



Full wwPDB X-ray Structure Validation Report i

Mar 31, 2014 – 03:52 PM BST

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

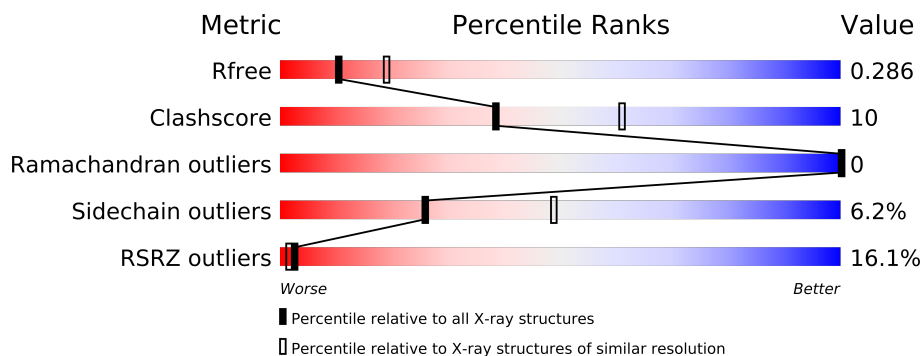
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23004
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

1 Overall quality at a glance

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}	66092	1940 (2.64-2.60)
Clashscore	79885	2404 (2.64-2.60)
Ramachandran outliers	78287	2360 (2.64-2.60)
Sidechain outliers	78261	2360 (2.64-2.60)
RSRZ outliers	66119	1939 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1372	
1	B	1372	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
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 deuterium.

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: O₄S).



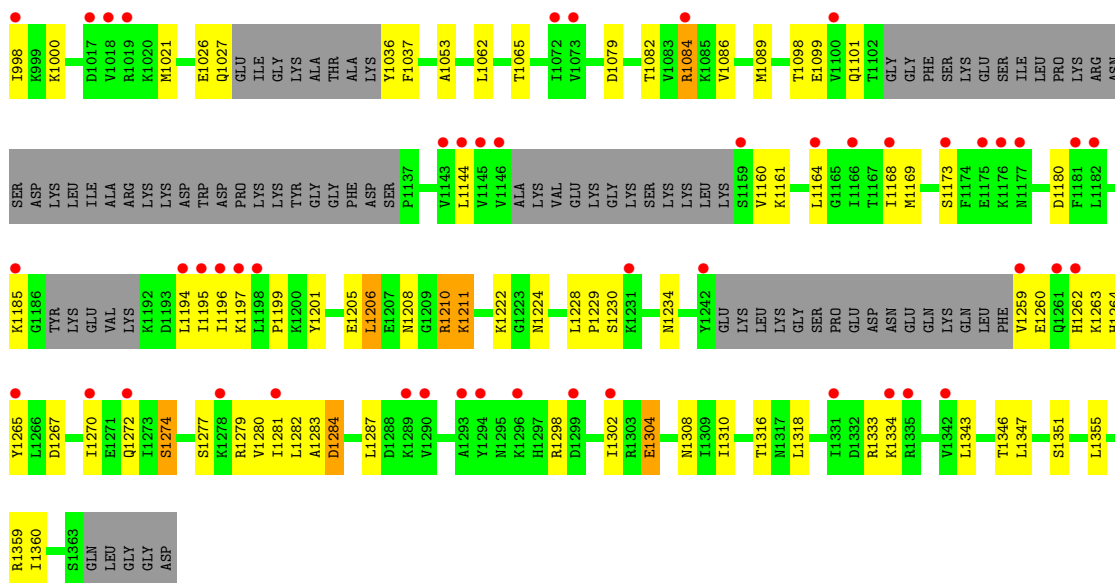
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- 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		

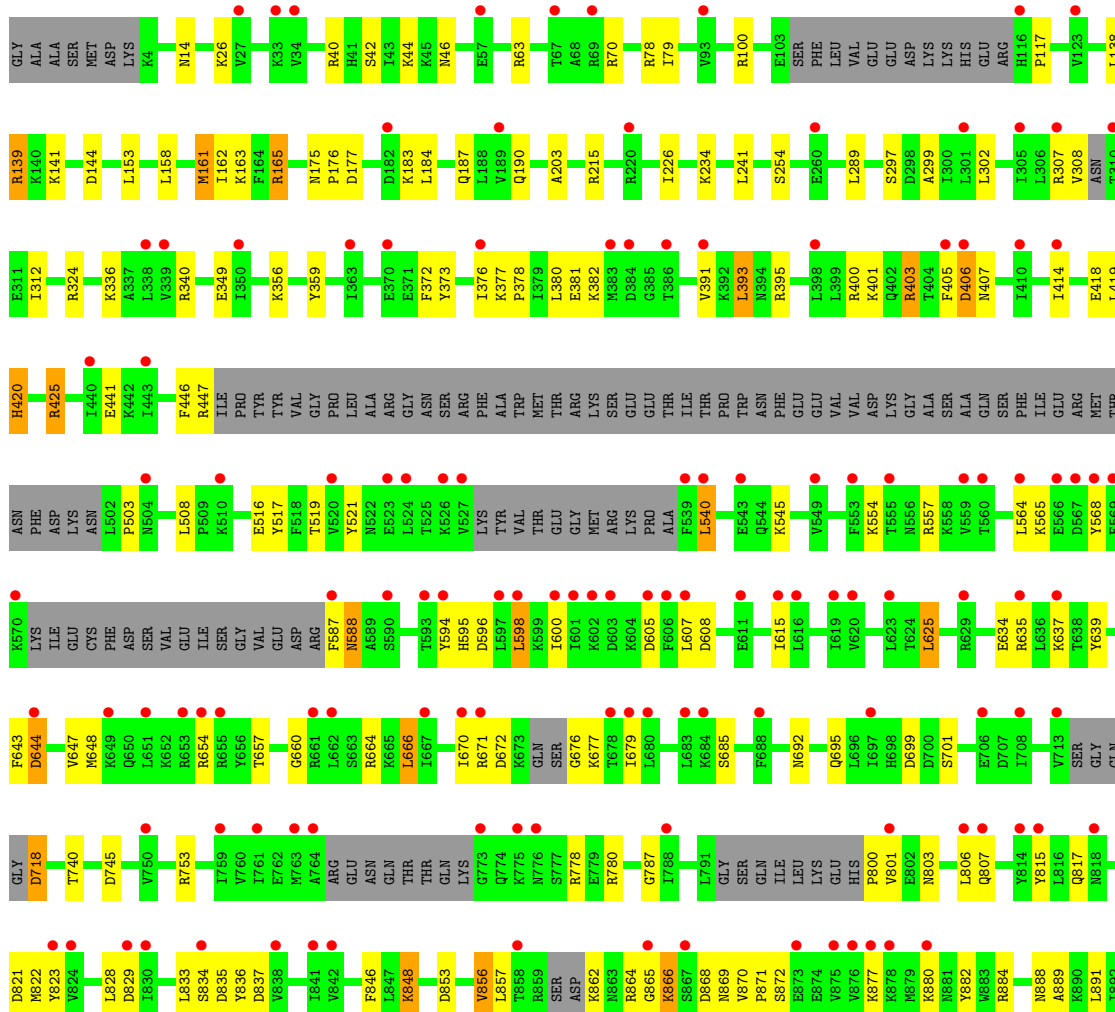
- Molecule 4 is water.

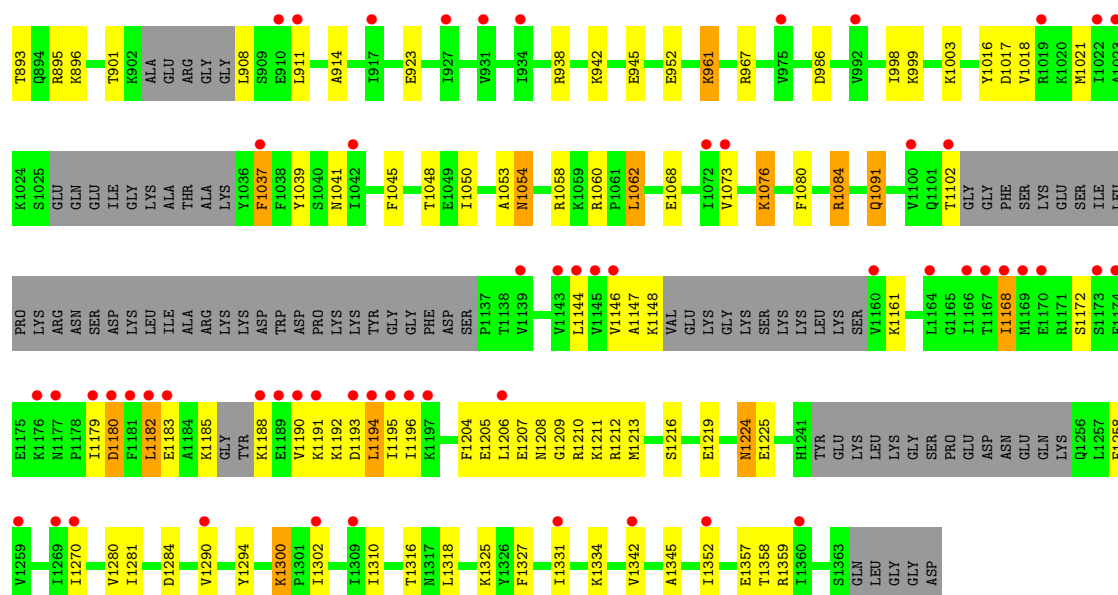
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	111	Total	O	0	0
			111	111		



• Molecule 1: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.252 , 0.286 0.252 , 0.286	Depositor DCC
R_{free} test set	2421 reflections (2.62%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 92492 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	38285	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9316	9456	0	168	0
1	B	9546	9738	0	206	0
2	A	10	0	0	0	0
2	B	15	0	0	5	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	92	0	0	7	0
4	B	111	0	0	13	0
All	All	19091	19194	0	374	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (374) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1179:ILE:O	1:B:1183:GLU:HG3	1.17	1.29
1:B:1191:LYS:HE2	1:B:1194:LEU:CD2	1.78	1.14
1:B:1179:ILE:HD12	1:B:1192:LYS:CD	1.80	1.12
1:B:1179:ILE:CD1	1:B:1192:LYS:HD2	1.81	1.10
1:B:1179:ILE:O	1:B:1183:GLU:CG	2.07	1.02
1:B:1191:LYS:CE	1:B:1194:LEU:HD22	1.91	1.00
1:B:1179:ILE:HD12	1:B:1192:LYS:HD2	0.98	0.95
1:A:46:ASN:ND2	1:A:1089:MET:SD	2.40	0.94
1:B:1045:PHE:HA	1:B:1060:ARG:NH2	1.82	0.94
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:HD22	2.03	0.89
1:B:1179:ILE:HG23	1:B:1183:GLU:OE2	1.72	0.88
1:B:1191:LYS:HE2	1:B:1194:LEU:HD22	1.48	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:1206:LEU:O	1:B:1207:GLU:HG2	1.73	0.87
1:B:1207:GLU:HG3	1:B:1208:ASN:H	1.38	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:B:1206:LEU:HD22	1:B:1345:ALA:HA	1.59	0.82
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:A:848:LYS:O	1:A:961:LYS:NZ	2.12	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: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:1191:LYS:HD3	1:B:1194:LEU:HD22	1.63	0.78
1:B:1334:LYS:NZ	4:B:2103:HOH:O	2.17	0.77
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.19	0.75
1:B:1045:PHE:HA	1:B:1060:ARG:CZ	2.17	0.75
1:B:554:LYS:NZ	1:B:608:ASP:OD1	2.21	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:GLU:OE1	1:A:437:ARG:NH1	2.21	0.74
1:B:672:ASP:O	1:B:676:GLY:N	2.21	0.73
1:A:1304:GLU:O	1:A:1308:ASN:ND2	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:HD13	2.03	0.72
1:B:1045:PHE:HA	1:B:1060:ARG:HH21	1.55	0.72
1:A:828:LEU:HA	1:A:833:LEU:HD11	1.71	0.72
1:B:254:SER:OG	4:B:2040:HOH:O	2.07	0.72
1:B:1206:LEU:CD2	1:B:1345:ALA:HA	2.22	0.70
1:B:1325:LYS:NZ	1:B:1327:PHE:O	2.24	0.70
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:A:218:LYS:NZ	1:A:406:ASP:OD1	2.25	0.69
1:B:866:LYS:NZ	1:B:870:VAL:O	2.25	0.69
1:A:870:VAL:HG13	1:A:871:PRO:HD2	1.74	0.69
1:B:1144:LEU:HD23	1:B:1196:ILE:HD11	1.75	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:A:1230:SER:O	1:A:1234:ASN:ND2	2.27	0.66
1:B:1206:LEU:HD22	1:B:1345:ALA:CA	2.25	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:B:596:ASP:O	1:B:654:ARG:NH2	2.30	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:B:1195:ILE:C	1:B:1196:ILE:HD13	2.18	0.64
1:A:1282:LEU:O	1:A:1334:LYS:NZ	2.30	0.64
1:A:21:ILE:HD13	1:A:991:ALA:HB1	1.80	0.64
1:A:977:GLU:HG3	1:A:1310:ILE:CG2	2.28	0.63
1:B:967:ARG:NH1	1:B:986:ASP:OD1	2.31	0.63
1:B:1207:GLU:HG3	1:B:1208:ASN:N	2.11	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:A:551:LEU:O	1:A:555:THR:OG1	2.18	0.62
1:B:165:ARG:NH2	1:B:446:PHE:O	2.31	0.61
1:B:540:LEU:HD23	1:B:545:LYS:CG	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	Distance(Å)	Clash(Å)
1:B:100:ARG:NH1	1:B:625:LEU:O	2.34	0.61
1:B:540:LEU:HD23	1:B:545:LYS:HG3	1.84	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:B:420:HIS:NE2	1:B:441:GLU:OE1	2.36	0.59
1:B:1179:ILE:CG1	1:B:1192:LYS:HD2	2.33	0.59
1:A:870:VAL:HG13	1:A:871:PRO:CD	2.32	0.59
1:B:643:PHE:CB	1:B:648:MET:HE1	2.32	0.59
1:A:158:LEU:HD23	1:A:419:LEU:HD13	1.84	0.59
1:A:1270:ILE:O	1:A:1274:SER:OG	2.19	0.59
1:B:1179:ILE:HG23	1:B:1183:GLU:CG	2.33	0.58
1:A:1206:LEU:CD1	1:A:1210:ARG:HG2	2.32	0.58
1:B:888:ASN:OD1	1:B:889:ALA:N	2.35	0.58
1:A:54:ASP:OD2	1:A:1201:TYR:OH	2.21	0.58
1:A:874:GLU:HA	1:A:877:LYS:HG3	1.82	0.58
1:A:1211:LYS:H	1:A:1224:ASN:HD22	1.51	0.58
1:B:1191:LYS:HE2	1:B:1194:LEU:HD21	1.76	0.58
1:B:780:ARG:NH1	1:B:806:LEU:O	2.35	0.58
1:B:600:ILE:HG23	1:B:647:VAL:HG11	1.85	0.58
1:A:1206:LEU:HD13	1:A:1210:ARG:HG2	1.86	0.58
1:B:837:ASP:OD2	1:B:862:LYS:N	2.37	0.58
1:A:150:ASP:OD2	1:A:152:ARG:NH2	2.36	0.58
1:B:177:ASP:OD1	1:B:183:LYS:NZ	2.37	0.57
1:A:1194:LEU:HD11	1:A:1196:ILE:HD12	1.85	0.57
1:B:187:GLN:NE2	1:B:190:GLN:OE1	2.37	0.57
1:A:887:LEU:HD12	1:A:897:PHE:CG	2.40	0.57
1:B:1179:ILE:HG23	1:B:1183:GLU:CD	2.24	0.57
1:A:247:GLY:HA2	1:A:407:ASN:HB2	1.86	0.57
1:B:817:GLN:O	1:B:882:TYR:OH	2.24	0.56
1:B:643:PHE:HB2	1:B:648:MET:HE1	1.87	0.56
1:B:588:ASN:OD1	1:B:588:ASN:N	2.37	0.56
1:B:308:VAL:HG23	1:B:312:ILE:HG22	1.86	0.56
1:B:139:ARG:NH1	1:B:418:GLU:OE1	2.38	0.56
1:A:780:ARG:NH1	1:A:806:LEU:O	2.36	0.56
1:B:165:ARG:NH1	2:B:2364:SO4:O4	2.38	0.56
1:B:1039:TYR:CD2	1:B:1058:ARG:NH1	2.73	0.56
1:B:1207:GLU:O	1:B:1209:GLY:N	2.35	0.56
1:A:781:MET:SD	1:A:803:ASN:HB2	2.46	0.56
1:B:828:LEU:HD23	1:B:833:LEU:HD12	1.88	0.56
1:A:1144:LEU:HD21	1:A:1196:ILE:HD13	1.88	0.55
1:A:339:VAL:HA	1:A:383:MET:HE2	1.87	0.55
1:A:139:ARG:NH1	1:A:418:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1086:VAL:HA	1:A:1089:MET:HE1	1.88	0.55
1:A:607:LEU:HD21	1:A:616:LEU:CD2	2.37	0.55
1:B:699:ASP:OD1	1:B:701:SER:OG	2.25	0.55
1:B:1191:LYS:CE	1:B:1194:LEU:CD2	2.54	0.55
1:A:66:ARG:NH1	4:A:2008:HOH:O	2.39	0.54
1:B:1179:ILE:HA	1:B:1182:LEU:HD13	1.88	0.54
1:A:874:GLU:HA	1:A:877:LYS:HE2	1.88	0.54
1:A:607:LEU:HD21	1:A:616:LEU:HD22	1.90	0.54
1:A:746:GLU:OE2	1:A:1351:SER:OG	2.25	0.54
1:B:70:ARG:NH1	1:B:718:ASP:OD2	2.40	0.54
1:B:1179:ILE:CG2	1:B:1183:GLU:OE2	2.49	0.54
1:A:799:HIS:CB	1:A:800:PRO:HD2	2.37	0.54
1:A:244:LEU:O	1:A:407:ASN:ND2	2.40	0.54
1:B:870:VAL:HG21	1:B:871:PRO:HD2	1.90	0.54
1:A:847:LEU:HD23	1:A:916:PHE:CG	2.43	0.53
1:B:1039:TYR:HD2	1:B:1058:ARG:NH1	2.06	0.53
1:A:1205:GLU:OE1	1:A:1359:ARG:NH2	2.37	0.53
1:A:46:ASN:N	1:A:46:ASN:OD1	2.41	0.53
1:B:800:PRO:N	1:B:815:TYR:HH	2.06	0.53
1:A:887:LEU:HD21	1:A:892:ILE:HG13	1.90	0.53
1:B:869:ASN:OD1	1:B:870:VAL:N	2.41	0.53
1:A:427:GLU:HB2	1:A:434:LYS:CG	2.38	0.53
1:B:403:ARG:NH2	2:B:2365:SO4:S	2.80	0.53
1:B:1102:THR:HA	1:B:1168:ILE:HD11	1.90	0.53
1:B:1281:ILE:HD12	1:B:1316:THR:HA	1.91	0.53
1:B:401:LYS:HB3	1:B:403:ARG:HE	1.74	0.52
1:A:401:LYS:HB3	1:A:403:ARG:HE	1.75	0.52
1:A:976:ARG:HH11	1:A:976:ARG:HG3	1.73	0.52
1:A:967:ARG:NH1	1:A:986:ASP:OD1	2.43	0.52
1:A:1263:LYS:HE2	1:A:1302:ILE:CD1	2.40	0.52
1:B:1146:VAL:HG23	1:B:1161:LYS:HG3	1.92	0.52
1:B:307:ARG:O	1:B:308:VAL:HB	2.10	0.52
1:A:1210:ARG:HB2	1:A:1280:VAL:HG11	1.92	0.52
1:B:215:ARG:HH21	1:B:395:ARG:CZ	2.23	0.52
1:A:349:GLU:HG3	1:A:356:LYS:HD3	1.92	0.52
1:A:825:ASP:HB2	1:A:879:MET:HE2	1.92	0.52
1:A:877:LYS:NZ	1:A:902:LYS:O	2.43	0.52
1:B:828:LEU:CD2	1:B:833:LEU:HD12	2.40	0.52
1:B:868:ASP:HA	1:B:1054:ASN:ND2	2.25	0.52
1:A:821:ASP:N	1:A:828:LEU:HG	2.26	0.51
1:B:648:MET:HE3	1:B:648:MET:HA	1.92	0.51
1:B:158:LEU:HA	1:B:161:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:877:LYS:HE2	1:B:880:LYS:NZ	2.26	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:508:LEU:HD22	1:B:664:ARG:CG	2.40	0.51
1:B:226:ILE:CD1	1:B:234:LYS:HG3	2.40	0.51
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.43	0.51
1:A:822:MET:HG2	1:A:856:VAL:HG12	1.92	0.51
1:A:1260:GLU:HB3	1:A:1263:LYS:HE3	1.93	0.51
1:A:1194:LEU:HB3	1:A:1196:ILE:CG1	2.41	0.51
1:B:565:LYS:HA	1:B:568:TYR:HD1	1.75	0.51
1:B:175:ASN:HB2	1:B:176:PRO:HD2	1.92	0.50
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:801:VAL:HB	1:B:815:TYR:CZ	2.46	0.50
1:A:45:LYS:HE3	1:A:1355:LEU:HA	1.94	0.50
1:B:14:ASN:ND2	4:B:2006:HOH:O	2.42	0.50
1:A:1160:VAL:HG13	1:A:1161:LYS:N	2.27	0.50
1:A:844:GLN:HG3	1:A:848:LYS:HG2	1.94	0.50
1:B:79:ILE:HD12	1:B:163:LYS:HG3	1.93	0.50
1:A:522:ASN:HA	1:A:525:THR:HG21	1.93	0.50
1:A:1194:LEU:HB3	1:A:1196:ILE:HD12	1.92	0.50
1:A:175:ASN:HB2	1:A:176:PRO:HD2	1.93	0.49
1:B:1062:LEU:HD21	1:B:1076:LYS:HB2	1.93	0.49
1:B:1300:LYS:HE2	1:B:1327:PHE:CE1	2.46	0.49
1:A:1224:ASN:ND2	1:A:1280:VAL:HG12	2.27	0.49
1:B:666:LEU:HD21	1:B:679:ILE:HD13	1.93	0.49
1:A:1144:LEU:HD21	1:A:1196:ILE:CD1	2.42	0.49
1:B:877:LYS:NZ	1:B:901:THR:O	2.34	0.49
1:A:1281:ILE:HD12	1:A:1316:THR:HA	1.95	0.49
1:A:867:SER:OG	1:A:868:ASP:N	2.46	0.49
1:A:1144:LEU:HB3	1:A:1196:ILE:HD13	1.95	0.49
1:A:677:LYS:HD2	1:A:681:ASP:HB3	1.95	0.48
1:B:644:ASP:N	1:B:644:ASP:OD1	2.46	0.48
1:A:847:LEU:HD23	1:A:916:PHE:CD1	2.48	0.48
1:B:942:LYS:NZ	1:B:952:GLU:OE2	2.47	0.48
1:A:150:ASP:OD1	1:A:151:LEU:N	2.46	0.48
1:A:822:MET:HE2	1:A:886:LEU:CD1	2.43	0.48
1:A:1164:LEU:HD22	1:A:1185:LYS:CD	2.44	0.48
1:B:1225:GLU:OE1	4:B:2080:HOH:O	2.20	0.48
1:B:241:LEU:HD11	1:B:289:LEU:HD23	1.95	0.48
1:B:1045:PHE:CA	1:B:1060:ARG:HH21	2.23	0.47
1:A:377:LYS:N	1:A:378:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:564:LEU:HG	1:B:568:TYR:HE1	1.78	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:866:LYS:HZ2	1:B:871:PRO:HA	1.78	0.47
1:A:184:LEU:CD1	1:A:299:ALA:HB3	2.43	0.47
1:A:601:ILE:HD13	1:A:643:PHE:CE1	2.50	0.47
1:A:866:LYS:HD3	1:A:1053:ALA:HB2	1.96	0.47
1:A:1079:ASP:O	1:A:1082:THR:OG1	2.31	0.47
1:A:11:ILE:HG12	1:A:740:THR:HG22	1.96	0.47
1:B:349:GLU:HG3	1:B:356:LYS:HD3	1.97	0.47
1:A:512:SER:OG	1:A:617:GLU:OE1	2.33	0.47
1:B:503:PRO:HD2	1:B:666:LEU:HD13	1.97	0.47
1:B:349:GLU:CG	1:B:356:LYS:HD3	2.45	0.47
1:A:125:GLU:OE2	1:A:129:HIS:NE2	2.47	0.47
1:B:1206:LEU:HD22	1:B:1345:ALA:CB	2.45	0.46
1:B:866:LYS:HD2	1:B:1053:ALA:HB2	1.96	0.46
1:A:416:LEU:HD21	1:A:419:LEU:HD21	1.96	0.46
1:B:848:LYS:O	1:B:961:LYS:NZ	2.48	0.46
1:A:1263:LYS:HE2	1:A:1302:ILE:HD12	1.98	0.46
1:B:557:ARG:HA	1:B:595:HIS:CD2	2.50	0.46
1:A:1282:LEU:N	1:A:1282:LEU:HD21	2.30	0.46
1:A:893:THR:HG21	1:A:896:LYS:H	1.80	0.46
1:B:1048:THR:HG23	1:B:1076:LYS:HG2	1.98	0.46
1:B:40:ARG:O	1:B:42:SER:N	2.46	0.46
1:B:670:ILE:HG23	1:B:671:ARG:N	2.31	0.46
1:B:1045:PHE:HA	1:B:1060:ARG:NE	2.30	0.46
1:B:1270:ILE:HD11	1:B:1294:TYR:CD2	2.51	0.46
1:B:1191:LYS:CD	1:B:1194:LEU:CD2	2.86	0.46
1:B:1302:ILE:HD13	1:B:1302:ILE:H	1.81	0.46
1:A:635:ARG:CG	1:A:635:ARG:HH11	2.28	0.46
1:B:203:ALA:N	4:B:2036:HOH:O	2.43	0.46
1:B:1207:GLU:CG	1:B:1208:ASN:N	2.73	0.46
1:A:828:LEU:HA	1:A:833:LEU:CD1	2.43	0.45
1:A:1021:MET:O	1:A:1036:TYR:N	2.49	0.45
1:B:226:ILE:HD12	1:B:234:LYS:CG	2.47	0.45
1:B:594:TYR:OH	1:B:608:ASP:OD2	2.34	0.45
1:A:803:ASN:HA	1:A:806:LEU:HD13	1.99	0.45
1:A:21:ILE:HD12	1:A:988:TYR:CD1	2.52	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:692:ASN:HB3	1:B:695:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:ILE:HG21	1:A:25:TYR:HA	1.98	0.45
1:B:870:VAL:CG2	1:B:871:PRO:HD2	2.47	0.45
1:A:822:MET:CG	1:A:856:VAL:HG12	2.47	0.45
1:B:822:MET:CG	1:B:856:VAL:HG22	2.46	0.45
1:A:972:PHE:HE1	1:A:1084:ARG:CG	2.30	0.45
1:A:820:ARG:HB2	1:A:882:TYR:OH	2.17	0.45
1:B:893:THR:HG21	1:B:896:LYS:H	1.82	0.45
1:A:821:ASP:CA	1:A:828:LEU:HG	2.47	0.44
1:A:1098:THR:HB	1:A:1199:PRO:HB2	1.99	0.44
1:B:1003:LYS:HB2	1:B:1021:MET:CE	2.48	0.44
1:B:46:ASN:ND2	1:B:1091:GLN:HG3	2.32	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:A:1206:LEU:HD13	1:A:1210:ARG:CG	2.45	0.44
1:B:822:MET:HG2	1:B:856:VAL:HG22	1.98	0.44
1:A:427:GLU:HB2	1:A:434:LYS:HG2	1.99	0.44
1:B:871:PRO:HD2	1:B:908:LEU:HG	2.00	0.44
1:A:887:LEU:HD22	1:A:897:PHE:HB2	1.99	0.44
1:B:391:VAL:HG13	1:B:395:ARG:HD3	2.00	0.44
1:B:1204:PHE:CE1	1:B:1342:VAL:HG11	2.52	0.44
1:B:1194:LEU:O	1:B:1194:LEU:HG	2.17	0.44
1:A:977:GLU:HG3	1:A:1310:ILE:HG21	1.97	0.44
1:A:823:TYR:CG	1:A:865:GLY:HA3	2.53	0.44
1:A:54:ASP:O	1:A:735:LYS:NZ	2.51	0.44
1:B:226:ILE:CD1	1:B:234:LYS:CG	2.95	0.44
1:B:666:LEU:HD21	1:B:679:ILE:CD1	2.48	0.44
1:A:866:LYS:HA	1:A:866:LYS:CE	2.47	0.44
1:B:184:LEU:HD11	1:B:299:ALA:HB3	1.99	0.44
1:B:1182:LEU:HD11	1:B:1190:VAL:HG22	2.00	0.43
1:B:508:LEU:O	1:B:660:GLY:N	2.46	0.43
1:B:380:LEU:HD13	1:B:393:LEU:HD13	2.00	0.43
1:A:1195:ILE:CG2	1:A:1197:LYS:HE2	2.48	0.43
1:A:1026:GLU:O	1:A:1027:GLN:HG3	2.18	0.43
1:A:825:ASP:N	1:A:879:MET:HE2	2.33	0.43
1:B:1270:ILE:HD11	1:B:1294:TYR:CG	2.53	0.43
1:A:1347:LEU:N	1:A:1360:ILE:O	2.51	0.43
1:A:978:ILE:HD13	1:A:1228:LEU:HB3	2.00	0.43
1:A:976:ARG:HH11	1:A:976:ARG:CG	2.32	0.43
1:A:829:ASP:H	1:A:833:LEU:CD1	2.31	0.43
1:B:871:PRO:CD	1:B:908:LEU:HG	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:339:VAL:CA	1:A:383:MET:HE2	2.49	0.43
1:B:835:ASP:N	1:B:835:ASP:OD1	2.51	0.43
1:B:778:ARG:HA	1:B:803:ASN:HD22	1.83	0.43
1:B:1045:PHE:CB	1:B:1060:ARG:HH21	2.32	0.43
1:A:373:TYR:O	1:A:377:LYS:HG3	2.18	0.43
1:B:823:TYR:CG	1:B:865:GLY:HA3	2.54	0.43
1:A:888:ASN:OD1	1:A:889:ALA:N	2.52	0.43
1:A:1283:ALA:HB3	1:A:1334:LYS:HE2	2.01	0.43
1:B:1037:PHE:CD1	1:B:1037:PHE:N	2.86	0.43
1:B:540:LEU:HD23	1:B:545:LYS:HG2	2.00	0.42
1:A:822:MET:CB	1:A:856:VAL:HG12	2.48	0.42
1:A:1228:LEU:HA	1:A:1272:GLN:HE22	1.84	0.42
1:B:634:GLU:HA	1:B:637:LYS:HE3	2.01	0.42
1:A:801:VAL:CG2	1:A:815:TYR:CE1	3.02	0.42
1:B:372:PHE:CZ	1:B:376:ILE:CD1	3.02	0.42
1:B:377:LYS:N	1:B:378:PRO:HD2	2.34	0.42
1:B:138:LEU:HD12	1:B:153:LEU:HB3	2.00	0.42
1:B:1224:ASN:CG	1:B:1280:VAL:HG12	2.38	0.42
1:B:834:SER:HG	1:B:835:ASP:N	2.17	0.42
1:B:373:TYR:CD2	1:B:393:LEU:HD21	2.54	0.42
1:B:1216:SER:OG	1:B:1219:GLU:N	2.52	0.42
1:A:158:LEU:HD23	1:A:419:LEU:CD1	2.49	0.42
1:A:368:SER:HB2	1:A:371:GLU:H	1.84	0.42
1:B:26:LYS:NZ	4:B:2008:HOH:O	2.52	0.42
1:A:704:PHE:O	1:A:707:ASP:N	2.52	0.42
1:A:427:GLU:HB2	1:A:434:LYS:HG3	1.99	0.42
1:B:1211:LYS:H	1:B:1224:ASN:HD22	1.68	0.42
1:B:1050:ILE:HD12	1:B:1060:ARG:HD2	2.00	0.42
1:A:869:ASN:HA	1:A:1053:ALA:HB1	2.01	0.42
1:A:202:ASN:OD1	1:A:204:SER:N	2.47	0.42
1:A:564:LEU:HD23	1:A:587:PHE:HE2	1.85	0.42
1:B:1180:ASP:N	1:B:1180:ASP:OD1	2.53	0.42
1:A:184:LEU:HD13	1:A:299:ALA:HB3	2.02	0.41
1:A:824:VAL:O	1:A:824:VAL:HG13	2.20	0.41
1:B:1213:MET:CE	1:B:1318:LEU:HD12	2.50	0.41
1:A:609:ASN:OD1	1:A:611:GLU:N	2.51	0.41
1:B:516:GLU:O	1:B:519:THR:HG23	2.20	0.41
1:B:1003:LYS:CE	1:B:1068:GLU:OE1	2.67	0.41
1:B:359:TYR:HA	1:B:372:PHE:CE1	2.55	0.41
1:B:745:ASP:OD2	1:B:938:ARG:NH2	2.53	0.41
1:A:801:VAL:HG23	1:A:815:TYR:CZ	2.55	0.41
1:B:540:LEU:CD2	1:B:545:LYS:HG3	2.49	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:MET:HE1	1:B:419:LEU:HB2	2.02	0.41
1:A:521:TYR:CE1	1:A:549:VAL:HG22	2.55	0.41
1:B:1281:ILE:CD1	1:B:1316:THR:HG23	2.50	0.41
1:B:615:ILE:HG21	1:B:639:TYR:CE1	2.55	0.41
1:A:1205:GLU:HB3	1:A:1346:THR:CG2	2.51	0.41
1:B:828:LEU:HD21	1:B:828:LEU:HA	1.91	0.41
1:B:117:PRO:HG2	1:B:635:ARG:NH2	2.36	0.41
1:A:881:ASN:N	1:A:881:ASN:OD1	2.52	0.41
1:A:240:ASN:ND2	1:A:255:ASN:OD1	2.52	0.41
1:B:1179:ILE:C	1:B:1183:GLU:HG3	2.18	0.41
1:A:427:GLU:HG3	1:A:434:LYS:HE3	2.03	0.41
1:B:833:LEU:C	1:B:836:TYR:H	2.24	0.41
1:B:184:LEU:CD1	1:B:299:ALA:HB3	2.50	0.41
1:B:378:PRO:O	1:B:382:LYS:HG2	2.21	0.41
1:B:999:LYS:HB3	1:B:1073:VAL:HG13	2.03	0.41
1:A:266:LEU:HD21	1:A:271:TYR:CZ	2.56	0.41
1:B:598:LEU:HG	1:B:607:LEU:HD13	2.02	0.41
1:A:828:LEU:HD23	1:A:833:LEU:HB3	2.03	0.41
1:A:882:TYR:CE2	1:A:886:LEU:HD12	2.55	0.41
1:B:372:PHE:CZ	1:B:376:ILE:HD13	2.56	0.41
1:B:1290:VAL:CG2	1:B:1331:ILE:CD1	2.99	0.41
1:A:1222:LYS:O	1:A:1318:LEU:HD13	2.21	0.41
1:B:600:ILE:CD1	1:B:654:ARG:NH2	2.84	0.40
1:A:635:ARG:NH1	1:A:635:ARG:HG2	2.35	0.40
1:B:1204:PHE:CD1	1:B:1342:VAL:HG11	2.56	0.40
1:A:763:MET:CG	1:A:928:THR:HG23	2.51	0.40
1:A:880:LYS:HA	1:A:883:TRP:CE3	2.55	0.40
1:B:1003:LYS:HD2	1:B:1016:TYR:CE2	2.56	0.40
1:A:892:ILE:HB	1:A:896:LYS:HD2	2.03	0.40
1:B:868:ASP:HA	1:B:1054:ASN:HD21	1.85	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:914:ALA:HA	1:B:1018:VAL:HG22	2.04	0.40
1:A:1194:LEU:CB	1:A:1196:ILE:HD12	2.51	0.40
1:B:828:LEU:CD2	1:B:833:LEU:HD22	2.51	0.40
1:A:787:GLY:HA3	1:A:891:LEU:HD22	2.02	0.40
1:B:677:LYS:NZ	1:B:685:SER:O	2.54	0.40
1:A:1086:VAL:HA	1:A:1089:MET:CE	2.50	0.40
1:B:139:ARG:CZ	1:B:161:MET:HG3	2.52	0.40
1:B:1146:VAL:HG23	1:B:1161:LYS:CG	2.51	0.40
1:A:1262:HIS:HB3	1:A:1265:TYR:CD1	2.56	0.40
1:A:1277:SER:HB2	1:A:1287:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:787:GLY:HA3	1:B:891:LEU:HD22	2.03	0.40
1:B:596:ASP:HB3	1:B:654:ARG:CZ	2.51	0.40
1:B:1284:ASP:OD1	4:B:2103:HOH:O	2.21	0.40
1:A:1229:PRO:CD	1:A:1272:GLN:HE22	2.35	0.40
1:B:336:LYS:NZ	4:B:2056:HOH:O	2.47	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	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 ⓘ

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%)	26	50
1	B	1050/1228 (86%)	984 (94%)	66 (6%)	25	48
All	All	2069/2456 (84%)	1941 (94%)	128 (6%)	26	49

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	1358	THR

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

Mol	Chain	Res	Type
1	A	83	GLN
1	A	224	ASN
1	A	228	GLN
1	A	240	ASN
1	A	285	GLN
1	A	412	HIS
1	A	436	ASN
1	A	504	ASN
1	A	612	ASN
1	A	721	HIS
1	A	723	HIS
1	A	726	ASN
1	A	807	GLN
1	A	982	HIS
1	A	1091	GLN
1	A	1101	GLN
1	A	1224	ASN
1	A	1234	ASN
1	A	1264	HIS
1	A	1272	GLN
1	A	1305	GLN
1	A	1308	ASN
1	A	1311	HIS
1	B	14	ASN
1	B	46	ASN
1	B	83	GLN
1	B	160	HIS
1	B	167	HIS
1	B	187	GLN
1	B	235	ASN
1	B	240	ASN
1	B	285	GLN
1	B	329	HIS
1	B	369	GLN
1	B	415	HIS
1	B	436	ASN
1	B	511	HIS

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Mol	Chain	Res	Type
1	B	612	ASN
1	B	641	HIS
1	B	690	ASN
1	B	726	ASN
1	B	982	HIS
1	B	1044	ASN
1	B	1093	ASN
1	B	1101	GLN
1	B	1177	ASN
1	B	1262	HIS
1	B	1297	HIS
1	B	1308	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	0.32	0	6,6,6	0.10	0
2	SO4	A	2365	-	4,4,4	0.21	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	2364	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	B	2365	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	B	2366	-	4,4,4	0.13	0	6,6,6	0.36	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1144/1372 (83%)	0.89	185 (16%) 2 1	17, 59, 125, 164	0
1	B	1166/1372 (84%)	0.93	188 (16%) 2 1	16, 54, 119, 162	0
All	All	2310/2744 (84%)	0.91	373 (16%) 2 1	16, 57, 122, 164	0

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	TYR	11.6
1	B	527	VAL	10.2
1	A	1195	ILE	7.9
1	B	1190	VAL	7.7
1	A	527	VAL	7.7
1	B	564	LEU	7.6
1	A	525	THR	7.6
1	B	801	VAL	7.3
1	B	570	LYS	7.2
1	A	1144	LEU	6.9
1	A	830	ILE	6.8
1	A	824	VAL	6.8
1	B	1302	ILE	6.7
1	B	830	ILE	6.6
1	A	801	VAL	6.6
1	B	1145	VAL	6.4
1	B	567	ASP	6.4
1	A	834	SER	6.4
1	B	1146	VAL	6.2
1	A	567	ASP	6.1
1	A	1145	VAL	6.1
1	A	1143	VAL	6.1
1	B	1259	VAL	6.1
1	B	504	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	407	ASN	5.9
1	A	549	VAL	5.8
1	B	653	ARG	5.8
1	A	601	ILE	5.7
1	A	828	LEU	5.7
1	A	838	VAL	5.7
1	B	773	GLY	5.6
1	B	858	THR	5.6
1	B	654	ARG	5.5
1	B	829	ASP	5.5
1	B	600	ILE	5.5
1	A	836	TYR	5.5
1	B	670	ILE	5.5
1	A	858	THR	5.4
1	A	1290	VAL	5.4
1	B	520	VAL	5.4
1	A	820	ARG	5.3
1	B	601	ILE	5.2
1	A	832	ARG	5.2
1	A	115	ARG	5.2
1	B	661	ARG	5.2
1	B	1195	ILE	5.0
1	A	670	ILE	5.0
1	A	818	ASN	5.0
1	B	1143	VAL	5.0
1	A	548	ILE	4.9
1	A	671	ARG	4.9
1	A	553	PHE	4.9
1	A	1146	VAL	4.9
1	B	566	GLU	4.8
1	B	688	PHE	4.8
1	A	815	TYR	4.8
1	B	560	THR	4.7
1	B	593	THR	4.7
1	B	569	PHE	4.7
1	B	1188	LYS	4.6
1	A	406	ASP	4.6
1	B	406	ASP	4.6
1	A	1177	ASN	4.6
1	B	603	ASP	4.6
1	A	870	VAL	4.5
1	A	123	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	829	ASP	4.5
1	A	564	LEU	4.5
1	B	597	LEU	4.5
1	B	594	TYR	4.4
1	B	1169	MET	4.4
1	A	814	TYR	4.4
1	B	619	ILE	4.4
1	A	1196	ILE	4.3
1	A	710	LYS	4.2
1	B	606	PHE	4.2
1	B	917	ILE	4.2
1	A	607	LEU	4.2
1	B	651	LEU	4.2
1	A	34	VAL	4.2
1	A	826	GLN	4.1
1	A	651	LEU	4.1
1	B	683	LEU	4.1
1	B	1100	VAL	4.1
1	B	602	LYS	4.0
1	A	307	ARG	4.0
1	B	1179	ILE	4.0
1	B	834	SER	4.0
1	A	857	LEU	4.0
1	A	1181	PHE	4.0
1	A	305	ILE	4.0
1	A	600	ILE	4.0
1	A	788	ILE	3.9
1	A	1342	VAL	3.9
1	B	1189	GLU	3.9
1	A	1084	ARG	3.9
1	A	1176	LYS	3.9
1	B	510	LYS	3.9
1	B	1168	ILE	3.9
1	B	1196	ILE	3.8
1	B	555	THR	3.8
1	B	842	VAL	3.8
1	A	697	ILE	3.8
1	A	1299	ASP	3.8
1	B	310	THR	3.8
1	B	1206	LEU	3.8
1	B	629	ARG	3.8
1	B	876	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	775	LYS	3.7
1	B	1177	ASN	3.7
1	A	708	ILE	3.7
1	A	504	ASN	3.7
1	A	876	VAL	3.7
1	A	784	ILE	3.6
1	A	552	LEU	3.6
1	B	815	TYR	3.6
1	A	597	LEU	3.6
1	A	558	LYS	3.6
1	A	524	LEU	3.6
1	A	835	ASP	3.6
1	B	655	ARG	3.6
1	B	384	ASP	3.6
1	B	644	ASP	3.6
1	A	118	ILE	3.5
1	A	865	GLY	3.5
1	A	679	ILE	3.5
1	B	697	ILE	3.5
1	A	677	LYS	3.5
1	B	713	VAL	3.5
1	B	559	VAL	3.5
1	B	1139	VAL	3.5
1	B	1170	GLU	3.5
1	B	1191	LYS	3.4
1	A	837	ASP	3.4
1	A	546	LYS	3.4
1	A	1019	ARG	3.4
1	B	1360	ILE	3.4
1	A	594	TYR	3.4
1	B	1193	ASP	3.4
1	A	619	ILE	3.4
1	B	607	LEU	3.4
1	B	788	ILE	3.4
1	B	911	LEU	3.4
1	B	543	GLU	3.3
1	B	764	ALA	3.3
1	B	838	VAL	3.3
1	B	1023	ALA	3.3
1	B	880	LYS	3.3
1	A	1265	TYR	3.3
1	B	305	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	GLU	3.3
1	A	748	VAL	3.2
1	A	809	GLU	3.2
1	B	841	ILE	3.2
1	A	206	VAL	3.2
1	A	917	ILE	3.2
1	B	1022	ILE	3.2
1	A	341	GLN	3.2
1	A	526	LYS	3.2
1	B	27	VAL	3.2
1	B	620	VAL	3.2
1	A	1242	TYR	3.2
1	B	1073	VAL	3.2
1	B	524	LEU	3.2
1	B	1181	PHE	3.1
1	B	667	ILE	3.1
1	B	1176	LYS	3.1
1	A	1168	ILE	3.1
1	B	616	LEU	3.1
1	B	1182	LEU	3.1
1	B	662	LEU	3.0
1	B	806	LEU	3.0
1	B	526	LYS	3.0
1	A	856	VAL	3.0
1	A	339	VAL	3.0
1	A	1072	ILE	3.0
1	A	1334	LYS	3.0
1	B	1290	VAL	3.0
1	B	553	PHE	3.0
1	B	1102	THR	3.0
1	B	383	MET	2.9
1	B	1194	LEU	2.9
1	B	1072	ILE	2.9
1	A	591	LEU	2.9
1	B	679	ILE	2.9
1	A	1261	GLN	2.9
1	B	523	GLU	2.9
1	B	587	PHE	2.9
1	A	661	ARG	2.9
1	B	637	LYS	2.9
1	A	691	ARG	2.8
1	B	540	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	649	LYS	2.8
1	B	123	VAL	2.8
1	A	615	ILE	2.8
1	B	539	PHE	2.8
1	B	761	ILE	2.8
1	A	593	THR	2.8
1	B	1342	VAL	2.8
1	A	405	PHE	2.8
1	B	615	ILE	2.8
1	A	1270	ILE	2.8
1	B	776	ASN	2.8
1	B	635	ARG	2.8
1	B	818	ASN	2.8
1	B	1173	SER	2.8
1	A	434	LYS	2.8
1	A	603	ASP	2.8
1	A	1194	LEU	2.7
1	A	563	GLN	2.7
1	A	1100	VAL	2.7
1	B	873	GLU	2.7
1	B	1166	ILE	2.7
1	A	1182	LEU	2.7
1	A	215	ARG	2.7
1	B	350	ILE	2.7
1	B	376	ILE	2.7
1	B	975	VAL	2.7
1	A	1231	LYS	2.7
1	A	667	ILE	2.7
1	A	1296	LYS	2.7
1	B	116	HIS	2.7
1	A	706	GLU	2.7
1	B	605	ASP	2.7
1	A	811	LEU	2.7
1	B	1174	PHE	2.7
1	B	680	LEU	2.7
1	A	545	LYS	2.7
1	A	666	LEU	2.6
1	A	776	ASN	2.6
1	B	67	THR	2.6
1	A	665	LYS	2.6
1	B	370	GLU	2.6
1	A	521	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	93	VAL	2.6
1	B	339	VAL	2.6
1	A	562	LYS	2.6
1	A	620	VAL	2.6
1	A	647	VAL	2.6
1	B	931	VAL	2.6
1	B	878	LYS	2.6
1	A	43	ILE	2.6
1	A	978	ILE	2.6
1	B	1019	ARG	2.6
1	A	632	ILE	2.6
1	A	1331	ILE	2.6
1	A	181	VAL	2.6
1	A	648	MET	2.6
1	A	587	PHE	2.5
1	A	507	VAL	2.5
1	A	1185	LYS	2.5
1	B	443	ILE	2.5
1	A	559	VAL	2.5
1	A	384	ASP	2.5
1	B	1183	GLU	2.5
1	A	21	ILE	2.5
1	B	708	ILE	2.5
1	B	598	LEU	2.5
1	A	211	ILE	2.5
1	B	678	THR	2.5
1	B	1270	ILE	2.5
1	B	877	LYS	2.5
1	B	623	LEU	2.5
1	A	1289	LYS	2.5
1	B	220	ARG	2.5
1	A	233	LYS	2.5
1	A	143	VAL	2.5
1	B	927	ILE	2.5
1	B	1309	ILE	2.4
1	A	1272	GLN	2.4
1	A	410	ILE	2.4
1	A	1164	LEU	2.4
1	A	901	THR	2.4
1	A	892	ILE	2.4
1	B	1164	LEU	2.4
1	A	1294	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1042	ILE	2.4
1	B	34	VAL	2.4
1	B	398	LEU	2.4
1	B	405	PHE	2.4
1	A	565	LYS	2.4
1	A	881	ASN	2.4
1	B	867	SER	2.4
1	A	598	LEU	2.4
1	A	1175	GLU	2.3
1	A	606	PHE	2.3
1	B	69	ARG	2.3
1	B	824	VAL	2.3
1	B	875	VAL	2.3
1	B	910	GLU	2.3
1	A	551	LEU	2.3
1	A	1281	ILE	2.3
1	A	678	THR	2.3
1	A	561	VAL	2.3
1	B	182	ASP	2.3
1	B	814	TYR	2.3
1	B	1144	LEU	2.3
1	B	1167	THR	2.3
1	A	376	ILE	2.3
1	B	611	GLU	2.3
1	B	823	TYR	2.3
1	B	671	ARG	2.3
1	A	733	ILE	2.3
1	A	1166	ILE	2.3
1	B	301	LEU	2.3
1	A	1017	ASP	2.2
1	B	410	ILE	2.2
1	A	789	LYS	2.2
1	A	1197	LYS	2.2
1	B	260	GLU	2.2
1	B	684	LYS	2.2
1	A	680	LEU	2.2
1	B	338	LEU	2.2
1	B	391	VAL	2.2
1	B	706	GLU	2.2
1	B	189	VAL	2.2
1	A	414	ILE	2.2
1	A	1018	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1262	HIS	2.2
1	B	992	VAL	2.2
1	A	998	ILE	2.2
1	A	653	ARG	2.2
1	A	975	VAL	2.2
1	A	201	ILE	2.2
1	B	759	ILE	2.2
1	A	1159	SER	2.2
1	A	220	ARG	2.2
1	B	386	THR	2.1
1	A	189	VAL	2.1
1	B	934	ILE	2.1
1	B	1352	ILE	2.1
1	B	1037	PHE	2.1
1	A	681	ASP	2.1
1	A	662	LEU	2.1
1	A	1198	LEU	2.1
1	B	33	LYS	2.1
1	B	307	ARG	2.1
1	B	363	ILE	2.1
1	B	763	MET	2.1
1	A	872	SER	2.1
1	A	35	LEU	2.1
1	A	520	VAL	2.1
1	A	1073	VAL	2.1
1	B	414	ILE	2.1
1	B	440	ILE	2.1
1	B	1269	ILE	2.1
1	A	93	VAL	2.1
1	A	750	VAL	2.1
1	A	1259	VAL	2.1
1	A	724	ILE	2.1
1	A	852	ILE	2.1
1	A	302	LEU	2.1
1	A	888	ASN	2.1
1	A	777	SER	2.1
1	B	57	GLU	2.1
1	B	1197	LYS	2.1
1	A	242	ILE	2.1
1	A	1302	ILE	2.1
1	A	40	ARG	2.1
1	A	1173	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	590	SER	2.0
1	B	807	GLN	2.0
1	B	1160	VAL	2.0
1	B	865	GLY	2.0
1	A	350	ILE	2.0
1	A	1293	ALA	2.0
1	B	1180	ASP	2.0
1	A	927	ILE	2.0
1	B	1331	ILE	2.0
1	A	1335	ARG	2.0
1	A	1278	LYS	2.0
1	B	549	VAL	2.0
1	B	750	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	B	2367	1/1	0.43	8.71	54,54,54,54	0
2	SO4	A	2365	5/5	0.24	1.58	88,99,106,106	0
2	SO4	A	2364	5/5	0.21	0.30	32,39,54,59	0
2	SO4	B	2365	5/5	0.20	0.07	80,91,102,103	0
2	SO4	B	2366	5/5	0.17	-0.18	30,30,30,30	0
2	SO4	B	2364	5/5	0.19	-0.34	21,25,39,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.