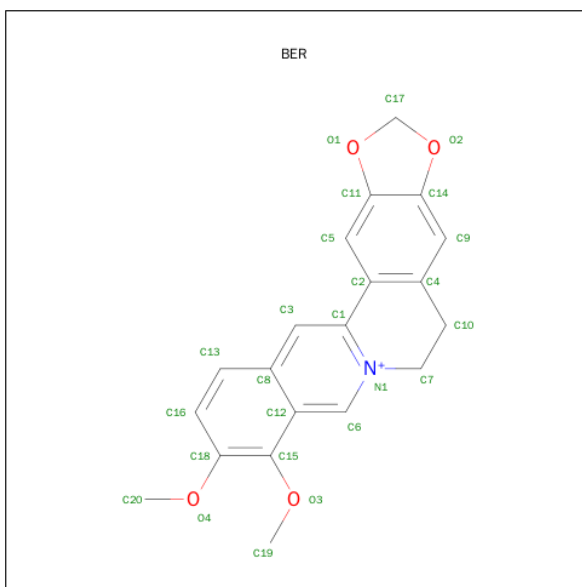
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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

- Molecule 3 is BERBERINE (three-letter code: BER) (formula: C<sub>20</sub>H<sub>18</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	20	1	4		

- Molecule 4 is water.

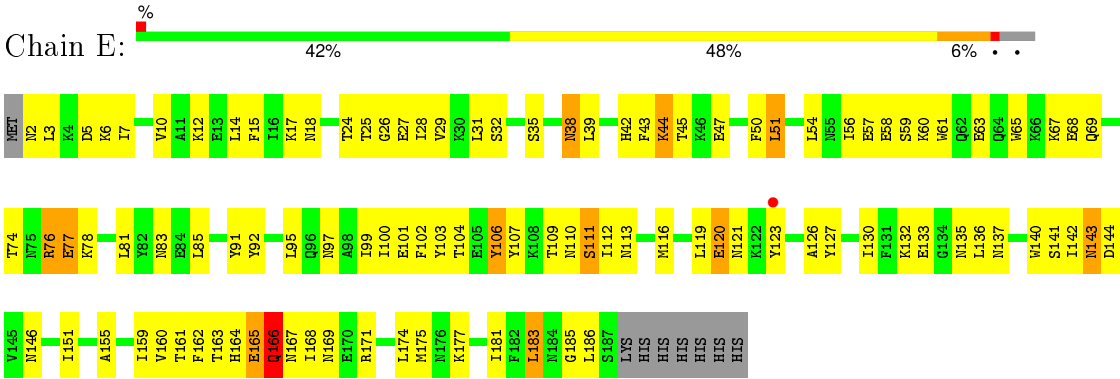
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	D	3	Total	O	0	0
			3	3		
4	E	1	Total	O	0	0
			1	1		



● Molecule 1: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION



● Molecule 1: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.30 Å   174.30 Å   96.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	84.29 – 2.98 84.29 – 2.57	Depositor EDS
% Data completeness (in resolution range)	92.7 (84.29-2.98) 67.3 (84.29-2.57)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.58 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.236   ,   0.284 0.219   ,   0.270	Depositor DCC
$R_{free}$ test set	2871 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 32177 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: BER, 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	0.66	0/1578	0.77	0/2126
1	B	0.60	0/1578	0.76	0/2126
1	D	0.63	0/1578	0.75	0/2126
1	E	0.70	0/1578	0.78	0/2126
All	All	0.65	0/6312	0.76	0/8504

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	TYR	Sidechain

### 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	1547	0	1536	74	0
1	B	1547	0	1536	125	0
1	D	1547	0	1536	89	0
1	E	1547	0	1536	97	0
2	A	30	0	0	1	0
2	B	25	0	0	1	0
2	D	20	0	0	0	0
2	E	35	0	0	2	0
3	A	25	0	18	3	0
4	A	3	0	0	0	0
4	D	3	0	0	1	0
4	E	1	0	0	0	0
All	All	6330	0	6162	369	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 30.

All (369) 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:2:ASN:ND2	1:D:3:LEU:H	1.49	1.10
1:B:45:THR:HG23	1:B:48:ASN:HB2	1.37	1.01
1:B:115:LYS:O	1:B:118:LYS:HG2	1.64	0.96
1:A:109:THR:HG22	1:A:111:SER:HB3	1.48	0.95
1:D:2:ASN:HD22	1:D:3:LEU:N	1.68	0.92
1:D:2:ASN:HD22	1:D:3:LEU:H	1.02	0.92
1:B:18:ASN:HD22	1:B:23:THR:HG22	1.33	0.92
1:E:24:THR:HG23	1:E:27:GLU:HB2	1.54	0.86
1:B:89:THR:HG22	1:B:90:GLU:H	1.38	0.86
1:D:24:THR:HG23	1:D:27:GLU:HB2	1.56	0.86
1:B:164:HIS:HB3	1:A:107:TYR:OH	1.75	0.85
1:B:39:LEU:H	1:B:39:LEU:HD22	1.43	0.84
1:B:62:GLN:HE22	1:B:126:ALA:HB2	1.43	0.84
1:A:68:GLU:HG2	1:A:85:LEU:HD11	1.58	0.84
1:B:29:VAL:HG22	1:B:39:LEU:HD21	1.59	0.83
1:D:165:GLU:HG2	1:D:166:GLN:OE1	1.78	0.83
1:A:103:TYR:O	1:A:107:TYR:HB2	1.78	0.83
1:B:66:LYS:HA	1:B:69:GLN:HE21	1.44	0.82
1:D:163:THR:HA	1:D:165:GLU:OE2	1.80	0.81
1:B:177:LYS:O	1:B:181:ILE:HG12	1.79	0.81
1:D:147:ALA:O	1:D:151:ILE:HG13	1.81	0.80
1:E:95:LEU:O	1:E:99:ILE:HG13	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:THR:HA	1:E:165:GLU:OE2	1.82	0.80
1:B:39:LEU:CD2	1:B:39:LEU:H	1.95	0.80
1:A:180:GLN:O	1:A:184:ASN:HB2	1.82	0.79
1:E:24:THR:CG2	1:E:27:GLU:HB2	2.14	0.78
1:A:30:LYS:O	1:A:30:LYS:HD3	1.84	0.78
1:A:147:ALA:O	1:A:151:ILE:HG12	1.84	0.77
1:E:143:ASN:CG	1:E:144:ASP:H	1.90	0.76
1:A:24:THR:OG1	1:A:27:GLU:HG3	1.86	0.75
1:D:2:ASN:ND2	1:D:3:LEU:N	2.28	0.75
1:E:3:LEU:O	1:E:7:ILE:HD13	1.86	0.74
1:A:167:ASN:ND2	1:A:169:ASN:H	1.86	0.74
1:D:10:VAL:HG21	1:D:32:SER:HB3	1.70	0.73
1:D:131:PHE:HB3	1:D:142:ILE:HD11	1.71	0.73
1:B:39:LEU:N	1:B:39:LEU:HD22	2.04	0.72
1:D:177:LYS:O	1:D:181:ILE:HG12	1.90	0.71
1:A:166:GLN:N	1:A:166:GLN:HE21	1.86	0.71
1:B:120:GLU:O	1:B:124:ILE:HG23	1.91	0.71
1:B:18:ASN:HB3	1:B:22:ALA:HB1	1.73	0.70
1:D:125:ASP:O	1:D:128:HIS:HB3	1.90	0.70
1:B:2:ASN:HB2	2:B:700:SO4:S	2.32	0.70
1:A:132:LYS:O	1:A:135:ASN:HB2	1.90	0.70
1:B:10:VAL:HG12	1:B:14:LEU:HD13	1.73	0.69
1:B:28:ILE:HD13	1:B:49:LEU:HD21	1.74	0.69
1:D:145:VAL:O	1:D:149:SER:HB2	1.92	0.69
1:B:62:GLN:NE2	1:B:126:ALA:HB2	2.07	0.69
1:A:114:GLU:HG2	1:A:118:LYS:HE3	1.75	0.68
1:B:106:TYR:O	1:B:112:ILE:HG13	1.93	0.68
1:E:26:GLY:O	1:E:29:VAL:HG22	1.93	0.68
1:E:58:GLU:HA	1:E:123:TYR:OH	1.92	0.68
1:B:96:GLN:HG2	1:B:157:ASN:HD21	1.59	0.68
1:A:179:SER:O	1:A:183:LEU:HB2	1.93	0.67
1:E:142:ILE:HD12	1:E:186:LEU:HD22	1.75	0.67
1:B:124:ILE:O	1:B:124:ILE:HG12	1.95	0.67
1:B:64:GLN:O	1:B:68:GLU:HG3	1.94	0.67
1:B:89:THR:HG22	1:B:90:GLU:N	2.09	0.66
1:B:11:ALA:HB3	1:B:53:ILE:HD11	1.77	0.66
1:A:76:ARG:HB3	1:A:76:ARG:NH1	2.11	0.66
1:B:4:LYS:HE3	1:B:42:HIS:CE1	2.31	0.66
1:E:24:THR:HG23	1:E:27:GLU:H	1.62	0.65
1:D:23:THR:HG22	1:D:23:THR:O	1.94	0.65
1:B:120:GLU:OE1	1:A:165:GLU:HG3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:THR:HG22	1:B:91:TYR:H	1.60	0.65
1:E:142:ILE:CD1	1:E:186:LEU:HD22	2.27	0.65
1:B:24:THR:H	1:B:27:GLU:HG3	1.61	0.65
1:B:106:TYR:HB3	1:B:112:ILE:HD11	1.78	0.64
1:B:18:ASN:HD22	1:B:23:THR:CG2	2.07	0.64
1:B:44:LYS:HA	1:B:44:LYS:HE3	1.80	0.64
1:D:155:ALA:HB1	1:E:155:ALA:HB1	1.80	0.64
1:B:3:LEU:HD11	1:B:38:ASN:HD22	1.62	0.64
1:E:164:HIS:HA	1:E:171:ARG:NH1	2.13	0.63
1:B:18:ASN:HB2	1:B:23:THR:HG23	1.79	0.63
1:D:184:ASN:O	1:E:185:GLY:HA2	1.97	0.63
1:A:146:ASN:O	1:A:150:LYS:HG3	1.99	0.63
1:D:73:LYS:NZ	1:D:73:LYS:HB2	2.14	0.63
1:D:6:LYS:O	1:D:10:VAL:HG23	1.99	0.63
1:B:105:GLU:HG2	1:B:105:GLU:O	1.99	0.62
1:A:25:THR:O	1:A:29:VAL:HG23	1.99	0.62
1:D:97:ASN:ND2	1:E:100:ILE:HD12	2.14	0.62
1:B:4:LYS:O	1:B:8:LEU:HD12	1.99	0.62
1:A:83:ASN:HB3	1:A:175:MET:CE	2.29	0.62
1:B:110:ASN:C	1:B:112:ILE:H	2.03	0.62
1:E:14:LEU:HD11	1:E:31:LEU:HD12	1.80	0.62
1:E:112:ILE:O	1:E:116:MET:HB2	1.99	0.62
1:B:24:THR:O	1:B:27:GLU:HB2	2.00	0.61
1:E:167:ASN:HD21	1:E:169:ASN:CB	2.13	0.61
1:D:107:TYR:HA	1:D:113:ASN:OD1	2.01	0.61
1:B:74:THR:OG1	1:B:77:GLU:HG3	2.01	0.61
1:D:100:ILE:O	1:D:104:THR:HG23	2.01	0.60
1:D:121:ASN:O	1:D:125:ASP:HB2	2.02	0.60
1:A:165:GLU:HG2	1:A:166:GLN:HE22	1.66	0.60
1:B:14:LEU:C	1:B:23:THR:HG21	2.22	0.60
1:E:143:ASN:CG	1:E:144:ASP:N	2.56	0.59
1:A:83:ASN:HB3	1:A:175:MET:HE3	1.84	0.59
1:D:167:ASN:ND2	1:D:169:ASN:H	2.00	0.59
1:D:164:HIS:HD2	1:E:104:THR:CG2	2.15	0.59
1:B:93:TYR:O	1:B:96:GLN:HB2	2.03	0.59
1:B:66:LYS:HA	1:B:69:GLN:NE2	2.16	0.58
1:B:7:ILE:HG21	1:B:43:PHE:HE1	1.68	0.58
1:B:70:ILE:N	1:B:70:ILE:HD13	2.18	0.58
1:B:156:VAL:O	1:B:160:VAL:HG23	2.04	0.58
1:E:165:GLU:O	1:E:166:GLN:O	2.21	0.58
1:E:163:THR:C	1:E:171:ARG:HH11	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:HZ2	1:D:73:LYS:HB2	1.68	0.58
1:B:6:LYS:O	1:B:10:VAL:HG23	2.05	0.57
1:A:132:LYS:HD3	2:A:801:SO4:O1	2.05	0.57
1:E:133:GLU:O	1:E:137:ASN:HB2	2.05	0.57
1:B:24:THR:HG22	1:B:27:GLU:HG3	1.87	0.56
1:D:164:HIS:HD2	1:E:104:THR:HG22	1.70	0.56
1:B:75:ASN:HB2	1:B:139:GLU:OE2	2.04	0.56
1:E:103:TYR:CD2	1:E:116:MET:HG2	2.40	0.56
1:B:15:PHE:CE1	1:B:50:PHE:HD2	2.24	0.56
1:B:3:LEU:HD11	1:B:38:ASN:ND2	2.21	0.56
1:B:14:LEU:HB3	1:B:23:THR:HG21	1.88	0.56
1:D:171:ARG:HH11	1:D:171:ARG:HG2	1.71	0.56
1:A:90:GLU:HG3	1:A:91:TYR:N	2.19	0.55
1:D:125:ASP:O	1:D:128:HIS:CB	2.55	0.55
1:D:167:ASN:C	1:D:167:ASN:HD22	2.09	0.55
1:D:66:LYS:HD2	1:D:69:GLN:HE21	1.69	0.55
1:B:103:TYR:O	1:B:107:TYR:HB3	2.06	0.55
1:B:81:LEU:HG	1:B:85:LEU:CD2	2.36	0.55
1:D:180:GLN:HG2	1:D:184:ASN:HD21	1.72	0.55
1:A:114:GLU:O	1:A:118:LYS:HG3	2.07	0.55
1:A:153:ALA:O	1:A:157:ASN:HB2	2.07	0.55
1:D:103:TYR:HE1	1:E:165:GLU:HB3	1.72	0.55
1:B:144:ASP:OD2	1:B:144:ASP:N	2.33	0.54
1:B:15:PHE:CD1	1:B:50:PHE:HD2	2.25	0.54
1:B:116:MET:HA	1:B:116:MET:CE	2.37	0.53
1:D:12:LYS:HD2	1:D:57:GLU:OE1	2.07	0.53
1:A:170:GLU:HA	1:A:170:GLU:OE2	2.07	0.53
1:B:66:LYS:HA	1:B:69:GLN:HG2	1.89	0.53
1:B:91:TYR:O	1:B:93:TYR:N	2.42	0.53
1:B:44:LYS:HA	1:B:44:LYS:CE	2.38	0.53
1:D:43:PHE:O	1:D:44:LYS:C	2.47	0.53
1:A:76:ARG:HG3	1:A:139:GLU:OE2	2.09	0.53
1:D:180:GLN:CG	1:D:184:ASN:HD21	2.22	0.53
1:E:126:ALA:O	1:E:130:ILE:HG12	2.09	0.53
1:B:28:ILE:HD13	1:B:49:LEU:CD2	2.39	0.52
1:A:144:ASP:N	1:A:144:ASP:OD1	2.43	0.52
1:D:66:LYS:HD2	1:D:69:GLN:NE2	2.24	0.52
1:A:165:GLU:HG2	1:A:166:GLN:NE2	2.24	0.52
1:E:43:PHE:O	1:E:45:THR:N	2.44	0.51
1:A:18:ASN:O	1:A:22:ALA:HB3	2.10	0.51
1:B:18:ASN:ND2	1:B:23:THR:HG22	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:PHE:CE1	1:E:50:PHE:HD2	2.27	0.51
1:D:183:LEU:C	1:D:185:GLY:H	2.14	0.51
1:A:89:THR:HB	3:A:803:BER:H161	1.93	0.51
1:B:80:TYR:O	1:B:84:GLU:HG3	2.11	0.51
1:A:134:GLY:HA3	1:A:140:TRP:CZ2	2.47	0.50
1:E:25:THR:O	1:E:29:VAL:HG13	2.10	0.50
1:E:103:TYR:HD2	1:E:116:MET:HG2	1.76	0.50
1:B:51:LEU:HD21	1:B:115:LYS:HB2	1.93	0.50
1:D:6:LYS:HE2	1:D:32:SER:HA	1.93	0.50
1:B:2:ASN:OD1	1:B:3:LEU:N	2.38	0.50
1:B:29:VAL:CG2	1:B:39:LEU:HD21	2.38	0.50
1:B:123:TYR:OH	1:B:157:ASN:HB2	2.11	0.50
1:B:11:ALA:O	1:B:12:LYS:C	2.50	0.50
1:D:135:ASN:OD1	1:D:141:SER:HA	2.11	0.50
1:D:177:LYS:HE3	1:D:181:ILE:HD11	1.94	0.50
1:B:107:TYR:CE1	1:B:108:LYS:HG3	2.47	0.50
1:D:75:ASN:HB2	1:D:139:GLU:OE2	2.11	0.50
1:E:136:LEU:O	1:E:136:LEU:HD12	2.12	0.50
1:E:106:TYR:N	1:E:106:TYR:CD2	2.79	0.50
1:B:14:LEU:O	1:B:23:THR:HG21	2.11	0.49
1:D:145:VAL:HG12	1:D:145:VAL:O	2.11	0.49
1:B:87:LEU:HD13	1:B:172:ILE:HD13	1.94	0.49
1:B:30:LYS:CD	1:B:31:LEU:HD13	2.42	0.49
1:E:144:ASP:OD2	1:E:146:ASN:HB3	2.12	0.49
1:B:115:LYS:HE2	1:B:118:LYS:NZ	2.27	0.49
1:B:45:THR:CG2	1:B:48:ASN:HB2	2.26	0.49
1:A:166:GLN:N	1:A:166:GLN:NE2	2.59	0.49
1:B:106:TYR:O	1:B:112:ILE:CG1	2.60	0.49
1:D:20:TYR:O	1:D:22:ALA:N	2.45	0.49
1:B:30:LYS:HD2	1:B:31:LEU:HD13	1.93	0.49
1:B:185:GLY:HA3	1:A:181:ILE:O	2.13	0.49
1:B:35:SER:HB3	1:B:38:ASN:OD1	2.13	0.48
1:B:134:GLY:HA3	1:B:140:TRP:CE2	2.48	0.48
1:D:163:THR:O	1:D:171:ARG:NH1	2.45	0.48
1:E:177:LYS:O	1:E:181:ILE:HG12	2.13	0.48
1:A:127:TYR:O	1:A:128:HIS:C	2.49	0.48
1:E:17:LYS:HG2	1:E:18:ASN:ND2	2.28	0.48
1:E:76:ARG:HD2	1:E:183:LEU:HD23	1.95	0.48
1:B:89:THR:CG2	1:B:91:TYR:H	2.25	0.48
1:D:177:LYS:O	1:D:181:ILE:CG1	2.61	0.48
1:B:109:THR:OG1	1:B:112:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:MET:HA	1:E:116:MET:CE	2.44	0.48
1:E:167:ASN:HD21	1:E:169:ASN:HB3	1.78	0.48
1:A:129:VAL:O	1:A:133:GLU:HG2	2.12	0.48
1:E:10:VAL:HG11	1:E:31:LEU:HB2	1.95	0.48
1:A:173:LYS:HD3	1:A:173:LYS:O	2.14	0.48
1:D:46:LYS:O	1:D:49:LEU:HB3	2.14	0.48
1:E:12:LYS:HD2	2:E:399:SO4:O4	2.14	0.48
1:D:167:ASN:O	1:D:169:ASN:N	2.47	0.47
1:E:159:ILE:HB	1:E:175:MET:HE1	1.96	0.47
1:B:89:THR:CG2	1:B:90:GLU:H	2.20	0.47
1:B:116:MET:HE2	1:B:116:MET:HA	1.96	0.47
1:B:132:LYS:O	1:B:136:LEU:HD13	2.14	0.47
1:A:135:ASN:HD21	1:A:142:ILE:H	1.63	0.47
1:A:58:GLU:OE1	3:A:803:BER:H102	2.15	0.47
1:E:160:VAL:HG12	1:E:161:THR:N	2.29	0.47
1:B:18:ASN:HB3	1:B:22:ALA:CB	2.42	0.47
1:B:61:TRP:HB2	1:B:91:TYR:HB2	1.96	0.47
1:D:142:ILE:HG13	1:D:145:VAL:HG22	1.97	0.47
1:E:58:GLU:HG3	1:E:59:SER:N	2.30	0.47
1:D:126:ALA:O	1:D:130:ILE:HG12	2.15	0.47
1:A:43:PHE:O	1:A:44:LYS:HB2	2.13	0.47
1:D:97:ASN:HD21	1:E:100:ILE:HD12	1.80	0.47
1:D:74:THR:HG23	1:D:77:GLU:OE2	2.15	0.47
1:A:156:VAL:O	1:A:160:VAL:HG23	2.14	0.47
1:A:83:ASN:HB3	1:A:175:MET:HE2	1.97	0.47
1:B:137:ASN:HD22	1:B:139:GLU:HG3	1.79	0.47
1:E:119:LEU:O	1:E:121:ASN:N	2.48	0.47
1:B:110:ASN:C	1:B:112:ILE:N	2.65	0.47
1:D:103:TYR:CE1	1:E:165:GLU:HG2	2.50	0.47
1:E:83:ASN:ND2	1:E:127:TYR:OH	2.48	0.47
1:B:18:ASN:C	1:B:22:ALA:HB3	2.35	0.46
1:D:100:ILE:HD11	1:E:162:PHE:CE2	2.50	0.46
1:A:172:ILE:O	1:A:172:ILE:HG22	2.13	0.46
1:E:47:GLU:CG	1:E:106:TYR:CE1	2.99	0.46
1:D:39:LEU:HD21	1:D:49:LEU:HD22	1.98	0.46
1:E:60:LYS:HD3	1:E:91:TYR:CZ	2.50	0.46
1:A:96:GLN:O	1:A:100:ILE:HG13	2.15	0.46
1:A:68:GLU:O	1:A:71:LYS:HG2	2.15	0.46
1:D:10:VAL:CG2	1:D:32:SER:HB3	2.40	0.46
1:B:173:LYS:HA	1:B:173:LYS:HE2	1.98	0.46
1:B:43:PHE:O	1:B:44:LYS:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LEU:HD12	1:D:38:ASN:HD21	1.80	0.46
1:E:2:ASN:HB2	1:E:5:ASP:HB2	1.98	0.46
1:D:20:TYR:C	1:D:22:ALA:H	2.20	0.46
1:B:81:LEU:O	1:B:85:LEU:HD22	2.16	0.46
1:A:123:TYR:CE2	3:A:803:BER:H172	2.50	0.46
1:A:117:ASN:C	1:A:119:LEU:N	2.69	0.46
1:B:24:THR:HG22	1:B:27:GLU:CG	2.46	0.46
1:E:65:TRP:O	1:E:69:GLN:HG2	2.15	0.46
1:B:130:ILE:O	1:B:140:TRP:HZ2	1.99	0.45
1:A:38:ASN:OD1	1:A:42:HIS:HD2	2.00	0.45
1:B:53:ILE:O	1:B:57:GLU:HG2	2.15	0.45
1:B:144:ASP:HB2	1:B:147:ALA:HB3	1.98	0.45
1:B:39:LEU:O	1:B:43:PHE:O	2.34	0.45
1:B:45:THR:OG1	1:B:47:GLU:HG2	2.16	0.45
1:E:54:LEU:HA	1:E:54:LEU:HD12	1.76	0.45
1:A:135:ASN:HA	1:A:135:ASN:HD22	1.50	0.45
1:D:34:SER:OG	1:D:35:SER:N	2.47	0.45
1:D:131:PHE:CE2	1:D:148:VAL:HG12	2.52	0.45
1:A:83:ASN:ND2	1:A:156:VAL:HG21	2.31	0.45
1:D:20:TYR:C	1:D:22:ALA:N	2.69	0.45
1:D:103:TYR:C	1:D:105:GLU:H	2.19	0.45
1:A:165:GLU:N	1:A:165:GLU:OE2	2.49	0.45
1:D:25:THR:HG23	1:D:39:LEU:HD13	1.99	0.45
1:A:76:ARG:HB3	1:A:76:ARG:HH11	1.81	0.44
1:E:50:PHE:CE1	1:E:54:LEU:HD22	2.52	0.44
1:B:3:LEU:HD13	1:B:4:LYS:N	2.32	0.44
1:E:164:HIS:HA	1:E:171:ARG:HH12	1.82	0.44
1:A:95:LEU:O	1:A:97:ASN:N	2.50	0.44
1:D:125:ASP:O	1:D:128:HIS:N	2.50	0.44
1:D:3:LEU:HD11	1:D:34:SER:HB3	1.99	0.44
1:E:57:GLU:HG3	1:E:95:LEU:HD12	1.99	0.44
1:D:164:HIS:O	1:D:164:HIS:CG	2.71	0.44
1:B:45:THR:OG1	1:B:46:LYS:N	2.51	0.44
1:E:92:TYR:CE2	1:E:123:TYR:CZ	3.06	0.44
1:B:144:ASP:O	1:B:147:ALA:N	2.45	0.44
1:B:104:THR:HG21	1:A:100:ILE:HD13	1.99	0.44
1:E:132:LYS:O	1:E:135:ASN:HB2	2.18	0.44
1:D:180:GLN:O	1:D:181:ILE:C	2.55	0.44
1:E:140:TRP:CD1	1:E:142:ILE:HG12	2.53	0.44
1:A:109:THR:C	1:A:111:SER:N	2.71	0.44
1:A:167:ASN:ND2	1:A:167:ASN:C	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HE2	1:B:118:LYS:HD3	2.00	0.44
1:B:137:ASN:HD22	1:B:139:GLU:CG	2.31	0.44
1:D:101:GLU:HG3	1:E:97:ASN:HD21	1.83	0.44
1:E:47:GLU:HG2	1:E:106:TYR:CE1	2.52	0.43
1:E:107:TYR:CD2	1:E:107:TYR:O	2.71	0.43
1:B:3:LEU:O	1:B:7:ILE:HG13	2.18	0.43
1:D:167:ASN:O	1:D:170:GLU:N	2.51	0.43
1:B:92:TYR:C	1:B:94:PRO:HD2	2.39	0.43
1:B:142:ILE:HD11	1:B:186:LEU:HD13	2.00	0.43
1:D:180:GLN:HG2	1:D:184:ASN:ND2	2.32	0.43
1:A:56:ILE:O	1:A:60:LYS:HG2	2.18	0.43
1:E:183:LEU:HD12	1:E:183:LEU:HA	1.77	0.43
1:A:105:GLU:C	1:A:107:TYR:H	2.21	0.43
1:E:162:PHE:O	1:E:163:THR:HG23	2.18	0.43
1:D:15:PHE:CD1	1:D:50:PHE:HD2	2.36	0.43
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.68	0.43
1:D:167:ASN:C	1:D:167:ASN:ND2	2.71	0.43
1:A:117:ASN:O	1:A:119:LEU:N	2.52	0.43
1:D:36:LYS:HG2	1:D:40:TYR:HE2	1.84	0.43
1:B:126:ALA:O	1:B:130:ILE:HG13	2.19	0.43
1:A:95:LEU:HA	1:A:95:LEU:HD23	1.84	0.43
1:A:8:LEU:HD13	1:A:56:ILE:CD1	2.49	0.43
1:A:30:LYS:C	1:A:30:LYS:HD3	2.36	0.43
1:E:43:PHE:O	1:E:44:LYS:C	2.56	0.43
1:D:29:VAL:CG2	1:D:39:LEU:HD12	2.49	0.43
1:B:55:ASN:CG	1:B:119:LEU:HD21	2.39	0.43
1:D:133:GLU:O	1:D:137:ASN:HB2	2.18	0.42
1:E:27:GLU:O	1:E:28:ILE:C	2.57	0.42
1:E:65:TRP:HZ3	1:E:81:LEU:HD23	1.84	0.42
1:B:7:ILE:HG21	1:B:43:PHE:CE1	2.52	0.42
1:A:163:THR:HB	1:A:171:ARG:HD2	2.01	0.42
1:B:166:GLN:HG2	1:B:166:GLN:H	1.72	0.42
1:E:106:TYR:HD2	1:E:106:TYR:H	1.67	0.42
1:E:65:TRP:CZ3	1:E:81:LEU:HD23	2.54	0.42
1:B:55:ASN:HD22	1:B:122:LYS:HE3	1.84	0.42
1:B:95:LEU:O	1:B:99:ILE:HG12	2.19	0.42
1:B:168:ILE:O	1:B:172:ILE:HG12	2.19	0.42
1:E:168:ILE:HG13	1:E:168:ILE:H	1.68	0.42
1:E:68:GLU:HG2	1:E:85:LEU:HD21	2.00	0.42
1:B:18:ASN:HB2	1:B:23:THR:CG2	2.45	0.42
1:D:73:LYS:HE3	1:D:77:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:O	1:B:69:GLN:HG2	2.19	0.42
1:E:43:PHE:N	1:E:43:PHE:CD1	2.86	0.42
1:B:165:GLU:OE2	1:B:166:GLN:NE2	2.53	0.42
1:D:135:ASN:HD21	1:D:142:ILE:HG12	1.85	0.42
1:A:156:VAL:HG22	1:A:175:MET:CE	2.50	0.41
1:D:163:THR:O	1:D:171:ARG:HD2	2.20	0.41
1:E:167:ASN:HD21	1:E:169:ASN:HB2	1.84	0.41
1:D:92:TYR:O	1:D:94:PRO:N	2.53	0.41
1:B:31:LEU:HD12	1:B:31:LEU:HA	1.80	0.41
1:E:121:ASN:HA	1:E:121:ASN:HD22	1.68	0.41
1:A:74:THR:O	1:A:77:GLU:HB2	2.20	0.41
1:A:68:GLU:O	1:A:68:GLU:HG3	2.19	0.41
1:D:11:ALA:O	1:D:12:LYS:C	2.59	0.41
1:A:94:PRO:O	1:A:95:LEU:C	2.58	0.41
1:E:6:LYS:O	1:E:10:VAL:HG23	2.21	0.41
1:A:8:LEU:HA	1:A:8:LEU:HD23	1.69	0.41
1:D:57:GLU:HB3	1:D:92:TYR:H	1.85	0.41
1:D:78:LYS:HB3	1:D:130:ILE:HD12	2.02	0.41
1:E:132:LYS:HD2	2:E:903:SO4:O3	2.21	0.41
1:B:186:LEU:HA	1:B:186:LEU:HD23	1.86	0.41
1:B:16:ILE:HG13	1:B:95:LEU:HD23	2.01	0.41
1:E:51:LEU:HD22	1:E:102:PHE:CZ	2.55	0.41
1:E:74:THR:H	1:E:77:GLU:HG3	1.86	0.41
1:E:99:ILE:HD13	1:E:99:ILE:HG21	1.87	0.41
1:E:155:ALA:O	1:E:159:ILE:HG12	2.21	0.41
1:B:127:TYR:O	1:B:131:PHE:CD2	2.74	0.41
1:D:52:GLU:O	1:D:55:ASN:N	2.50	0.41
1:E:35:SER:OG	1:E:38:ASN:HB2	2.21	0.41
1:D:124:ILE:HD12	1:D:153:ALA:CB	2.51	0.41
1:B:7:ILE:O	1:B:10:VAL:N	2.52	0.41
1:D:171:ARG:HG2	1:D:171:ARG:NH1	2.34	0.41
1:E:56:ILE:O	1:E:57:GLU:C	2.59	0.41
1:D:122:LYS:O	1:D:125:ASP:HB3	2.21	0.41
1:A:135:ASN:ND2	1:A:141:SER:HA	2.36	0.41
1:A:142:ILE:HD11	1:A:186:LEU:HD13	2.03	0.41
1:E:100:ILE:O	1:E:101:GLU:C	2.59	0.41
1:A:156:VAL:HG22	1:A:175:MET:HE1	2.03	0.41
1:E:61:TRP:HH2	1:E:85:LEU:HB3	1.86	0.41
1:A:92:TYR:CD1	1:A:92:TYR:O	2.74	0.41
1:A:14:LEU:HG	1:A:23:THR:HG23	2.02	0.41
1:B:4:LYS:HA	1:B:7:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:LEU:C	1:E:121:ASN:N	2.73	0.40
1:E:74:THR:OG1	1:E:77:GLU:CG	2.70	0.40
1:E:38:ASN:O	1:E:42:HIS:CD2	2.74	0.40
1:E:174:LEU:HD23	1:E:174:LEU:HA	1.75	0.40
1:D:60:LYS:HE3	4:D:1002:HOH:O	2.20	0.40
1:E:111:SER:C	1:E:113:ASN:N	2.75	0.40
1:E:74:THR:O	1:E:78:LYS:HG3	2.21	0.40
1:A:177:LYS:O	1:A:180:GLN:HB3	2.21	0.40
1:E:109:THR:O	1:E:110:ASN:HB2	2.22	0.40
1:B:37:GLY:O	1:B:40:TYR:N	2.54	0.40
1:B:44:LYS:N	1:B:48:ASN:HD22	2.20	0.40
1:E:110:ASN:HB3	1:E:111:SER:H	1.52	0.40
1:D:178:PHE:HB2	1:E:151:ILE:CG2	2.51	0.40
1:B:61:TRP:HB2	1:B:91:TYR:CB	2.51	0.40
1:D:121:ASN:HD22	1:D:121:ASN:N	2.19	0.40
1:E:47:GLU:HG2	1:E:106:TYR:CD1	2.57	0.40
1:D:186:LEU:HD23	1:E:181:ILE:HG23	2.03	0.40
1:E:119:LEU:O	1:E:120:GLU:C	2.60	0.40
1:B:163:THR:O	1:B:166:GLN:HG2	2.22	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	184/194 (95%)	155 (84%)	24 (13%)	5 (3%)	6	30
1	B	184/194 (95%)	148 (80%)	30 (16%)	6 (3%)	5	24
1	D	184/194 (95%)	154 (84%)	24 (13%)	6 (3%)	5	24
1	E	184/194 (95%)	153 (83%)	27 (15%)	4 (2%)	8	36
All	All	736/776 (95%)	610 (83%)	105 (14%)	21 (3%)	6	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	LYS
1	B	165	GLU
1	A	89	THR
1	A	144	ASP
1	E	44	LYS
1	E	166	GLN
1	B	28	ILE
1	B	92	TYR
1	B	145	VAL
1	A	96	GLN
1	A	164	HIS
1	B	27	GLU
1	D	44	LYS
1	D	93	TYR
1	D	104	THR
1	D	92	TYR
1	D	111	SER
1	E	143	ASN
1	E	120	GLU
1	D	168	ILE
1	A	145	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	169/177 (96%)	150 (89%)	19 (11%)	7	27
1	B	169/177 (96%)	148 (88%)	21 (12%)	6	23
1	D	169/177 (96%)	155 (92%)	14 (8%)	14	44
1	E	169/177 (96%)	155 (92%)	14 (8%)	14	44
All	All	676/708 (96%)	608 (90%)	68 (10%)	9	33

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	LYS
1	B	6	LYS
1	B	13	GLU
1	B	31	LEU
1	B	42	HIS
1	B	44	LYS
1	B	45	THR
1	B	85	LEU
1	B	88	THR
1	B	89	THR
1	B	95	LEU
1	B	110	ASN
1	B	116	MET
1	B	124	ILE
1	B	129	VAL
1	B	143	ASN
1	B	144	ASP
1	B	157	ASN
1	B	169	ASN
1	B	173	LYS
1	B	184	ASN
1	D	2	ASN
1	D	3	LEU
1	D	23	THR
1	D	24	THR
1	D	31	LEU
1	D	45	THR
1	D	47	GLU
1	D	97	ASN
1	D	107	TYR
1	D	108	LYS
1	D	129	VAL
1	D	149	SER
1	D	165	GLU
1	D	167	ASN
1	A	3	LEU
1	A	14	LEU
1	A	21	ASN
1	A	25	THR
1	A	49	LEU
1	A	63	GLU
1	A	90	GLU
1	A	91	TYR

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Mol	Chain	Res	Type
1	A	108	LYS
1	A	111	SER
1	A	116	MET
1	A	130	ILE
1	A	135	ASN
1	A	141	SER
1	A	146	ASN
1	A	163	THR
1	A	166	GLN
1	A	167	ASN
1	A	184	ASN
1	E	32	SER
1	E	38	ASN
1	E	39	LEU
1	E	51	LEU
1	E	63	GLU
1	E	67	LYS
1	E	76	ARG
1	E	77	GLU
1	E	106	TYR
1	E	111	SER
1	E	141	SER
1	E	165	GLU
1	E	166	GLN
1	E	183	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	42	HIS
1	B	48	ASN
1	B	55	ASN
1	B	62	GLN
1	B	69	GLN
1	B	83	ASN
1	B	96	GLN
1	B	110	ASN
1	B	137	ASN
1	B	146	ASN
1	B	154	ASN
1	B	157	ASN

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Mol	Chain	Res	Type
1	B	166	GLN
1	D	2	ASN
1	D	38	ASN
1	D	48	ASN
1	D	55	ASN
1	D	69	GLN
1	D	83	ASN
1	D	121	ASN
1	D	154	ASN
1	D	164	HIS
1	D	167	ASN
1	D	176	ASN
1	D	180	GLN
1	D	184	ASN
1	A	42	HIS
1	A	48	ASN
1	A	55	ASN
1	A	83	ASN
1	A	96	GLN
1	A	121	ASN
1	A	135	ASN
1	A	166	GLN
1	A	167	ASN
1	A	180	GLN
1	A	184	ASN
1	E	18	ASN
1	E	48	ASN
1	E	64	GLN
1	E	83	ASN
1	E	97	ASN
1	E	110	ASN
1	E	117	ASN
1	E	121	ASN
1	E	166	GLN
1	E	167	ASN
1	E	184	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

23 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	299	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	A	699	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	799	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	A	800	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	A	801	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	A	802	-	4,4,4	0.07	0	6,6,6	0.17	0
3	BER	A	803	-	29,29,29	4.01	21 (72%)	38,43,43	1.84	10 (26%)
2	SO4	B	1000	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	B	195	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	B	199	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	B	499	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	700	-	4,4,4	0.30	0	6,6,6	0.13	0
2	SO4	D	1000	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	D	899	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	D	900	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO4	D	999	-	4,4,4	0.60	0	6,6,6	0.24	0
2	SO4	E	399	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	E	579	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	E	639	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	E	900	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	E	901	-	4,4,4	0.35	0	6,6,6	0.15	0
2	SO4	E	902	-	4,4,4	0.20	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	903	-	4,4,4	0.27	0	6,6,6	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	299	-	-	0/0/0/0	0/0/0/0
2	SO4	A	699	-	-	0/0/0/0	0/0/0/0
2	SO4	A	799	-	-	0/0/0/0	0/0/0/0
2	SO4	A	800	-	-	0/0/0/0	0/0/0/0
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	BER	A	803	-	-	0/4/19/19	0/5/5/5
2	SO4	B	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	B	195	-	-	0/0/0/0	0/0/0/0
2	SO4	B	199	-	-	0/0/0/0	0/0/0/0
2	SO4	B	499	-	-	0/0/0/0	0/0/0/0
2	SO4	B	700	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1000	-	-	0/0/0/0	0/0/0/0
2	SO4	D	899	-	-	0/0/0/0	0/0/0/0
2	SO4	D	900	-	-	0/0/0/0	0/0/0/0
2	SO4	D	999	-	-	0/0/0/0	0/0/0/0
2	SO4	E	399	-	-	0/0/0/0	0/0/0/0
2	SO4	E	579	-	-	0/0/0/0	0/0/0/0
2	SO4	E	639	-	-	0/0/0/0	0/0/0/0
2	SO4	E	900	-	-	0/0/0/0	0/0/0/0
2	SO4	E	901	-	-	0/0/0/0	0/0/0/0
2	SO4	E	902	-	-	0/0/0/0	0/0/0/0
2	SO4	E	903	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	BER	C2-C1	2.08	1.51	1.47
3	A	803	BER	C12-C8	2.33	1.47	1.42
3	A	803	BER	O1-C17	2.33	1.47	1.43
3	A	803	BER	C15-C12	2.45	1.48	1.43
3	A	803	BER	C5-C11	2.59	1.43	1.38
3	A	803	BER	C10-C4	2.68	1.55	1.51
3	A	803	BER	C16-C18	2.95	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	BER	C14-C11	3.01	1.47	1.39
3	A	803	BER	C9-C4	3.28	1.45	1.39
3	A	803	BER	C13-C16	3.51	1.44	1.36
3	A	803	BER	O3-C15	3.63	1.43	1.38
3	A	803	BER	C5-C2	3.67	1.45	1.39
3	A	803	BER	C3-C1	4.24	1.45	1.36
3	A	803	BER	C9-C14	4.45	1.47	1.38
3	A	803	BER	C7-N1	4.48	1.55	1.48
3	A	803	BER	C7-C10	4.64	1.58	1.51
3	A	803	BER	C18-C15	4.78	1.48	1.38
3	A	803	BER	O4-C18	4.81	1.44	1.37
3	A	803	BER	C1-N1	4.88	1.46	1.37
3	A	803	BER	C2-C4	7.55	1.51	1.40
3	A	803	BER	C6-N1	12.01	1.45	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	BER	O4-C18-C16	-2.38	120.34	124.35
3	A	803	BER	C16-C18-C15	-2.23	118.07	119.86
3	A	803	BER	O1-C11-C5	2.10	130.90	127.88
3	A	803	BER	O2-C14-C9	2.52	131.49	127.88
3	A	803	BER	O4-C18-C15	2.60	121.59	116.46
3	A	803	BER	C7-C10-C4	2.79	112.98	109.66
3	A	803	BER	C10-C4-C2	2.85	121.47	118.78
3	A	803	BER	C20-O4-C18	3.58	122.97	117.54
3	A	803	BER	C19-O3-C15	3.73	124.34	115.06
3	A	803	BER	C10-C7-N1	5.34	116.60	109.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SO4	1	0
3	A	803	BER	3	0
2	B	700	SO4	1	0
2	E	399	SO4	1	0
2	E	903	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, 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	186/194 (95%)	-0.26	0 <span>100</span> <span>100</span>	25, 46, 82, 103	0
1	B	186/194 (95%)	0.18	9 (4%) <span>34</span> <span>19</span>	29, 60, 115, 130	0
1	D	186/194 (95%)	-0.16	0 <span>100</span> <span>100</span>	34, 57, 91, 105	0
1	E	186/194 (95%)	-0.16	1 (0%) <span>91</span> <span>80</span>	28, 48, 85, 97	0
All	All	744/776 (95%)	-0.10	10 (1%) <span>79</span> <span>59</span>	25, 52, 98, 130	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	41	TYR	6.2
1	B	42	HIS	5.3
1	B	40	TYR	4.9
1	E	123	TYR	4.5
1	B	43	PHE	3.0
1	B	34	SER	2.9
1	B	28	ILE	2.9
1	B	36	LYS	2.7
1	B	107	TYR	2.5
1	B	29	VAL	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	199	5/5	0.89	0.57	18.24	146,147,147,147	0
2	SO4	A	799	5/5	0.90	0.51	17.94	134,134,134,134	0
2	SO4	D	1000	5/5	0.20	1.17	15.75	173,173,173,174	0
2	SO4	E	639	5/5	0.64	0.68	15.33	188,188,189,189	0
2	SO4	E	399	5/5	0.86	0.77	15.14	194,194,195,195	0
3	BER	A	803	25/25	0.77	0.62	9.14	47,53,61,62	0
2	SO4	D	999	5/5	0.76	0.31	3.27	123,123,124,126	0
2	SO4	A	802	5/5	0.95	0.30	3.03	152,153,154,154	0
2	SO4	E	901	5/5	0.79	0.31	2.44	145,145,145,146	0
2	SO4	A	800	5/5	0.83	0.20	1.60	134,135,135,135	0
2	SO4	A	699	5/5	0.84	0.18	1.23	143,143,143,143	0
2	SO4	D	899	5/5	0.79	0.23	0.84	147,148,148,149	0
2	SO4	E	900	5/5	0.90	0.21	0.71	138,138,138,138	0
2	SO4	D	900	5/5	0.88	0.16	-0.83	135,135,136,136	0
2	SO4	B	700	5/5	0.45	0.60	-	199,200,200,200	0
2	SO4	B	195	5/5	0.86	0.30	-	177,177,177,178	0
2	SO4	B	499	5/5	0.84	0.47	-	157,157,157,157	0
2	SO4	A	299	5/5	0.79	0.23	-	148,148,148,149	0
2	SO4	B	1000	5/5	0.81	0.22	-	176,176,176,176	0
2	SO4	E	902	5/5	0.71	0.24	-	181,182,182,182	0
2	SO4	E	579	5/5	0.48	0.32	-	176,176,176,177	0
2	SO4	A	801	5/5	0.86	0.39	-	161,161,161,161	0
2	SO4	E	903	5/5	0.60	0.47	-	174,174,174,175	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.