



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:44 AM UTC

PDB ID : 4CMP / pdb\_00004cmp  
Title : Crystal structure of *S. pyogenes* Cas9  
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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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

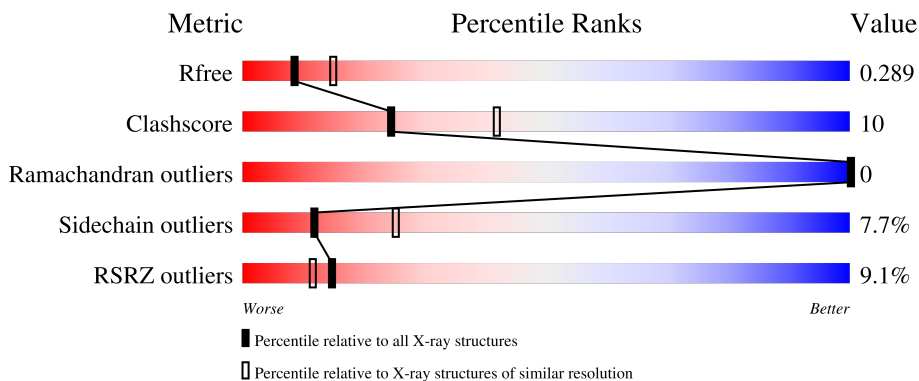
# 1 Overall quality at a glance

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))
$R_{free}$	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1372	 9% 63% 18% • 17%
1	B	1372	 7% 65% 17% • 15%

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	B	2365	-	-	X	-
2	SO4	B	2366	-	-	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
			Total	C	H	N	O	S			
1	A	1144	18772	5949	9456	1610	1738	19	0	0	0
1	B	1166	19284	6101	9738	1648	1778	19	0	0	0

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 (CCD ID: 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	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

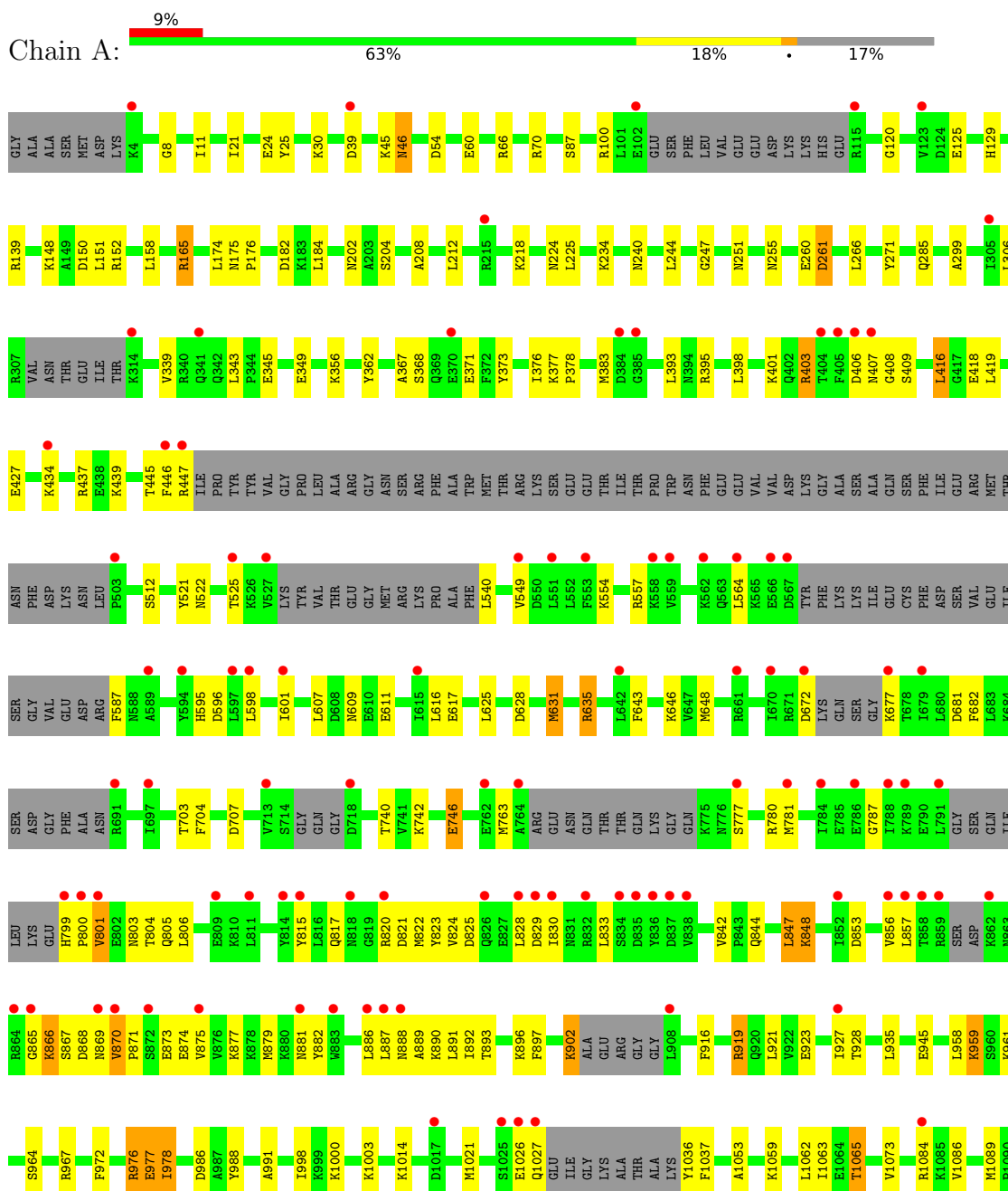
- Molecule 4 is water.

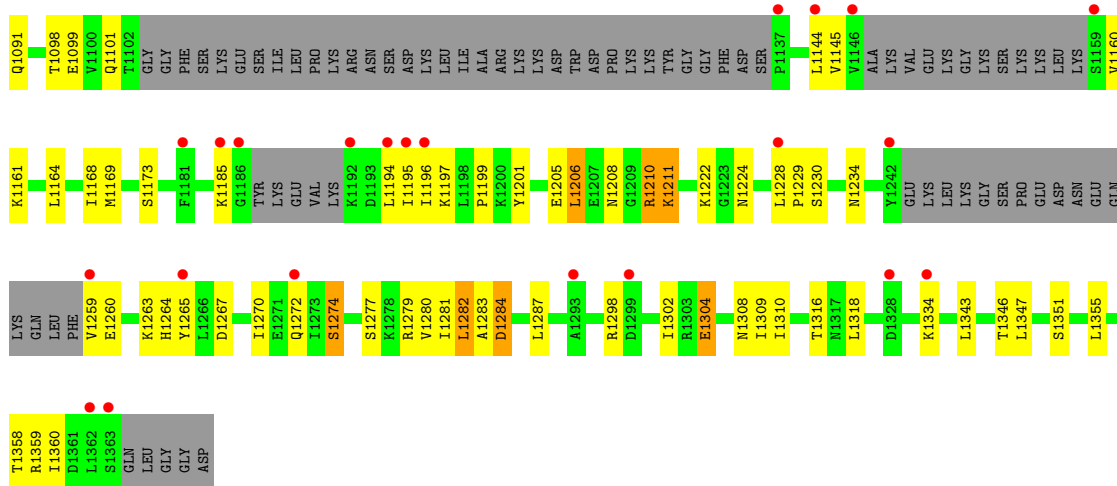
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	92	Total O 92 92	0	0
4	B	111	Total O 111 111	0	0

### 3 Residue-property plots

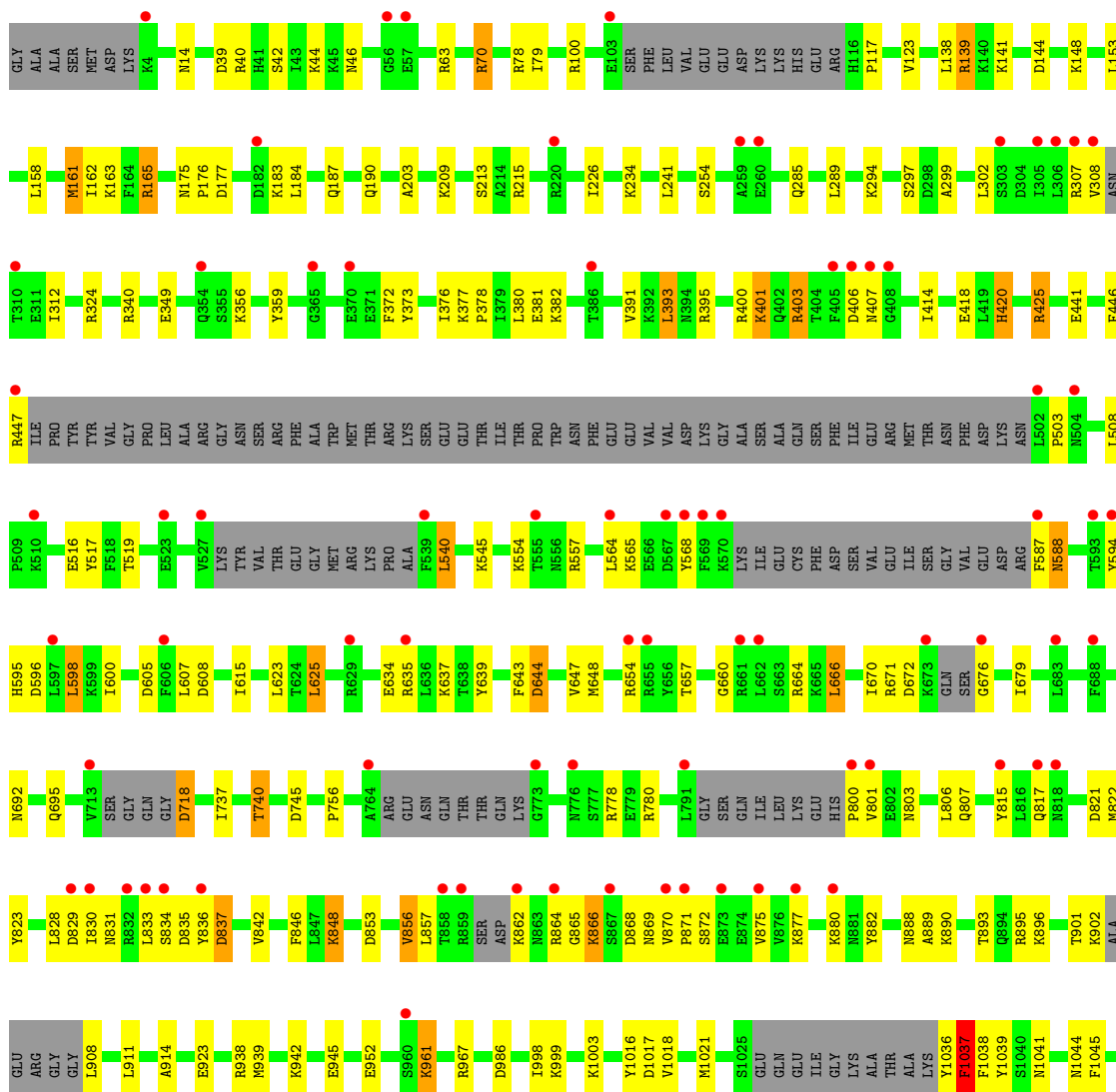
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

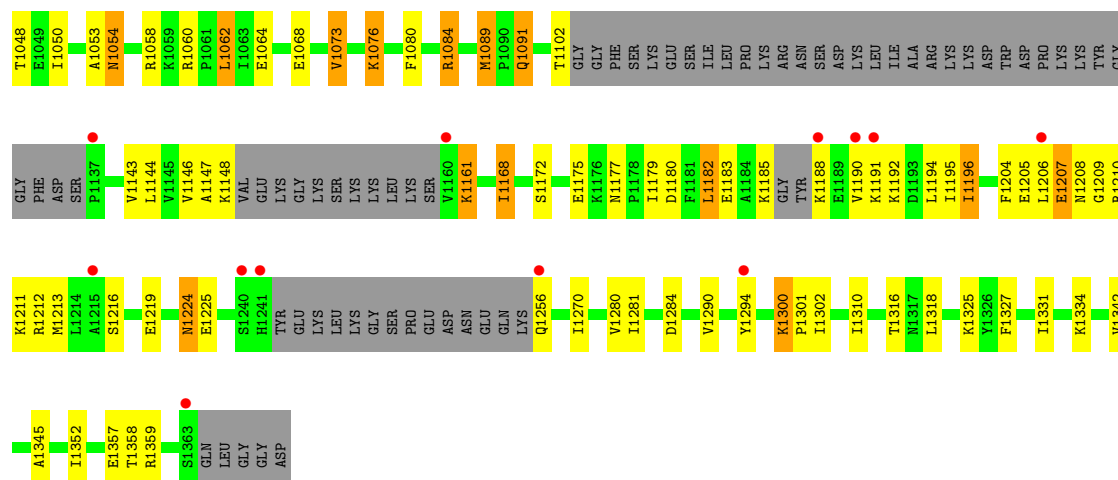
#### • Molecule 1: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1





● 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)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.252 , 0.286 0.258 , 0.289	Depositor DCC
$R_{free}$ test set	2424 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtrriage
Anisotropy	0.232	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	38285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage'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: SO4, MG

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	0.36	0/9463	0.74	4/12717 (0.0%)
1	B	0.38	0/9698	0.74	7/13022 (0.1%)
All	All	0.37	0/19161	0.74	11/25739 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	834	SER	N-CA-C	-7.00	102.71	111.11
1	A	830	ILE	N-CA-C	6.64	116.79	110.42
1	B	831	ASN	N-CA-C	5.78	117.66	111.36
1	B	837	ASP	N-CA-C	5.69	116.79	108.14
1	B	830	ILE	N-CA-C	5.53	115.72	110.42
1	B	1038	PHE	N-CA-C	-5.45	106.68	113.55
1	A	873	GLU	N-CA-C	5.40	117.50	110.43
1	A	409	SER	N-CA-C	-5.39	100.98	109.50
1	B	1037	PHE	N-CA-C	5.23	117.33	109.23
1	A	408	GLY	N-CA-C	5.09	118.71	110.87
1	B	1207	GLU	N-CA-C	5.06	115.49	108.00

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	172	0
1	B	9546	9738	9714	204	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	6	0
4	B	111	0	0	11	0
All	All	19091	19194	19140	376	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 (376) 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:400:ARG:NH2	4:B:2052:HOH:O	2.05	0.88
1:B:1205:GLU:OE1	1:B:1359:ARG:NH2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:254:SER:OG	4:B:2040:HOH:O	2.07	0.72
1:B:1196:ILE:N	1:B:1196:ILE:HD12	2.03	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:866:LYS:NZ	1:B:870:VAL:O	2.25	0.69
1:B:1144:LEU:HD22	1:B:1196:ILE:HD13	1.74	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:B:1195:ILE:C	1:B:1196:ILE:HD12	2.19	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:218:LYS:NZ	1:A:406:ASP:OD1	2.25	0.64
1:A:977:GLU:HG3	1:A:1310:ILE:CG2	2.27	0.64
1:B:1003:LYS:NZ	1:B:1068:GLU:OE1	2.26	0.64
1:B:1045:PHE:CA	1:B:1060:ARG:NH2	2.60	0.64
1:A:1282:LEU:O	1:A:1334:LYS:NZ	2.30	0.64
1:B:967:ARG:NH1	1:B:986:ASP:OD1	2.31	0.63
1:B:540:LEU:HD22	1:B:545:LYS:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:GLU:HG3	1:B:1208:ASN:N	2.10	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:1179:ILE:HG22	1:B:1183:GLU:CD	2.24	0.62
1:B:165:ARG:NH2	1:B:446:PHE:O	2.31	0.61
1:B:100:ARG:NH1	1:B:625:LEU:O	2.34	0.61
1:B:1084:ARG:N	4:B:2087:HOH:O	2.33	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:158:LEU:HD22	1:A:419:LEU:HD12	1.83	0.60
1:A:1206:LEU:CD1	1:A:1210:ARG:HG2	2.31	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:643:PHE:CB	1:B:648:MET:HE3	2.32	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:A:339:VAL:HA	1:A:383:MET:HE1	1.84	0.58
1:A:150:ASP:OD2	1:A:152:ARG:NH2	2.36	0.58
1:B:643:PHE:HB2	1:B:648:MET:HE3	1.85	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: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: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:828:LEU:HD22	1:B:833:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:1191:LYS:CE	1:B:1194:LEU:CD2	2.54	0.55
1:B:588:ASN:N	1:B:588:ASN:OD1	2.37	0.54
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:70:ARG:NH1	1:B:718:ASP:OD2	2.40	0.54
1:B:1146:VAL:HG22	1:B:1161:LYS:HG3	1.90	0.54
1:A:1086:VAL:HA	1:A:1089:MET:HE3	1.89	0.54
1:B:870:VAL:HG23	1:B:871:PRO:HD2	1.89	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:825:ASP:HB2	1:A:879:MET:HE1	1.91	0.52
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:158:LEU:HA	1:B:161:MET:HE2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:1210:ARG:HB2	1:A:1280:VAL:HG13	1.93	0.51
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.43	0.51
1:B:508:LEU:HD21	1:B:664:ARG:CG	2.41	0.51
1:B:1102:THR:HA	1:B:1168:ILE:HD13	1.92	0.51
1:A:522:ASN:HA	1:A:525:THR:HG23	1.92	0.51
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:1045:PHE:CB	1:B:1060:ARG:NH2	2.75	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:B:648:MET:HE2	1:B:648:MET:HA	1.93	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:847:LEU:HD22	1:A:916:PHE:CD1	2.47	0.49
1:A:867:SER:OG	1:A:868:ASP:N	2.46	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:644:ASP:N	1:B:644:ASP:OD1	2.46	0.48
1:B:1045:PHE:CA	1:B:1060:ARG:HH21	2.22	0.48
1:A:822:MET:HE1	1:A:886:LEU:CD1	2.42	0.48
1:B:1224:ASN:CG	1:B:1280:VAL:HG11	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1281:ILE:HD11	1:B:1316:THR:HA	1.95	0.48
1:B:692:ASN:HB3	1:B:695:GLN:HG3	1.95	0.48
1:B:1300:LYS:HE2	1:B:1327:PHE:CE1	2.47	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
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: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: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:557:ARG:HA	1:B:595:HIS:CD2	2.50	0.46
1:B:1045:PHE:HA	1:B:1060:ARG:NE	2.30	0.46
1:B:40:ARG:O	1:B:42:SER:N	2.46	0.46
1:B:1206:LEU:HD21	1:B:1345:ALA:CB	2.46	0.46
1:A:893:THR:HG23	1:A:896:LYS:H	1.81	0.46
1:A:635:ARG:HH11	1:A:635:ARG:CG	2.28	0.46
1:B:203:ALA:N	4:B:2036:HOH:O	2.43	0.46
1:B:1191:LYS:CD	1:B:1194:LEU:CD2	2.86	0.46
1:A:427:GLU:HB2	1:A:434:LYS:HG2	1.97	0.46
1:B:670:ILE:HG22	1:B:671:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:GLU:CG	1:B:1208:ASN:N	2.73	0.46
1:A:1021:MET:O	1:A:1036:TYR:N	2.49	0.45
1:B:833:LEU:C	1:B:836:TYR:H	2.24	0.45
1:B:391:VAL:HG12	1:B:395:ARG:HD3	1.98	0.45
1:A:822:MET:CG	1:A:856:VAL:HG11	2.47	0.45
1:A:1282:LEU:HD23	1:A:1282:LEU:N	2.31	0.45
1:A:820:ARG:HB2	1:A:882:TYR:OH	2.17	0.45
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:A:1206:LEU:HD12	1:A:1210:ARG:CG	2.45	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:822:MET:CG	1:B:856:VAL:HG21	2.46	0.45
1:B:1194:LEU:O	1:B:1194:LEU:HG	2.16	0.45
1:B:540:LEU:HD22	1:B:545:LYS:HG2	1.97	0.45
1:B:46:ASN:ND2	1:B:1091:GLN:HG3	2.31	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:1302:ILE:HD12	1:B:1302:ILE:H	1.82	0.45
1:A:21:ILE:HD11	1:A:988:TYR:CD1	2.52	0.45
1:B:870:VAL:CG2	1:B:871:PRO:HD2	2.47	0.45
1:B:1204:PHE:CE1	1:B:1342:VAL:HG13	2.52	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:1179:ILE:C	1:B:1183:GLU:HG3	2.20	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:799:HIS:CB	1:A:800:PRO:CD	2.95	0.44
1:A:1206:LEU:CD1	1:A:1210:ARG:CG	2.95	0.44
1:B:46:ASN:CG	1:B:1089:MET:CE	2.91	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: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:226:ILE:CD1	1:B:234:LYS:CG	2.95	0.44
1:B:1045:PHE:CB	1:B:1060:ARG:HH21	2.31	0.44
1:B:1325:LYS:NZ	1:B:1327:PHE:O	2.24	0.44
1:B:508:LEU:O	1:B:660:GLY:N	2.46	0.43
1:A:339:VAL:CA	1:A:383:MET:HE1	2.49	0.43
1:A:822:MET:CB	1:A:856:VAL:HG11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ILE:HD12	1:A:1228:LEU:HB3	1.99	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:1347:LEU:N	1:A:1360:ILE:O	2.51	0.43
1:A:368:SER:HB2	1:A:371:GLU:H	1.83	0.43
1:A:825:ASP:N	1:A:879:MET:HE1	2.33	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:OD1	1:B:835:ASP:N	2.51	0.43
1:A:427:GLU:HB2	1:A:434:LYS:HG3	1.98	0.43
1:A:746:GLU:OE2	1:A:1351:SER:OG	2.25	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
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: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:138:LEU:HD11	1:B:153:LEU:HB3	2.00	0.42
1:B:1064:GLU:HG2	1:B:1076:LYS:HE2	2.01	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:117:PRO:HG2	1:B:635:ARG:NH2	2.35	0.42
1:B:372:PHE:CZ	1:B:376:ILE:CD1	3.02	0.42
1:B:999:LYS:HB3	1:B:1073:VAL:HG12	2.02	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:B:1041:ASN:HB3	1:B:1044:ASN:CG	2.44	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:888:ASN:OD1	1:B:888:ASN:C	2.63	0.42
1:B:1216:SER:OG	1:B:1219:GLU:N	2.52	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:A:1228:LEU:HA	1:A:1272:GLN:HE22	1.85	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:914:ALA:HA	1:B:1018:VAL:HG21	2.02	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:202:ASN:OD1	1:A:204:SER:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD22	1:A:587:PHE:HE2	1.85	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:B:1050:ILE:HD11	1:B:1060:ARG:HD2	2.00	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:598:LEU:HG	1:B:607:LEU:HD12	2.02	0.42
1:B:1180:ASP:OD1	1:B:1180:ASP:N	2.53	0.42
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:A:1026:GLU:O	1:A:1027:GLN:HG3	2.20	0.41
1:B:615:ILE:HG23	1:B:639:TYR:CE1	2.55	0.41
1:A:824:VAL:C	1:A:879:MET:HE1	2.45	0.41
1:B:745:ASP:OD2	1:B:938:ARG:NH2	2.53	0.41
1:B:1003:LYS:HD2	1:B:1016:TYR:CE2	2.54	0.41
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: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:184:LEU:CD1	1:B:299:ALA:HB2	2.50	0.41
1:B:1300:LYS:HD2	1:B:1301:PRO:HD2	2.02	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:A:777:SER:C	1:A:803:ASN:OD1	2.64	0.41
1:B:596:ASP:HB3	1:B:654:ARG:CZ	2.50	0.41
1:B:1003:LYS:HG2	1:B:1036:TYR:OH	2.21	0.41
1:A:824:VAL:O	1:A:824:VAL:HG12	2.20	0.41
1:A:1281:ILE:HD11	1:A:1316:THR:HG22	2.03	0.41
1:B:373:TYR:O	1:B:377:LYS:HG3	2.21	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:A:1205:GLU:HB3	1:A:1346:THR:CG2	2.51	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:877:LYS:NZ	1:A:902:LYS:C	2.78	0.41
1:B:1204:PHE:CD1	1:B:1342:VAL:HG13	2.56	0.41
1:A:763:MET:CG	1:A:928:THR:HG22	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:TYR:CE2	1:A:886:LEU:HD11	2.55	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:643:PHE:HB2	1:A:648:MET:HE1	2.03	0.40
1:A:828:LEU:CA	1:A:833:LEU:HD13	2.47	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:8:GLY:HA3	1:A:991:ALA:HB2	2.04	0.40
1:A:512:SER:OG	1:A:617:GLU:OE1	2.33	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:B:1003:LYS:HB2	1:B:1021:MET:HE2	2.04	0.40
1:A:635:ARG:NH1	1:A:635:ARG:HG2	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:1229:PRO:CD	1:A:1272:GLN:HE22	2.35	0.40
1:A:120:GLY:C	1:A:631:MET:HE3	2.46	0.40
1:A:362:TYR:HA	1:A:367:ALA:HB3	2.04	0.40
1:B:828:LEU:CD2	1:B:833:LEU:HD21	2.52	0.40
1:B:1284:ASP:OD1	4:B:2103:HOH:O	2.21	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%)	937 (92%)	82 (8%)	11	23
1	B	1050/1228 (86%)	972 (93%)	78 (7%)	13	27
All	All	2069/2456 (84%)	1909 (92%)	160 (8%)	12	25

All (160) 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	70	ARG
1	A	87	SER
1	A	148	LYS
1	A	165	ARG
1	A	174	LEU
1	A	182	ASP
1	A	212	LEU
1	A	224	ASN
1	A	225	LEU
1	A	234	LYS
1	A	260	GLU
1	A	261	ASP
1	A	285	GLN
1	A	306	LEU
1	A	343	LEU
1	A	345	GLU
1	A	395	ARG
1	A	403	ARG
1	A	416	LEU
1	A	439	LYS
1	A	445	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	447	ARG
1	A	540	LEU
1	A	628	ASP
1	A	631	MET
1	A	635	ARG
1	A	646	LYS
1	A	746	GLU
1	A	801	VAL
1	A	804	THR
1	A	805	GLN
1	A	842	VAL
1	A	847	LEU
1	A	848	LYS
1	A	853	ASP
1	A	857	LEU
1	A	866	LYS
1	A	870	VAL
1	A	875	VAL
1	A	890	LYS
1	A	902	LYS
1	A	919	ARG
1	A	921	LEU
1	A	923	GLU
1	A	927	ILE
1	A	935	LEU
1	A	945	GLU
1	A	958	LEU
1	A	959	LYS
1	A	964	SER
1	A	976	ARG
1	A	977	GLU
1	A	978	ILE
1	A	998	ILE
1	A	1003	LYS
1	A	1014	LYS
1	A	1037	PHE
1	A	1059	LYS
1	A	1062	LEU
1	A	1063	ILE
1	A	1065	THR
1	A	1073	VAL
1	A	1091	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1099	GLU
1	A	1101	GLN
1	A	1145	VAL
1	A	1168	ILE
1	A	1173	SER
1	A	1206	LEU
1	A	1210	ARG
1	A	1211	LYS
1	A	1274	SER
1	A	1282	LEU
1	A	1284	ASP
1	A	1304	GLU
1	A	1309	ILE
1	A	1343	LEU
1	A	1358	THR
1	B	39	ASP
1	B	44	LYS
1	B	63	ARG
1	B	70	ARG
1	B	123	VAL
1	B	139	ARG
1	B	141	LYS
1	B	148	LYS
1	B	161	MET
1	B	165	ARG
1	B	285	GLN
1	B	294	LYS
1	B	302	LEU
1	B	340	ARG
1	B	381	GLU
1	B	393	LEU
1	B	401	LYS
1	B	403	ARG
1	B	414	ILE
1	B	420	HIS
1	B	425	ARG
1	B	447	ARG
1	B	517	TYR
1	B	540	LEU
1	B	587	PHE
1	B	588	ASN
1	B	598	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	605	ASP
1	B	623	LEU
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	807	GLN
1	B	829	ASP
1	B	842	VAL
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	875	VAL
1	B	890	LYS
1	B	895	ARG
1	B	902	LYS
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	1073	VAL
1	B	1076	LYS
1	B	1084	ARG
1	B	1089	MET
1	B	1091	GLN
1	B	1143	VAL
1	B	1148	LYS
1	B	1161	LYS
1	B	1168	ILE
1	B	1172	SER
1	B	1175	GLU
1	B	1177	ASN

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Mol	Chain	Res	Type
1	B	1182	LEU
1	B	1185	LYS
1	B	1196	ILE
1	B	1210	ARG
1	B	1224	ASN
1	B	1256	GLN
1	B	1300	LYS
1	B	1352	ILE
1	B	1358	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	GLN
1	A	412	HIS
1	A	420	HIS
1	A	556	ASN
1	A	721	HIS
1	A	723	HIS
1	A	726	ASN
1	A	807	GLN
1	A	885	GLN
1	A	920	GLN
1	A	983	HIS
1	A	1224	ASN
1	A	1234	ASN
1	A	1264	HIS
1	A	1272	GLN
1	A	1305	GLN
1	A	1311	HIS
1	A	1350	GLN
1	B	14	ASN
1	B	160	HIS
1	B	178	ASN
1	B	187	GLN
1	B	235	ASN
1	B	281	GLN
1	B	285	GLN
1	B	329	HIS
1	B	330	GLN
1	B	412	HIS
1	B	426	GLN

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Mol	Chain	Res	Type
1	B	641	HIS
1	B	721	HIS
1	B	803	ASN
1	B	807	GLN
1	B	980	ASN
1	B	982	HIS
1	B	1044	ASN
1	B	1262	HIS

### 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 oligosaccharides 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	2365	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	B	2365	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	2366	-	4,4,4	0.27	0	6,6,6	0.31	0
2	SO4	A	2364	-	4,4,4	0.19	0	6,6,6	0.09	0
2	SO4	B	2364	-	4,4,4	0.21	0	6,6,6	0.16	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	2365	SO4	2	0
2	B	2366	SO4	2	0
2	B	2364	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

### 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%)	0.49	121 (10%) <b>11</b> <b>9</b>	18, 65, 134, 180	0
1	B	1166/1372 (84%)	0.40	90 (7%) <b>19</b> <b>15</b>	17, 59, 129, 174	0
All	All	2310/2744 (84%)	0.45	211 (9%) <b>15</b> <b>11</b>	17, 62, 132, 180	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	TYR	8.8
1	A	567	ASP	7.5
1	B	564	LEU	5.8
1	A	407	ASN	5.7
1	A	527	VAL	5.6
1	A	1159	SER	5.6
1	A	838	VAL	5.4
1	B	1206	LEU	5.2
1	B	310	THR	5.1
1	B	567	ASP	5.1
1	A	834	SER	5.0
1	A	870	VAL	5.0
1	B	858	THR	4.9
1	A	788	ILE	4.9
1	A	406	ASP	4.8
1	B	859	ARG	4.7
1	A	799	HIS	4.6
1	A	836	TYR	4.6
1	B	539	PHE	4.6
1	A	503	PRO	4.6
1	B	502	LEU	4.5
1	A	1362	LEU	4.4
1	B	510	LYS	4.4
1	B	406	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1242	TYR	4.2
1	B	764	ALA	4.2
1	B	504	ASN	4.2
1	B	569	PHE	4.2
1	A	829	ASP	4.1
1	B	365	GLY	4.0
1	B	527	VAL	4.0
1	B	103	GLU	3.8
1	A	815	TYR	3.8
1	A	858	THR	3.7
1	A	1192	LYS	3.6
1	B	654	ARG	3.6
1	A	1363	SER	3.6
1	A	786	GLU	3.5
1	B	1240	SER	3.5
1	A	830	ILE	3.5
1	A	525	THR	3.5
1	B	791	LEU	3.5
1	B	570	LYS	3.4
1	A	791	LEU	3.4
1	A	1272	GLN	3.4
1	A	553	PHE	3.4
1	A	837	ASP	3.3
1	A	820	ARG	3.3
1	A	1146	VAL	3.3
1	B	829	ASP	3.3
1	A	4	LYS	3.3
1	B	1160	VAL	3.3
1	A	789	LYS	3.3
1	A	818	ASN	3.3
1	A	691	ARG	3.2
1	A	598	LEU	3.2
1	B	688	PHE	3.2
1	A	864	ARG	3.2
1	B	594	TYR	3.2
1	B	308	VAL	3.2
1	B	629	ARG	3.2
1	A	341	GLN	3.2
1	B	836	TYR	3.2
1	B	1191	LYS	3.1
1	A	1186	GLY	3.1
1	A	115	ARG	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	864	ARG	3.1
1	B	386	THR	3.1
1	A	814	TYR	3.1
1	A	718	ASP	3.1
1	A	404	THR	3.1
1	A	865	GLY	3.1
1	A	405	PHE	3.1
1	B	447	ARG	3.0
1	A	828	LEU	3.0
1	B	1241	HIS	3.0
1	A	564	LEU	3.0
1	A	551	LEU	2.9
1	B	877	LYS	2.9
1	B	555	THR	2.9
1	B	4	LYS	2.9
1	B	713	VAL	2.9
1	A	857	LEU	2.9
1	B	867	SER	2.9
1	B	407	ASN	2.9
1	B	587	PHE	2.9
1	B	834	SER	2.9
1	B	606	PHE	2.9
1	A	102	GLU	2.8
1	A	869	ASN	2.8
1	B	306	LEU	2.8
1	A	762	GLU	2.8
1	A	859	ARG	2.8
1	A	615	ILE	2.8
1	A	886	LEU	2.8
1	A	1144	LEU	2.8
1	A	1084	ARG	2.8
1	A	434	LYS	2.8
1	B	818	ASN	2.8
1	A	1181	PHE	2.8
1	B	260	GLU	2.8
1	B	661	ARG	2.8
1	B	815	TYR	2.8
1	A	777	SER	2.7
1	A	1265	TYR	2.7
1	B	801	VAL	2.7
1	A	781	MET	2.7
1	B	832	ARG	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1190	VAL	2.7
1	B	833	LEU	2.7
1	A	809	GLU	2.7
1	A	1334	LYS	2.7
1	B	1137	PRO	2.7
1	A	1195	ILE	2.6
1	A	832	ARG	2.6
1	A	677	LYS	2.6
1	A	1025	SER	2.6
1	B	875	VAL	2.6
1	B	593	THR	2.6
1	B	662	LEU	2.6
1	A	862	LYS	2.6
1	B	405	PHE	2.6
1	A	697	ILE	2.6
1	A	927	ILE	2.6
1	B	305	ILE	2.6
1	A	801	VAL	2.6
1	B	1363	SER	2.5
1	A	559	VAL	2.5
1	B	220	ARG	2.5
1	B	370	GLU	2.5
1	A	215	ARG	2.5
1	A	811	LEU	2.5
1	B	259	ALA	2.5
1	A	856	VAL	2.5
1	B	817	GLN	2.5
1	A	642	LEU	2.4
1	A	1026	GLU	2.4
1	A	594	TYR	2.4
1	A	1027	GLN	2.4
1	B	1188	LYS	2.4
1	A	1293	ALA	2.4
1	A	1194	LEU	2.4
1	A	1185	LYS	2.4
1	B	655	ARG	2.4
1	A	670	ILE	2.4
1	B	773	GLY	2.4
1	B	871	PRO	2.4
1	A	305	ILE	2.4
1	B	597	LEU	2.4
1	B	873	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	672	ASP	2.4
1	A	597	LEU	2.3
1	A	1299	ASP	2.3
1	A	883	TRP	2.3
1	B	408	GLY	2.3
1	A	1328	ASP	2.3
1	A	123	VAL	2.3
1	A	713	VAL	2.3
1	B	673	LYS	2.3
1	B	880	LYS	2.3
1	B	182	ASP	2.3
1	B	676	GLY	2.3
1	A	589	ALA	2.3
1	A	679	ILE	2.3
1	A	1137	PRO	2.3
1	A	549	VAL	2.3
1	A	887	LEU	2.3
1	A	446	PHE	2.3
1	B	830	ILE	2.2
1	B	776	ASN	2.2
1	B	307	ARG	2.2
1	A	835	ASP	2.2
1	A	764	ALA	2.2
1	A	784	ILE	2.2
1	B	862	LYS	2.2
1	B	1294	TYR	2.2
1	A	558	LYS	2.2
1	A	852	ILE	2.2
1	A	370	GLU	2.2
1	B	523	GLU	2.2
1	A	908	LEU	2.2
1	A	1017	ASP	2.2
1	A	875	VAL	2.2
1	A	1259	VAL	2.2
1	A	826	GLN	2.2
1	A	314	LYS	2.2
1	B	1215	ALA	2.1
1	A	1228	LEU	2.1
1	B	56	GLY	2.1
1	B	303	SER	2.1
1	A	800	PRO	2.1
1	A	1196	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	57	GLU	2.1
1	A	447	ARG	2.1
1	A	385	GLY	2.1
1	A	601	ILE	2.1
1	B	354	GLN	2.1
1	A	39	ASP	2.0
1	A	566	GLU	2.0
1	A	661	ARG	2.0
1	A	562	LYS	2.0
1	B	800	PRO	2.0
1	B	1256	GLN	2.0
1	A	881	ASN	2.0
1	B	870	VAL	2.0
1	B	635	ARG	2.0
1	A	384	ASP	2.0
1	A	872	SER	2.0
1	B	960	SER	2.0
1	B	683	LEU	2.0
1	A	888	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	2367	1/1	0.32	0.19	54,54,54,54	0
2	SO4	B	2366	5/5	0.86	0.20	30,30,30,30	0
2	SO4	A	2365	5/5	0.88	0.12	88,99,106,106	0
2	SO4	B	2365	5/5	0.88	0.13	80,91,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	2364	5/5	0.96	0.10	21,25,39,57	0
2	SO4	A	2364	5/5	0.96	0.10	32,39,54,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.