



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:35 PM BST

PDB ID : 4AU5
Title : Structure of the NhaA dimer, crystallised at low pH
Authors : Drew, D.; Lee, C.; Iwata, S.; Cameron, A.D.
Deposited on : 2012-05-14
Resolution : 3.70 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

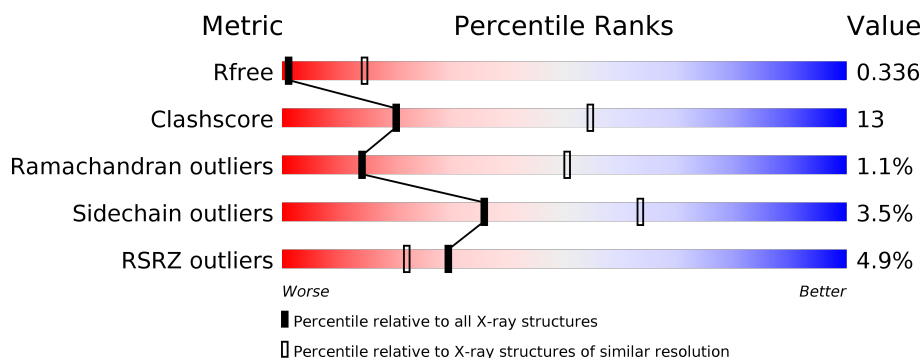
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	401	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• 5%</div> </div> </div>
1	B	401	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• 7%</div> </div> </div>
1	C	401	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	D	401	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• 7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	1385	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11343 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 NA(+)/H(+) ANTIPORTER NHAA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2853	1895	465	480	13			
1	B	374	Total	C	N	O	S	0	0	0
			2794	1856	455	470	13			
1	C	381	Total	C	N	O	S	0	0	0
			2853	1895	465	480	13			
1	D	374	Total	C	N	O	S	0	0	0
			2794	1856	455	470	13			

There are 52 discrepancies between the modelled and reference sequences:

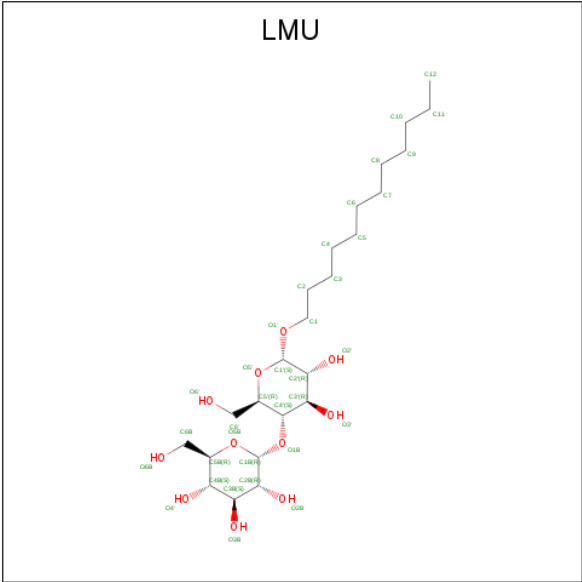
Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLU	-	expression tag	UNP P13738
A	390	PHE	-	expression tag	UNP P13738
A	391	ARG	-	expression tag	UNP P13738
A	392	VAL	-	expression tag	UNP P13738
A	393	PRO	-	expression tag	UNP P13738
A	394	GLY	-	expression tag	UNP P13738
A	395	SER	-	expression tag	UNP P13738
A	396	GLU	-	expression tag	UNP P13738
A	397	ASN	-	expression tag	UNP P13738
A	398	LEU	-	expression tag	UNP P13738
A	399	TYR	-	expression tag	UNP P13738
A	400	PHE	-	expression tag	UNP P13738
A	401	GLN	-	expression tag	UNP P13738
B	389	GLU	-	expression tag	UNP P13738
B	390	PHE	-	expression tag	UNP P13738
B	391	ARG	-	expression tag	UNP P13738
B	392	VAL	-	expression tag	UNP P13738
B	393	PRO	-	expression tag	UNP P13738
B	394	GLY	-	expression tag	UNP P13738
B	395	SER	-	expression tag	UNP P13738
B	396	GLU	-	expression tag	UNP P13738

Continued on next page...

Continued from previous page...

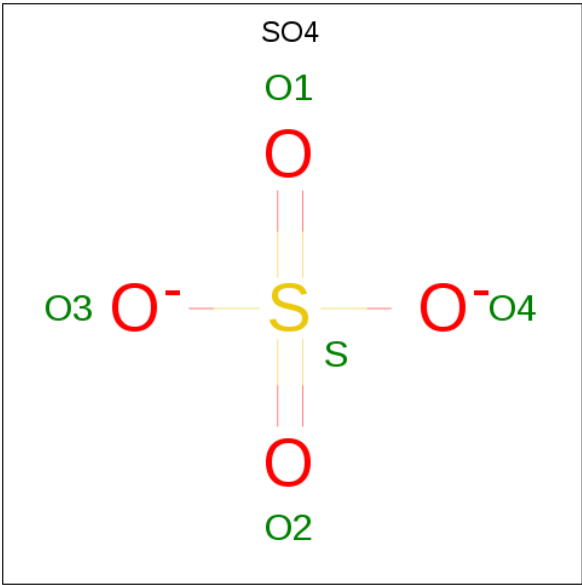
Chain	Residue	Modelled	Actual	Comment	Reference
B	397	ASN	-	expression tag	UNP P13738
B	398	LEU	-	expression tag	UNP P13738
B	399	TYR	-	expression tag	UNP P13738
B	400	PHE	-	expression tag	UNP P13738
B	401	GLN	-	expression tag	UNP P13738
C	389	GLU	-	expression tag	UNP P13738
C	390	PHE	-	expression tag	UNP P13738
C	391	ARG	-	expression tag	UNP P13738
C	392	VAL	-	expression tag	UNP P13738
C	393	PRO	-	expression tag	UNP P13738
C	394	GLY	-	expression tag	UNP P13738
C	395	SER	-	expression tag	UNP P13738
C	396	GLU	-	expression tag	UNP P13738
C	397	ASN	-	expression tag	UNP P13738
C	398	LEU	-	expression tag	UNP P13738
C	399	TYR	-	expression tag	UNP P13738
C	400	PHE	-	expression tag	UNP P13738
C	401	GLN	-	expression tag	UNP P13738
D	389	GLU	-	expression tag	UNP P13738
D	390	PHE	-	expression tag	UNP P13738
D	391	ARG	-	expression tag	UNP P13738
D	392	VAL	-	expression tag	UNP P13738
D	393	PRO	-	expression tag	UNP P13738
D	394	GLY	-	expression tag	UNP P13738
D	395	SER	-	expression tag	UNP P13738
D	396	GLU	-	expression tag	UNP P13738
D	397	ASN	-	expression tag	UNP P13738
D	398	LEU	-	expression tag	UNP P13738
D	399	TYR	-	expression tag	UNP P13738
D	400	PHE	-	expression tag	UNP P13738
D	401	GLN	-	expression tag	UNP P13738

- Molecule 2 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			29	18	11		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

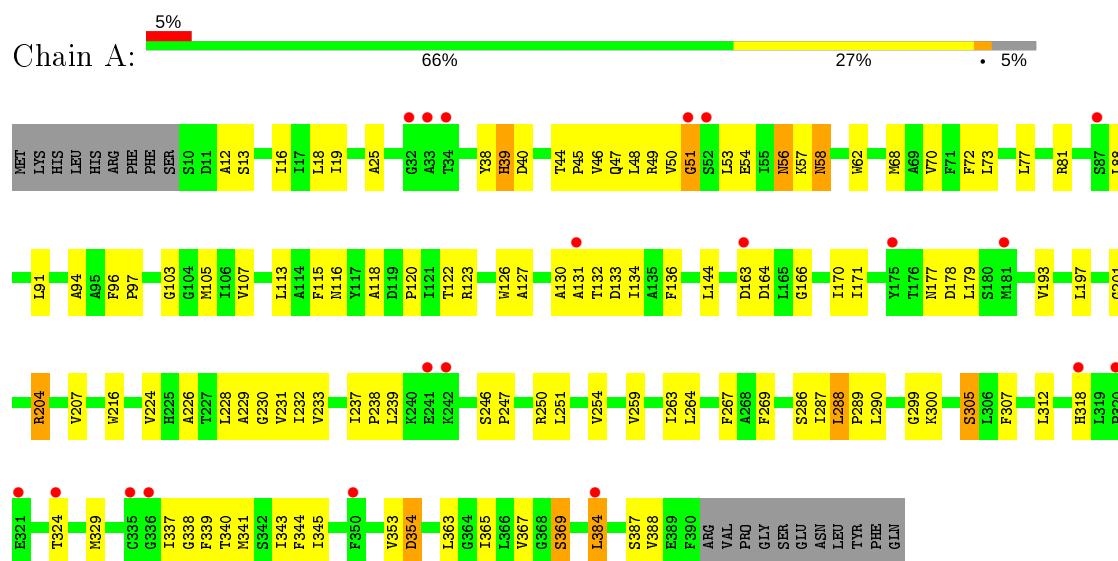
Continued from previous page...

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

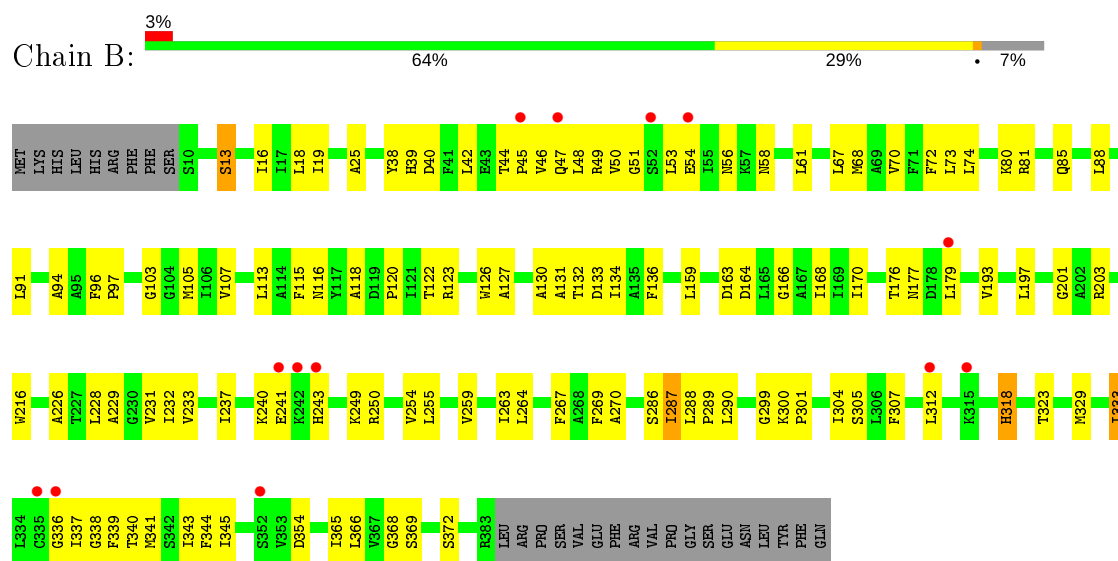
3 Residue-property plots

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: NA(+)/H(+) ANTIPORTER NHAA

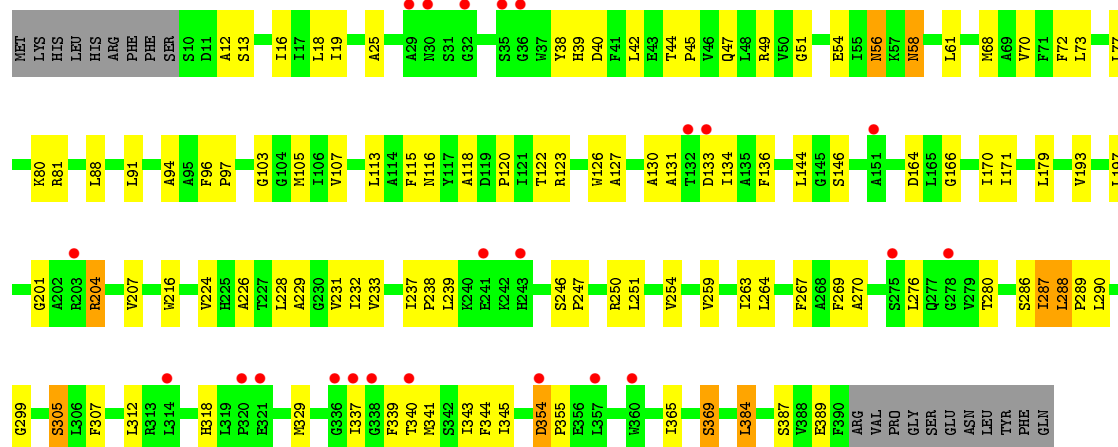


- Molecule 1: NA(+)/H(+) ANTIPORTER NHAA



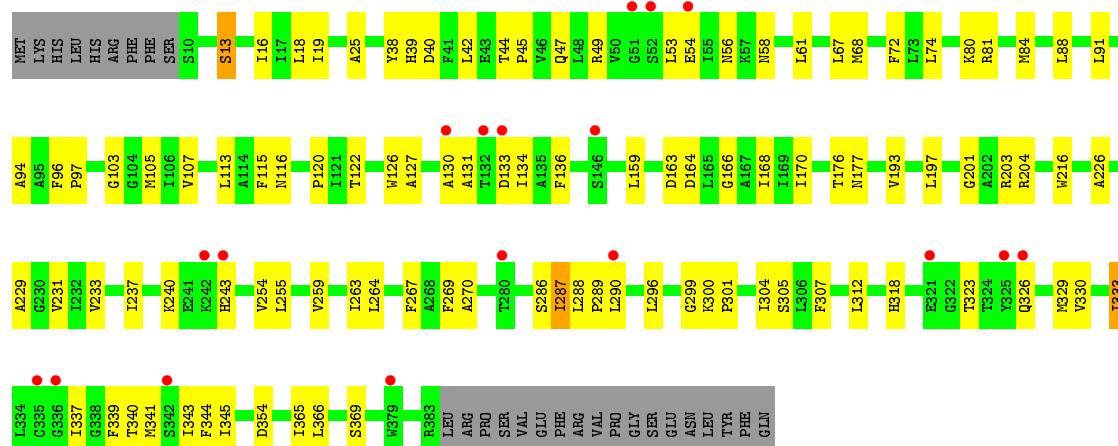
- Molecule 1: NA(+)/H(+) ANTIPORTER NHAA

Chain C: 6% 68% 25% 5%



• Molecule 1: NA(+)/H(+) ANTIPTORER NHAA

Chain D: 4% 67% 25% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	115.80Å 100.56Å 141.61Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	29.64 – 3.70 29.64 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.64-3.70) 98.3 (29.64-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.318 , 0.342 0.315 , 0.336	Depositor DCC
R_{free} test set	1879 reflections (5.49%)	wwPDB-VP
Wilson B-factor (Å ²)	135.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11343	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: SO4, LMU

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	0.54	1/2914 (0.0%)	0.66	2/3974 (0.1%)
1	B	0.53	0/2853	0.60	0/3891
1	C	0.47	0/2914	0.63	2/3974 (0.1%)
1	D	0.45	0/2853	0.60	1/3891 (0.0%)
All	All	0.50	1/11534 (0.0%)	0.62	5/15730 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	ASN	N-CA	5.26	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	LEU	CA-CB-CG	-6.68	99.95	115.30
1	C	384	LEU	CA-CB-CG	-6.40	100.59	115.30
1	D	296	LEU	CB-CG-CD2	-5.67	101.37	111.00
1	C	288	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	A	288	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	HIS	Sidechain

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	2853	0	3037	90	0
1	B	2794	0	2977	89	0
1	C	2853	0	3037	68	0
1	D	2794	0	2977	67	0
2	B	29	0	31	2	0
3	B	10	0	0	3	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
All	All	11343	0	12059	293	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 13.

All (293) 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:47:GLN:HG3	1:B:49:ARG:HB2	1.39	1.03
1:A:49:ARG:HB2	1:B:47:GLN:HG3	1.40	1.02
1:B:38:TYR:HD2	1:B:39:HIS:HD2	1.23	0.84
1:A:343:ILE:HG13	1:A:365:ILE:HD11	1.60	0.82
1:D:38:TYR:HD2	1:D:39:HIS:HD2	1.27	0.80
2:B:1384:LMU:O6'	3:B:1385:SO4:S	2.40	0.79
1:C:343:ILE:HG13	1:C:365:ILE:HD11	1.66	0.78
1:A:49:ARG:N	1:B:47:GLN:O	2.12	0.76
1:A:51:GLY:N	1:B:45:PRO:O	2.19	0.75
1:B:312:LEU:HD21	1:B:318:HIS:HB3	1.66	0.75
1:D:259:VAL:HA	1:D:263:ILE:HB	1.70	0.73
1:A:47:GLN:O	1:B:49:ARG:N	2.16	0.73
1:A:49:ARG:O	1:B:47:GLN:N	2.13	0.73
1:C:312:LEU:HD21	1:C:318:HIS:HB3	1.71	0.72
1:D:312:LEU:HD21	1:D:318:HIS:HB3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:HD21	1:A:318:HIS:HB3	1.72	0.72
1:A:13:SER:HA	1:A:16:ILE:HG12	1.73	0.71
1:B:47:GLN:HB3	1:B:56:ASN:HB3	1.73	0.70
1:C:13:SER:HA	1:C:16:ILE:HG12	1.72	0.70
1:B:116:ASN:OD1	1:B:122:THR:OG1	2.09	0.69
1:A:259:VAL:HA	1:A:263:ILE:HB	1.73	0.69
1:C:259:VAL:HA	1:C:263:ILE:HB	1.73	0.69
1:B:305:SER:HB2	1:B:329:MET:HG2	1.75	0.68
1:C:305:SER:HB2	1:C:329:MET:HG2	1.75	0.68
1:A:49:ARG:HB2	1:B:47:GLN:CG	2.21	0.68
1:D:116:ASN:OD1	1:D:122:THR:OG1	2.11	0.68
1:C:116:ASN:OD1	1:C:122:THR:OG1	2.12	0.68
1:C:122:THR:HB	1:C:288:LEU:HD11	1.75	0.67
1:B:38:TYR:HD2	1:B:39:HIS:CD2	2.10	0.67
1:A:46:VAL:HG22	1:B:50:VAL:HG13	1.76	0.67
1:A:122:THR:HB	1:A:288:LEU:HD11	1.77	0.67
1:A:116:ASN:OD1	1:A:122:THR:OG1	2.13	0.66
1:D:305:SER:HB2	1:D:329:MET:HG2	1.78	0.66
1:A:305:SER:HB2	1:A:329:MET:HG2	1.77	0.66
1:A:47:GLN:HB3	1:A:56:ASN:HB3	1.77	0.66
1:A:50:VAL:HG13	1:B:46:VAL:HG22	1.77	0.65
1:B:259:VAL:HA	1:B:263:ILE:HB	1.78	0.65
1:D:38:TYR:HD2	1:D:39:HIS:CD2	2.12	0.64
1:A:72:PHE:HB3	1:A:231:VAL:HG23	1.79	0.63
1:D:47:GLN:HB3	1:D:56:ASN:HB3	1.80	0.63
1:B:72:PHE:HB3	1:B:231:VAL:HG23	1.81	0.62
1:C:72:PHE:HB3	1:C:231:VAL:HG23	1.80	0.61
1:B:38:TYR:CD2	1:B:39:HIS:HD2	2.13	0.61
1:C:239:LEU:O	1:C:246:SER:OG	2.17	0.61
1:C:47:GLN:HB3	1:C:56:ASN:HB3	1.84	0.60
1:B:105:MET:HG3	1:B:130:ALA:HB1	1.83	0.60
1:B:343:ILE:HG13	1:B:365:ILE:HD11	1.83	0.60
1:A:47:GLN:CG	1:B:49:ARG:HB2	2.24	0.60
1:D:105:MET:HG3	1:D:130:ALA:HB1	1.84	0.60
1:B:49:ARG:HG2	1:B:54:GLU:HG2	1.82	0.60
1:D:38:TYR:CD2	1:D:39:HIS:HD2	2.14	0.60
1:A:45:PRO:O	1:B:51:GLY:N	2.34	0.60
1:A:105:MET:HG3	1:A:130:ALA:HB1	1.83	0.59
1:C:105:MET:HG3	1:C:130:ALA:HB1	1.83	0.59
1:D:343:ILE:HG13	1:D:365:ILE:HD11	1.84	0.59
1:D:72:PHE:HB3	1:D:231:VAL:HG23	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LYS:NZ	1:B:237:ILE:O	2.33	0.59
1:C:19:ILE:HD13	1:C:136:PHE:CE1	2.38	0.58
1:D:49:ARG:HG2	1:D:54:GLU:HG2	1.84	0.58
2:B:1384:LMU:O6'	3:B:1385:SO4:O1	2.22	0.58
1:A:12:ALA:O	1:A:16:ILE:HG23	2.04	0.57
1:B:365:ILE:O	1:B:369:SER:HB2	2.05	0.57
1:A:19:ILE:HD13	1:A:136:PHE:CE1	2.40	0.57
1:B:88:LEU:HD12	1:B:94:ALA:HB1	1.88	0.56
1:A:144:LEU:HD13	1:A:384:LEU:HD11	1.88	0.56
1:B:122:THR:HB	1:B:288:LEU:HD11	1.88	0.56
1:A:49:ARG:HG2	1:A:54:GLU:HG2	1.88	0.55
1:C:144:LEU:HD13	1:C:384:LEU:HD11	1.87	0.55
1:D:13:SER:HA	1:D:16:ILE:HG12	1.88	0.55
1:A:77:LEU:HD11	1:A:251:LEU:HD23	1.89	0.55
1:C:25:ALA:HB2	1:C:269:PHE:HA	1.89	0.55
1:D:40:ASP:O	1:D:44:THR:OG1	2.24	0.55
1:A:267:PHE:CE1	1:A:340:THR:HG23	2.42	0.55
1:A:47:GLN:N	1:B:49:ARG:O	2.17	0.54
1:A:239:LEU:O	1:A:246:SER:OG	2.16	0.54
1:D:80:LYS:NZ	1:D:237:ILE:O	2.40	0.54
1:C:267:PHE:CE1	1:C:340:THR:HG23	2.42	0.54
1:D:88:LEU:HD12	1:D:94:ALA:HB1	1.89	0.54
1:A:25:ALA:HB2	1:A:269:PHE:HA	1.90	0.54
1:D:122:THR:HB	1:D:288:LEU:HD11	1.91	0.53
1:A:387:SER:HA	1:D:84:MET:O	2.08	0.53
1:C:19:ILE:HD13	1:C:136:PHE:HE1	1.72	0.53
1:D:164:ASP:OD2	1:D:341:MET:HG2	2.08	0.53
1:A:103:GLY:HA3	1:A:307:PHE:CG	2.44	0.53
1:D:25:ALA:HB2	1:D:269:PHE:HA	1.89	0.53
1:A:19:ILE:HD13	1:A:136:PHE:HE1	1.74	0.52
1:A:96:PHE:HB3	1:A:97:PRO:HD3	1.92	0.52
1:B:267:PHE:CE1	1:B:340:THR:HG23	2.44	0.52
1:D:203:ARG:HD3	1:D:243:HIS:ND1	2.24	0.52
1:B:13:SER:HA	1:B:16:ILE:HG12	1.90	0.52
1:C:12:ALA:O	1:C:16:ILE:HG23	2.09	0.52
1:A:197:LEU:HD21	1:A:207:VAL:HG12	1.92	0.52
1:B:25:ALA:HB2	1:B:269:PHE:HA	1.91	0.52
1:D:204:ARG:NE	3:D:1384:SO4:O1	2.42	0.52
1:A:91:LEU:H	1:A:91:LEU:HD12	1.75	0.52
1:C:77:LEU:HD11	1:C:251:LEU:HD23	1.92	0.52
1:C:91:LEU:HD12	1:C:91:LEU:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:SER:HB3	1:D:289:PRO:HD2	1.91	0.52
1:A:88:LEU:HD12	1:A:94:ALA:HB1	1.92	0.52
1:B:203:ARG:HD3	1:B:243:HIS:ND1	2.25	0.51
1:B:287:ILE:HD12	1:B:288:LEU:HD12	1.92	0.51
1:D:103:GLY:HA3	1:D:307:PHE:CG	2.45	0.51
1:D:365:ILE:O	1:D:369:SER:HB2	2.11	0.51
1:C:88:LEU:HD12	1:C:94:ALA:HB1	1.92	0.51
1:A:388:VAL:N	1:D:84:MET:O	2.39	0.51
1:B:67:LEU:HD22	1:B:263:ILE:HG13	1.92	0.51
1:B:103:GLY:HA3	1:B:307:PHE:CG	2.45	0.51
1:B:164:ASP:OD2	1:B:341:MET:HG2	2.10	0.51
1:C:40:ASP:O	1:C:44:THR:OG1	2.26	0.51
1:C:103:GLY:HA3	1:C:307:PHE:CG	2.46	0.51
1:C:365:ILE:O	1:C:369:SER:HB2	2.11	0.51
1:D:166:GLY:O	1:D:170:ILE:HG13	2.11	0.50
1:B:70:VAL:O	1:B:73:LEU:HB3	2.11	0.50
1:C:96:PHE:HB3	1:C:97:PRO:HD3	1.93	0.50
1:C:49:ARG:HG2	1:C:54:GLU:HG2	1.93	0.50
1:C:70:VAL:O	1:C:73:LEU:HB3	2.12	0.50
1:A:88:LEU:HA	1:A:94:ALA:HB2	1.93	0.50
1:C:16:ILE:HA	1:C:19:ILE:HG22	1.92	0.50
1:A:107:VAL:HG12	1:A:299:GLY:HA2	1.93	0.50
1:A:204:ARG:NE	3:B:1385:SO4:O3	2.35	0.49
1:D:107:VAL:HG12	1:D:299:GLY:HA2	1.93	0.49
1:D:19:ILE:HD13	1:D:136:PHE:CE1	2.46	0.49
1:B:286:SER:HB3	1:B:289:PRO:HD2	1.92	0.49
1:C:131:ALA:HB1	1:C:341:MET:HB3	1.93	0.49
1:C:88:LEU:HA	1:C:94:ALA:HB2	1.95	0.49
1:A:16:ILE:HA	1:A:19:ILE:HG22	1.94	0.49
1:B:74:LEU:HB2	1:B:255:LEU:HD13	1.94	0.49
1:B:85:GLN:HG2	1:C:387:SER:HA	1.95	0.49
1:A:70:VAL:O	1:A:73:LEU:HB3	2.13	0.48
1:D:68:MET:HG3	1:D:344:PHE:CE1	2.48	0.48
1:A:365:ILE:O	1:A:369:SER:HB2	2.13	0.48
1:C:107:VAL:HG12	1:C:299:GLY:HA2	1.95	0.48
1:B:19:ILE:HD13	1:B:136:PHE:CE1	2.48	0.48
1:A:50:VAL:HA	1:B:46:VAL:HA	1.95	0.48
1:B:68:MET:HG3	1:B:344:PHE:CE1	2.49	0.48
1:A:193:VAL:O	1:A:197:LEU:HB2	2.13	0.48
1:B:241:GLU:OE2	1:B:249:LYS:HE2	2.13	0.48
1:C:204:ARG:NE	3:C:1391:SO4:O3	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PHE:CZ	1:A:290:LEU:HD23	2.49	0.47
1:B:42:LEU:HD21	1:B:270:ALA:O	2.14	0.47
1:B:47:GLN:CB	1:B:56:ASN:HB3	2.44	0.47
1:C:115:PHE:CZ	1:C:290:LEU:HD23	2.48	0.47
1:C:204:ARG:HH21	1:D:254:VAL:HG13	1.79	0.47
1:D:42:LEU:HD21	1:D:270:ALA:O	2.14	0.47
1:A:113:LEU:HD21	1:A:126:TRP:HB3	1.96	0.47
1:C:80:LYS:NZ	1:C:237:ILE:O	2.46	0.47
1:D:229:ALA:O	1:D:233:VAL:HG23	2.13	0.47
1:A:118:ALA:HA	1:A:123:ARG:HE	1.79	0.47
1:A:131:ALA:HB1	1:A:341:MET:HB3	1.97	0.47
1:B:96:PHE:HB3	1:B:97:PRO:HD3	1.97	0.47
1:C:113:LEU:HD21	1:C:126:TRP:HB3	1.96	0.47
1:A:229:ALA:O	1:A:233:VAL:HG23	2.15	0.47
1:B:107:VAL:HG12	1:B:299:GLY:HA2	1.96	0.47
1:C:197:LEU:HD21	1:C:207:VAL:HG12	1.97	0.47
1:A:47:GLN:CB	1:A:56:ASN:HB3	2.46	0.46
1:D:113:LEU:HD21	1:D:126:TRP:HB3	1.97	0.46
1:B:40:ASP:O	1:B:44:THR:OG1	2.27	0.46
1:C:115:PHE:HZ	1:C:290:LEU:HD23	1.80	0.46
1:C:144:LEU:HD13	1:C:384:LEU:CD1	2.45	0.46
1:C:58:ASN:N	1:C:58:ASN:OD1	2.48	0.46
1:D:267:PHE:CE1	1:D:340:THR:HG23	2.50	0.46
1:A:115:PHE:HZ	1:A:290:LEU:HD23	1.80	0.46
1:B:368:GLY:O	1:B:372:SER:OG	2.32	0.46
1:D:74:LEU:HB2	1:D:255:LEU:HD13	1.96	0.46
1:A:228:LEU:O	1:A:232:ILE:HG12	2.16	0.46
1:B:115:PHE:CZ	1:B:290:LEU:HD23	2.51	0.46
1:B:113:LEU:HD21	1:B:126:TRP:HB3	1.98	0.46
1:C:254:VAL:HG13	1:D:204:ARG:HH21	1.81	0.45
1:A:250:ARG:O	1:A:254:VAL:HG23	2.16	0.45
1:B:18:LEU:HD13	1:B:264:LEU:HB3	1.98	0.45
1:B:118:ALA:HA	1:B:123:ARG:HE	1.80	0.45
1:A:216:TRP:CD1	1:A:226:ALA:HB1	2.50	0.45
1:C:238:PRO:O	1:C:247:PRO:HG2	2.16	0.45
1:D:287:ILE:HD12	1:D:288:LEU:HD12	1.98	0.45
1:B:216:TRP:NE1	1:B:226:ALA:HB1	2.32	0.45
1:D:193:VAL:O	1:D:197:LEU:HB2	2.17	0.45
1:A:18:LEU:HD13	1:A:264:LEU:HB3	1.99	0.45
1:A:238:PRO:O	1:A:247:PRO:HG2	2.17	0.45
1:B:159:LEU:HD13	1:B:304:ILE:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASP:OD2	1:D:300:LYS:NZ	2.49	0.45
1:D:131:ALA:HB1	1:D:341:MET:HB3	1.98	0.45
1:C:166:GLY:O	1:C:170:ILE:HG13	2.17	0.45
1:A:133:ASP:N	1:A:337:ILE:O	2.42	0.44
1:A:40:ASP:O	1:A:44:THR:OG1	2.32	0.44
1:B:127:ALA:O	1:B:345:ILE:HG21	2.17	0.44
1:C:133:ASP:N	1:C:337:ILE:O	2.42	0.44
1:D:115:PHE:CZ	1:D:290:LEU:HD23	2.51	0.44
1:B:115:PHE:HZ	1:B:290:LEU:HD23	1.82	0.44
1:B:19:ILE:HD13	1:B:136:PHE:HE1	1.82	0.44
1:B:88:LEU:HA	1:B:94:ALA:HB2	1.99	0.44
1:C:118:ALA:HA	1:C:123:ARG:HE	1.81	0.44
1:D:19:ILE:HD13	1:D:136:PHE:HE1	1.82	0.44
1:D:67:LEU:HD22	1:D:263:ILE:HG13	2.00	0.44
1:B:240:LYS:HE2	1:C:389:GLU:OE1	2.17	0.44
1:B:131:ALA:HB1	1:B:341:MET:HB3	2.00	0.44
1:B:241:GLU:HB2	1:C:146:SER:HB2	2.00	0.44
1:C:193:VAL:O	1:C:197:LEU:HB2	2.17	0.44
1:C:42:LEU:HD21	1:C:270:ALA:O	2.17	0.44
1:D:96:PHE:HB3	1:D:97:PRO:HD3	1.99	0.44
1:C:286:SER:HB3	1:C:289:PRO:HD2	2.00	0.44
1:D:127:ALA:O	1:D:345:ILE:HG21	2.18	0.44
1:A:49:ARG:HA	1:A:53:LEU:O	2.18	0.43
1:B:229:ALA:O	1:B:233:VAL:HG23	2.17	0.43
1:A:48:LEU:HA	1:B:48:LEU:HA	1.99	0.43
1:D:16:ILE:HA	1:D:19:ILE:HG22	2.00	0.43
1:A:286:SER:HB3	1:A:289:PRO:HD2	2.00	0.43
1:B:166:GLY:O	1:B:170:ILE:HG13	2.18	0.43
1:B:193:VAL:O	1:B:197:LEU:HB2	2.18	0.43
1:D:159:LEU:HD13	1:D:304:ILE:HD12	2.00	0.43
1:C:77:LEU:HD21	1:C:237:ILE:HD12	2.00	0.43
1:C:61:LEU:HD23	1:C:61:LEU:HA	1.93	0.43
1:A:164:ASP:OD2	1:A:341:MET:HG2	2.19	0.43
1:C:68:MET:HG3	1:C:344:PHE:CE1	2.53	0.43
1:D:133:ASP:N	1:D:337:ILE:O	2.47	0.43
1:B:228:LEU:O	1:B:232:ILE:HG12	2.18	0.43
1:C:171:ILE:HG22	1:C:224:VAL:HG21	2.01	0.43
1:D:216:TRP:NE1	1:D:226:ALA:HB1	2.33	0.43
1:A:166:GLY:O	1:A:170:ILE:HG13	2.19	0.43
1:D:18:LEU:HD13	1:D:264:LEU:HB3	2.01	0.43
1:D:115:PHE:HZ	1:D:290:LEU:HD23	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:HG22	1:A:369:SER:HA	2.00	0.43
1:C:164:ASP:OD2	1:C:341:MET:HG2	2.19	0.43
1:C:250:ARG:O	1:C:254:VAL:HG23	2.19	0.43
1:D:88:LEU:HA	1:D:94:ALA:HB2	2.00	0.43
1:A:197:LEU:HD21	1:A:207:VAL:CG1	2.49	0.42
1:A:216:TRP:NE1	1:A:226:ALA:HB1	2.33	0.42
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.88	0.42
1:B:163:ASP:OD2	1:B:300:LYS:NZ	2.52	0.42
1:B:133:ASP:N	1:B:337:ILE:O	2.45	0.42
1:B:341:MET:O	1:B:345:ILE:HG12	2.19	0.42
1:A:132:THR:HA	1:A:338:GLY:HA2	2.00	0.42
1:B:105:MET:HG3	1:B:130:ALA:CB	2.50	0.42
1:D:301:PRO:HB3	1:D:333:ILE:HG12	2.01	0.42
1:A:73:LEU:HA	1:A:230:GLY:O	2.19	0.42
1:C:276:LEU:O	1:C:280:THR:OG1	2.37	0.42
1:D:91:LEU:HD12	1:D:91:LEU:H	1.85	0.42
1:B:255:LEU:HD23	1:B:255:LEU:HA	1.85	0.42
1:C:38:TYR:HD2	1:C:39:HIS:CD2	2.38	0.42
1:D:105:MET:HG3	1:D:130:ALA:CB	2.50	0.42
1:A:312:LEU:HD11	1:A:324:THR:HG21	2.02	0.42
1:C:229:ALA:O	1:C:233:VAL:HG23	2.20	0.42
1:A:178:ASP:N	1:A:178:ASP:OD1	2.49	0.42
1:A:58:ASN:N	1:A:58:ASN:OD1	2.52	0.42
1:A:57:LYS:HB2	1:A:62:TRP:CD1	2.55	0.42
1:C:233:VAL:O	1:C:237:ILE:HG13	2.19	0.42
1:C:337:ILE:HG22	1:C:369:SER:HA	2.00	0.42
1:A:127:ALA:O	1:A:345:ILE:HG21	2.20	0.42
1:A:144:LEU:HD13	1:A:384:LEU:CD1	2.50	0.41
1:D:61:LEU:HD23	1:D:61:LEU:HA	1.89	0.41
1:B:318:HIS:ND1	1:B:318:HIS:C	2.73	0.41
1:B:38:TYR:CD2	1:B:39:HIS:CD2	2.99	0.41
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.87	0.41
1:C:18:LEU:HD13	1:C:264:LEU:HB3	2.01	0.41
1:A:77:LEU:HD21	1:A:237:ILE:HD12	2.02	0.41
1:B:301:PRO:HB3	1:B:333:ILE:HG12	2.02	0.41
1:D:53:LEU:HA	1:D:53:LEU:HD23	1.90	0.41
1:A:290:LEU:HA	1:A:290:LEU:HD12	1.94	0.41
1:B:300:LYS:HG3	1:B:336:GLY:HA2	2.03	0.41
1:A:171:ILE:HG22	1:A:224:VAL:HG21	2.03	0.41
1:B:16:ILE:HA	1:B:19:ILE:HG22	2.03	0.41
1:B:336:GLY:O	1:B:372:SER:OG	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ALA:O	1:C:345:ILE:HG21	2.21	0.41
1:C:354:ASP:OD1	1:C:355:PRO:HD2	2.20	0.41
1:B:168:ILE:HD13	1:B:168:ILE:HA	1.91	0.41
1:B:243:HIS:H	1:B:243:HIS:CD2	2.38	0.41
1:D:44:THR:HA	1:D:45:PRO:HD3	1.88	0.41
1:A:233:VAL:O	1:A:237:ILE:HG13	2.21	0.41
1:B:250:ARG:O	1:B:254:VAL:HG23	2.21	0.41
1:C:228:LEU:O	1:C:232:ILE:HG12	2.21	0.41
1:D:233:VAL:O	1:D:237:ILE:HG13	2.21	0.41
1:D:243:HIS:H	1:D:243:HIS:CD2	2.39	0.41
1:A:363:LEU:O	1:A:367:VAL:HG23	2.21	0.41
1:A:38:TYR:HD1	1:A:39:HIS:CD2	2.39	0.40
1:C:44:THR:HA	1:C:45:PRO:HD3	1.94	0.40
1:D:168:ILE:HA	1:D:168:ILE:HD13	1.91	0.40
1:A:163:ASP:OD2	1:A:300:LYS:NZ	2.55	0.40
1:A:312:LEU:CD1	1:A:324:THR:HG21	2.52	0.40
1:A:68:MET:HG3	1:A:344:PHE:CE1	2.57	0.40
1:A:44:THR:HA	1:A:45:PRO:HD3	1.95	0.40
1:A:46:VAL:HA	1:B:50:VAL:HA	2.03	0.40
1:B:91:LEU:H	1:B:91:LEU:HD12	1.87	0.40
1:B:179:LEU:HA	1:B:179:LEU:HD12	1.84	0.40
1:A:204:ARG:HH21	1:B:254:VAL:HG13	1.86	0.40
1:C:216:TRP:CD1	1:C:226:ALA:HB1	2.56	0.40
1:A:53:LEU:HA	1:A:53:LEU:HD23	1.89	0.40
1:B:132:THR:HA	1:B:338:GLY:HA2	2.04	0.40
1:D:326:GLN:O	1:D:330:VAL:HG23	2.22	0.40
1:D:337:ILE:HG22	1:D:369:SER:HA	2.03	0.40
1:D:341:MET:O	1:D:345:ILE:HG12	2.21	0.40
1:A:353:VAL:HG12	1:A:354:ASP:HB2	2.03	0.40
1:C:287:ILE:HG13	1:C:287:ILE:H	1.62	0.40
1:D:240:LYS:HD3	1:D:240:LYS:HA	1.93	0.40
1:D:286:SER:O	1:D:289:PRO:HD2	2.21	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	379/401 (94%)	348 (92%)	27 (7%)	4 (1%)	14	50
1	B	372/401 (93%)	344 (92%)	24 (6%)	4 (1%)	14	50
1	C	379/401 (94%)	349 (92%)	26 (7%)	4 (1%)	14	50
1	D	372/401 (93%)	344 (92%)	24 (6%)	4 (1%)	14	50
All	All	1502/1604 (94%)	1385 (92%)	101 (7%)	16 (1%)	14	50

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PHE
1	B	339	PHE
1	C	339	PHE
1	D	339	PHE
1	D	177	ASN
1	A	201	GLY
1	B	177	ASN
1	B	201	GLY
1	C	201	GLY
1	D	201	GLY
1	B	120	PRO
1	D	120	PRO
1	A	51	GLY
1	C	51	GLY
1	C	120	PRO
1	A	120	PRO

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	296/315 (94%)	286 (97%)	10 (3%)	37	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	289/315 (92%)	278 (96%)	11 (4%)	33	61
1	C	296/315 (94%)	286 (97%)	10 (3%)	37	64
1	D	289/315 (92%)	279 (96%)	10 (4%)	36	63
All	All	1170/1260 (93%)	1129 (96%)	41 (4%)	36	63

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	58	ASN
1	A	81	ARG
1	A	134	ILE
1	A	179	LEU
1	A	204	ARG
1	A	287	ILE
1	A	305	SER
1	A	354	ASP
1	A	369	SER
1	B	13	SER
1	B	58	ASN
1	B	81	ARG
1	B	134	ILE
1	B	176	THR
1	B	287	ILE
1	B	318	HIS
1	B	323	THR
1	B	333	ILE
1	B	354	ASP
1	B	366	LEU
1	C	56	ASN
1	C	58	ASN
1	C	81	ARG
1	C	134	ILE
1	C	179	LEU
1	C	204	ARG
1	C	287	ILE
1	C	305	SER
1	C	354	ASP
1	C	369	SER
1	D	13	SER
1	D	58	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	81	ARG
1	D	134	ILE
1	D	176	THR
1	D	287	ILE
1	D	323	THR
1	D	333	ILE
1	D	354	ASP
1	D	366	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	116	ASN
1	B	39	HIS
1	C	39	HIS
1	C	116	ASN
1	D	39	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
3	SO4	C	1391	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	B	1385	-	4,4,4	0.26	0	6,6,6	0.59	0
3	SO4	D	1384	-	4,4,4	0.16	0	6,6,6	0.42	0
2	LMU	B	1384	-	30,30,36	1.38	4 (13%)	41,41,47	1.43	6 (14%)
3	SO4	B	1386	-	4,4,4	0.19	0	6,6,6	0.37	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	LMU	B	1384	-	-	7/15/55/61	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1384	LMU	O5B-C1B	4.00	1.52	1.41
2	B	1384	LMU	C3'-C4'	-3.11	1.44	1.52
2	B	1384	LMU	C3B-C2B	-2.52	1.45	1.52
2	B	1384	LMU	O1B-C1B	-2.18	1.35	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1384	LMU	C1-O1'-C1'	3.89	120.29	113.84
2	B	1384	LMU	C1B-O1B-C4'	-2.49	111.81	117.96
2	B	1384	LMU	C1'-C2'-C3'	2.32	114.83	110.00
2	B	1384	LMU	O3B-C3B-C2B	-2.26	105.13	110.35
2	B	1384	LMU	O6B-C6B-C5B	2.26	119.03	111.29
2	B	1384	LMU	O5B-C5B-C6B	2.10	111.65	106.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1384	LMU	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

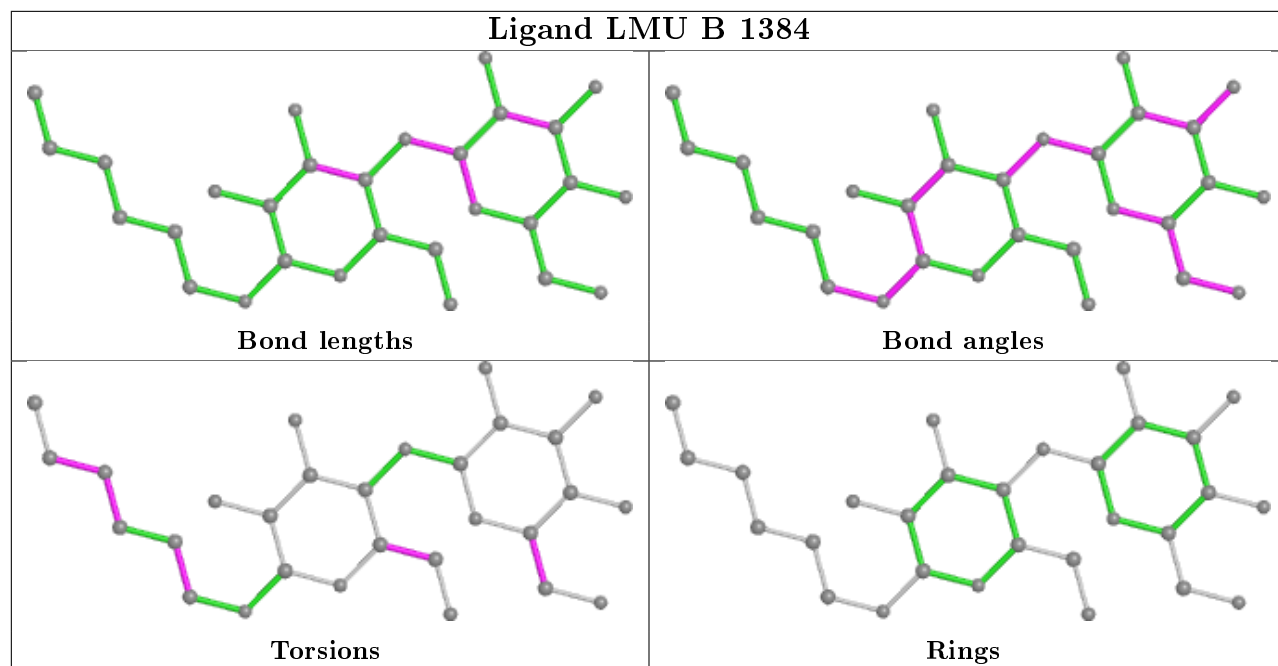
Mol	Chain	Res	Type	Atoms
2	B	1384	LMU	C2-C3-C4-C5
2	B	1384	LMU	C4'-C5'-C6'-O6'
2	B	1384	LMU	O5B-C5B-C6B-O6B
2	B	1384	LMU	C4B-C5B-C6B-O6B
2	B	1384	LMU	O1'-C1-C2-C3
2	B	1384	LMU	C3-C4-C5-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1391	SO4	1	0
3	B	1385	SO4	3	0
3	D	1384	SO4	1	0
2	B	1384	LMU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	381/401 (95%)	-0.12	20 (5%)	27 20	89, 177, 292, 416	0
1	B	374/401 (93%)	-0.23	13 (3%)	44 33	82, 173, 300, 490	0
1	C	381/401 (95%)	-0.01	23 (6%)	21 15	123, 206, 330, 463	0
1	D	374/401 (93%)	-0.09	18 (4%)	30 22	119, 216, 357, 483	0
All	All	1510/1604 (94%)	-0.11	74 (4%)	29 22	82, 194, 326, 490	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	GLU	7.6
1	B	243	HIS	6.5
1	B	242	LYS	6.4
1	A	181	MET	6.2
1	A	51	GLY	5.9
1	D	242	LYS	5.6
1	A	241	GLU	5.5
1	D	52	SER	5.1
1	D	336	GLY	5.1
1	C	320	PRO	4.7
1	C	132	THR	4.2
1	C	203	ARG	4.1
1	A	87	SER	4.0
1	D	243	HIS	3.8
1	A	175	TYR	3.8
1	C	32	GLY	3.8
1	B	315	LYS	3.5
1	A	384	LEU	3.5
1	B	336	GLY	3.5
1	B	52	SER	3.5
1	B	241	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	33	ALA	3.4
1	A	52	SER	3.4
1	D	335	CYS	3.3
1	C	321	GLU	3.3
1	C	241	GLU	3.2
1	D	54	GLU	3.0
1	D	325	TYR	3.0
1	D	342	SER	2.9
1	B	179	LEU	2.9
1	C	360	TRP	2.9
1	B	54	GLU	2.8
1	C	36	GLY	2.8
1	C	133	ASP	2.7
1	C	338	GLY	2.7
1	A	335	CYS	2.7
1	A	324	THR	2.7
1	C	243	HIS	2.7
1	A	336	GLY	2.7
1	A	321	GLU	2.6
1	C	354	ASP	2.6
1	C	314	LEU	2.6
1	B	335	CYS	2.5
1	B	45	PRO	2.5
1	C	357	LEU	2.5
1	C	278	GLY	2.5
1	C	275	SER	2.5
1	D	132	THR	2.5
1	D	326	GLN	2.4
1	D	280	THR	2.4
1	B	352	SER	2.3
1	C	340	THR	2.3
1	D	290	LEU	2.3
1	A	242	LYS	2.3
1	D	51	GLY	2.3
1	C	29	ALA	2.3
1	C	151	ALA	2.3
1	A	320	PRO	2.3
1	D	146	SER	2.3
1	A	350	PHE	2.3
1	C	35	SER	2.2
1	C	30	ASN	2.2
1	D	379	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	130	ALA	2.2
1	D	133	ASP	2.1
1	C	336	GLY	2.1
1	C	337	ILE	2.1
1	A	163	ASP	2.1
1	B	312	LEU	2.1
1	B	47	GLN	2.1
1	A	34	THR	2.1
1	A	32	GLY	2.1
1	A	131	ALA	2.1
1	A	318	HIS	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

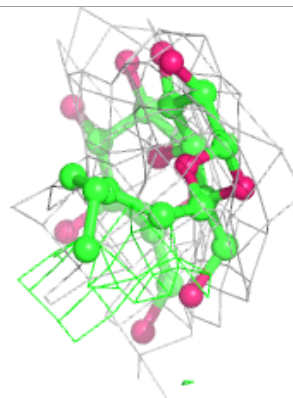
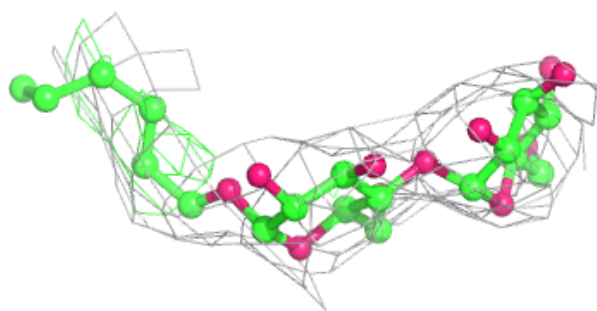
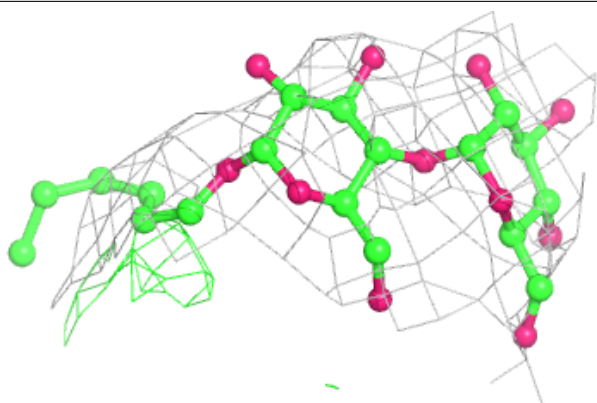
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LMU	B	1384	29/35	0.79	0.36	242,242,242,242	0
3	SO4	C	1391	5/5	0.84	0.12	171,171,171,171	0
3	SO4	D	1384	5/5	0.85	0.17	158,158,158,158	0
3	SO4	B	1385	5/5	0.87	0.13	149,149,149,149	0
3	SO4	B	1386	5/5	0.90	0.14	146,146,146,146	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMU B 1384:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.