



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:50 AM UTC

PDB ID : 4CMQ / pdb_00004cmq
Title : Crystal structure of Mn-bound *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 : 2014-01-17
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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

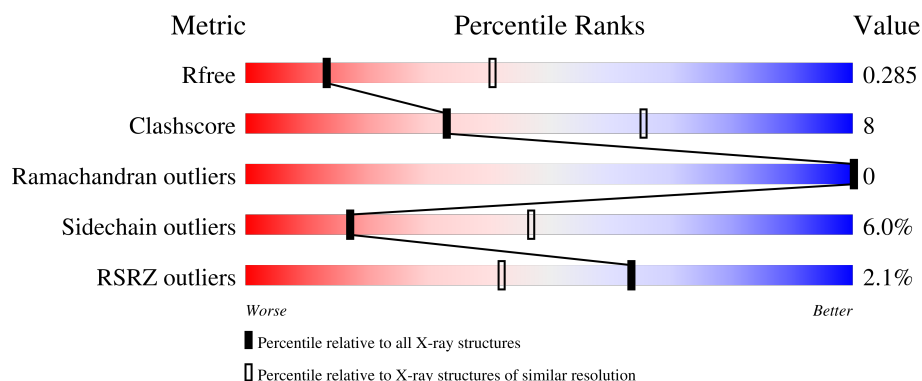
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	1372	

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
3	SO4	B	2372	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18904 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1156	Total	C	N	O	S	0	0	0
			9407	6011	1629	1748	19			
1	B	1168	Total	C	N	O	S	0	0	0
			9454	6038	1638	1759	19			

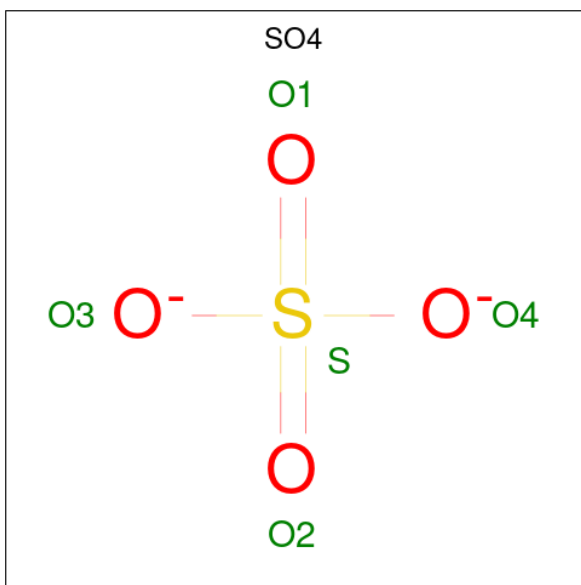
There are 8 discrepancies between the modelled and reference sequences:

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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Mn	0	0
			7	7		
2	B	6	Total	Mn	0	0
			6	6		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

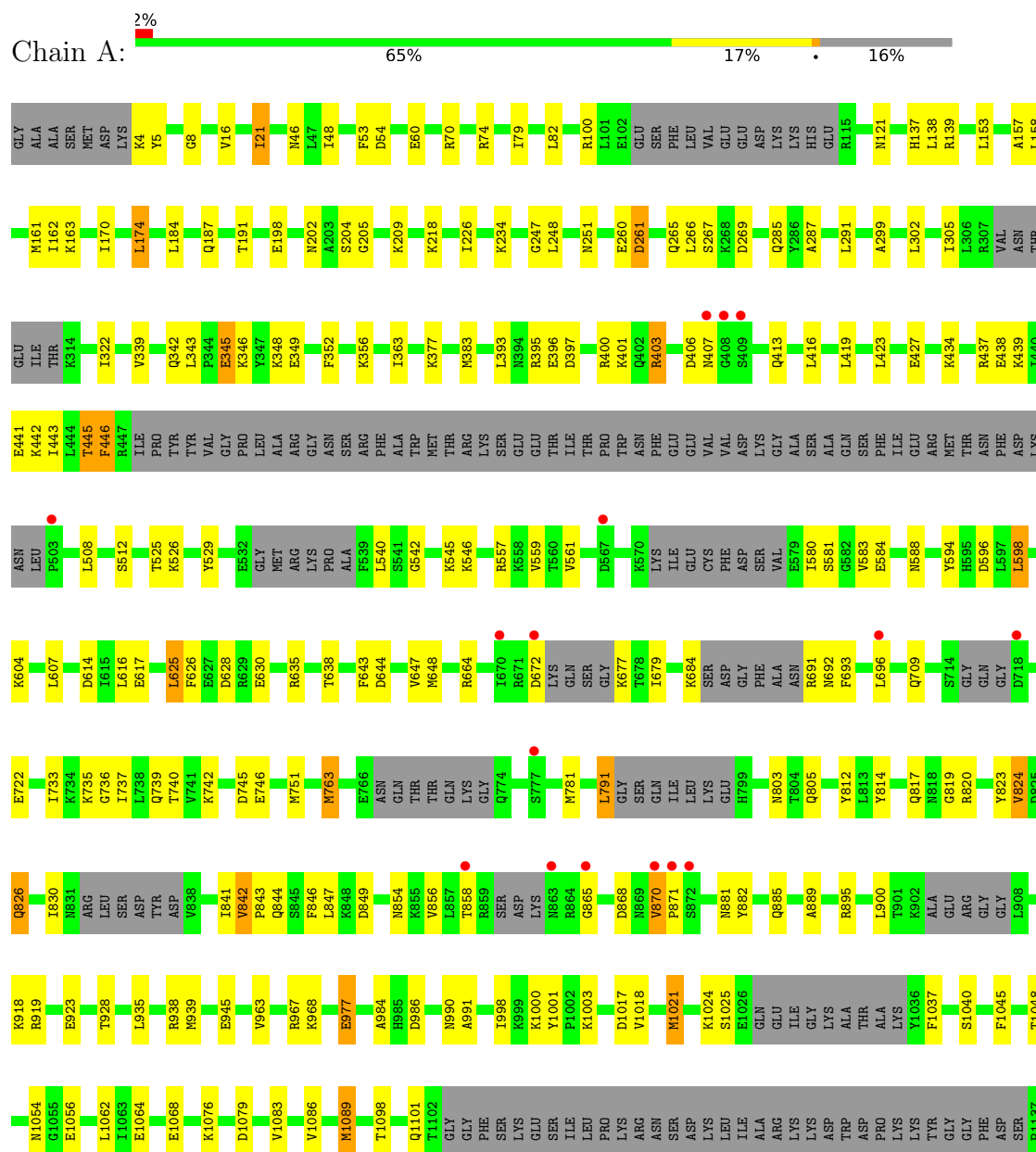


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

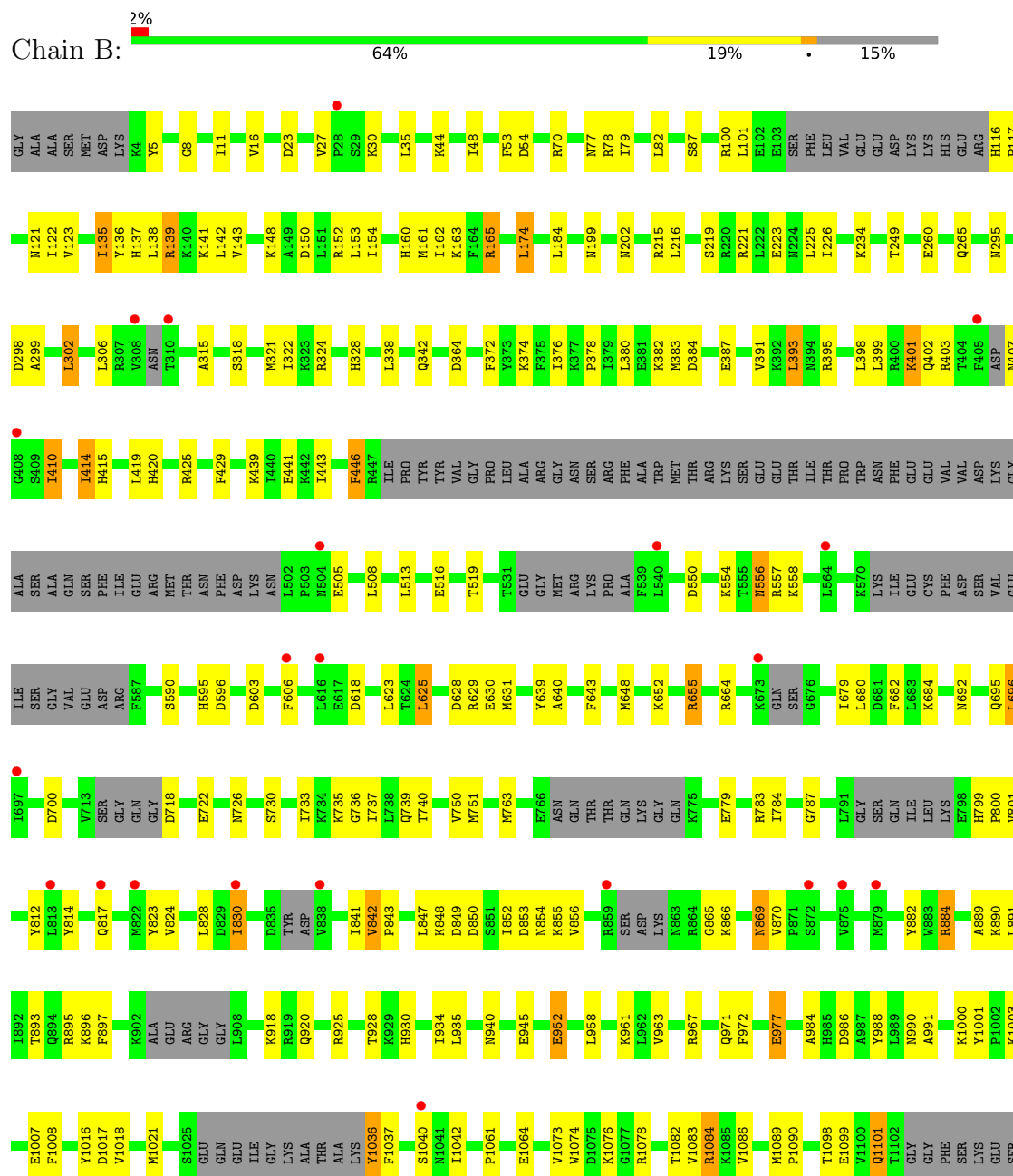
3 Residue-property plots

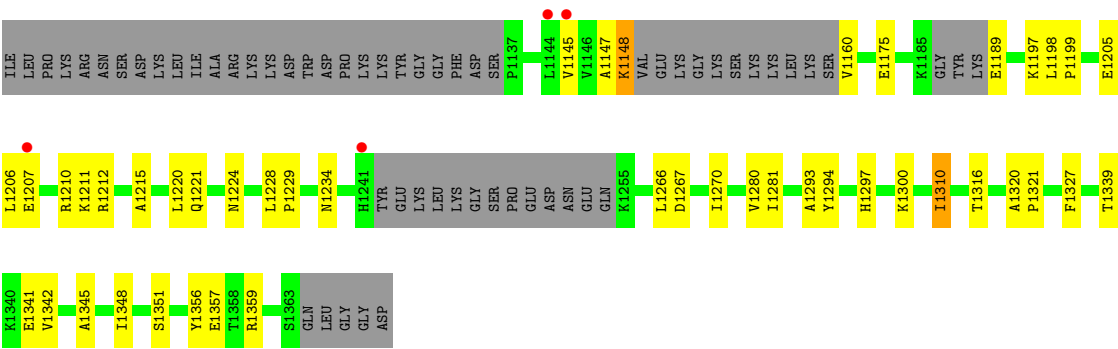
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	159.88Å 210.12Å 90.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 3.09 47.53 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.53-3.09) 99.0 (47.53-3.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.07Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.249 , 0.277 0.256 , 0.285	Depositor DCC
R_{free} test set	1500 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18904	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	0.30	0/9555	0.70	4/12836 (0.0%)
1	B	0.30	0/9601	0.71	7/12909 (0.1%)
All	All	0.30	0/19156	0.70	11/25745 (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	A	1089	MET	CA-C-N	7.18	127.18	119.28
1	A	1089	MET	C-N-CA	7.18	127.18	119.28
1	A	803	ASN	N-CA-C	6.81	119.54	111.71
1	B	1198	LEU	CA-C-N	6.39	126.36	119.78
1	B	1198	LEU	C-N-CA	6.39	126.36	119.78
1	B	842	VAL	CA-C-N	5.84	125.80	119.78
1	B	842	VAL	C-N-CA	5.84	125.80	119.78
1	B	1207	GLU	CB-CA-C	-5.84	109.82	116.54
1	B	87	SER	N-CA-C	5.76	117.24	111.07
1	A	1327	PHE	CB-CA-C	-5.06	110.72	116.54
1	B	869	ASN	N-CA-C	5.01	117.63	111.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9407	0	9528	140	0
1	B	9454	0	9536	157	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
3	A	15	0	0	2	0
3	B	15	0	0	3	0
All	All	18904	0	19064	297	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 8.

All (297) 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:A:1207:GLU:HG3	1:A:1208:ASN:H	1.04	1.16
1:A:1207:GLU:HG3	1:A:1208:ASN:N	1.84	0.90
1:A:1207:GLU:CG	1:A:1208:ASN:H	1.82	0.84
1:A:184:LEU:HD12	1:A:299:ALA:HB2	1.64	0.79
1:B:967:ARG:NH1	1:B:986:ASP:OD1	2.16	0.78
1:B:1205:GLU:OE1	1:B:1359:ARG:NH2	2.19	0.76
1:A:977:GLU:HG3	1:A:1310:ILE:HG23	1.68	0.73
1:A:247:GLY:HA2	1:A:407:ASN:HB2	1.71	0.73
1:A:349:GLU:HG3	1:A:356:LYS:HD3	1.71	0.73
1:B:1224:ASN:ND2	3:B:2372:SO4:O2	2.23	0.72
1:B:165:ARG:NH2	1:B:446:PHE:O	2.23	0.72
1:B:893:THR:HG23	1:B:896:LYS:H	1.54	0.71
1:B:963:VAL:HG21	1:B:990:ASN:HD22	1.54	0.71
1:B:199:ASN:ND2	1:B:779:GLU:OE1	2.25	0.70
1:B:82:LEU:HD22	1:B:162:ILE:HD12	1.74	0.69
1:B:977:GLU:HG3	1:B:1310:ILE:HG23	1.75	0.69
1:A:598:LEU:HD21	1:A:604:LYS:HG2	1.74	0.69
1:B:640:ALA:HA	1:B:648:MET:HE3	1.73	0.69
1:A:343:LEU:HD23	1:A:346:LYS:HD2	1.75	0.68
1:A:100:ARG:NH1	1:A:625:LEU:O	2.27	0.68
1:A:1207:GLU:CG	1:A:1208:ASN:N	2.46	0.67
1:A:342:GLN:HB2	1:A:383:MET:HE3	1.76	0.67
1:A:158:LEU:HD22	1:A:419:LEU:HD22	1.75	0.67
1:A:1098:THR:HB	1:A:1199:PRO:HB2	1.77	0.66
1:B:1357:GLU:OE2	1:B:1359:ARG:NH1	2.27	0.66
1:B:165:ARG:NH1	3:B:2370:SO4:O4	2.28	0.66
1:B:184:LEU:HD13	1:B:299:ALA:HB2	1.76	0.66
1:A:401:LYS:HB3	1:A:403:ARG:HE	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:LYS:NZ	1:B:870:VAL:O	2.30	0.65
1:B:849:ASP:HB3	1:B:854:ASN:HD22	1.63	0.64
1:B:100:ARG:NH1	1:B:625:LEU:O	2.30	0.64
1:B:787:GLY:HA2	1:B:889:ALA:HB1	1.79	0.64
1:A:967:ARG:NH1	1:A:986:ASP:OD1	2.30	0.64
1:A:174:LEU:HD21	1:A:302:LEU:HD21	1.78	0.64
1:B:848:LYS:O	1:B:961:LYS:NZ	2.31	0.63
1:A:79:ILE:HD11	1:A:163:LYS:HG3	1.82	0.62
1:B:78:ARG:NH1	1:B:162:ILE:O	2.32	0.62
1:A:614:ASP:OD1	1:A:664:ARG:NH2	2.32	0.62
1:A:791:LEU:HD21	1:A:889:ALA:HB2	1.81	0.61
1:B:629:ARG:HG3	1:B:655:ARG:HH12	1.65	0.61
1:A:1357:GLU:OE1	1:A:1359:ARG:NH1	2.33	0.61
1:B:380:LEU:HD12	1:B:393:LEU:HD12	1.83	0.61
1:A:849:ASP:OD2	1:A:895:ARG:NH2	2.33	0.61
1:B:79:ILE:HD11	1:B:163:LYS:HG3	1.83	0.60
1:B:410:ILE:HD12	1:B:414:ILE:HD11	1.83	0.60
1:B:8:GLY:HA3	1:B:991:ALA:HB2	1.83	0.60
1:A:427:GLU:HB2	1:A:434:LYS:HB2	1.85	0.59
1:A:817:GLN:O	1:A:882:TYR:OH	2.21	0.59
1:B:1212:ARG:NH2	1:B:1280:VAL:O	2.30	0.59
1:B:249:THR:HG23	1:B:265:GLN:HB2	1.85	0.59
1:A:396:GLU:O	1:A:400:ARG:NH1	2.36	0.58
1:A:1212:ARG:NH2	1:A:1280:VAL:O	2.37	0.58
1:B:1147:ALA:O	1:B:1189:GLU:N	2.37	0.58
1:A:868:ASP:HA	1:A:1054:ASN:HB3	1.86	0.58
1:B:817:GLN:O	1:B:882:TYR:OH	2.21	0.57
1:A:1351:SER:HB2	1:A:1356:TYR:HB2	1.86	0.57
1:B:557:ARG:NH2	1:B:596:ASP:OD1	2.32	0.57
1:B:1293:ALA:O	1:B:1297:HIS:ND1	2.35	0.57
1:B:54:ASP:O	1:B:735:LYS:NZ	2.38	0.56
1:B:652:LYS:O	1:B:655:ARG:NH2	2.38	0.56
1:A:736:GLY:O	1:A:740:THR:HG23	2.04	0.56
1:A:21:ILE:HD12	1:A:991:ALA:HB3	1.87	0.56
1:A:54:ASP:O	1:A:735:LYS:NZ	2.32	0.56
1:B:324:ARG:NH1	1:B:401:LYS:O	2.39	0.56
1:B:722:GLU:O	1:B:726:ASN:ND2	2.39	0.56
1:A:377:LYS:HE2	1:A:393:LEU:HD21	1.88	0.55
1:B:121:ASN:HA	1:B:628:ASP:HB2	1.88	0.55
1:B:226:ILE:HD11	1:B:234:LYS:HG3	1.88	0.55
1:B:11:ILE:HB	1:B:763:MET:HG3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:MET:HE1	1:B:419:LEU:N	2.22	0.55
1:B:223:GLU:HG2	1:B:234:LYS:HE2	1.88	0.55
1:B:138:LEU:HD11	1:B:153:LEU:HB3	1.89	0.55
1:B:763:MET:O	1:B:925:ARG:NH1	2.39	0.55
1:B:391:VAL:HG12	1:B:395:ARG:HH11	1.72	0.55
1:B:1061:PRO:O	1:B:1076:LYS:NZ	2.40	0.55
1:A:48:ILE:HG12	1:A:984:ALA:HB1	1.89	0.55
1:B:30:LYS:NZ	1:B:750:VAL:O	2.39	0.55
1:B:963:VAL:HG21	1:B:990:ASN:ND2	2.20	0.54
1:A:1284:ASP:N	1:A:1284:ASP:OD1	2.37	0.54
1:B:216:LEU:O	1:B:221:ARG:NH1	2.39	0.54
1:A:60:GLU:OE2	1:A:742:LYS:NZ	2.41	0.54
1:A:139:ARG:NH2	1:A:161:MET:HG2	2.23	0.54
1:B:1211:LYS:N	1:B:1224:ASN:OD1	2.37	0.54
1:B:338:LEU:HB3	1:B:383:MET:HE1	1.90	0.54
1:B:420:HIS:ND1	1:B:441:GLU:OE2	2.41	0.54
1:B:1084:ARG:HH22	1:B:1234:ASN:HD21	1.56	0.54
1:A:745:ASP:OD2	1:A:938:ARG:NH2	2.40	0.53
1:B:850:ASP:O	1:B:855:LYS:NZ	2.41	0.53
1:A:138:LEU:HD11	1:A:153:LEU:HB3	1.90	0.53
1:A:1230:SER:O	1:A:1234:ASN:ND2	2.42	0.53
1:A:198:GLU:OE1	1:A:812:TYR:OH	2.23	0.53
1:B:787:GLY:HA3	1:B:891:LEU:HD21	1.91	0.53
1:B:48:ILE:HG12	1:B:984:ALA:HB1	1.90	0.52
1:B:298:ASP:OD1	1:B:407:ASN:ND2	2.39	0.52
1:A:849:ASP:HB3	1:A:854:ASN:HD22	1.74	0.52
1:A:247:GLY:HA2	1:A:407:ASN:CB	2.39	0.52
1:A:1018:VAL:HA	1:A:1021:MET:HE2	1.92	0.52
1:A:267:SER:HB3	1:A:407:ASN:H	1.74	0.52
1:A:735:LYS:O	1:A:739:GLN:HG2	2.10	0.52
1:B:972:PHE:HE1	1:B:1084:ARG:HG2	1.75	0.52
1:B:378:PRO:O	1:B:382:LYS:HG2	2.10	0.51
1:A:1171:ARG:O	1:A:1175:GLU:HG2	2.09	0.51
1:B:1281:ILE:HD11	1:B:1316:THR:HG22	1.93	0.51
1:A:870:VAL:HG22	1:A:871:PRO:HD2	1.93	0.51
1:B:143:VAL:HG11	1:B:315:ALA:HB2	1.93	0.51
1:B:1064:GLU:OE2	1:B:1076:LYS:NZ	2.43	0.51
1:A:82:LEU:HD22	1:A:162:ILE:HD12	1.92	0.51
1:A:814:TYR:CZ	1:A:830:ILE:HG12	2.46	0.50
1:B:823:TYR:HB3	1:B:865:GLY:HA3	1.92	0.50
1:B:1220:LEU:HG	1:B:1339:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ARG:HH22	1:B:415:HIS:CE1	2.29	0.50
1:B:618:ASP:OD2	1:B:639:TYR:OH	2.25	0.50
1:B:679:ILE:HG23	1:B:696:LEU:HD23	1.92	0.50
1:B:1211:LYS:NZ	3:B:2372:SO4:O4	2.44	0.50
1:A:46:ASN:ND2	1:A:1089:MET:SD	2.85	0.50
1:A:226:ILE:HD12	1:A:234:LYS:HA	1.94	0.50
1:B:5:TYR:CZ	1:B:751:MET:HG3	2.47	0.49
1:B:814:TYR:CZ	1:B:830:ILE:HG23	2.47	0.49
1:A:1277:SER:HA	1:A:1281:ILE:HB	1.94	0.49
1:A:1062:LEU:HD12	1:A:1076:LYS:HB2	1.93	0.49
1:A:626:PHE:CE2	1:A:635:ARG:HD2	2.47	0.49
1:B:139:ARG:HH21	1:B:160:HIS:CE1	2.30	0.49
1:B:342:GLN:HB2	1:B:383:MET:HE3	1.95	0.49
1:A:187:GLN:O	1:A:191:THR:HG23	2.13	0.49
1:A:442:LYS:O	1:A:446:PHE:HB3	2.13	0.49
1:A:607:LEU:HD23	1:A:616:LEU:HD21	1.95	0.49
1:A:1229:PRO:HD2	1:A:1232:TYR:HD2	1.77	0.48
1:B:556:ASN:N	1:B:556:ASN:OD1	2.45	0.48
1:A:1054:ASN:OD1	1:A:1056:GLU:HB2	2.12	0.48
1:B:391:VAL:O	1:B:395:ARG:HD3	2.14	0.48
1:B:1175:GLU:OE2	1:B:1197:LYS:NZ	2.46	0.48
1:B:1267:ASP:OD1	1:B:1294:TYR:OH	2.31	0.48
1:A:251:ASN:ND2	1:A:261:ASP:OD1	2.46	0.48
1:A:269:ASP:OD1	1:A:269:ASP:N	2.46	0.48
1:A:692:ASN:OD1	1:A:693:PHE:N	2.47	0.48
1:B:643:PHE:HB2	1:B:648:MET:HE2	1.96	0.48
1:B:783:ARG:NE	1:B:890:LYS:O	2.46	0.48
1:A:16:VAL:HG23	1:A:53:PHE:HE2	1.79	0.48
1:B:849:ASP:HB3	1:B:854:ASN:ND2	2.27	0.48
1:B:1064:GLU:HB2	1:B:1074:TRP:HB3	1.96	0.48
1:A:170:ILE:O	1:A:413:GLN:NE2	2.45	0.48
1:A:266:LEU:HD12	1:A:407:ASN:HB3	1.96	0.48
1:A:881:ASN:OD1	1:A:885:GLN:NE2	2.47	0.48
1:B:1224:ASN:HB2	1:B:1280:VAL:HG11	1.96	0.48
1:A:423:LEU:HD13	1:A:437:ARG:HG3	1.95	0.47
1:A:679:ILE:HG23	1:A:696:LEU:HD23	1.96	0.47
1:A:733:ILE:O	1:A:737:ILE:HG13	2.14	0.47
1:B:516:GLU:HA	1:B:519:THR:HG22	1.96	0.47
1:B:733:ILE:O	1:B:737:ILE:HG13	2.13	0.47
1:B:852:ILE:HA	1:B:855:LYS:HB2	1.96	0.47
1:A:963:VAL:HG21	1:A:990:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ARG:O	1:B:590:SER:HB2	2.14	0.47
1:B:692:ASN:HB3	1:B:695:GLN:HG3	1.97	0.47
1:B:150:ASP:OD2	1:B:152:ARG:NH2	2.47	0.47
1:B:321:MET:O	1:B:402:GLN:NE2	2.42	0.47
1:B:298:ASP:O	1:B:302:LEU:HB2	2.14	0.47
1:A:814:TYR:CE1	1:A:819:GLY:HA2	2.50	0.47
1:B:735:LYS:O	1:B:739:GLN:HG2	2.14	0.47
1:A:849:ASP:OD2	1:A:919:ARG:NH2	2.48	0.47
1:A:1048:THR:HG22	1:A:1076:LYS:HD3	1.96	0.47
1:A:1168:ILE:O	1:A:1171:ARG:HG2	2.15	0.47
1:B:930:HIS:O	1:B:934:ILE:HG13	2.15	0.47
1:A:512:SER:OG	1:A:617:GLU:OE1	2.30	0.46
1:B:398:LEU:HG	1:B:399:LEU:HG	1.96	0.46
1:B:513:LEU:H	1:B:513:LEU:HD12	1.81	0.46
1:B:249:THR:OG1	1:B:265:GLN:OE1	2.30	0.46
1:B:1210:ARG:NH2	1:B:1341:GLU:OE1	2.48	0.46
1:A:583:VAL:HG12	1:A:584:GLU:O	2.15	0.46
1:A:74:ARG:HD2	3:A:2371:SO4:O2	2.16	0.46
1:A:342:GLN:NE2	1:A:383:MET:O	2.43	0.46
1:B:508:LEU:HD21	1:B:664:ARG:HB2	1.98	0.46
1:B:843:PRO:HG2	1:B:869:ASN:O	2.15	0.46
1:B:682:PHE:HB2	1:B:696:LEU:HD21	1.98	0.46
1:A:823:TYR:CD2	1:A:858:THR:HG21	2.51	0.46
1:B:439:LYS:O	1:B:443:ILE:HG13	2.16	0.46
1:A:287:ALA:O	1:A:291:LEU:HG	2.16	0.45
1:A:1325:LYS:HG3	1:A:1330:THR:HG22	1.97	0.45
1:B:226:ILE:HD11	1:B:234:LYS:HE3	1.98	0.45
1:B:842:VAL:HA	1:B:843:PRO:HD3	1.73	0.45
1:A:648:MET:HE2	1:A:648:MET:HB2	1.84	0.45
1:B:27:VAL:HG12	1:B:1086:VAL:HG22	1.99	0.45
1:B:550:ASP:HA	1:B:554:LYS:HG3	1.99	0.45
1:B:1084:ARG:HH22	1:B:1234:ASN:ND2	2.13	0.45
1:B:174:LEU:HD21	1:B:302:LEU:HD11	1.98	0.45
1:B:1300:LYS:HE2	1:B:1327:PHE:CE1	2.52	0.45
1:A:161:MET:HE1	1:A:419:LEU:HA	1.99	0.45
1:A:70:ARG:HG2	1:A:722:GLU:CD	2.42	0.44
1:A:439:LYS:O	1:A:443:ILE:HG13	2.17	0.44
1:B:184:LEU:HD22	1:B:295:ASN:HB3	1.98	0.44
1:B:557:ARG:HG2	1:B:558:LYS:HG3	2.00	0.44
1:A:1000:LYS:HG3	1:A:1001:TYR:CE1	2.52	0.44
1:B:1101:GLN:H	1:B:1101:GLN:HG2	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1215:ALA:HB2	1:B:1221:GLN:HG3	2.00	0.44
1:B:784:ILE:HD11	1:B:812:TYR:CD1	2.52	0.44
1:A:121:ASN:HA	1:A:628:ASP:HB2	1.99	0.44
1:A:525:THR:HA	1:A:545:LYS:HE2	1.99	0.44
1:A:594:TYR:O	1:A:598:LEU:HB2	2.17	0.44
1:B:219:SER:O	1:B:223:GLU:HG3	2.17	0.44
1:B:1351:SER:HB3	1:B:1356:TYR:HB2	1.99	0.44
1:A:1232:TYR:CE1	1:A:1265:TYR:HD2	2.36	0.44
1:A:1220:LEU:HG	1:A:1339:THR:HG22	1.98	0.44
1:B:5:TYR:CE2	1:B:751:MET:HG3	2.52	0.44
1:B:814:TYR:HE2	1:B:828:LEU:O	2.00	0.44
1:B:1082:THR:O	1:B:1086:VAL:HG23	2.18	0.44
1:A:542:GLY:O	1:A:546:LYS:HG3	2.18	0.44
1:A:918:LYS:HE3	1:A:1018:VAL:HG11	1.99	0.44
1:A:508:LEU:HD21	1:A:664:ARG:HB2	2.00	0.43
1:A:526:LYS:HE3	1:A:692:ASN:HB2	2.00	0.43
1:B:847:LEU:HD12	1:B:848:LYS:N	2.33	0.43
1:B:1098:THR:HB	1:B:1199:PRO:HB2	2.00	0.43
1:A:1086:VAL:HG13	1:A:1089:MET:HE2	1.99	0.43
1:B:401:LYS:HB3	1:B:403:ARG:HE	1.83	0.43
1:B:1205:GLU:HB2	1:B:1348:ILE:HD11	1.99	0.43
1:A:339:VAL:HA	1:A:383:MET:HE1	2.00	0.43
1:A:403:ARG:NH2	3:A:2372:SO4:O2	2.34	0.43
1:A:1045:PHE:O	1:A:1064:GLU:HG3	2.18	0.43
1:B:1000:LYS:HG3	1:B:1001:TYR:CE1	2.54	0.43
1:A:842:VAL:HA	1:A:843:PRO:HD3	1.79	0.43
1:B:16:VAL:HG23	1:B:53:PHE:HE1	1.82	0.43
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.50	0.43
1:B:382:LYS:HA	1:B:382:LYS:HD3	1.92	0.43
1:A:218:LYS:HB2	1:A:248:LEU:HD21	2.00	0.43
1:A:895:ARG:NH2	1:A:919:ARG:HH22	2.16	0.43
1:A:137:HIS:HA	1:A:322:ILE:HD11	2.00	0.43
1:A:202:ASN:OD1	1:A:204:SER:HB3	2.19	0.43
1:A:583:VAL:CG1	1:A:584:GLU:N	2.82	0.43
1:A:841:ILE:HD13	1:A:900:LEU:HG	2.00	0.43
1:A:856:VAL:HG12	1:A:858:THR:HG23	1.99	0.42
1:B:1206:LEU:HD21	1:B:1345:ALA:HB2	2.01	0.42
1:A:5:TYR:CZ	1:A:751:MET:HG3	2.54	0.42
1:A:1280:VAL:HG23	1:A:1281:ILE:HD12	2.01	0.42
1:B:122:ILE:HG12	1:B:631:MET:HG3	2.01	0.42
1:B:784:ILE:HD11	1:B:812:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:HG2	1:A:407:ASN:OD1	2.19	0.42
1:B:139:ARG:CZ	1:B:161:MET:HG2	2.50	0.42
1:B:410:ILE:HD11	1:B:415:HIS:CE1	2.54	0.42
1:B:763:MET:HB3	1:B:928:THR:HG22	2.01	0.42
1:A:644:ASP:HB2	1:A:647:VAL:HG23	2.01	0.42
1:A:823:TYR:HB3	1:A:865:GLY:HA3	2.00	0.42
1:B:137:HIS:HA	1:B:322:ILE:HD11	2.01	0.42
1:B:1021:MET:O	1:B:1036:TYR:N	2.52	0.42
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.83	0.42
1:A:1024:LYS:HG2	1:A:1025:SER:H	1.84	0.42
1:A:348:LYS:HA	1:A:352:PHE:HD2	1.85	0.42
1:B:841:ILE:HD11	1:B:896:LYS:HE3	1.99	0.42
1:A:546:LYS:HE2	1:A:684:LYS:HG2	2.02	0.42
1:A:824:VAL:HB	1:A:826:GLN:HG2	2.02	0.42
1:B:1266:LEU:O	1:B:1270:ILE:HG12	2.19	0.42
1:A:672:ASP:H	1:A:677:LYS:N	2.17	0.42
1:A:763:MET:HB2	1:A:928:THR:HG22	2.02	0.42
1:B:1089:MET:HA	1:B:1090:PRO:HD2	1.86	0.41
1:A:8:GLY:HA3	1:A:991:ALA:HB2	2.02	0.41
1:B:8:GLY:CA	1:B:991:ALA:HB2	2.49	0.41
1:B:136:TYR:HA	1:B:139:ARG:HB2	2.02	0.41
1:B:410:ILE:HD11	1:B:415:HIS:NE2	2.35	0.41
1:B:920:GLN:NE2	1:B:1042:ILE:HG12	2.34	0.41
1:B:1320:ALA:HA	1:B:1321:PRO:HD3	1.89	0.41
1:A:598:LEU:HD23	1:A:607:LEU:HD12	2.02	0.41
1:B:603:ASP:OD1	1:B:606:PHE:N	2.49	0.41
1:B:1148:LYS:C	1:B:1160:VAL:HA	2.45	0.41
1:A:204:SER:OG	1:A:205:GLY:N	2.53	0.41
1:A:345:GLU:CD	1:A:345:GLU:H	2.27	0.41
1:A:583:VAL:HG12	1:A:584:GLU:N	2.35	0.41
1:A:643:PHE:HB2	1:A:648:MET:HE1	2.03	0.41
1:A:625:LEU:HD12	1:A:625:LEU:HA	1.87	0.41
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.93	0.41
1:B:318:SER:O	1:B:322:ILE:HG13	2.20	0.41
1:B:799:HIS:HA	1:B:800:PRO:HD2	1.97	0.41
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.82	0.41
1:A:1300:LYS:HD3	1:A:1327:PHE:CE1	2.55	0.41
1:B:116:HIS:HA	1:B:117:PRO:HD3	1.91	0.41
1:B:135:ILE:HG21	1:B:160:HIS:CD2	2.56	0.41
1:B:142:LEU:HD13	1:B:154:ILE:HA	2.02	0.41
1:B:372:PHE:CZ	1:B:376:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ALA:O	1:A:161:MET:HG3	2.20	0.41
1:A:302:LEU:HD12	1:A:305:ILE:HD11	2.03	0.41
1:A:626:PHE:HE2	1:A:635:ARG:HD2	1.86	0.41
1:A:1221:GLN:NE2	1:A:1320:ALA:HB2	2.35	0.41
1:A:1262:HIS:HB3	1:A:1265:TYR:CD1	2.56	0.41
1:B:328:HIS:CE1	1:B:399:LEU:HB3	2.56	0.41
1:B:680:LEU:HG	1:B:684:LYS:HE3	2.01	0.41
1:A:529:TYR:HA	1:A:580:ILE:HA	2.03	0.41
1:A:846:PHE:O	1:A:1040:SER:HB2	2.21	0.41
1:A:1079:ASP:O	1:A:1083:VAL:HG23	2.21	0.41
1:A:1203:LEU:O	1:A:1347:LEU:HD12	2.19	0.41
1:A:1293:ALA:HA	1:A:1296:LYS:HD2	2.03	0.41
1:B:148:LYS:HB2	1:B:429:PHE:CD2	2.57	0.40
1:B:557:ARG:HA	1:B:595:HIS:CD2	2.57	0.40
1:B:730:SER:O	1:B:733:ILE:HG22	2.22	0.40
1:B:884:ARG:HD2	1:B:897:PHE:CZ	2.56	0.40
1:B:940:ASN:OD1	1:B:952:GLU:N	2.54	0.40
1:B:1003:LYS:HD2	1:B:1016:TYR:CE2	2.57	0.40
1:A:441:GLU:O	1:A:445:THR:OG1	2.38	0.40
1:B:736:GLY:O	1:B:740:THR:HG22	2.22	0.40
1:B:988:TYR:HE2	1:B:1083:VAL:HG13	1.86	0.40
1:B:918:LYS:HE2	1:B:1018:VAL:HG11	2.02	0.40
1:B:1228:LEU:HA	1:B:1229:PRO:HD3	1.94	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	1118/1372 (82%)	1088 (97%)	30 (3%)	0	100	100
1	B	1130/1372 (82%)	1104 (98%)	26 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2248/2744 (82%)	2192 (98%)	56 (2%)	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	1026/1228 (84%)	967 (94%)	59 (6%)	18	48
1	B	1026/1228 (84%)	961 (94%)	65 (6%)	16	45
All	All	2052/2456 (84%)	1928 (94%)	124 (6%)	17	47

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	21	ILE
1	A	174	LEU
1	A	209	LYS
1	A	260	GLU
1	A	261	ASP
1	A	285	GLN
1	A	345	GLU
1	A	363	ILE
1	A	395	ARG
1	A	397	ASP
1	A	403	ARG
1	A	406	ASP
1	A	416	LEU
1	A	438	GLU
1	A	445	THR
1	A	446	PHE
1	A	540	LEU
1	A	559	VAL
1	A	561	VAL

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Mol	Chain	Res	Type
1	A	581	SER
1	A	588	ASN
1	A	598	LEU
1	A	625	LEU
1	A	630	GLU
1	A	638	THR
1	A	691	ARG
1	A	709	GLN
1	A	746	GLU
1	A	763	MET
1	A	781	MET
1	A	791	LEU
1	A	805	GLN
1	A	820	ARG
1	A	824	VAL
1	A	826	GLN
1	A	842	VAL
1	A	844	GLN
1	A	847	LEU
1	A	870	VAL
1	A	923	GLU
1	A	935	LEU
1	A	939	MET
1	A	945	GLU
1	A	968	LYS
1	A	977	GLU
1	A	998	ILE
1	A	1003	LYS
1	A	1017	ASP
1	A	1021	MET
1	A	1037	PHE
1	A	1068	GLU
1	A	1101	GLN
1	A	1206	LEU
1	A	1270	ILE
1	A	1284	ASP
1	A	1305	GLN
1	A	1312	LEU
1	A	1328	ASP
1	B	23	ASP
1	B	35	LEU
1	B	44	LYS

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Mol	Chain	Res	Type
1	B	70	ARG
1	B	77	ASN
1	B	101	LEU
1	B	123	VAL
1	B	135	ILE
1	B	139	ARG
1	B	141	LYS
1	B	165	ARG
1	B	174	LEU
1	B	202	ASN
1	B	215	ARG
1	B	225	LEU
1	B	260	GLU
1	B	302	LEU
1	B	306	LEU
1	B	364	ASP
1	B	374	LYS
1	B	384	ASP
1	B	387	GLU
1	B	393	LEU
1	B	401	LYS
1	B	410	ILE
1	B	414	ILE
1	B	425	ARG
1	B	446	PHE
1	B	505	GLU
1	B	556	ASN
1	B	623	LEU
1	B	625	LEU
1	B	630	GLU
1	B	655	ARG
1	B	696	LEU
1	B	700	ASP
1	B	718	ASP
1	B	801	VAL
1	B	824	VAL
1	B	830	ILE
1	B	853	ASP
1	B	856	VAL
1	B	884	ARG
1	B	895	ARG
1	B	935	LEU

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Mol	Chain	Res	Type
1	B	945	GLU
1	B	952	GLU
1	B	958	LEU
1	B	971	GLN
1	B	977	GLU
1	B	1007	GLU
1	B	1008	PHE
1	B	1017	ASP
1	B	1036	TYR
1	B	1037	PHE
1	B	1040	SER
1	B	1073	VAL
1	B	1078	ARG
1	B	1084	ARG
1	B	1099	GLU
1	B	1101	GLN
1	B	1145	VAL
1	B	1148	LYS
1	B	1310	ILE
1	B	1342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	99	HIS
1	A	199	ASN
1	A	281	GLN
1	A	420	HIS
1	A	844	GLN
1	A	920	GLN
1	A	1305	GLN
1	B	77	ASN
1	B	160	HIS
1	B	178	ASN
1	B	199	ASN
1	B	255	ASN
1	B	342	GLN
1	B	650	GLN
1	B	698	HIS
1	B	723	HIS
1	B	739	GLN

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Mol	Chain	Res	Type
1	B	758	ASN
1	B	803	ASN
1	B	990	ASN
1	B	1044	ASN
1	B	1054	ASN
1	B	1221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 13 are monoatomic - leaving 6 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	$\# Z > 2$
3	SO4	B	2370	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	B	2371	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	2372	-	4,4,4	0.19	0	6,6,6	0.18	0
3	SO4	A	2371	-	4,4,4	0.22	0	6,6,6	0.06	0
3	SO4	A	2372	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	2373	-	4,4,4	0.24	0	6,6,6	0.09	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2370	SO4	1	0
3	B	2372	SO4	2	0
3	A	2371	SO4	1	0
3	A	2372	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, 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	1156/1372 (84%)	-0.06	22 (1%) 66 45	13, 54, 96, 149	0
1	B	1168/1372 (85%)	0.09	26 (2%) 62 41	12, 61, 113, 147	0
All	All	2324/2744 (84%)	0.02	48 (2%) 63 42	12, 57, 106, 149	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	ASN	5.5
1	A	863	ASN	4.1
1	B	564	LEU	4.1
1	B	813	LEU	3.9
1	B	1040	SER	3.8
1	B	697	ILE	3.7
1	A	503	PRO	3.7
1	B	817	GLN	3.6
1	B	540	LEU	3.1
1	A	870	VAL	3.1
1	A	871	PRO	3.0
1	B	310	THR	3.0
1	B	879	MET	2.9
1	B	606	PHE	2.7
1	B	830	ILE	2.7
1	B	308	VAL	2.7
1	A	567	ASP	2.7
1	A	1299	ASP	2.6
1	A	1259	VAL	2.6
1	B	1241	HIS	2.5
1	A	672	ASP	2.5
1	B	875	VAL	2.5
1	B	872	SER	2.5
1	B	1144	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	504	ASN	2.4
1	A	858	THR	2.3
1	A	1196	ILE	2.3
1	A	696	LEU	2.3
1	B	1145	VAL	2.3
1	A	670	ILE	2.2
1	B	408	GLY	2.2
1	B	1207	GLU	2.2
1	B	673	LYS	2.2
1	A	1159	SER	2.1
1	B	28	PRO	2.1
1	A	718	ASP	2.1
1	B	822	MET	2.1
1	A	872	SER	2.1
1	B	405	PHE	2.1
1	A	1362	LEU	2.1
1	A	777	SER	2.1
1	A	865	GLY	2.1
1	A	409	SER	2.1
1	B	838	VAL	2.1
1	A	1326	TYR	2.1
1	A	408	GLY	2.1
1	B	859	ARG	2.0
1	B	616	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	2369	1/1	0.71	0.16	104,104,104,104	0
3	SO4	A	2373	5/5	0.74	0.19	100,100,102,103	0
3	SO4	A	2372	5/5	0.81	0.19	122,123,123,124	0
2	MN	A	2370	1/1	0.81	0.16	98,98,98,98	0
3	SO4	B	2372	5/5	0.81	0.10	87,87,89,89	0
3	SO4	B	2371	5/5	0.84	0.16	111,112,112,112	0
2	MN	B	2367	1/1	0.84	0.13	96,96,96,96	0
2	MN	B	2368	1/1	0.86	0.06	98,98,98,98	0
2	MN	A	2367	1/1	0.88	0.08	84,84,84,84	0
2	MN	B	2366	1/1	0.89	0.08	98,98,98,98	0
2	MN	A	2368	1/1	0.90	0.07	136,136,136,136	0
3	SO4	B	2370	5/5	0.92	0.08	46,48,49,50	0
3	SO4	A	2371	5/5	0.93	0.07	36,41,42,43	0
2	MN	B	2369	1/1	0.93	0.09	69,69,69,69	0
2	MN	A	2364	1/1	0.94	0.09	31,31,31,31	0
2	MN	A	2365	1/1	0.95	0.05	36,36,36,36	0
2	MN	B	2364	1/1	0.97	0.05	30,30,30,30	0
2	MN	B	2365	1/1	0.97	0.10	38,38,38,38	0
2	MN	A	2366	1/1	0.97	0.07	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.