



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:19 AM UTC

PDB ID : 2O7C / pdb\_00002o7c  
Title : Crystal structure of L-methionine-lyase from Pseudomonas  
Authors : Misaki, S.; Takimoto, A.; Takakura, T.; Yoshioka, T.; Yamashita, M.; Tamura, T.; Tanaka, H.; Inagaki, K.  
Deposited on : 2006-12-10  
Resolution : 1.70 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)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

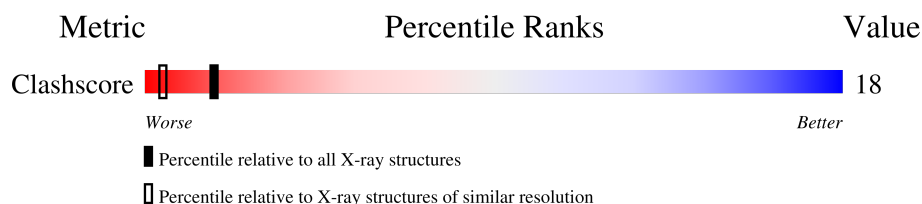
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
Clashscore	190562	5924 (1.70-1.70)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	 68% 32% .
1	B	398	 71% 28% .
1	C	398	 69% 30% .
1	D	398	 74% 24% .

## 2 Entry composition [i](#)

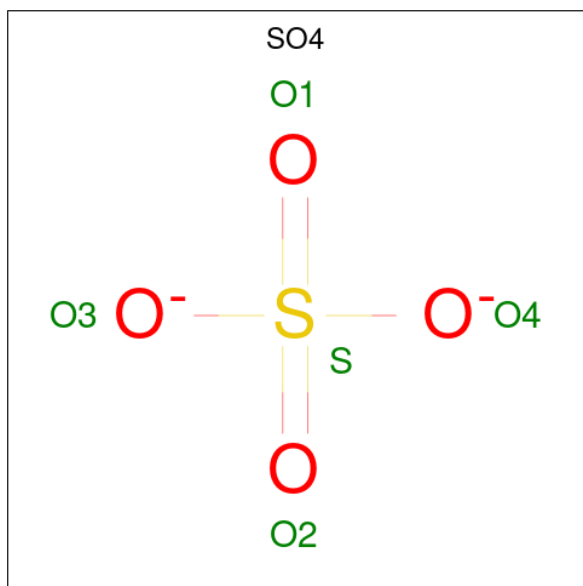
There are 3 unique types of molecules in this entry. The entry contains 12783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	B	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	C	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			
1	D	398	Total	C	N	O	P	S	0	0	0
			3011	1897	533	562	1	18			

- 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	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is water.

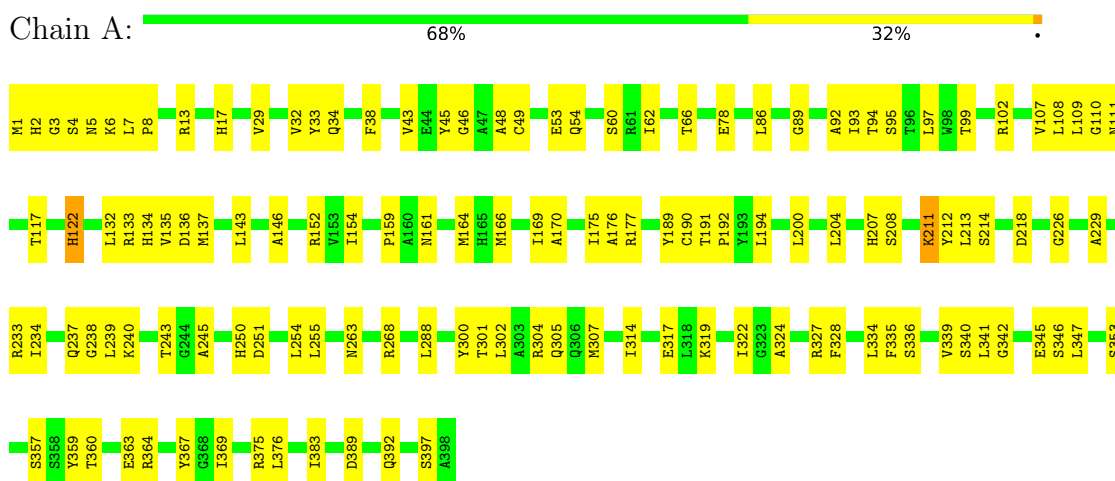
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total	O	0	0
			165	165		
3	B	172	Total	O	0	0
			172	172		
3	C	197	Total	O	0	0
			197	197		
3	D	185	Total	O	0	0
			185	185		

### 3 Residue-property plots

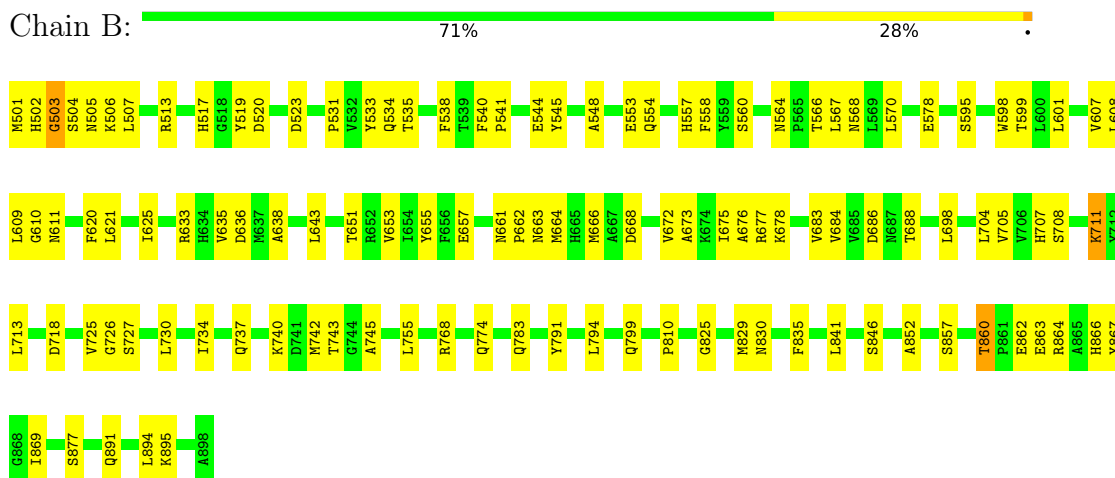
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: Methionine gamma-lyase



#### • Molecule 1: Methionine gamma-lyase



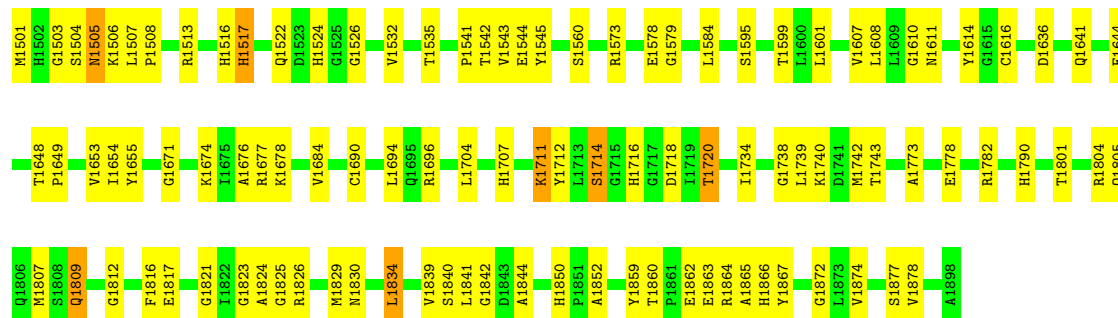
#### • Molecule 1: Methionine gamma-lyase





• Molecule 1: Methionine gamma-lyase

Chain D: 74% 24%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.13Å 133.13Å 215.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LLP

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	0.45	0/3051	0.90	9/4139 (0.2%)
1	B	0.45	0/3051	0.92	15/4139 (0.4%)
1	C	0.47	0/3051	0.91	9/4139 (0.2%)
1	D	0.45	0/3051	0.91	13/4139 (0.3%)
All	All	0.45	0/12204	0.91	46/16556 (0.3%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1505	ASN	N-CA-C	-7.50	102.31	113.72
1	B	610	GLY	N-CA-C	-7.44	104.15	112.33
1	C	1214	SER	N-CA-C	-6.81	103.78	111.14
1	D	1877	SER	N-CA-C	-6.51	96.46	107.99
1	A	208	SER	N-CA-C	-6.43	95.79	107.75
1	C	1017	HIS	N-CA-C	6.15	119.29	110.24
1	A	60	SER	N-CA-C	6.11	119.57	111.75
1	D	1824	ALA	N-CA-C	-6.05	104.76	111.36
1	D	1834	LEU	N-CA-C	-6.04	104.89	112.93
1	A	319	LYS	N-CA-C	-6.04	100.91	109.96
1	D	1517	HIS	N-CA-C	6.01	119.20	110.42
1	B	560	SER	N-CA-C	6.01	119.71	112.38
1	A	214	SER	N-CA-C	-6.00	104.66	111.14
1	D	1560	SER	N-CA-C	6.00	119.69	112.38
1	D	1809	GLN	CA-C-N	5.98	125.68	119.82
1	D	1809	GLN	C-N-CA	5.98	125.68	119.82
1	A	169	ILE	N-CA-C	5.88	116.53	110.36
1	C	1060	SER	N-CA-C	5.87	118.46	111.71
1	C	1125	ILE	CB-CA-C	-5.79	104.45	112.04
1	B	519	TYR	N-CA-C	5.78	117.83	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ILE	CB-CA-C	-5.77	104.48	112.04
1	B	708	SER	N-CA-C	-5.73	96.46	107.57
1	B	742	MET	N-CA-C	5.63	120.15	113.28
1	A	189	TYR	N-CA-C	5.55	117.01	111.07
1	A	334	LEU	N-CA-C	-5.51	105.35	112.68
1	B	503	GLY	N-CA-C	5.46	115.18	110.21
1	B	517	HIS	N-CA-C	5.45	118.24	110.24
1	B	688	THR	N-CA-C	5.41	116.86	111.07
1	B	860	THR	N-CA-C	-5.37	102.21	110.58
1	D	1720	THR	N-CA-C	-5.35	100.18	108.90
1	D	1844	ALA	N-CA-C	-5.26	105.71	111.82
1	C	1208	SER	N-CA-C	-5.23	97.43	107.57
1	D	1610	GLY	N-CA-C	-5.16	106.66	112.33
1	C	1241	ASP	N-CA-C	5.14	120.20	113.88
1	B	540	PHE	CA-C-N	5.14	124.83	119.64
1	B	540	PHE	C-N-CA	5.14	124.83	119.64
1	B	740	LYS	N-CA-C	5.13	116.56	111.07
1	A	122	HIS	N-CA-C	5.12	117.99	111.69
1	C	1242	MET	N-CA-C	5.11	119.66	113.38
1	C	1360	THR	N-CA-C	-5.09	103.73	110.40
1	D	1740	LYS	N-CA-C	5.08	116.50	110.97
1	B	877	SER	N-CA-C	-5.07	97.64	107.62
1	D	1714	SER	N-CA-C	-5.03	105.71	111.14
1	C	1138	ALA	N-CA-C	-5.01	107.02	113.23
1	B	638	ALA	N-CA-C	-5.01	107.22	113.38
1	B	810	PRO	N-CA-C	5.00	120.20	114.20

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	3011	0	2971	120	0
1	B	3011	0	2968	102	0
1	C	3011	0	2968	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3011	0	2968	97	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	165	0	0	8	0
3	B	172	0	0	8	0
3	C	197	0	0	10	0
3	D	185	0	0	5	0
All	All	12783	0	11875	420	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 18.

All (420) 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:29:VAL:HB	1:D:1535:THR:HG22	1.15	1.07
1:B:663:ASN:HD22	1:B:663:ASN:H	1.07	1.01
1:C:1003:GLY:HA2	1:C:1013:ARG:HG2	1.44	0.97
1:D:1507:LEU:HB2	1:D:1508:PRO:HD3	1.50	0.94
1:B:533:TYR:HB3	3:B:993:HOH:O	1.68	0.93
1:D:1542:THR:HG22	1:D:1545:TYR:H	1.41	0.86
1:C:1043:VAL:H	1:D:1830:ASN:HD21	1.24	0.84
1:C:1061:ARG:NH2	1:D:1616:CYS:SG	2.50	0.84
1:C:1061:ARG:HG3	1:C:1246:VAL:CG2	2.07	0.83
1:C:1211:LLP:HD3	1:C:1341:LEU:HD13	1.58	0.83
1:A:43:VAL:H	1:B:830:ASN:HD21	1.23	0.83
1:A:29:VAL:HB	1:D:1535:THR:CG2	2.07	0.82
1:B:860:THR:C	1:B:862:GLU:H	1.86	0.82
1:C:1166:MET:HE2	1:C:1303:ALA:HA	1.63	0.81
1:B:663:ASN:H	1:B:663:ASN:ND2	1.78	0.81
1:C:1219:ILE:HD11	1:C:1251:ASP:HA	1.64	0.80
1:B:666:MET:H	1:B:799:GLN:HE22	1.29	0.80
1:B:663:ASN:HD22	1:B:663:ASN:N	1.78	0.79
1:C:1276:LEU:HB2	3:C:1585:HOH:O	1.81	0.79
1:C:1166:MET:H	1:C:1299:GLN:HE22	1.30	0.78
3:A:526:HOH:O	1:D:1522:GLN:HG3	1.81	0.78
1:B:863:GLU:HA	1:B:866:HIS:HB3	1.65	0.78
1:C:1243:THR:OG1	1:D:1743:THR:HA	1.83	0.77
1:B:501:MET:HE2	1:B:501:MET:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1095:SER:O	1:C:1099:THR:HG23	1.86	0.75
1:B:535:THR:HG22	3:B:993:HOH:O	1.86	0.75
1:A:33:TYR:H	1:A:66:THR:HG21	1.52	0.74
1:A:93:ILE:HG13	1:A:94:THR:N	2.01	0.74
1:B:894:LEU:HB3	1:B:895:LYS:HZ2	1.53	0.74
1:A:239:LEU:O	1:A:240:LYS:HB3	1.88	0.73
1:A:99:THR:HG21	1:A:234:ILE:HA	1.70	0.73
1:A:33:TYR:H	1:A:66:THR:CG2	2.01	0.73
1:C:1277:ALA:HB3	3:C:1403:HOH:O	1.87	0.73
1:D:1501:MET:N	1:D:1516:HIS:HB3	2.04	0.72
1:A:110:GLY:O	1:A:134:HIS:HD2	1.72	0.72
1:B:502:HIS:HB2	1:D:1834:LEU:HD13	1.70	0.72
1:A:3:GLY:O	1:A:13:ARG:HG2	1.90	0.72
1:D:1812:GLY:O	1:D:1878:VAL:HG12	1.89	0.71
1:C:1219:ILE:HD12	1:C:1254:LEU:HD23	1.73	0.71
1:A:5:ASN:N	1:A:5:ASN:HD22	1.89	0.71
1:C:1061:ARG:HG3	1:C:1246:VAL:HG21	1.71	0.71
1:A:302:LEU:HA	1:A:305:GLN:HG3	1.73	0.70
1:C:1093:ILE:HG13	1:C:1094:THR:N	2.06	0.70
1:C:1276:LEU:HD22	3:C:1585:HOH:O	1.92	0.70
1:D:1773:ALA:HB2	1:D:1878:VAL:HG11	1.74	0.69
1:D:1738:GLY:O	1:D:1742:MET:O	2.11	0.69
1:A:111:ASN:ND2	1:A:136:ASP:HA	2.07	0.69
1:B:891:GLN:HE21	1:B:891:GLN:HA	1.57	0.69
1:B:620:PHE:CZ	1:B:625:ILE:HG12	2.28	0.69
1:D:1595:SER:O	1:D:1599:THR:HG23	1.92	0.69
1:D:1504:SER:HB2	1:D:1517:HIS:CD2	2.27	0.68
1:A:2:HIS:HB2	1:C:1334:LEU:HD13	1.74	0.68
1:C:1166:MET:CE	1:C:1303:ALA:HA	2.24	0.68
1:B:599:THR:HG21	1:B:734:ILE:HA	1.75	0.67
1:B:666:MET:H	1:B:799:GLN:NE2	1.90	0.67
1:D:1542:THR:HG22	1:D:1545:TYR:N	2.10	0.67
1:C:1001:MET:HA	1:C:1008:PRO:HG3	1.77	0.67
1:C:1329:MET:HE3	1:C:1374:VAL:HB	1.75	0.66
1:C:1114:TYR:HB3	1:C:1117:THR:CG2	2.25	0.66
1:C:1114:TYR:HB3	1:C:1117:THR:HG23	1.76	0.66
1:A:95:SER:O	1:A:99:THR:HG23	1.96	0.66
1:C:1370:SER:HB3	1:C:1373:LEU:HB2	1.77	0.65
1:C:1276:LEU:O	1:C:1280:LEU:HD23	1.95	0.65
1:C:1121:LEU:HD23	1:C:1125:ILE:CD1	2.27	0.65
3:C:1444:HOH:O	1:D:1720:THR:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1542:THR:HG23	1:D:1544:GLU:H	1.62	0.65
1:B:507:LEU:O	1:B:507:LEU:HD23	1.97	0.65
1:C:1169:ILE:H	1:C:1306:GLN:HE22	1.45	0.65
1:D:1507:LEU:HB2	1:D:1508:PRO:CD	2.26	0.65
1:B:774:GLN:HG2	3:B:909:HOH:O	1.97	0.65
1:C:1121:LEU:HA	1:C:1125:ILE:HD12	1.77	0.64
1:D:1517:HIS:O	1:D:1573:ARG:HD3	1.97	0.64
1:B:860:THR:O	1:B:862:GLU:N	2.30	0.64
1:D:1504:SER:C	1:D:1506:LYS:H	2.04	0.64
1:D:1542:THR:CG2	1:D:1545:TYR:H	2.11	0.64
1:D:1711:LLP:HD3	1:D:1841:LEU:HG	1.80	0.64
1:A:135:VAL:HG23	1:A:137:MET:HE2	1.80	0.63
3:A:427:HOH:O	1:D:1535:THR:HG23	1.97	0.63
1:B:894:LEU:HB3	1:B:895:LYS:NZ	2.12	0.63
1:D:1542:THR:HG23	1:D:1544:GLU:N	2.13	0.63
1:C:1099:THR:HG21	1:C:1234:ILE:HA	1.80	0.62
1:A:263:ASN:H	1:A:263:ASN:HD22	1.45	0.62
1:C:1089:GLY:O	1:C:1093:ILE:HG23	2.00	0.62
1:A:29:VAL:CB	1:D:1535:THR:HG22	2.10	0.61
1:B:860:THR:C	1:B:862:GLU:N	2.54	0.61
1:C:1117:THR:HG21	3:C:1460:HOH:O	2.00	0.61
1:A:108:LEU:HD23	1:A:133:ARG:HB3	1.80	0.61
1:A:109:LEU:HB2	1:A:134:HIS:CD2	2.36	0.60
1:D:1504:SER:HA	1:D:1513:ARG:HD3	1.84	0.60
1:A:29:VAL:O	1:D:1535:THR:HG21	1.99	0.60
1:A:250:HIS:HD2	1:A:251:ASP:OD2	1.84	0.60
1:A:239:LEU:O	1:A:240:LYS:CB	2.49	0.60
1:B:867:TYR:HB3	1:B:869:ILE:CD1	2.31	0.60
1:D:1599:THR:HG21	1:D:1734:ILE:HA	1.83	0.60
1:C:1135:VAL:HG21	1:C:1143:LEU:HD23	1.83	0.60
1:C:1219:ILE:CD1	1:C:1254:LEU:HD23	2.32	0.59
1:A:345:GLU:HG3	1:C:1028:LEU:HD11	1.84	0.59
1:C:1098:TRP:CZ3	1:C:1125:ILE:HG23	2.38	0.59
1:C:1243:THR:CG2	1:C:1245:ALA:H	2.15	0.59
1:A:111:ASN:HD22	1:A:136:ASP:HA	1.67	0.59
1:B:598:TRP:CZ3	1:B:625:ILE:HG23	2.37	0.58
1:D:1524:HIS:HD2	3:D:2034:HOH:O	1.85	0.58
1:A:339:VAL:HG22	3:B:936:HOH:O	2.04	0.58
1:B:655:TYR:CD1	1:B:684:VAL:HG22	2.39	0.58
1:B:704:LEU:HD12	1:B:726:GLY:HA3	1.85	0.58
1:C:1121:LEU:HA	1:C:1125:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD21	1:A:133:ARG:HH21	1.68	0.58
1:A:211:LLP:HD3	1:A:341:LEU:HG	1.84	0.58
1:B:601:LEU:HD21	1:B:653:VAL:HG13	1.86	0.58
1:B:863:GLU:OE2	1:B:867:TYR:HB2	2.04	0.58
1:D:1595:SER:O	1:D:1599:THR:CG2	2.51	0.58
1:D:1860:THR:H	1:D:1863:GLU:HB2	1.69	0.58
1:C:1166:MET:H	1:C:1299:GLN:NE2	1.99	0.57
1:D:1504:SER:C	1:D:1506:LYS:N	2.59	0.57
1:B:727:SER:OG	1:B:730:LEU:HB2	2.05	0.57
1:A:143:LEU:HD23	1:A:175:ILE:HD12	1.87	0.57
1:B:595:SER:O	1:B:599:THR:CG2	2.53	0.57
1:A:108:LEU:CD2	1:A:133:ARG:HB3	2.35	0.56
1:A:48:ALA:CB	1:A:54:GLN:HB2	2.35	0.56
1:B:599:THR:HB	1:B:737:GLN:HG2	1.86	0.56
1:B:608:LEU:HD22	1:B:651:THR:HG21	1.86	0.56
1:A:288:LEU:HB3	1:A:317:GLU:HG3	1.87	0.56
1:A:359:TYR:HB2	1:A:364:ARG:HG3	1.87	0.56
1:A:389:ASP:O	1:A:392:GLN:HG3	2.05	0.56
1:C:1360:THR:OG1	1:C:1362:GLU:HG2	2.06	0.56
1:A:322:ILE:HG13	3:A:559:HOH:O	2.06	0.56
1:B:768:ARG:NH1	3:B:988:HOH:O	2.36	0.56
1:B:867:TYR:HB3	1:B:869:ILE:HD11	1.88	0.56
1:D:1865:ALA:C	1:D:1867:TYR:H	2.14	0.56
1:A:3:GLY:HA2	1:A:13:ARG:HG2	1.88	0.56
1:C:1290:HIS:HD2	3:C:1466:HOH:O	1.88	0.56
1:A:110:GLY:O	1:A:134:HIS:CD2	2.57	0.55
1:A:154:ILE:HD12	1:A:176:ALA:HB2	1.88	0.55
1:B:668:ASP:O	1:B:672:VAL:HG13	2.06	0.55
1:C:1285:GLN:H	1:C:1285:GLN:HE21	1.54	0.55
1:C:1262:LEU:HD22	1:C:1266:MET:HG2	1.89	0.55
1:A:327:ARG:NH2	1:A:397:SER:O	2.40	0.55
1:B:676:ALA:HB3	1:B:677:ARG:HH21	1.72	0.55
1:B:570:LEU:HD21	1:B:755:LEU:HD13	1.88	0.55
1:C:1003:GLY:CA	1:C:1013:ARG:HG2	2.28	0.55
1:C:1108:LEU:HD22	1:C:1151:THR:HG21	1.88	0.55
1:A:78:GLU:HG2	1:A:192:PRO:HB3	1.88	0.54
1:B:548:ALA:CB	1:B:554:GLN:HB2	2.37	0.54
1:C:1204:LEU:HD23	1:C:1226:GLY:HA3	1.87	0.54
1:D:1839:VAL:O	1:D:1840:SER:CB	2.55	0.54
1:B:675:ILE:HA	1:B:678:LYS:HE3	1.90	0.54
1:C:1002:HIS:O	1:C:1017:HIS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1091:GLY:HA2	1:D:1743:THR:O	2.08	0.54
1:A:78:GLU:OE2	1:A:207:HIS:HE1	1.91	0.54
1:B:607:VAL:HG22	1:B:609:LEU:HD13	1.89	0.54
1:A:32:VAL:HB	1:D:1532:VAL:HG12	1.89	0.53
1:A:300:TYR:O	1:A:304:ARG:HG2	2.08	0.53
1:C:1320:GLY:HA3	1:C:1324:ALA:HB2	1.90	0.53
1:C:1011:ALA:O	1:C:1015:ILE:HG23	2.09	0.53
1:A:78:GLU:OE2	1:A:207:HIS:CE1	2.61	0.53
1:C:1194:LEU:HD22	1:C:1309:GLN:HB2	1.90	0.53
1:A:8:PRO:O	1:A:13:ARG:HD3	2.09	0.53
1:C:1047:ALA:HA	1:C:1050:PHE:HD1	1.73	0.53
1:D:1504:SER:O	1:D:1507:LEU:HG	2.08	0.53
1:D:1677:ARG:HA	1:D:1677:ARG:NE	2.23	0.53
1:D:1694:LEU:HD22	1:D:1809:GLN:HB2	1.91	0.53
1:D:1778:GLU:O	1:D:1782:ARG:HG3	2.09	0.53
1:B:548:ALA:HB1	1:B:554:GLN:HB2	1.90	0.52
1:B:860:THR:OG1	1:B:862:GLU:HG2	2.09	0.52
1:C:1169:ILE:H	1:C:1306:GLN:NE2	2.07	0.52
1:A:48:ALA:HB1	1:A:54:GLN:HB2	1.90	0.52
1:A:339:VAL:O	1:A:340:SER:CB	2.58	0.52
1:D:1696:ARG:NH2	3:D:2043:HOH:O	2.42	0.52
1:D:1816:PHE:CE1	1:D:1874:VAL:HG22	2.44	0.52
1:B:608:LEU:HD22	1:B:651:THR:CG2	2.39	0.52
1:D:1503:GLY:C	1:D:1517:HIS:HD2	2.17	0.52
1:A:238:GLY:O	1:A:243:THR:HB	2.10	0.52
1:B:502:HIS:CB	1:D:1834:LEU:HD13	2.39	0.52
1:C:1120:PHE:CZ	1:C:1125:ILE:HG12	2.44	0.52
1:C:1168:ASP:O	1:C:1172:VAL:HG13	2.09	0.52
1:C:1395:LYS:HD3	1:C:1395:LYS:N	2.25	0.52
1:D:1507:LEU:CB	1:D:1508:PRO:HD3	2.32	0.52
1:D:1601:LEU:HD21	1:D:1607:VAL:HG21	1.90	0.52
1:D:1578:GLU:OE1	1:D:1707:HIS:HE1	1.92	0.52
1:B:863:GLU:O	1:B:863:GLU:HG3	2.09	0.52
1:C:1250:HIS:HD2	1:C:1251:ASP:OD2	1.93	0.52
1:D:1821:GLY:HA2	1:D:1872:GLY:HA3	1.91	0.52
1:B:663:ASN:ND2	1:B:663:ASN:N	2.45	0.52
1:B:743:THR:HG22	1:B:745:ALA:HB2	1.92	0.52
1:C:1166:MET:HE2	1:C:1303:ALA:CA	2.36	0.52
1:B:862:GLU:CG	1:B:863:GLU:H	2.21	0.51
1:A:135:VAL:HG23	1:A:137:MET:CE	2.39	0.51
1:A:229:ALA:O	1:A:233:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1328:PHE:CD2	1:C:1329:MET:HE2	2.46	0.51
1:A:3:GLY:HA2	1:A:13:ARG:CG	2.41	0.51
1:A:34:GLN:HG3	1:B:718:ASP:O	2.11	0.51
1:B:538:PHE:HB2	1:B:558:PHE:HA	1.92	0.51
1:D:1641:GLN:H	1:D:1641:GLN:NE2	2.09	0.51
1:C:1114:TYR:CE2	1:C:1116:CYS:HB2	2.45	0.51
1:B:705:VAL:HG23	1:B:725:VAL:HB	1.93	0.51
1:D:1866:HIS:C	1:D:1867:TYR:HD1	2.19	0.51
1:C:1328:PHE:HD2	1:C:1329:MET:HE2	1.76	0.50
1:B:768:ARG:NH2	3:B:1072:HOH:O	2.39	0.50
1:A:122:HIS:NE2	1:A:134:HIS:HE1	2.09	0.50
1:A:133:ARG:NH2	1:A:146:ALA:O	2.45	0.50
1:C:1285:GLN:H	1:C:1285:GLN:NE2	2.09	0.50
1:C:1287:GLU:HB2	1:C:1319:LYS:HG2	1.92	0.50
1:B:673:ALA:O	1:B:677:ARG:NE	2.45	0.50
1:B:705:VAL:CG2	1:B:725:VAL:HB	2.42	0.50
1:B:502:HIS:HB2	1:D:1834:LEU:CD1	2.41	0.50
1:B:611:ASN:OD1	1:B:636:ASP:HA	2.11	0.50
1:B:557:HIS:HE1	1:B:568:ASN:ND2	2.09	0.50
1:B:891:GLN:HE21	1:B:891:GLN:CA	2.23	0.50
1:C:1200:LEU:HD11	1:C:1306:GLN:HG2	1.94	0.50
1:D:1716:HIS:HB2	3:D:2059:HOH:O	2.11	0.50
1:C:1349:GLN:NE2	3:C:1532:HOH:O	2.44	0.50
1:D:1648:THR:HB	1:D:1649:PRO:HD2	1.94	0.50
1:A:360:THR:OG1	1:A:363:GLU:HG3	2.12	0.50
1:A:213:LEU:HB3	1:A:255:LEU:HD11	1.93	0.49
1:C:1243:THR:HG23	1:C:1245:ALA:H	1.77	0.49
1:C:1243:THR:HG23	1:C:1245:ALA:CB	2.42	0.49
1:D:1578:GLU:OE1	1:D:1707:HIS:CE1	2.66	0.49
1:B:711:LLP:HD3	1:B:841:LEU:HG	1.94	0.49
1:D:1541:PRO:HD2	1:D:1545:TYR:CD1	2.47	0.49
1:D:1601:LEU:HD11	1:D:1653:VAL:HG13	1.94	0.49
1:D:1504:SER:CB	1:D:1517:HIS:CD2	2.94	0.49
1:A:194:LEU:O	1:A:307:MET:HA	2.13	0.48
1:D:1790:HIS:HE1	1:D:1817:GLU:OE1	1.96	0.48
1:C:1061:ARG:HG3	1:C:1246:VAL:HG22	1.91	0.48
1:A:161:ASN:HD21	1:A:375:ARG:HD2	1.76	0.48
1:A:32:VAL:HB	1:D:1532:VAL:CG1	2.44	0.48
1:B:595:SER:O	1:B:599:THR:HG23	2.13	0.48
1:B:676:ALA:CB	1:B:677:ARG:HH21	2.26	0.48
1:C:1219:ILE:HD13	1:C:1254:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1825:GLY:O	1:D:1829:MET:HG2	2.13	0.48
1:B:507:LEU:HD22	3:B:1022:HOH:O	2.13	0.48
1:A:345:GLU:HG3	1:C:1028:LEU:CD1	2.44	0.48
1:C:1243:THR:HG1	1:D:1743:THR:HA	1.76	0.48
1:D:1860:THR:HG23	1:D:1863:GLU:OE2	2.13	0.48
1:A:367:TYR:HB3	1:A:369:ILE:HD12	1.96	0.48
1:B:503:GLY:O	1:B:513:ARG:HG2	2.14	0.48
1:B:677:ARG:HE	1:B:677:ARG:N	2.12	0.48
3:C:1434:HOH:O	1:D:1839:VAL:HG22	2.13	0.48
1:D:1859:TYR:HB2	1:D:1864:ARG:HG3	1.94	0.48
1:D:1865:ALA:C	1:D:1867:TYR:N	2.72	0.48
1:C:1211:LLP:HD3	1:C:1341:LEU:CD1	2.38	0.47
1:A:48:ALA:HB1	1:A:53:GLU:HG3	1.96	0.47
1:C:1364:ARG:HG2	1:C:1369:ILE:HB	1.96	0.47
1:A:164:MET:O	1:A:166:MET:HE2	2.14	0.47
1:B:783:GLN:HG3	1:B:894:LEU:CD2	2.45	0.47
1:D:1654:ILE:HD12	1:D:1676:ALA:HB2	1.96	0.47
1:C:1135:VAL:HG22	1:C:1137:MET:HE2	1.95	0.47
1:C:1339:VAL:O	1:C:1340:SER:HB3	2.13	0.47
1:C:1057:HIS:HE1	1:C:1068:ASN:HD21	1.62	0.47
1:D:1584:LEU:HD11	1:D:1739:LEU:HD12	1.97	0.47
1:A:43:VAL:HG22	1:B:830:ASN:HD21	1.79	0.47
1:A:95:SER:OG	1:A:243:THR:HG21	2.14	0.47
1:B:608:LEU:HD12	1:B:633:ARG:HB3	1.97	0.47
1:C:1108:LEU:HD22	1:C:1151:THR:CG2	2.45	0.47
1:C:1180:GLY:O	1:C:1181:ALA:O	2.33	0.47
1:D:1671:GLY:O	1:D:1674:LYS:HE2	2.15	0.47
1:D:1714:SER:OG	3:D:2059:HOH:O	2.21	0.47
1:C:1187:ASN:ND2	1:C:1195:GLN:HE21	2.12	0.47
1:A:328:PHE:HB2	1:A:397:SER:HB2	1.97	0.47
1:C:1177:ARG:NH2	1:C:1203:ASP:OD1	2.48	0.47
1:A:3:GLY:HA2	1:A:13:ARG:HA	1.96	0.46
1:A:190:CYS:O	1:A:194:LEU:HB2	2.14	0.46
1:B:657:GLU:HG2	1:B:686:ASP:HB3	1.96	0.46
1:C:1198:LEU:HD11	1:C:1225:VAL:HG12	1.97	0.46
1:A:218:ASP:O	1:B:534:GLN:HG3	2.16	0.46
1:A:301:THR:O	1:A:305:GLN:HG2	2.14	0.46
1:B:661:ASN:HB3	1:B:662:PRO:HA	1.97	0.46
1:B:698:LEU:HB2	3:B:975:HOH:O	2.15	0.46
1:C:1352:ALA:O	1:C:1357:SER:HA	2.16	0.46
1:A:62:ILE:HG13	1:A:240:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:GLU:H	1:B:544:GLU:HG2	1.39	0.46
1:C:1243:THR:HG22	1:C:1245:ALA:H	1.80	0.46
1:C:1318:LEU:HD12	1:C:1325:GLY:HA2	1.96	0.46
1:C:1353:SER:C	1:C:1357:SER:HB2	2.41	0.46
1:D:1862:GLU:H	1:D:1862:GLU:CD	2.22	0.46
1:C:1057:HIS:HE1	1:C:1068:ASN:ND2	2.14	0.46
1:D:1614:TYR:CE2	1:D:1616:CYS:HB2	2.51	0.46
1:A:2:HIS:C	1:A:4:SER:H	2.24	0.46
1:A:345:GLU:H	1:A:345:GLU:HG2	1.49	0.46
1:C:1034:GLN:HG3	1:D:1718:ASP:O	2.16	0.46
1:B:564:ASN:ND2	1:B:566:THR:HB	2.30	0.46
1:C:1288:LEU:HB3	1:C:1317:GLU:HG3	1.98	0.46
1:D:1506:LYS:HE3	1:D:1579:GLY:HA2	1.98	0.46
1:B:621:LEU:HD13	1:B:625:ILE:HD11	1.98	0.46
1:C:1114:TYR:HD2	1:C:1117:THR:HG22	1.81	0.46
1:D:1505:ASN:O	1:D:1506:LYS:HB2	2.16	0.46
1:A:159:PRO:HB3	1:A:166:MET:CE	2.46	0.45
1:A:3:GLY:C	1:A:17:HIS:HD2	2.24	0.45
1:C:1003:GLY:O	1:C:1008:PRO:HD2	2.17	0.45
1:A:3:GLY:O	1:A:17:HIS:HD2	1.98	0.45
1:C:1004:SER:O	1:C:1005:ASN:C	2.60	0.45
1:A:170:ALA:HA	1:A:200:LEU:O	2.16	0.45
1:B:564:ASN:ND2	1:B:566:THR:H	2.15	0.45
1:B:663:ASN:O	1:B:664:MET:HB2	2.17	0.45
1:C:1090:MET:HE1	1:C:1117:THR:HA	1.98	0.45
1:C:1003:GLY:O	1:C:1013:ARG:HD3	2.17	0.45
1:C:1243:THR:HG23	1:C:1245:ALA:HB2	1.98	0.45
1:B:564:ASN:HD22	1:B:567:LEU:H	1.65	0.45
1:B:578:GLU:OE2	1:B:707:HIS:CE1	2.70	0.45
1:A:2:HIS:CE1	1:A:5:ASN:HB2	2.52	0.45
1:C:1326:ARG:HG2	1:D:1543:VAL:HG11	1.99	0.45
1:A:93:ILE:HD13	1:A:117:THR:HG23	1.98	0.45
1:B:864:ARG:HA	1:B:869:ILE:HD12	1.98	0.45
1:D:1862:GLU:HB3	1:D:1866:HIS:NE2	2.32	0.45
1:C:1356:HIS:O	1:C:1359:TYR:HB2	2.16	0.44
1:A:108:LEU:CD2	1:A:133:ARG:HD2	2.47	0.44
1:B:852:ALA:HA	1:B:864:ARG:HD3	1.99	0.44
1:C:1238:GLY:O	1:C:1243:THR:HB	2.17	0.44
1:A:324:ALA:HA	1:A:327:ARG:NH2	2.32	0.44
1:A:6:LYS:O	1:A:7:LEU:C	2.60	0.44
1:A:212:TYR:CD1	1:A:342:GLY:HA2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1690:CYS:SG	1:D:1807:MET:HE3	2.57	0.44
1:A:46:GLY:O	1:A:49:CYS:HB2	2.18	0.44
1:A:89:GLY:O	1:A:93:ILE:HG23	2.17	0.44
1:A:335:PHE:CE1	1:A:346:SER:HB3	2.52	0.44
1:C:1238:GLY:HA2	1:C:1242:MET:HE3	1.98	0.44
1:A:2:HIS:HB3	1:A:3:GLY:H	1.48	0.44
1:A:152:ARG:NH1	3:A:552:HOH:O	2.49	0.44
1:A:314:ILE:CG2	1:A:376:LEU:HB2	2.48	0.44
1:B:791:TYR:HB3	1:B:794:LEU:HD22	2.00	0.44
1:C:1046:GLY:O	1:C:1050:PHE:CD1	2.71	0.44
1:C:1219:ILE:CD1	1:C:1254:LEU:HB3	2.48	0.44
1:A:233:ARG:O	1:A:237:GLN:HB2	2.18	0.44
1:D:1601:LEU:HD21	1:D:1607:VAL:CG2	2.48	0.44
1:A:243:THR:HG23	1:A:245:ALA:H	1.83	0.43
1:C:1281:ALA:HA	1:C:1289:ILE:HD11	1.99	0.43
1:B:505:ASN:HA	1:B:513:ARG:HD2	2.00	0.43
1:B:713:LEU:HB3	1:B:755:LEU:HD21	2.00	0.43
1:D:1711:LLP:NZ	1:D:1711:LLP:O3	2.50	0.43
1:D:1801:THR:O	1:D:1805:GLN:HG3	2.17	0.43
1:D:1866:HIS:ND1	1:D:1866:HIS:N	2.67	0.43
1:A:2:HIS:CG	1:A:5:ASN:HB2	2.53	0.43
1:C:1006:LYS:HE2	1:C:1007:LEU:H	1.83	0.43
1:C:1350:HIS:HD2	1:C:1373:LEU:O	2.02	0.43
1:A:66:THR:HB	3:A:508:HOH:O	2.18	0.43
1:A:336:SER:HB2	1:A:347:LEU:HD12	2.00	0.43
1:A:1:MET:HE2	3:C:1424:HOH:O	2.18	0.43
1:C:1200:LEU:CD1	1:C:1306:GLN:HG2	2.49	0.43
1:C:1243:THR:HG23	1:C:1245:ALA:N	2.34	0.43
1:C:1341:LEU:HD13	1:C:1341:LEU:N	2.34	0.43
1:A:99:THR:HG22	1:A:238:GLY:CA	2.49	0.43
1:C:1339:VAL:O	1:C:1340:SER:CB	2.67	0.43
1:D:1644:GLU:OE1	1:D:1678:LYS:HE3	2.19	0.43
1:B:553:GLU:H	1:B:553:GLU:HG2	1.67	0.42
1:B:677:ARG:NH2	1:B:683:VAL:HG23	2.33	0.42
1:C:1163:ASN:HB2	3:C:1580:HOH:O	2.19	0.42
1:A:322:ILE:HG13	1:A:322:ILE:H	1.49	0.42
1:C:1007:LEU:N	1:C:1008:PRO:HD3	2.35	0.42
1:A:359:TYR:N	1:A:359:TYR:CD1	2.87	0.42
1:D:1684:VAL:HA	1:D:1704:LEU:O	2.19	0.42
1:D:1850:HIS:NE2	1:D:1852:ALA:HB3	2.34	0.42
1:A:107:VAL:CG1	1:A:132:LEU:HD12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:SER:C	1:A:357:SER:HB2	2.45	0.42
1:C:1210:THR:HG23	1:C:1219:ILE:O	2.19	0.42
1:C:1360:THR:H	1:C:1363:GLU:HB2	1.84	0.42
1:C:1004:SER:HB2	1:C:1017:HIS:HE1	1.85	0.42
1:C:1276:LEU:O	1:C:1280:LEU:CD2	2.65	0.42
1:D:1712:TYR:CE1	1:D:1842:GLY:HA2	2.55	0.42
1:B:743:THR:CG2	1:B:745:ALA:HB2	2.50	0.42
1:A:43:VAL:HG22	1:B:830:ASN:ND2	2.35	0.42
1:A:108:LEU:HD21	1:A:133:ARG:HD2	2.02	0.42
1:B:643:LEU:HD13	1:B:675:ILE:HG21	2.01	0.42
1:B:891:GLN:O	1:B:895:LYS:HD2	2.19	0.42
1:A:111:ASN:ND2	3:A:499:HOH:O	2.52	0.42
1:B:506:LYS:H	1:B:513:ARG:CZ	2.31	0.42
1:B:531:PRO:HB2	1:C:1031:PRO:HB2	2.00	0.42
1:B:852:ALA:O	1:B:857:SER:HA	2.20	0.42
1:C:1125:ILE:H	1:C:1125:ILE:HG13	1.32	0.42
1:A:177:ARG:HD2	3:A:525:HOH:O	2.20	0.42
1:B:835:PHE:CE2	1:B:846:SER:HB3	2.55	0.42
1:D:1599:THR:HG22	1:D:1738:GLY:CA	2.50	0.42
1:A:191:THR:HB	1:A:192:PRO:HD2	2.02	0.41
1:A:211:LLP:NZ	1:A:211:LLP:O3	2.53	0.41
1:C:1095:SER:OG	1:C:1243:THR:HG21	2.20	0.41
1:C:1102:ARG:HD3	1:C:1102:ARG:HA	1.90	0.41
1:D:1542:THR:CG2	1:D:1545:TYR:N	2.79	0.41
1:A:102:ARG:HD3	1:A:102:ARG:HA	1.88	0.41
1:B:635:VAL:HG11	1:B:643:LEU:HA	2.01	0.41
1:D:1611:ASN:HD21	1:D:1636:ASP:HB2	1.85	0.41
1:A:3:GLY:CA	1:A:13:ARG:HG2	2.50	0.41
1:A:268:ARG:HB2	1:A:268:ARG:NH1	2.35	0.41
1:A:86:LEU:HD13	1:A:92:ALA:HA	2.02	0.41
1:B:704:LEU:HD13	1:B:730:LEU:HD23	2.02	0.41
1:C:1219:ILE:HG12	1:C:1251:ASP:HB3	2.01	0.41
1:C:1006:LYS:HE2	1:C:1006:LYS:HB3	1.86	0.41
1:A:107:VAL:HG13	1:A:107:VAL:O	2.21	0.41
1:C:1317:GLU:HA	1:C:1372:GLY:O	2.21	0.41
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.93	0.41
1:B:541:PRO:HD2	1:B:545:TYR:CD2	2.55	0.41
1:C:1057:HIS:CE1	1:C:1068:ASN:HD21	2.38	0.41
1:C:1190:CYS:C	1:C:1191:THR:HG23	2.46	0.41
1:C:1288:LEU:HD12	1:C:1289:ILE:H	1.86	0.41
1:A:45:TYR:CE2	1:A:49:CYS:SG	3.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:TYR:N	1:A:359:TYR:HD1	2.19	0.41
1:B:557:HIS:CE1	1:B:568:ASN:ND2	2.89	0.41
1:C:1177:ARG:HH22	1:C:1183:VAL:HG23	1.86	0.41
1:D:1504:SER:N	1:D:1517:HIS:CD2	2.89	0.41
1:D:1608:LEU:HD12	1:D:1608:LEU:HA	1.92	0.41
1:A:7:LEU:HD23	3:A:509:HOH:O	2.20	0.41
1:B:862:GLU:HG3	1:B:863:GLU:H	1.83	0.41
1:B:891:GLN:NE2	1:B:895:LYS:NZ	2.69	0.41
1:C:1093:ILE:HD13	1:C:1117:THR:HB	2.02	0.41
1:A:204:LEU:HD23	1:A:226:GLY:HA3	2.02	0.41
1:A:243:THR:CG2	1:A:245:ALA:H	2.34	0.41
1:B:863:GLU:HA	1:B:866:HIS:CB	2.43	0.41
1:D:1773:ALA:CB	1:D:1878:VAL:HG11	2.49	0.41
1:C:1329:MET:CE	1:C:1374:VAL:HB	2.48	0.40
1:D:1804:ARG:NH2	3:D:1943:HOH:O	2.55	0.40
1:A:93:ILE:HD12	1:A:97:LEU:CD2	2.50	0.40
1:A:301:THR:O	1:A:305:GLN:CG	2.70	0.40
1:B:825:GLY:O	1:B:829:MET:HG2	2.21	0.40
1:B:520:ASP:HB3	1:B:523:ASP:OD2	2.21	0.40
1:C:1007:LEU:HD13	1:C:1007:LEU:HA	1.87	0.40
1:C:1340:SER:N	2:C:1400:SO4:O1	2.43	0.40
1:C:1341:LEU:CD1	1:C:1341:LEU:N	2.84	0.40
1:D:1823:GLY:HA2	1:D:1826:ARG:NH2	2.36	0.40
1:A:38:PHE:HA	1:D:1526:GLY:O	2.21	0.40
1:B:504:SER:O	1:B:513:ARG:HD3	2.21	0.40
1:D:1655:TYR:CD1	1:D:1684:VAL:HG22	2.56	0.40
1:D:1839:VAL:O	1:D:1840:SER:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	A	211	-	23,24,25	2.93	7 (30%)	25,32,34	1.66	3 (12%)
1	LLP	C	1211	-	23,24,25	2.96	8 (34%)	25,32,34	1.63	4 (16%)
1	LLP	D	1711	-	23,24,25	2.95	7 (30%)	25,32,34	1.70	5 (20%)
1	LLP	B	711	-	23,24,25	2.95	7 (30%)	25,32,34	1.68	5 (20%)

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
1	LLP	A	211	-	-	4/16/17/19	0/1/1/1
1	LLP	C	1211	-	-	5/16/17/19	0/1/1/1
1	LLP	D	1711	-	-	4/16/17/19	0/1/1/1
1	LLP	B	711	-	-	5/16/17/19	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	711	LLP	C6-C5	7.84	1.53	1.37
1	D	1711	LLP	C6-C5	7.77	1.53	1.37
1	C	1211	LLP	C6-C5	7.74	1.53	1.37
1	A	211	LLP	C6-C5	7.57	1.52	1.37
1	B	711	LLP	C6-N1	6.11	1.46	1.34
1	D	1711	LLP	C6-N1	5.89	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1211	LLP	C6-N1	5.88	1.46	1.34
1	A	211	LLP	C4'-NZ	5.88	1.46	1.27
1	C	1211	LLP	C4'-NZ	5.81	1.46	1.27
1	D	1711	LLP	C4'-NZ	5.79	1.46	1.27
1	B	711	LLP	C4'-NZ	5.77	1.46	1.27
1	A	211	LLP	C6-N1	5.76	1.46	1.34
1	C	1211	LLP	O3-C3	-5.71	1.23	1.36
1	B	711	LLP	O3-C3	-5.65	1.24	1.36
1	A	211	LLP	O3-C3	-5.57	1.24	1.36
1	D	1711	LLP	O3-C3	-5.51	1.24	1.36
1	C	1211	LLP	C4-C4'	3.61	1.54	1.46
1	A	211	LLP	P-OP4	-3.61	1.48	1.60
1	A	211	LLP	C4-C4'	3.57	1.54	1.46
1	D	1711	LLP	P-OP4	-3.57	1.49	1.60
1	C	1211	LLP	P-OP4	-3.32	1.49	1.60
1	B	711	LLP	P-OP4	-3.26	1.50	1.60
1	B	711	LLP	C4-C4'	3.23	1.53	1.46
1	D	1711	LLP	C4-C4'	3.22	1.53	1.46
1	D	1711	LLP	C2'-C2	2.25	1.54	1.50
1	C	1211	LLP	C2'-C2	2.08	1.53	1.50
1	B	711	LLP	C2'-C2	2.04	1.53	1.50
1	C	1211	LLP	P-OP2	-2.00	1.47	1.54
1	A	211	LLP	C2'-C2	2.00	1.53	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LLP	C5-C6-N1	-6.16	113.81	123.83
1	D	1711	LLP	C5-C6-N1	-6.06	113.97	123.83
1	B	711	LLP	C5-C6-N1	-6.01	114.06	123.83
1	C	1211	LLP	C5-C6-N1	-5.88	114.26	123.83
1	A	211	LLP	C6-N1-C2	2.51	123.76	119.20
1	D	1711	LLP	C4-C4'-NZ	-2.46	112.69	124.04
1	D	1711	LLP	C4-C3-C2	2.38	121.48	120.14
1	B	711	LLP	C4-C4'-NZ	-2.37	113.09	124.04
1	C	1211	LLP	C4-C4'-NZ	-2.34	113.25	124.04
1	B	711	LLP	C6-N1-C2	2.33	123.43	119.20
1	A	211	LLP	C4-C4'-NZ	-2.33	113.28	124.04
1	B	711	LLP	C4-C3-C2	2.33	121.45	120.14
1	D	1711	LLP	C6-N1-C2	2.26	123.31	119.20
1	D	1711	LLP	C2'-C2-C3	-2.26	118.15	120.80
1	C	1211	LLP	C6-N1-C2	2.23	123.25	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1211	LLP	C4-C3-C2	2.21	121.39	120.14
1	B	711	LLP	C2'-C2-C3	-2.16	118.27	120.80

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	211	LLP	O-C-CA-CB
1	B	711	LLP	O-C-CA-CB
1	C	1211	LLP	C4-C4'-NZ-CE
1	C	1211	LLP	O-C-CA-CB
1	D	1711	LLP	O-C-CA-CB
1	A	211	LLP	C4-C4'-NZ-CE
1	D	1711	LLP	C4-C4'-NZ-CE
1	B	711	LLP	C4-C4'-NZ-CE
1	B	711	LLP	CG-CD-CE-NZ
1	D	1711	LLP	C4-C5-C5'-OP4
1	C	1211	LLP	CD-CE-NZ-C4'
1	A	211	LLP	CD-CE-NZ-C4'
1	C	1211	LLP	C3-C4-C4'-NZ
1	B	711	LLP	CD-CE-NZ-C4'
1	A	211	LLP	N-CA-CB-CG
1	C	1211	LLP	N-CA-CB-CG
1	B	711	LLP	C3-C4-C4'-NZ
1	D	1711	LLP	CD-CE-NZ-C4'

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	211	LLP	2	0
1	C	1211	LLP	2	0
1	D	1711	LLP	2	0
1	B	711	LLP	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	D	1900	-	4,4,4	0.54	0	6,6,6	0.09	0
2	SO4	C	1400	-	4,4,4	0.53	0	6,6,6	0.08	0
2	SO4	A	400	-	4,4,4	0.59	0	6,6,6	0.09	0
2	SO4	B	900	-	4,4,4	0.43	0	6,6,6	0.07	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1400	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.