



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:32 am GMT

PDB ID : 4CMP  
Title : Crystal structure of *S. pyogenes* Cas9  
Authors : Jinek, M.; Jiang, F.; Taylor, D.W.; Sternberg, S.H.; Kaya, E.; Ma, E.; Anders, C.; Hauer, M.; Zhou, K.; Lin, S.; Kaplan, M.; Iavarone, A.T.; Charpentier, E.; Nogales, E.; Doudna, J.A.  
Deposited on : 2014-01-16  
Resolution : 2.62 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

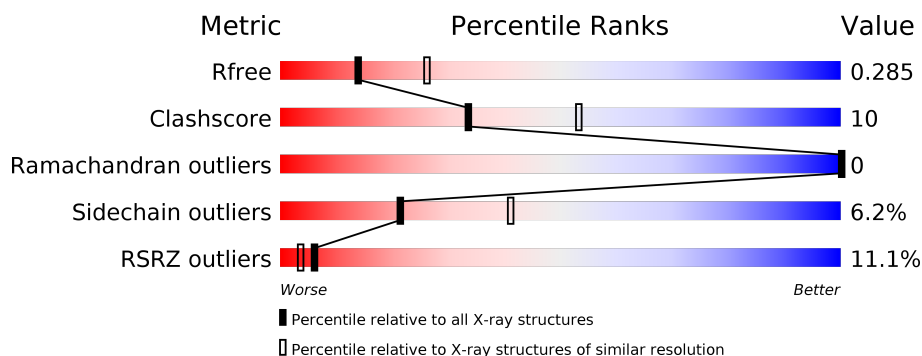
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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	1372	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>16%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	1372	<div> <div>9%</div> <div> <div></div> <div>66%</div> <div>17%</div> <div>•</div> <div>15%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2365	-	-	-	X
2	SO4	B	2365	-	-	X	-
2	SO4	B	2366	-	-	X	-
3	MG	B	2367	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 38285 atoms, of which 19194 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 CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1144	Total	C	H	N	O	S	0	0	0
			18772	5949	9456	1610	1738	19			
1	B	1166	Total	C	H	N	O	S	0	0	0
			19284	6101	9738	1648	1778	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q99ZW2
A	-2	ALA	-	EXPRESSION TAG	UNP Q99ZW2
A	-1	ALA	-	EXPRESSION TAG	UNP Q99ZW2
A	0	SER	-	EXPRESSION TAG	UNP Q99ZW2
B	-3	GLY	-	EXPRESSION TAG	UNP Q99ZW2
B	-2	ALA	-	EXPRESSION TAG	UNP Q99ZW2
B	-1	ALA	-	EXPRESSION TAG	UNP Q99ZW2
B	0	SER	-	EXPRESSION TAG	UNP Q99ZW2

- 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	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		

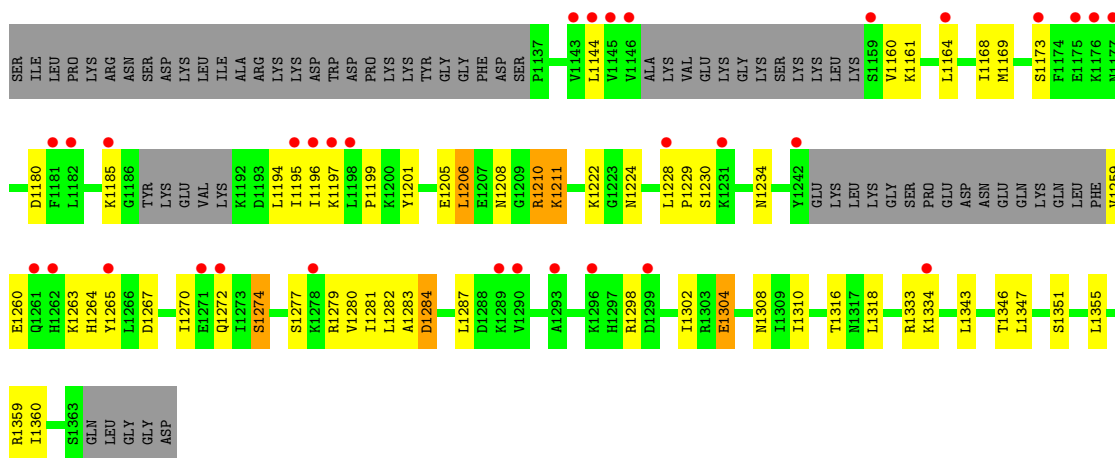
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

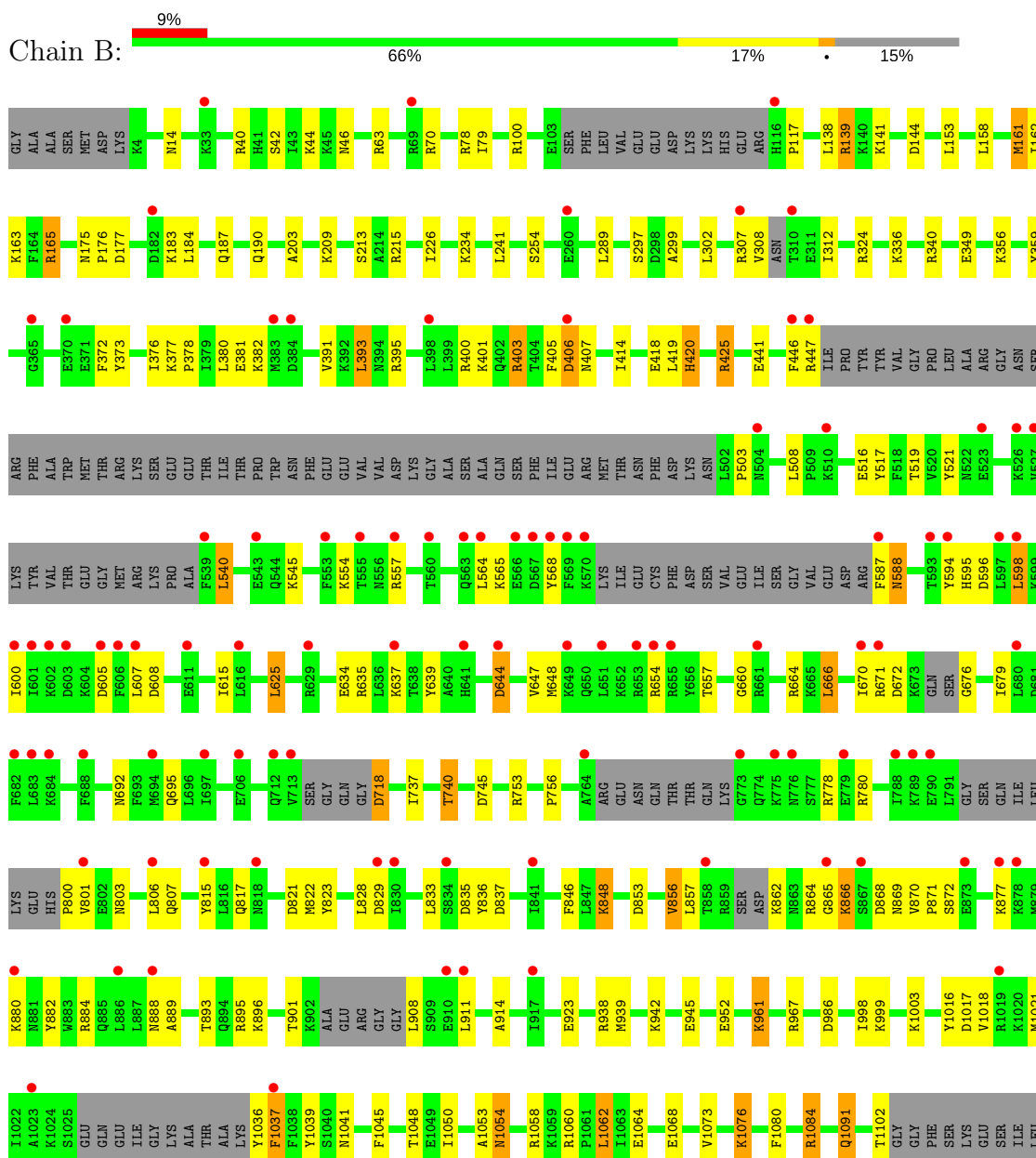
- Molecule 4 is water.

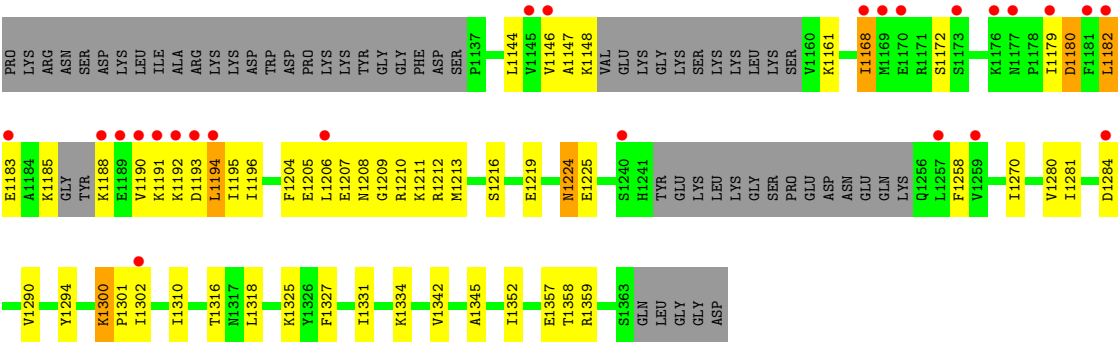
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	111	Total	O	0	0
			111	111		





- Molecule 1: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.78Å 209.62Å 91.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.48 – 2.62 47.48 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.48-2.62) 99.6 (47.48-2.62)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.252 , 0.286 0.252 , 0.285	Depositor DCC
$R_{free}$ test set	2420 reflections (2.62%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	38285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.7554e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.28	0/9463	0.51	1/12717 (0.0%)
1	B	0.30	0/9698	0.50	1/13022 (0.0%)
All	All	0.29	0/19161	0.50	2/25739 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1084	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	1193	ASP	CB-CG-OD2	5.17	122.95	118.30

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	9316	9456	9426	169	0
1	B	9546	9738	9714	199	0
2	A	10	0	0	0	0
2	B	15	0	0	5	0
3	B	1	0	0	0	0
4	A	92	0	0	7	0
4	B	111	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19091	19194	19140	368	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 10.

All (368) 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:1179:ILE:O	1:B:1183:GLU:HG3	1.18	1.31
1:B:1191:LYS:HE2	1:B:1194:LEU:CD2	1.79	1.12
1:B:1179:ILE:HD11	1:B:1192:LYS:CD	1.80	1.12
1:B:1179:ILE:CD1	1:B:1192:LYS:HD2	1.80	1.11
1:B:1179:ILE:O	1:B:1183:GLU:CG	2.07	1.02
1:B:1191:LYS:CE	1:B:1194:LEU:HD21	1.90	1.01
1:A:46:ASN:ND2	1:A:1089:MET:SD	2.40	0.94
1:B:1179:ILE:HD11	1:B:1192:LYS:HD2	0.97	0.94
1:B:1045:PHE:HA	1:B:1060:ARG:NH2	1.82	0.93
1:B:78:ARG:NH1	1:B:162:ILE:O	2.03	0.91
1:A:1208:ASN:O	1:A:1279:ARG:NH1	2.06	0.89
1:B:1191:LYS:CD	1:B:1194:LEU:HD21	2.03	0.89
1:B:1206:LEU:O	1:B:1207:GLU:HG2	1.72	0.88
1:B:1205:GLU:OE1	1:B:1359:ARG:NH2	2.05	0.88
1:B:400:ARG:NH2	4:B:2052:HOH:O	2.05	0.88
1:B:1179:ILE:HG22	1:B:1183:GLU:OE2	1.72	0.88
1:B:1207:GLU:HG3	1:B:1208:ASN:H	1.37	0.87
1:B:1191:LYS:HE2	1:B:1194:LEU:HD21	1.49	0.86
1:B:297:SER:OG	1:B:407:ASN:OD1	1.94	0.85
1:B:1080:PHE:O	4:B:2087:HOH:O	1.95	0.83
1:A:165:ARG:NH2	1:A:446:PHE:O	2.12	0.82
1:B:557:ARG:NH2	1:B:596:ASP:OD1	2.11	0.82
1:B:1147:ALA:O	1:B:1188:LYS:N	2.14	0.80
1:A:1169:MET:O	4:A:2082:HOH:O	2.00	0.80
1:B:1206:LEU:HD21	1:B:1345:ALA:HA	1.64	0.79
1:A:100:ARG:NH1	1:A:625:LEU:O	2.16	0.79
1:A:919:ARG:O	1:A:959:LYS:NZ	2.15	0.78
1:B:1334:LYS:NZ	4:B:2103:HOH:O	2.17	0.77
1:A:848:LYS:O	1:A:961:LYS:NZ	2.12	0.76
1:B:1045:PHE:HA	1:B:1060:ARG:CZ	2.16	0.75
1:B:1191:LYS:HD3	1:B:1194:LEU:HD21	1.66	0.75
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.19	0.75
1:A:427:GLU:OE1	1:A:437:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:GLU:O	1:A:1308:ASN:ND2	2.21	0.73
1:B:672:ASP:O	1:B:676:GLY:N	2.21	0.73
1:B:821:ASP:OD2	1:B:864:ARG:NH2	2.21	0.73
1:B:1196:ILE:N	1:B:1196:ILE:HD12	2.03	0.72
1:B:254:SER:OG	4:B:2040:HOH:O	2.07	0.72
1:B:1045:PHE:HA	1:B:1060:ARG:HH21	1.55	0.71
1:A:870:VAL:HG12	1:A:871:PRO:HD2	1.71	0.71
1:B:1211:LYS:NZ	2:B:2366:SO4:S	2.64	0.69
1:A:799:HIS:O	1:A:815:TYR:OH	2.10	0.69
1:B:1144:LEU:HD22	1:B:1196:ILE:HD13	1.74	0.69
1:B:866:LYS:NZ	1:B:870:VAL:O	2.25	0.69
1:A:828:LEU:HA	1:A:833:LEU:HD13	1.74	0.69
1:B:1191:LYS:HE2	1:B:1194:LEU:HD23	1.76	0.68
1:A:557:ARG:NH1	4:A:2051:HOH:O	2.26	0.68
1:B:1211:LYS:NZ	2:B:2366:SO4:O4	2.27	0.67
1:A:398:LEU:O	4:A:2040:HOH:O	2.13	0.67
1:B:1357:GLU:OE2	1:B:1359:ARG:NH1	2.27	0.67
1:A:251:ASN:ND2	1:A:261:ASP:OD1	2.28	0.67
1:B:1206:LEU:HD21	1:B:1345:ALA:CA	2.25	0.66
1:A:1230:SER:O	1:A:1234:ASN:ND2	2.27	0.66
1:A:1259:VAL:N	4:A:2089:HOH:O	2.29	0.66
1:B:324:ARG:NH1	1:B:401:LYS:O	2.29	0.66
1:B:406:ASP:N	4:B:2052:HOH:O	2.27	0.66
1:A:21:ILE:HD12	1:A:991:ALA:HB3	1.79	0.65
1:B:554:LYS:NZ	1:B:608:ASP:OD1	2.21	0.65
1:B:1206:LEU:CD2	1:B:1345:ALA:HA	2.27	0.65
1:B:596:ASP:O	1:B:654:ARG:NH2	2.30	0.64
1:A:977:GLU:HG3	1:A:1310:ILE:CG2	2.27	0.64
1:B:1045:PHE:CA	1:B:1060:ARG:NH2	2.60	0.64
1:B:1003:LYS:NZ	1:B:1068:GLU:OE1	2.26	0.64
1:A:1282:LEU:O	1:A:1334:LYS:NZ	2.30	0.64
1:B:1195:ILE:C	1:B:1196:ILE:HD12	2.19	0.64
1:B:967:ARG:NH1	1:B:986:ASP:OD1	2.31	0.63
1:B:1207:GLU:HG3	1:B:1208:ASN:N	2.10	0.62
1:B:540:LEU:HD22	1:B:545:LYS:HG3	1.81	0.62
1:A:1284:ASP:N	1:A:1284:ASP:OD1	2.33	0.62
1:A:60:GLU:OE2	1:A:742:LYS:NZ	2.33	0.62
1:B:144:ASP:O	1:B:425:ARG:NH2	2.32	0.62
1:B:540:LEU:HD22	1:B:545:LYS:CG	2.30	0.62
1:B:165:ARG:NH2	1:B:446:PHE:O	2.31	0.61
1:B:1084:ARG:N	4:B:2087:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ARG:NH1	1:B:625:LEU:O	2.34	0.61
1:A:1206:LEU:HD12	1:A:1210:ARG:HG2	1.83	0.61
1:A:874:GLU:HA	1:A:877:LYS:HG3	1.81	0.61
1:A:1206:LEU:CD1	1:A:1210:ARG:HG2	2.31	0.60
1:A:158:LEU:HD22	1:A:419:LEU:HD12	1.83	0.60
1:A:598:LEU:CD2	1:A:607:LEU:CD1	2.79	0.60
1:A:208:ALA:N	4:A:2027:HOH:O	2.33	0.60
1:A:1270:ILE:O	1:A:1274:SER:OG	2.19	0.59
1:B:420:HIS:NE2	1:B:441:GLU:OE1	2.36	0.59
1:A:1211:LYS:H	1:A:1224:ASN:HD21	1.50	0.59
1:B:1179:ILE:HG22	1:B:1183:GLU:CG	2.33	0.58
1:A:870:VAL:HG12	1:A:871:PRO:CD	2.33	0.58
1:B:888:ASN:OD1	1:B:889:ALA:N	2.35	0.58
1:B:600:ILE:HG22	1:B:647:VAL:HG13	1.84	0.58
1:A:874:GLU:HA	1:A:877:LYS:HE2	1.84	0.58
1:B:1179:ILE:CG1	1:B:1192:LYS:HD2	2.33	0.58
1:B:780:ARG:NH1	1:B:806:LEU:O	2.35	0.58
1:B:158:LEU:HA	1:B:161:MET:HE2	1.85	0.58
1:A:150:ASP:OD2	1:A:152:ARG:NH2	2.36	0.58
1:B:837:ASP:OD2	1:B:862:LYS:N	2.37	0.58
1:B:177:ASP:OD1	1:B:183:LYS:NZ	2.37	0.57
1:A:1194:LEU:HD13	1:A:1196:ILE:HD11	1.85	0.57
1:B:187:GLN:NE2	1:B:190:GLN:OE1	2.37	0.57
1:A:887:LEU:HD11	1:A:897:PHE:CG	2.40	0.57
1:B:1179:ILE:HG22	1:B:1183:GLU:CD	2.24	0.57
1:B:308:VAL:HG22	1:B:312:ILE:HG21	1.85	0.57
1:B:817:GLN:O	1:B:882:TYR:OH	2.24	0.56
1:B:588:ASN:OD1	1:B:588:ASN:N	2.37	0.56
1:A:780:ARG:NH1	1:A:806:LEU:O	2.36	0.56
1:B:139:ARG:NH1	1:B:418:GLU:OE1	2.38	0.56
1:B:165:ARG:NH1	2:B:2364:SO4:O4	2.38	0.56
1:A:1144:LEU:HD23	1:A:1196:ILE:HD12	1.88	0.56
1:B:1039:TYR:CD2	1:B:1058:ARG:NH1	2.73	0.56
1:B:1179:ILE:HA	1:B:1182:LEU:HD12	1.87	0.56
1:B:828:LEU:HD22	1:B:833:LEU:HD11	1.87	0.56
1:A:247:GLY:HA2	1:A:407:ASN:HB2	1.87	0.56
1:B:1207:GLU:O	1:B:1209:GLY:N	2.35	0.56
1:A:607:LEU:HD23	1:A:616:LEU:CD2	2.36	0.56
1:A:139:ARG:NH1	1:A:418:GLU:OE1	2.39	0.55
1:A:607:LEU:HD23	1:A:616:LEU:HD21	1.88	0.55
1:A:887:LEU:HD23	1:A:892:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:LYS:NZ	1:B:901:THR:O	2.34	0.55
1:B:800:PRO:N	1:B:815:TYR:HH	2.05	0.55
1:A:825:ASP:N	1:A:879:MET:HE3	2.21	0.55
1:B:1325:LYS:NZ	1:B:1327:PHE:O	2.24	0.55
1:B:1191:LYS:CE	1:B:1194:LEU:CD2	2.54	0.55
1:B:161:MET:HE1	1:B:419:LEU:HA	1.88	0.55
1:A:66:ARG:NH1	4:A:2008:HOH:O	2.39	0.54
1:A:847:LEU:HD22	1:A:916:PHE:CG	2.42	0.54
1:A:799:HIS:CB	1:A:800:PRO:HD2	2.37	0.54
1:B:1146:VAL:HG22	1:B:1161:LYS:HG3	1.90	0.54
1:B:70:ARG:NH1	1:B:718:ASP:OD2	2.40	0.54
1:B:870:VAL:HG23	1:B:871:PRO:HD2	1.89	0.54
1:A:218:LYS:NZ	1:A:406:ASP:OD1	2.25	0.54
1:A:781:MET:SD	1:A:803:ASN:HB2	2.48	0.54
1:B:1179:ILE:CG2	1:B:1183:GLU:OE2	2.49	0.54
1:A:244:LEU:O	1:A:407:ASN:ND2	2.40	0.54
1:A:1205:GLU:OE1	1:A:1359:ARG:NH2	2.37	0.53
1:B:1039:TYR:HD2	1:B:1058:ARG:NH1	2.06	0.53
1:A:46:ASN:N	1:A:46:ASN:OD1	2.41	0.53
1:A:1263:LYS:HE2	1:A:1302:ILE:CD1	2.38	0.53
1:B:226:ILE:CD1	1:B:234:LYS:HG3	2.38	0.53
1:A:401:LYS:HB3	1:A:403:ARG:HE	1.74	0.53
1:B:869:ASN:OD1	1:B:870:VAL:N	2.41	0.53
1:B:403:ARG:NH2	2:B:2365:SO4:S	2.80	0.53
1:A:349:GLU:HG3	1:A:356:LYS:HD3	1.91	0.53
1:B:565:LYS:HA	1:B:568:TYR:HD1	1.73	0.53
1:A:677:LYS:HD2	1:A:681:ASP:HB3	1.91	0.52
1:B:307:ARG:O	1:B:308:VAL:HB	2.09	0.52
1:A:967:ARG:NH1	1:A:986:ASP:OD1	2.43	0.52
1:A:976:ARG:HH11	1:A:976:ARG:HG3	1.73	0.52
1:B:401:LYS:HB3	1:B:403:ARG:HE	1.75	0.52
1:B:79:ILE:HD11	1:B:163:LYS:HG3	1.91	0.52
1:B:215:ARG:HH21	1:B:395:ARG:CZ	2.23	0.52
1:B:877:LYS:HE2	1:B:880:LYS:NZ	2.25	0.52
1:A:45:LYS:HE3	1:A:1355:LEU:HA	1.92	0.52
1:B:828:LEU:CD2	1:B:833:LEU:HD11	2.40	0.52
1:A:427:GLU:HB2	1:A:434:LYS:CG	2.39	0.51
1:A:877:LYS:NZ	1:A:902:LYS:O	2.43	0.51
1:B:1062:LEU:HD23	1:B:1076:LYS:HB2	1.91	0.51
1:A:1194:LEU:HB3	1:A:1196:ILE:CG1	2.41	0.51
1:A:844:GLN:HG3	1:A:848:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:ARG:HB2	1:A:1280:VAL:HG13	1.93	0.51
1:A:349:GLU:HG3	1:A:356:LYS:CD	2.41	0.51
1:A:554:LYS:O	1:A:595:HIS:NE2	2.43	0.51
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.43	0.51
1:B:1102:THR:HA	1:B:1168:ILE:HD13	1.92	0.51
1:B:508:LEU:HD21	1:B:664:ARG:CG	2.41	0.51
1:A:522:ASN:HA	1:A:525:THR:HG23	1.92	0.51
1:B:1045:PHE:CB	1:B:1060:ARG:NH2	2.75	0.50
1:B:403:ARG:NH2	2:B:2365:SO4:O2	2.41	0.50
1:B:666:LEU:HD23	1:B:679:ILE:HD12	1.92	0.50
1:B:868:ASP:HA	1:B:1054:ASN:ND2	2.27	0.50
1:A:1224:ASN:ND2	1:A:1280:VAL:HG11	2.27	0.50
1:B:14:ASN:ND2	4:B:2006:HOH:O	2.42	0.50
1:B:503:PRO:HD2	1:B:666:LEU:HD12	1.94	0.50
1:A:821:ASP:N	1:A:828:LEU:HG	2.27	0.50
1:A:1160:VAL:HG12	1:A:1161:LYS:N	2.27	0.50
1:A:1194:LEU:HB3	1:A:1196:ILE:HD11	1.93	0.49
1:B:175:ASN:HB2	1:B:176:PRO:HD2	1.93	0.49
1:B:801:VAL:HB	1:B:815:TYR:CZ	2.47	0.49
1:B:349:GLU:HG3	1:B:356:LYS:HD3	1.95	0.49
1:A:1260:GLU:HB3	1:A:1263:LYS:HE3	1.94	0.49
1:A:1144:LEU:HD23	1:A:1196:ILE:CD1	2.42	0.49
1:A:175:ASN:HB2	1:A:176:PRO:HD2	1.94	0.49
1:A:822:MET:HG2	1:A:856:VAL:HG11	1.94	0.49
1:A:746:GLU:OE2	1:A:1351:SER:OG	2.25	0.49
1:A:867:SER:OG	1:A:868:ASP:N	2.46	0.49
1:A:847:LEU:HD22	1:A:916:PHE:CD1	2.47	0.49
1:A:54:ASP:OD2	1:A:1201:TYR:OH	2.21	0.49
1:B:241:LEU:HD13	1:B:289:LEU:HD22	1.94	0.49
1:B:1045:PHE:CA	1:B:1060:ARG:HH21	2.22	0.48
1:B:644:ASP:N	1:B:644:ASP:OD1	2.46	0.48
1:B:1281:ILE:HD11	1:B:1316:THR:HA	1.95	0.48
1:B:1300:LYS:HE2	1:B:1327:PHE:CE1	2.47	0.48
1:B:692:ASN:HB3	1:B:695:GLN:HG3	1.95	0.48
1:A:150:ASP:OD1	1:A:151:LEU:N	2.46	0.48
1:B:349:GLU:CG	1:B:356:LYS:HD3	2.44	0.48
1:A:1164:LEU:HD21	1:A:1185:LYS:CD	2.44	0.48
1:A:184:LEU:CD1	1:A:299:ALA:HB2	2.42	0.48
1:A:601:ILE:HD12	1:A:643:PHE:CE1	2.49	0.48
1:A:1144:LEU:HB3	1:A:1196:ILE:HD12	1.96	0.48
1:B:1225:GLU:OE1	4:B:2080:HOH:O	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:LYS:O	1:B:213:SER:OG	2.28	0.47
1:A:1000:LYS:NZ	1:A:1065:THR:O	2.47	0.47
1:A:314:LYS:NZ	4:A:2021:HOH:O	2.46	0.47
1:B:846:PHE:O	1:B:1041:ASN:N	2.47	0.47
1:B:1048:THR:HG22	1:B:1076:LYS:HG2	1.96	0.47
1:A:21:ILE:HG23	1:A:25:TYR:HA	1.96	0.47
1:B:564:LEU:HG	1:B:568:TYR:HE1	1.77	0.47
1:A:377:LYS:N	1:A:378:PRO:HD2	2.29	0.47
1:A:1098:THR:HB	1:A:1199:PRO:HB2	1.97	0.47
1:A:1281:ILE:HD11	1:A:1316:THR:HA	1.96	0.47
1:B:871:PRO:HD2	1:B:908:LEU:HG	1.96	0.47
1:A:125:GLU:OE2	1:A:129:HIS:NE2	2.47	0.47
1:A:416:LEU:HD23	1:A:419:LEU:HD23	1.96	0.47
1:A:1263:LYS:HE2	1:A:1302:ILE:HD11	1.97	0.47
1:B:866:LYS:HD2	1:B:1053:ALA:HB1	1.96	0.47
1:A:866:LYS:HD3	1:A:1053:ALA:HB1	1.97	0.46
1:A:977:GLU:HG3	1:A:1310:ILE:HG23	1.95	0.46
1:B:1270:ILE:HD13	1:B:1294:TYR:CD2	2.51	0.46
1:A:338:LEU:C	1:A:383:MET:HE1	2.36	0.46
1:B:226:ILE:HD11	1:B:234:LYS:CG	2.46	0.46
1:B:848:LYS:O	1:B:961:LYS:NZ	2.48	0.46
1:A:803:ASN:HA	1:A:806:LEU:HD12	1.98	0.46
1:B:1003:LYS:HB2	1:B:1021:MET:CE	2.46	0.46
1:B:1045:PHE:HA	1:B:1060:ARG:NE	2.30	0.46
1:B:557:ARG:HA	1:B:595:HIS:CD2	2.50	0.46
1:B:1206:LEU:HD21	1:B:1345:ALA:CB	2.46	0.46
1:B:40:ARG:O	1:B:42:SER:N	2.46	0.46
1:A:893:THR:HG23	1:A:896:LYS:H	1.81	0.46
1:A:339:VAL:N	1:A:383:MET:HE1	2.30	0.46
1:A:635:ARG:CG	1:A:635:ARG:HH11	2.28	0.46
1:B:1191:LYS:CD	1:B:1194:LEU:CD2	2.86	0.46
1:B:203:ALA:N	4:B:2036:HOH:O	2.43	0.46
1:A:427:GLU:HB2	1:A:434:LYS:HG2	1.97	0.46
1:B:1207:GLU:CG	1:B:1208:ASN:N	2.73	0.46
1:B:670:ILE:HG22	1:B:671:ARG:N	2.31	0.46
1:A:1021:MET:O	1:A:1036:TYR:N	2.49	0.45
1:B:391:VAL:HG12	1:B:395:ARG:HD3	1.98	0.45
1:A:1282:LEU:N	1:A:1282:LEU:HD23	2.31	0.45
1:A:822:MET:CG	1:A:856:VAL:HG11	2.47	0.45
1:A:1206:LEU:HD12	1:A:1210:ARG:CG	2.45	0.45
1:A:820:ARG:HB2	1:A:882:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:LEU:HD21	1:A:897:PHE:HB2	1.98	0.45
1:A:972:PHE:HE1	1:A:1084:ARG:CG	2.30	0.45
1:B:594:TYR:OH	1:B:608:ASP:OD2	2.34	0.45
1:A:817:GLN:O	1:A:882:TYR:OH	2.34	0.45
1:B:1270:ILE:CD1	1:B:1294:TYR:CE1	3.00	0.45
1:B:1194:LEU:O	1:B:1194:LEU:HG	2.16	0.45
1:B:822:MET:CG	1:B:856:VAL:HG21	2.46	0.45
1:B:540:LEU:HD22	1:B:545:LYS:HG2	1.97	0.45
1:B:1302:ILE:HD12	1:B:1302:ILE:H	1.82	0.45
1:B:184:LEU:HD13	1:B:299:ALA:HB2	1.98	0.45
1:B:380:LEU:HD12	1:B:393:LEU:HD12	1.99	0.45
1:B:46:ASN:ND2	1:B:1091:GLN:HG3	2.31	0.45
1:A:21:ILE:HD11	1:A:988:TYR:CD1	2.52	0.45
1:B:1204:PHE:CE1	1:B:1342:VAL:HG13	2.52	0.45
1:B:870:VAL:CG2	1:B:871:PRO:HD2	2.47	0.45
1:A:11:ILE:HG12	1:A:740:THR:HG21	1.98	0.44
1:A:823:TYR:CG	1:A:865:GLY:HA3	2.53	0.44
1:B:1310:ILE:O	4:B:2104:HOH:O	2.21	0.44
1:B:1196:ILE:N	1:B:1196:ILE:CD1	2.73	0.44
1:A:1206:LEU:CD1	1:A:1210:ARG:CG	2.95	0.44
1:A:799:HIS:CB	1:A:800:PRO:CD	2.95	0.44
1:B:893:THR:HG23	1:B:896:LYS:H	1.82	0.44
1:A:1195:ILE:CG2	1:A:1197:LYS:HE2	2.47	0.44
1:A:339:VAL:HA	1:A:383:MET:HE1	1.99	0.44
1:B:666:LEU:HD23	1:B:679:ILE:CD1	2.48	0.44
1:B:1270:ILE:HD13	1:B:1294:TYR:CG	2.53	0.44
1:B:1045:PHE:CB	1:B:1060:ARG:HH21	2.31	0.44
1:B:226:ILE:CD1	1:B:234:LYS:CG	2.95	0.44
1:B:508:LEU:O	1:B:660:GLY:N	2.46	0.43
1:A:978:ILE:HD12	1:A:1228:LEU:HB3	1.99	0.43
1:A:822:MET:CB	1:A:856:VAL:HG11	2.48	0.43
1:A:1347:LEU:N	1:A:1360:ILE:O	2.51	0.43
1:A:829:ASP:H	1:A:833:LEU:CD1	2.31	0.43
1:A:976:ARG:HH11	1:A:976:ARG:CG	2.32	0.43
1:A:368:SER:HB2	1:A:371:GLU:H	1.83	0.43
1:B:540:LEU:CD2	1:B:545:LYS:HG3	2.47	0.43
1:B:1182:LEU:HD13	1:B:1190:VAL:HG21	2.01	0.43
1:B:835:ASP:N	1:B:835:ASP:OD1	2.51	0.43
1:A:427:GLU:HB2	1:A:434:LYS:HG3	1.98	0.43
1:B:373:TYR:CD2	1:B:393:LEU:HD23	2.54	0.43
1:A:184:LEU:HD12	1:A:299:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:ASN:OD1	1:A:889:ALA:N	2.52	0.43
1:B:1037:PHE:CD1	1:B:1037:PHE:N	2.86	0.43
1:B:1224:ASN:CG	1:B:1280:VAL:HG11	2.38	0.42
1:B:823:TYR:CG	1:B:865:GLY:HA3	2.54	0.42
1:B:871:PRO:CD	1:B:908:LEU:HG	2.49	0.42
1:A:1277:SER:HB2	1:A:1287:LEU:HD22	2.01	0.42
1:B:1064:GLU:HG2	1:B:1076:LYS:HE2	2.01	0.42
1:B:138:LEU:HD11	1:B:153:LEU:HB3	2.00	0.42
1:A:158:LEU:HD22	1:A:419:LEU:CD1	2.49	0.42
1:A:801:VAL:CG2	1:A:815:TYR:CE1	3.02	0.42
1:B:999:LYS:HB3	1:B:1073:VAL:HG12	2.02	0.42
1:B:372:PHE:CZ	1:B:376:ILE:CD1	3.02	0.42
1:B:117:PRO:HG2	1:B:635:ARG:NH2	2.35	0.42
1:A:672:ASP:HA	1:A:703:THR:HG21	2.01	0.42
1:B:756:PRO:HD2	1:B:939:MET:CE	2.50	0.42
1:A:801:VAL:HG22	1:A:815:TYR:CZ	2.55	0.42
1:A:821:ASP:CA	1:A:828:LEU:HG	2.50	0.42
1:B:1216:SER:OG	1:B:1219:GLU:N	2.52	0.42
1:A:1228:LEU:HA	1:A:1272:GLN:HE22	1.85	0.42
1:A:521:TYR:CE1	1:A:549:VAL:HG21	2.54	0.42
1:A:704:PHE:O	1:A:707:ASP:N	2.52	0.42
1:B:914:ALA:HA	1:B:1018:VAL:HG21	2.02	0.42
1:B:634:GLU:HA	1:B:637:LYS:HE3	2.02	0.42
1:B:778:ARG:HA	1:B:803:ASN:HD21	1.84	0.42
1:B:359:TYR:HA	1:B:372:PHE:CE1	2.55	0.42
1:A:1283:ALA:HB2	1:A:1334:LYS:HE2	2.01	0.42
1:A:824:VAL:C	1:A:879:MET:HE3	2.40	0.42
1:A:202:ASN:OD1	1:A:204:SER:N	2.47	0.42
1:A:564:LEU:HD22	1:A:587:PHE:HE2	1.85	0.42
1:B:1050:ILE:HD11	1:B:1060:ARG:HD2	2.00	0.42
1:B:377:LYS:N	1:B:378:PRO:HD2	2.35	0.42
1:B:942:LYS:NZ	1:B:952:GLU:OE2	2.47	0.42
1:A:828:LEU:HD22	1:A:833:LEU:HB3	2.02	0.42
1:A:892:ILE:HB	1:A:896:LYS:HD2	2.02	0.42
1:B:1180:ASP:N	1:B:1180:ASP:OD1	2.53	0.42
1:B:598:LEU:HG	1:B:607:LEU:HD12	2.02	0.42
1:A:1026:GLU:O	1:A:1027:GLN:HG3	2.20	0.41
1:A:427:GLU:HG3	1:A:434:LYS:HE3	2.02	0.41
1:A:609:ASN:OD1	1:A:611:GLU:N	2.51	0.41
1:B:615:ILE:HG23	1:B:639:TYR:CE1	2.55	0.41
1:B:1003:LYS:HD2	1:B:1016:TYR:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1003:LYS:CE	1:B:1068:GLU:OE1	2.67	0.41
1:B:1281:ILE:CD1	1:B:1316:THR:HG22	2.50	0.41
1:B:745:ASP:OD2	1:B:938:ARG:NH2	2.53	0.41
1:A:373:TYR:O	1:A:377:LYS:HG3	2.20	0.41
1:A:828:LEU:HA	1:A:833:LEU:CD1	2.47	0.41
1:B:1300:LYS:HD2	1:B:1301:PRO:HD2	2.02	0.41
1:B:184:LEU:CD1	1:B:299:ALA:HB2	2.50	0.41
1:A:266:LEU:HD23	1:A:271:TYR:CZ	2.56	0.41
1:B:516:GLU:O	1:B:519:THR:HG22	2.21	0.41
1:B:822:MET:HG2	1:B:856:VAL:HG21	2.01	0.41
1:A:1222:LYS:O	1:A:1318:LEU:HD12	2.21	0.41
1:B:1213:MET:CE	1:B:1318:LEU:HD11	2.50	0.41
1:A:677:LYS:HB2	1:A:682:PHE:CZ	2.56	0.41
1:B:1003:LYS:HG2	1:B:1036:TYR:OH	2.21	0.41
1:B:596:ASP:HB3	1:B:654:ARG:CZ	2.50	0.41
1:A:1281:ILE:HD11	1:A:1316:THR:HG22	2.03	0.41
1:A:824:VAL:O	1:A:824:VAL:HG12	2.20	0.41
1:B:373:TYR:O	1:B:377:LYS:HG3	2.21	0.41
1:A:1205:GLU:HB3	1:A:1346:THR:CG2	2.51	0.41
1:A:240:ASN:ND2	1:A:255:ASN:OD1	2.52	0.41
1:A:881:ASN:N	1:A:881:ASN:OD1	2.52	0.41
1:B:372:PHE:CZ	1:B:376:ILE:HD12	2.56	0.41
1:B:378:PRO:O	1:B:382:LYS:HG2	2.21	0.41
1:A:1086:VAL:HA	1:A:1089:MET:CE	2.51	0.41
1:B:1204:PHE:CD1	1:B:1342:VAL:HG13	2.56	0.41
1:B:833:LEU:C	1:B:836:TYR:H	2.24	0.41
1:A:882:TYR:CE2	1:A:886:LEU:HD11	2.55	0.41
1:A:763:MET:CG	1:A:928:THR:HG22	2.51	0.41
1:B:1290:VAL:CG2	1:B:1331:ILE:CD1	2.99	0.41
1:A:376:ILE:HD12	1:A:393:LEU:CD1	2.51	0.40
1:A:828:LEU:CA	1:A:833:LEU:HD13	2.47	0.40
1:B:648:MET:HA	1:B:648:MET:HE2	2.04	0.40
1:B:600:ILE:CD1	1:B:654:ARG:NH2	2.84	0.40
1:B:737:ILE:HA	1:B:740:THR:HG23	2.04	0.40
1:A:1004:LEU:HD21	1:A:1021:MET:HE1	2.03	0.40
1:A:869:ASN:HA	1:A:1053:ALA:HB3	2.03	0.40
1:A:1264:HIS:CE1	1:A:1265:TYR:CE1	3.09	0.40
1:A:1267:ASP:OD1	1:A:1298:ARG:NH1	2.49	0.40
1:A:512:SER:OG	1:A:617:GLU:OE1	2.33	0.40
1:A:8:GLY:HA3	1:A:991:ALA:HB2	2.04	0.40
1:A:635:ARG:HG2	1:A:635:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:PRO:CD	1:A:1272:GLN:HE22	2.35	0.40
1:A:595:HIS:HA	1:A:598:LEU:HG	2.03	0.40
1:A:787:GLY:HA3	1:A:891:LEU:HD21	2.02	0.40
1:A:362:TYR:HA	1:A:367:ALA:HB3	2.04	0.40
1:B:1284:ASP:OD1	4:B:2103:HOH:O	2.21	0.40
1:B:336:LYS:NZ	4:B:2056:HOH:O	2.47	0.40
1:B:828:LEU:CD2	1:B:833:LEU:HD21	2.52	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	1108/1372 (81%)	1064 (96%)	44 (4%)	0	100	100
1	B	1132/1372 (82%)	1095 (97%)	37 (3%)	0	100	100
All	All	2240/2744 (82%)	2159 (96%)	81 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1019/1228 (83%)	957 (94%)	62 (6%)	22	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1050/1228 (86%)	984 (94%)	66 (6%)	21	40
All	All	2069/2456 (84%)	1941 (94%)	128 (6%)	21	41

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	30	LYS
1	A	39	ASP
1	A	46	ASN
1	A	87	SER
1	A	165	ARG
1	A	174	LEU
1	A	182	ASP
1	A	224	ASN
1	A	261	ASP
1	A	285	GLN
1	A	288	ASP
1	A	306	LEU
1	A	395	ARG
1	A	403	ARG
1	A	416	LEU
1	A	425	ARG
1	A	445	THR
1	A	446	PHE
1	A	447	ARG
1	A	517	TYR
1	A	521	TYR
1	A	628	ASP
1	A	635	ARG
1	A	646	LYS
1	A	668	ASN
1	A	746	GLU
1	A	801	VAL
1	A	804	THR
1	A	805	GLN
1	A	822	MET
1	A	842	VAL
1	A	847	LEU
1	A	848	LYS
1	A	853	ASP
1	A	857	LEU

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Mol	Chain	Res	Type
1	A	866	LYS
1	A	868	ASP
1	A	870	VAL
1	A	919	ARG
1	A	935	LEU
1	A	959	LYS
1	A	964	SER
1	A	967	ARG
1	A	976	ARG
1	A	977	GLU
1	A	998	ILE
1	A	1037	PHE
1	A	1062	LEU
1	A	1099	GLU
1	A	1101	GLN
1	A	1168	ILE
1	A	1173	SER
1	A	1180	ASP
1	A	1206	LEU
1	A	1210	ARG
1	A	1211	LYS
1	A	1274	SER
1	A	1284	ASP
1	A	1304	GLU
1	A	1333	ARG
1	A	1343	LEU
1	B	44	LYS
1	B	63	ARG
1	B	139	ARG
1	B	141	LYS
1	B	161	MET
1	B	165	ARG
1	B	302	LEU
1	B	340	ARG
1	B	381	GLU
1	B	393	LEU
1	B	403	ARG
1	B	405	PHE
1	B	406	ASP
1	B	414	ILE
1	B	420	HIS
1	B	425	ARG

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Mol	Chain	Res	Type
1	B	447	ARG
1	B	517	TYR
1	B	521	TYR
1	B	540	LEU
1	B	587	PHE
1	B	588	ASN
1	B	598	LEU
1	B	605	ASP
1	B	625	LEU
1	B	644	ASP
1	B	657	THR
1	B	666	LEU
1	B	718	ASP
1	B	740	THR
1	B	753	ARG
1	B	807	GLN
1	B	829	ASP
1	B	848	LYS
1	B	853	ASP
1	B	856	VAL
1	B	857	LEU
1	B	866	LYS
1	B	872	SER
1	B	884	ARG
1	B	895	ARG
1	B	911	LEU
1	B	923	GLU
1	B	945	GLU
1	B	961	LYS
1	B	998	ILE
1	B	1017	ASP
1	B	1037	PHE
1	B	1054	ASN
1	B	1062	LEU
1	B	1076	LYS
1	B	1084	ARG
1	B	1091	GLN
1	B	1148	LYS
1	B	1168	ILE
1	B	1172	SER
1	B	1180	ASP
1	B	1182	LEU

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Mol	Chain	Res	Type
1	B	1185	LYS
1	B	1194	LEU
1	B	1210	ARG
1	B	1224	ASN
1	B	1258	PHE
1	B	1300	LYS
1	B	1352	ILE
1	B	1358	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	285	GLN
1	A	721	HIS
1	A	807	GLN
1	A	1101	GLN
1	A	1224	ASN
1	A	1234	ASN
1	A	1264	HIS
1	A	1272	GLN
1	A	1311	HIS
1	B	160	HIS
1	B	187	GLN
1	B	235	ASN
1	B	285	GLN
1	B	556	ASN
1	B	563	GLN
1	B	641	HIS
1	B	982	HIS
1	B	1044	ASN
1	B	1177	ASN
1	B	1262	HIS
1	B	1297	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	2364	-	4,4,4	0.08	0	6,6,6	0.09	0
2	SO4	A	2365	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	2364	-	4,4,4	0.11	0	6,6,6	0.15	0
2	SO4	B	2365	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	2366	-	4,4,4	0.21	0	6,6,6	0.33	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	2364	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2365	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2364	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2365	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2366	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2364	SO4	1	0
2	B	2365	SO4	2	0
2	B	2366	SO4	2	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<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	1144/1372 (83%)	0.73	131 (11%) 5 3	17, 59, 124, 164	0
1	B	1166/1372 (84%)	0.76	125 (10%) 7 4	16, 54, 118, 162	0
All	All	2310/2744 (84%)	0.75	256 (11%) 6 4	16, 56, 121, 164	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	TYR	11.8
1	B	564	LEU	9.3
1	B	567	ASP	7.4
1	B	773	GLY	7.1
1	B	570	LYS	7.1
1	A	828	LEU	6.9
1	A	407	ASN	6.7
1	B	527	VAL	6.6
1	A	1144	LEU	6.6
1	A	820	ARG	6.2
1	A	834	SER	6.1
1	A	836	TYR	6.0
1	A	115	ARG	5.9
1	A	525	THR	5.9
1	B	661	ARG	5.7
1	A	567	ASP	5.7
1	A	564	LEU	5.5
1	A	1299	ASP	5.5
1	A	671	ARG	5.5
1	B	566	GLU	5.5
1	A	1177	ASN	5.4
1	A	832	ARG	5.4
1	B	602	LYS	5.4
1	A	814	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	1190	VAL	5.2
1	A	601	ILE	5.0
1	B	654	ARG	5.0
1	A	818	ASN	4.9
1	A	527	VAL	4.8
1	A	1181	PHE	4.7
1	B	569	PHE	4.7
1	A	815	TYR	4.7
1	A	870	VAL	4.7
1	B	594	TYR	4.6
1	B	1169	MET	4.6
1	A	1176	LYS	4.6
1	B	653	ARG	4.6
1	B	829	ASP	4.5
1	A	563	GLN	4.4
1	B	600	ILE	4.4
1	B	603	ASP	4.4
1	B	384	ASP	4.4
1	A	1195	ILE	4.4
1	A	307	ARG	4.4
1	A	553	PHE	4.3
1	A	829	ASP	4.3
1	A	1261	GLN	4.3
1	B	560	THR	4.2
1	B	1193	ASP	4.2
1	A	710	LYS	4.2
1	B	644	ASP	4.2
1	A	558	LYS	4.2
1	B	310	THR	4.2
1	B	1206	LEU	4.2
1	B	670	ILE	4.1
1	A	826	GLN	4.1
1	B	801	VAL	4.1
1	A	858	THR	4.1
1	B	649	LYS	4.1
1	B	504	ASN	4.0
1	A	651	LEU	4.0
1	A	830	ILE	4.0
1	B	1188	LYS	4.0
1	B	1259	VAL	4.0
1	A	552	LEU	3.9
1	B	383	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	607	LEU	3.9
1	B	510	LYS	3.9
1	A	1084	ARG	3.9
1	B	1189	GLU	3.9
1	A	1145	VAL	3.9
1	A	857	LEU	3.8
1	B	597	LEU	3.8
1	B	1146	VAL	3.8
1	A	837	ASP	3.7
1	B	629	ARG	3.7
1	B	1191	LYS	3.7
1	A	835	ASP	3.7
1	A	838	VAL	3.6
1	A	1146	VAL	3.6
1	A	406	ASP	3.6
1	A	1182	LEU	3.6
1	B	593	THR	3.5
1	A	1242	TYR	3.5
1	B	764	ALA	3.5
1	B	873	GLU	3.5
1	B	688	PHE	3.5
1	B	815	TYR	3.5
1	A	1334	LYS	3.5
1	B	834	SER	3.5
1	B	1177	ASN	3.4
1	B	880	LYS	3.4
1	A	526	LYS	3.4
1	B	775	LYS	3.4
1	A	881	ASN	3.4
1	B	526	LYS	3.4
1	A	549	VAL	3.3
1	B	1179	ILE	3.3
1	B	683	LEU	3.3
1	A	341	GLN	3.3
1	A	648	MET	3.3
1	B	1183	GLU	3.3
1	B	1023	ALA	3.3
1	A	591	LEU	3.2
1	A	370	GLU	3.2
1	B	1302	ILE	3.2
1	A	384	ASP	3.2
1	B	607	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	406	ASP	3.2
1	B	606	PHE	3.2
1	B	806	LEU	3.2
1	A	824	VAL	3.1
1	A	788	ILE	3.1
1	A	220	ARG	3.1
1	A	434	LYS	3.1
1	B	911	LEU	3.1
1	B	917	ILE	3.1
1	A	865	GLY	3.1
1	A	233	LYS	3.1
1	A	546	LYS	3.0
1	B	858	THR	3.0
1	A	1143	VAL	3.0
1	A	811	LEU	3.0
1	A	1231	LYS	3.0
1	A	670	ILE	3.0
1	A	1290	VAL	2.9
1	B	1173	SER	2.9
1	A	706	GLU	2.9
1	B	543	GLU	2.9
1	A	801	VAL	2.9
1	B	1194	LEU	2.8
1	A	809	GLU	2.8
1	A	603	ASP	2.8
1	A	1296	LYS	2.8
1	B	370	GLU	2.8
1	A	711	ALA	2.8
1	B	655	ARG	2.8
1	A	1017	ASP	2.8
1	B	776	ASN	2.8
1	A	868	ASP	2.8
1	A	597	LEU	2.8
1	B	601	ILE	2.8
1	A	1265	TYR	2.7
1	A	548	ILE	2.7
1	B	651	LEU	2.7
1	B	555	THR	2.7
1	A	789	LYS	2.7
1	B	1176	LYS	2.7
1	A	776	ASN	2.7
1	B	1257	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	779	GLU	2.7
1	B	878	LYS	2.7
1	A	1185	LYS	2.7
1	B	307	ARG	2.7
1	B	1145	VAL	2.6
1	A	777	SER	2.6
1	B	712	GLN	2.6
1	A	1289	LYS	2.6
1	A	565	LYS	2.6
1	A	1159	SER	2.6
1	B	910	GLU	2.6
1	A	691	ARG	2.6
1	B	69	ARG	2.6
1	A	545	LYS	2.5
1	A	524	LEU	2.5
1	B	557	ARG	2.5
1	A	901	THR	2.5
1	A	661	ARG	2.5
1	A	1271	GLU	2.5
1	A	1196	ILE	2.5
1	B	1037	PHE	2.5
1	B	611	GLU	2.5
1	A	598	LEU	2.5
1	A	1173	SER	2.5
1	B	605	ASP	2.5
1	B	877	LYS	2.5
1	B	1170	GLU	2.4
1	A	876	VAL	2.4
1	B	539	PHE	2.4
1	B	680	LEU	2.4
1	B	182	ASP	2.4
1	A	1198	LEU	2.4
1	B	1182	LEU	2.4
1	A	649	LYS	2.4
1	B	713	VAL	2.4
1	A	594	TYR	2.4
1	A	812	TYR	2.4
1	A	258	LEU	2.4
1	B	830	ILE	2.4
1	B	865	GLY	2.4
1	B	684	LYS	2.4
1	B	1019	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1262	HIS	2.4
1	A	1272	GLN	2.4
1	B	563	GLN	2.4
1	A	600	ILE	2.4
1	A	866	LYS	2.4
1	B	616	LEU	2.4
1	B	637	LYS	2.4
1	B	706	GLU	2.3
1	B	682	PHE	2.3
1	A	1228	LEU	2.3
1	A	123	VAL	2.3
1	B	33	LYS	2.3
1	B	1181	PHE	2.3
1	B	598	LEU	2.3
1	A	562	LYS	2.3
1	B	790	GLU	2.3
1	A	1293	ALA	2.3
1	B	641	HIS	2.3
1	B	523	GLU	2.3
1	A	637	LYS	2.3
1	A	677	LYS	2.3
1	B	587	PHE	2.3
1	A	888	ASN	2.2
1	A	305	ILE	2.2
1	A	697	ILE	2.2
1	A	708	ILE	2.2
1	B	697	ILE	2.2
1	B	446	PHE	2.2
1	A	872	SER	2.2
1	A	1278	LYS	2.2
1	B	789	LYS	2.2
1	B	1284	ASP	2.2
1	A	968	LYS	2.2
1	A	1197	LYS	2.2
1	B	841	ILE	2.2
1	A	116	HIS	2.2
1	B	553	PHE	2.2
1	B	867	SER	2.1
1	B	888	ASN	2.1
1	B	1192	LYS	2.1
1	A	543	GLU	2.1
1	B	886	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	671	ARG	2.1
1	B	694	MET	2.1
1	A	551	LEU	2.1
1	A	978	ILE	2.1
1	A	1164	LEU	2.1
1	B	116	HIS	2.1
1	A	802	GLU	2.1
1	B	260	GLU	2.1
1	A	215	ARG	2.1
1	B	365	GLY	2.1
1	B	398	LEU	2.1
1	A	764	ALA	2.1
1	A	1175	GLU	2.1
1	A	680	LEU	2.0
1	B	788	ILE	2.0
1	B	1168	ILE	2.0
1	A	557	ARG	2.0
1	B	447	ARG	2.0
1	B	1240	SER	2.0
1	A	886	LEU	2.0
1	A	1019	ARG	2.0
1	B	818	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
3	MG	B	2367	1/1	0.23	0.46	11.11	54,54,54,54	0
2	SO4	A	2365	5/5	0.79	0.33	4.19	88,99,106,106	0
2	SO4	A	2364	5/5	0.98	0.23	0.39	32,39,54,59	0
2	SO4	B	2365	5/5	0.89	0.22	0.06	80,91,102,103	0
2	SO4	B	2366	5/5	0.90	0.19	-0.01	30,30,30,30	0
2	SO4	B	2364	5/5	0.97	0.19	-0.46	21,25,39,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.