



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:07 PM EDT

PDB ID : 6SS6 / pdb_00006ss6
Title : Structure of arginase-2 in complex with the inhibitory human antigen-binding fragment Fab C0020187
Authors : Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; See-wooruthun, C.; Carr, M.
Deposited on : 2019-09-06
Resolution : 3.25 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:

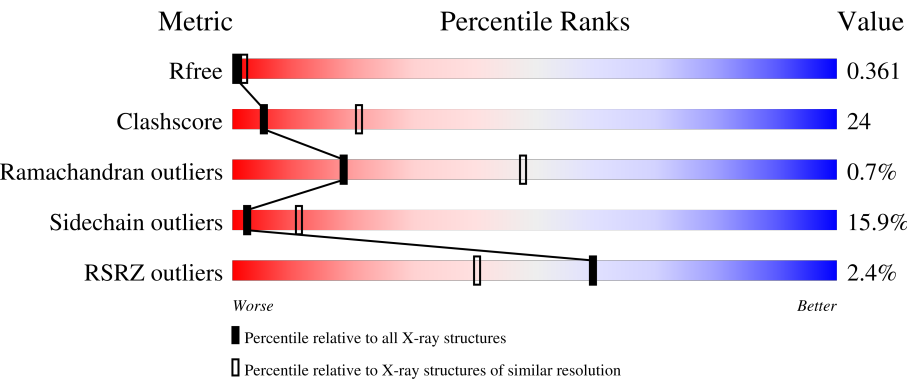
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	AAA	346	3% 52%30%10%8%
1	BBB	346	% 57%24%8%11%
1	CCC	346	3% 56%26%8%8%
2	HHH	233	67%23%5%5%
2	III	233	3% 61%29%6%5%

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Mol	Chain	Length	Quality of chain
2	JJJ	233	3% 60% 29% 5% 6%
3	LLL	220	% 71% 21% 5% •
3	MMM	220	4% 72% 16% 8% •
3	NNN	220	2% 49% 37% 10% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33558 atoms, of which 16603 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 Arginase-2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	318	Total	C	H	N	O	S	121	0	0
			4848	1534	2419	422	464	9			
1	BBB	308	Total	C	H	N	O	S	116	0	0
			4691	1482	2341	411	448	9			
1	CCC	317	Total	C	H	N	O	S	120	0	0
			4837	1531	2414	421	462	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	MET	-	initiating methionine	UNP P78540
AAA	355	GLY	-	expression tag	UNP P78540
AAA	356	GLY	-	expression tag	UNP P78540
AAA	357	GLY	-	expression tag	UNP P78540
AAA	358	HIS	-	expression tag	UNP P78540
AAA	359	HIS	-	expression tag	UNP P78540
AAA	360	HIS	-	expression tag	UNP P78540
AAA	361	HIS	-	expression tag	UNP P78540
AAA	362	HIS	-	expression tag	UNP P78540
AAA	363	HIS	-	expression tag	UNP P78540
AAA	364	HIS	-	expression tag	UNP P78540
AAA	365	HIS	-	expression tag	UNP P78540
AAA	366	HIS	-	expression tag	UNP P78540
AAA	367	HIS	-	expression tag	UNP P78540
BBB	22	MET	-	initiating methionine	UNP P78540
BBB	355	GLY	-	expression tag	UNP P78540
BBB	356	GLY	-	expression tag	UNP P78540
BBB	357	GLY	-	expression tag	UNP P78540
BBB	358	HIS	-	expression tag	UNP P78540
BBB	359	HIS	-	expression tag	UNP P78540
BBB	360	HIS	-	expression tag	UNP P78540
BBB	361	HIS	-	expression tag	UNP P78540
BBB	362	HIS	-	expression tag	UNP P78540

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	363	HIS	-	expression tag	UNP P78540
BBB	364	HIS	-	expression tag	UNP P78540
BBB	365	HIS	-	expression tag	UNP P78540
BBB	366	HIS	-	expression tag	UNP P78540
BBB	367	HIS	-	expression tag	UNP P78540
CCC	22	MET	-	initiating methionine	UNP P78540
CCC	355	GLY	-	expression tag	UNP P78540
CCC	356	GLY	-	expression tag	UNP P78540
CCC	357	GLY	-	expression tag	UNP P78540
CCC	358	HIS	-	expression tag	UNP P78540
CCC	359	HIS	-	expression tag	UNP P78540
CCC	360	HIS	-	expression tag	UNP P78540
CCC	361	HIS	-	expression tag	UNP P78540
CCC	362	HIS	-	expression tag	UNP P78540
CCC	363	HIS	-	expression tag	UNP P78540
CCC	364	HIS	-	expression tag	UNP P78540
CCC	365	HIS	-	expression tag	UNP P78540
CCC	366	HIS	-	expression tag	UNP P78540
CCC	367	HIS	-	expression tag	UNP P78540

- Molecule 2 is a protein called Fab C0020187 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	HHH	222	Total	C	H	N	O	S	93	0	0
			3267	1032	1624	280	324	7			
2	III	222	Total	C	H	N	O	S	93	0	0
			3267	1032	1624	280	324	7			
2	JJJ	218	Total	C	H	N	O	S	92	0	0
			3205	1013	1593	275	317	7			

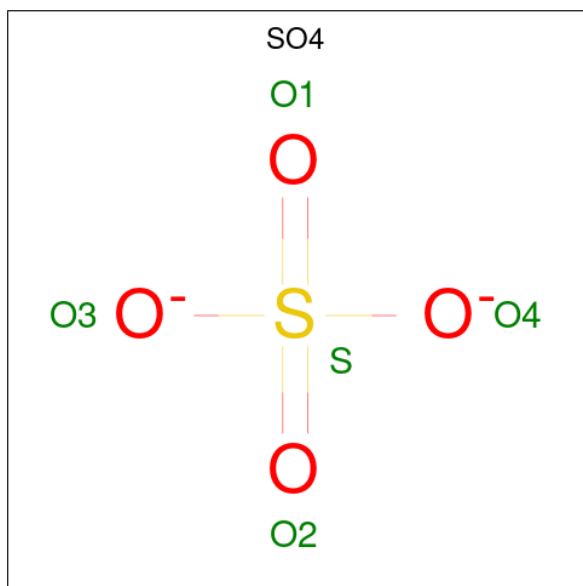
- Molecule 3 is a protein called Fab C0020187 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	LLL	214	Total	C	H	N	O	S	103	0	0
			3120	990	1538	262	326	4			
3	MMM	213	Total	C	H	N	O	S	103	0	0
			3105	985	1532	261	323	4			
3	NNN	211	Total	C	H	N	O	S	102	0	0
			3077	976	1518	259	320	4			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	2	Total Mn 2 2	0	0
4	BBB	2	Total Mn 2 2	0	0
4	CCC	2	Total Mn 2 2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	BBB	1	Total O S 5 4 1	0	0
5	CCC	1	Total O S 5 4 1	0	0
5	CCC	1	Total O S 5 4 1	0	0
5	CCC	1	Total O S 5 4 1	0	0

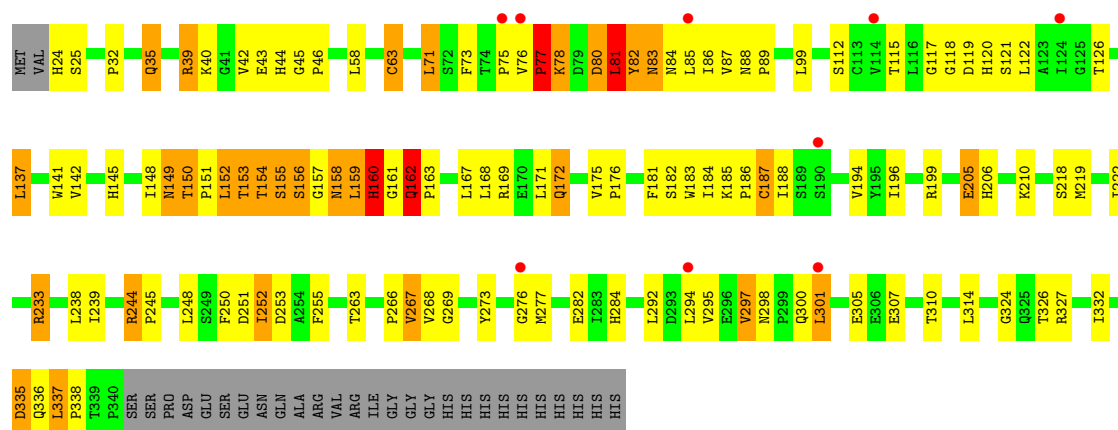
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	JJJ	1	Total	O	S	0	0
			5	4	1		
5	LLL	1	Total	O	S	0	0
			5	4	1		
5	LLL	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		

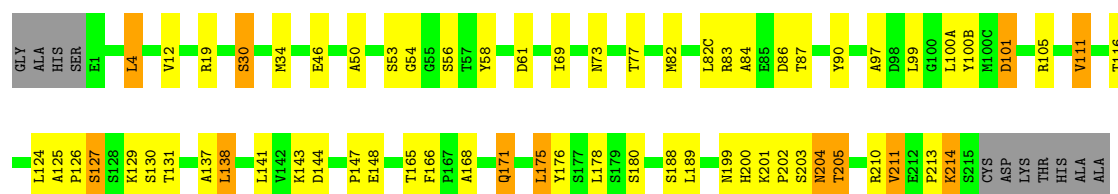
- Molecule 1: Arginase-2, mitochondrial





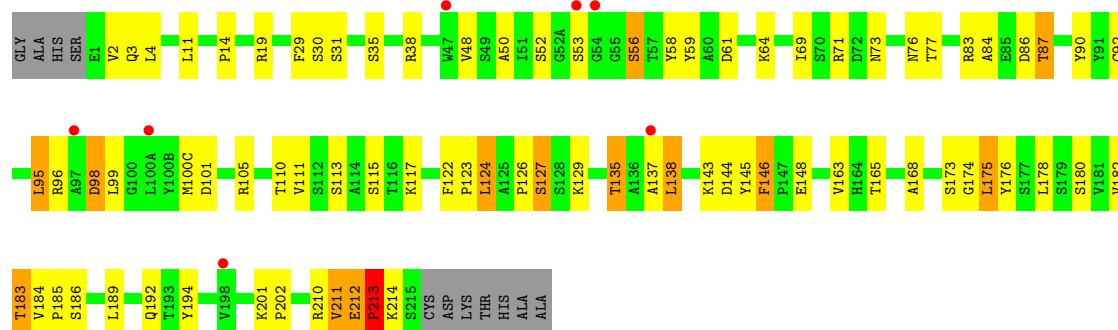
• Molecule 2: Fab C0020187 heavy chain (IgG1)

Chain HHH: 67% 23% 5% 5%



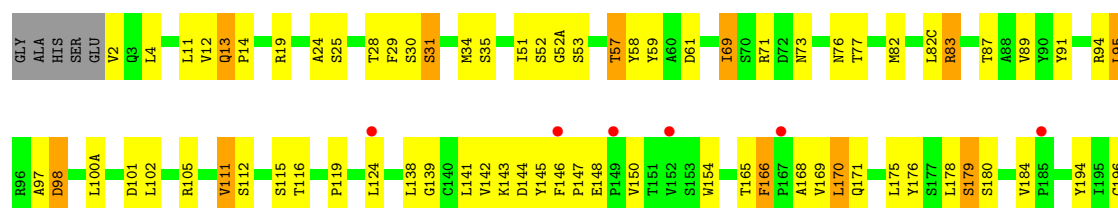
• Molecule 2: Fab C0020187 heavy chain (IgG1)

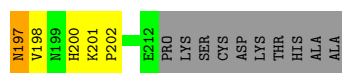
Chain III: 3% 61% 29% 6% 5%



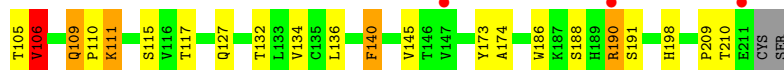
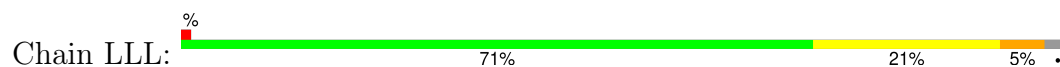
• Molecule 2: Fab C0020187 heavy chain (IgG1)

Chain JJJ: 3% 60% 29% 5% 6%

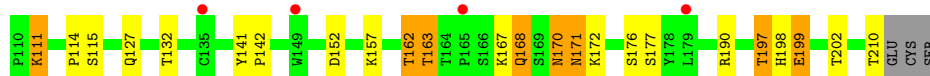
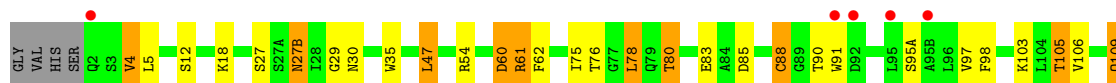
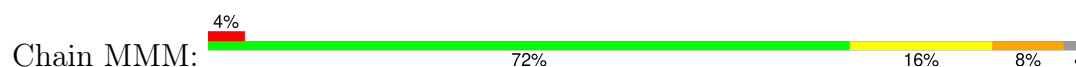




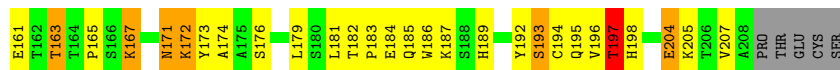
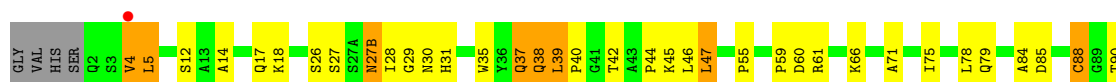
• Molecule 3: Fab C0020187 light chain (IgG1)



• Molecule 3: Fab C0020187 light chain (IgG1)



• Molecule 3: Fab C0020187 light chain (IgG1)



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.13Å 138.13Å 551.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.76 – 3.25 48.76 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-3.25) 99.9 (48.76-3.25)	Depositor EDS
R_{merge}	0.78	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.300 , 0.361 0.300 , 0.361	Depositor DCC
R_{free} test set	2549 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	33558	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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	AAA	1.01	0/2483	1.52	3/3380 (0.1%)
1	BBB	1.02	0/2401	1.56	6/3265 (0.2%)
1	CCC	1.02	0/2477	1.57	5/3372 (0.1%)
2	HHH	1.05	0/1679	1.34	1/2283 (0.0%)
2	III	1.03	0/1679	1.40	7/2283 (0.3%)
2	JJJ	1.06	0/1647	1.35	0/2240
3	LLL	1.03	0/1621	1.34	1/2216 (0.0%)
3	MMM	1.03	0/1612	1.29	0/2204
3	NNN	1.05	0/1597	1.40	2/2182 (0.1%)
All	All	1.03	0/17196	1.44	25/23425 (0.1%)

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	CCC	0	2

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	III	212	GLU	CA-C-N	9.78	132.06	119.84
2	III	212	GLU	C-N-CA	9.78	132.06	119.84
1	CCC	77	PRO	N-CA-CB	-9.11	93.69	103.25
1	BBB	82	TYR	CB-CA-C	8.84	129.25	117.23
2	III	213	PRO	CA-N-CD	-6.25	103.25	112.00
3	NNN	197	THR	CB-CA-C	6.08	120.29	109.65
2	III	123	PRO	CB-CA-C	-5.98	106.85	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	III	213	PRO	N-CA-C	5.92	124.66	112.47
1	BBB	82	TYR	CA-CB-CG	5.66	124.09	113.90
1	BBB	75	PRO	CA-C-N	5.59	132.47	122.13
1	BBB	75	PRO	C-N-CA	5.59	132.47	122.13
3	NNN	152	ASP	CA-CB-CG	5.40	118.00	112.60
1	CCC	160	HIS	CB-CA-C	5.36	119.69	110.79
1	CCC	154	THR	CA-CB-OG1	-5.27	101.70	109.60
1	BBB	297	VAL	CA-C-O	-5.21	116.18	121.70
1	AAA	300	GLN	CA-C-N	5.20	127.98	120.38
1	AAA	300	GLN	C-N-CA	5.20	127.98	120.38
1	BBB	88	ASN	CB-CA-C	5.20	120.41	110.17
2	HHH	54	GLY	CA-C-O	-5.19	118.72	122.45
3	LLL	111	LYS	CA-C-O	-5.13	115.75	121.81
2	III	122	PHE	CA-C-N	5.10	127.42	120.79
2	III	122	PHE	C-N-CA	5.10	127.42	120.79
1	CCC	81	LEU	CB-CA-C	-5.08	109.22	116.34
1	CCC	150	THR	CA-CB-OG1	-5.06	102.01	109.60
1	AAA	44	HIS	N-CA-C	-5.05	107.18	113.19

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	157	GLY	Peptide
1	CCC	158	ASN	Peptide

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	AAA	2429	2419	2406	154	4
1	BBB	2350	2341	2328	133	4
1	CCC	2423	2414	2399	137	0
2	HHH	1643	1624	1624	61	1
2	III	1643	1624	1624	75	1
2	JJJ	1612	1593	1590	87	0
3	LLL	1582	1538	1534	51	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	MMM	1573	1532	1528	36	0
3	NNN	1559	1518	1514	137	7
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
5	AAA	15	0	0	1	0
5	BBB	15	0	0	0	0
5	CCC	30	0	0	1	0
5	HHH	25	0	0	0	0
5	III	20	0	0	0	0
5	JJJ	5	0	0	0	0
5	LLL	10	0	0	0	0
5	MMM	15	0	0	0	0
All	All	16955	16603	16547	819	12

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 24.

All (819) 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)
3:NNN:149:TRP:CZ3	3:NNN:194:CYS:CB	2.11	1.33
1:BBB:149:ASN:HB3	1:BBB:154:THR:CG2	1.58	1.32
1:BBB:149:ASN:CB	1:BBB:154:THR:HG21	1.62	1.30
1:CCC:88:ASN:OD1	1:CCC:89:PRO:HD3	1.41	1.19
1:AAA:150:THR:HG23	1:AAA:153:THR:HG21	1.25	1.18
3:NNN:149:TRP:CZ3	3:NNN:194:CYS:HB2	1.73	1.17
3:NNN:135:CYS:HB3	3:NNN:149:TRP:CH2	1.80	1.15
3:NNN:167:LYS:HD3	3:NNN:173:TYR:CZ	1.82	1.13
1:BBB:35:GLN:HE21	1:BBB:39:ARG:HG2	1.10	1.12
3:NNN:39:LEU:HB3	3:NNN:40:PRO:HD2	1.23	1.11
2:III:87:THR:HG22	2:III:110:THR:HA	1.25	1.09
2:III:87:THR:CG2	2:III:110:THR:HA	1.81	1.09
2:III:184:VAL:HG21	2:III:194:TYR:OH	1.51	1.09
2:HHH:144:ASP:HA	2:HHH:175:LEU:HD11	1.28	1.09
1:CCC:119:ASP:OD1	1:CCC:121:SER:OG	1.70	1.08
3:NNN:149:TRP:CE3	3:NNN:194:CYS:HA	1.87	1.08
3:NNN:135:CYS:HB3	3:NNN:149:TRP:HH2	0.98	1.08
3:NNN:149:TRP:CZ3	3:NNN:194:CYS:CA	2.37	1.07
2:HHH:87:THR:OG1	2:HHH:111:VAL:HG23	1.52	1.07
3:NNN:149:TRP:CH2	3:NNN:194:CYS:SG	2.48	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:199:ARG:NE	1:CCC:267:VAL:HG12	1.71	1.05
3:NNN:135:CYS:CB	3:NNN:149:TRP:HH2	1.70	1.05
1:AAA:102:VAL:O	1:AAA:105:ARG:HG3	1.57	1.04
1:BBB:149:ASN:HB3	1:BBB:154:THR:HG22	1.37	1.04
1:CCC:199:ARG:HE	1:CCC:267:VAL:HG12	1.20	1.03
1:CCC:159:LEU:HD12	1:CCC:159:LEU:H	1.22	1.00
3:NNN:118:LEU:HD21	3:NNN:207:VAL:HG13	1.44	1.00
2:III:144:ASP:HA	2:III:175:LEU:CD1	1.91	0.98
3:NNN:149:TRP:HZ3	3:NNN:194:CYS:HB2	1.06	0.98
1:BBB:34:SER:HB3	1:BBB:43:GLU:OE2	1.63	0.98
3:NNN:149:TRP:CZ3	3:NNN:194:CYS:SG	2.56	0.97
3:NNN:149:TRP:HZ3	3:NNN:194:CYS:CB	1.58	0.97
1:AAA:150:THR:OG1	1:AAA:153:THR:HG22	1.64	0.97
2:III:144:ASP:CA	2:III:175:LEU:CD1	2.43	0.96
1:BBB:46:PRO:HD3	1:BBB:117:GLY:O	1.65	0.95
1:CCC:199:ARG:HE	1:CCC:267:VAL:CG1	1.79	0.95
1:CCC:39:ARG:NH1	1:CCC:160:HIS:ND1	2.14	0.95
1:AAA:150:THR:HG23	1:AAA:153:THR:CG2	1.96	0.93
3:NNN:140:PHE:CE2	3:NNN:174:ALA:HA	2.02	0.93
3:MMM:80:THR:HA	3:MMM:106:VAL:HG21	1.50	0.93
3:NNN:39:LEU:HB3	3:NNN:40:PRO:CD	1.98	0.92
1:BBB:150:THR:O	1:BBB:162:GLN:NE2	2.03	0.92
1:BBB:159:LEU:HA	1:BBB:162:GLN:HB3	1.52	0.91
1:BBB:149:ASN:CB	1:BBB:154:THR:CG2	2.32	0.91
3:NNN:149:TRP:CZ3	3:NNN:194:CYS:HA	2.04	0.90
1:AAA:159:LEU:HD23	1:AAA:162:GLN:CD	1.99	0.87
1:CCC:35:GLN:NE2	1:CCC:35:GLN:HA	1.89	0.87
2:III:144:ASP:C	2:III:175:LEU:CD1	2.47	0.87
1:BBB:149:ASN:HB2	1:BBB:154:THR:HG21	1.55	0.86
1:CCC:39:ARG:HB3	1:CCC:39:ARG:CZ	2.05	0.86
2:III:144:ASP:CA	2:III:175:LEU:HD12	2.05	0.86
2:HHH:175:LEU:HD13	2:HHH:175:LEU:C	2.00	0.86
2:III:126:PRO:HA	2:III:138:LEU:HD21	1.55	0.86
1:AAA:42:VAL:HG12	1:AAA:118:GLY:HA2	1.56	0.86
1:CCC:82:TYR:HA	1:CCC:85:LEU:HD23	1.55	0.85
1:CCC:162:GLN:H	1:CCC:163:PRO:CD	1.89	0.85
2:III:144:ASP:HA	2:III:175:LEU:HD12	1.57	0.85
2:III:144:ASP:HA	2:III:175:LEU:HD13	1.58	0.85
1:BBB:35:GLN:NE2	1:BBB:39:ARG:HG2	1.92	0.84
3:MMM:162:THR:OG1	3:MMM:177:SER:HB2	1.77	0.84
1:AAA:162:GLN:N	1:AAA:163:PRO:HD3	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HHH:214:LYS:H	2:HHH:214:LYS:CE	1.91	0.83
1:BBB:251:ASP:OD2	1:BBB:296:GLU:OE1	1.96	0.82
2:HHH:125:ALA:HB1	2:HHH:214:LYS:NZ	1.95	0.82
3:NNN:150:LYS:HD2	3:NNN:195:GLN:NE2	1.94	0.82
1:CCC:199:ARG:NE	1:CCC:267:VAL:CG1	2.40	0.82
2:III:144:ASP:CB	2:III:175:LEU:HD12	2.10	0.82
3:MMM:162:THR:OG1	3:MMM:177:SER:CB	2.28	0.81
1:BBB:46:PRO:HD3	1:BBB:117:GLY:C	2.06	0.81
1:AAA:73:PHE:HB3	1:AAA:75:PRO:HD3	1.61	0.81
1:AAA:162:GLN:H	1:AAA:163:PRO:HD3	1.47	0.80
3:NNN:120:PRO:HB2	3:NNN:121:PRO:HD2	1.63	0.80
1:AAA:42:VAL:HG12	1:AAA:118:GLY:CA	2.11	0.80
1:AAA:159:LEU:CD2	1:AAA:162:GLN:NE2	2.44	0.80
2:III:87:THR:HG23	2:III:111:VAL:N	1.95	0.80
1:AAA:159:LEU:HD23	1:AAA:162:GLN:NE2	1.97	0.80
3:NNN:167:LYS:HD3	3:NNN:173:TYR:OH	1.82	0.80
1:AAA:83:ASN:HA	1:AAA:87:VAL:HG13	1.63	0.79
2:III:144:ASP:C	2:III:175:LEU:HD13	2.06	0.79
3:NNN:118:LEU:HD21	3:NNN:207:VAL:CG1	2.12	0.79
1:CCC:162:GLN:N	1:CCC:163:PRO:CD	2.45	0.79
3:NNN:167:LYS:HD3	3:NNN:173:TYR:CE1	2.18	0.79
1:BBB:90:ARG:HG3	1:BBB:179:PRO:O	1.83	0.79
2:JJJ:124:LEU:HD13	3:NNN:119:PHE:HD2	1.48	0.79
1:BBB:162:GLN:N	1:BBB:163:PRO:HD3	1.97	0.79
1:AAA:42:VAL:CG1	1:AAA:118:GLY:CA	2.60	0.78
2:III:87:THR:HG23	2:III:111:VAL:H	1.49	0.78
1:BBB:85:LEU:HD22	1:BBB:85:LEU:H	1.47	0.78
1:BBB:81:LEU:O	1:BBB:81:LEU:HD23	1.84	0.78
1:BBB:147:ASP:O	1:BBB:163:PRO:HD2	1.83	0.77
3:NNN:118:LEU:HB2	3:NNN:135:CYS:HB2	1.66	0.77
1:CCC:39:ARG:NE	1:CCC:160:HIS:CE1	2.53	0.76
2:JJJ:124:LEU:HD13	3:NNN:119:PHE:CD2	2.20	0.76
1:CCC:162:GLN:N	1:CCC:163:PRO:HD2	2.00	0.76
1:CCC:199:ARG:HB2	1:CCC:267:VAL:HG11	1.66	0.76
1:CCC:337:LEU:HD12	1:CCC:337:LEU:H	1.50	0.76
3:NNN:31:HIS:CE1	3:NNN:93:SER:OG	2.39	0.76
1:CCC:159:LEU:HD12	1:CCC:159:LEU:N	2.00	0.76
3:NNN:39:LEU:CB	3:NNN:40:PRO:HD2	2.12	0.76
1:AAA:145:HIS:HB2	1:AAA:147:ASP:OD1	1.85	0.76
1:AAA:221:ASP:OD2	1:AAA:221:ASP:N	2.18	0.76
1:CCC:159:LEU:H	1:CCC:159:LEU:CD1	1.88	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HHH:87:THR:OG1	2:HHH:111:VAL:CG2	2.31	0.75
1:CCC:83:ASN:HA	1:CCC:87:VAL:HB	1.69	0.74
2:JJJ:13:GLN:NE2	2:JJJ:14:PRO:HD2	2.02	0.74
1:CCC:159:LEU:HA	1:CCC:162:GLN:HE22	1.53	0.74
2:III:144:ASP:CA	2:III:175:LEU:HD13	2.16	0.74
3:MMM:78:LEU:HD23	3:MMM:106:VAL:HG12	1.70	0.73
2:HHH:214:LYS:H	2:HHH:214:LYS:HE2	1.53	0.73
2:JJJ:35:SER:HB2	2:JJJ:95:LEU:HD22	1.71	0.73
1:BBB:159:LEU:HD12	1:BBB:159:LEU:H	1.52	0.73
1:CCC:199:ARG:CB	1:CCC:267:VAL:HG11	2.18	0.73
1:BBB:159:LEU:HB3	1:BBB:162:GLN:HG2	1.69	0.73
1:CCC:150:THR:OG1	1:CCC:153:THR:OG1	2.06	0.73
3:NNN:4:VAL:HG21	3:NNN:97:VAL:HG12	1.71	0.72
1:CCC:149:ASN:OD1	1:CCC:205:GLU:OE2	2.07	0.72
1:AAA:150:THR:H	1:AAA:153:THR:HG23	1.55	0.72
3:NNN:78:LEU:HG	3:NNN:106:VAL:CG2	2.20	0.71
2:JJJ:94:ARG:NH1	2:JJJ:101:ASP:OD2	2.17	0.71
2:JJJ:165:THR:OG1	2:JJJ:180:SER:CB	2.38	0.71
3:NNN:149:TRP:HZ3	3:NNN:194:CYS:CA	1.87	0.71
1:BBB:30:GLY:O	1:BBB:71:LEU:HD23	1.89	0.71
1:AAA:159:LEU:HB3	1:AAA:162:GLN:HB2	1.72	0.71
2:III:184:VAL:CG2	2:III:194:TYR:OH	2.37	0.71
3:NNN:133:LEU:HD12	3:NNN:179:LEU:HD23	1.73	0.71
1:AAA:150:THR:H	1:AAA:153:THR:CG2	2.04	0.70
1:BBB:84:ASN:H	1:BBB:84:ASN:HD22	1.36	0.70
3:NNN:149:TRP:CH2	3:NNN:194:CYS:HB2	2.24	0.70
3:LLL:4:VAL:HG21	3:LLL:97:VAL:HG12	1.72	0.70
1:AAA:150:THR:CG2	1:AAA:153:THR:CG2	2.68	0.70
1:AAA:150:THR:CB	1:AAA:153:THR:HG22	2.21	0.70
1:BBB:198:LEU:O	1:BBB:218:SER:HB2	1.90	0.70
2:HHH:138:LEU:HD21	2:HHH:211:VAL:HB	1.73	0.69
2:HHH:87:THR:HG1	2:HHH:111:VAL:HG23	1.57	0.69
1:BBB:34:SER:CB	1:BBB:43:GLU:OE2	2.38	0.69
1:CCC:85:LEU:HB3	2:JJJ:97:ALA:CB	2.22	0.69
1:AAA:84:ASN:ND2	1:AAA:84:ASN:H	1.88	0.69
2:III:126:PRO:HB3	2:III:213:PRO:HA	1.74	0.69
3:NNN:135:CYS:O	3:NNN:135:CYS:SG	2.50	0.69
1:CCC:298:ASN:OD1	1:CCC:301:LEU:N	2.20	0.69
3:LLL:83:GLU:CD	3:LLL:106:VAL:HG23	2.17	0.69
3:NNN:145:VAL:HG12	3:NNN:198:HIS:CD2	2.28	0.69
3:NNN:149:TRP:CH2	3:NNN:194:CYS:CB	2.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:156:SER:HB3	2:JJJ:52:SER:HB2	1.75	0.69
2:JJJ:145:TYR:OH	2:JJJ:178:LEU:HD23	1.92	0.69
1:BBB:159:LEU:O	1:BBB:162:GLN:N	2.24	0.68
1:CCC:80:ASP:HB3	1:CCC:81:LEU:HD13	1.75	0.68
1:CCC:199:ARG:CZ	1:CCC:267:VAL:HG12	2.22	0.68
3:LLL:140:PHE:HD2	3:LLL:198:HIS:HD2	1.41	0.68
1:BBB:42:VAL:HB	1:BBB:298:ASN:HB2	1.74	0.68
3:NNN:140:PHE:CZ	3:NNN:174:ALA:HA	2.27	0.68
1:BBB:178:LEU:HG	1:BBB:179:PRO:HD2	1.75	0.68
1:BBB:32:PRO:HB3	1:BBB:43:GLU:HB3	1.75	0.68
3:NNN:38:GLN:O	3:NNN:84:ALA:HB1	1.94	0.67
3:MMM:171:ASN:O	3:MMM:171:ASN:ND2	2.26	0.67
1:BBB:84:ASN:ND2	2:III:58:TYR:OH	2.27	0.67
3:NNN:107:LEU:HD11	3:NNN:142:PRO:HG3	1.75	0.67
1:CCC:46:PRO:HD3	1:CCC:117:GLY:C	2.19	0.67
1:AAA:42:VAL:CG1	1:AAA:118:GLY:C	2.68	0.67
1:AAA:42:VAL:CG1	1:AAA:118:GLY:HA2	2.23	0.67
1:CCC:154:THR:O	2:JJJ:31:SER:HA	1.95	0.67
3:NNN:150:LYS:HD2	3:NNN:195:GLN:HE21	1.59	0.66
1:CCC:305:GLU:N	1:CCC:305:GLU:OE1	2.28	0.66
1:BBB:159:LEU:HD12	1:BBB:159:LEU:N	2.10	0.66
2:JJJ:165:THR:OG1	2:JJJ:180:SER:OG	2.13	0.66
3:LLL:46:LEU:O	3:LLL:58:ILE:HD11	1.94	0.66
1:AAA:35:GLN:HB3	1:AAA:39:ARG:HD2	1.77	0.66
1:CCC:199:ARG:HG2	1:CCC:219:MET:HG2	1.78	0.66
1:AAA:43:GLU:HG2	1:AAA:73:PHE:CE1	2.31	0.66
1:AAA:251:ASP:CG	1:AAA:296:GLU:HG3	2.20	0.66
3:NNN:144:ALA:HB2	3:NNN:165:PRO:HG3	1.78	0.66
1:CCC:39:ARG:NE	1:CCC:160:HIS:HE1	1.94	0.65
3:NNN:150:LYS:CD	3:NNN:195:GLN:HE21	2.09	0.65
3:NNN:135:CYS:CB	3:NNN:149:TRP:CH2	2.57	0.65
1:CCC:58:LEU:O	1:CCC:63:CYS:SG	2.54	0.65
1:AAA:199:ARG:HB3	1:AAA:267:VAL:HG11	1.79	0.65
2:HHH:125:ALA:HB1	2:HHH:214:LYS:HZ3	1.61	0.65
1:AAA:92:VAL:HG21	1:AAA:158:ASN:OD1	1.97	0.65
1:CCC:120:HIS:NE2	1:CCC:141:TRP:CZ2	2.65	0.64
2:JJJ:144:ASP:HA	2:JJJ:175:LEU:HB3	1.80	0.64
1:AAA:199:ARG:HD3	1:AAA:219:MET:HG2	1.80	0.64
2:III:137:ALA:HB2	2:III:183:THR:HG23	1.79	0.64
2:JJJ:196:CYS:O	2:JJJ:196:CYS:SG	2.55	0.64
1:BBB:71:LEU:HD23	1:BBB:71:LEU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:337:LEU:HD21	1:BBB:174:LYS:NZ	2.13	0.64
2:HHH:144:ASP:HA	2:HHH:175:LEU:CD1	2.16	0.64
2:III:144:ASP:HB3	2:III:175:LEU:HD12	1.78	0.64
1:AAA:162:GLN:N	1:AAA:163:PRO:CD	2.61	0.64
1:CCC:78:LYS:HB3	1:CCC:81:LEU:HD21	1.80	0.64
1:CCC:149:ASN:CG	1:CCC:205:GLU:OE2	2.41	0.64
1:CCC:39:ARG:CZ	1:CCC:160:HIS:ND1	2.61	0.63
2:III:50:ALA:C	2:III:69:ILE:HD13	2.23	0.63
1:CCC:46:PRO:HD3	1:CCC:117:GLY:O	1.97	0.63
2:JJJ:166:PHE:HE1	3:NNN:136:LEU:HD13	1.63	0.63
2:JJJ:197:ASN:OD1	2:JJJ:197:ASN:N	2.32	0.63
3:NNN:172:LYS:HA	3:NNN:172:LYS:CE	2.28	0.63
2:HHH:175:LEU:HD13	2:HHH:176:TYR:N	2.13	0.63
2:III:52:SER:HB3	2:III:56:SER:HB2	1.80	0.63
2:III:184:VAL:HG21	2:III:194:TYR:CZ	2.32	0.63
1:CCC:39:ARG:HB3	1:CCC:39:ARG:NH2	2.13	0.63
2:III:87:THR:CG2	2:III:110:THR:CA	2.70	0.63
1:AAA:198:LEU:HD12	1:AAA:216:TYR:CD1	2.34	0.63
1:CCC:151:PRO:HG2	1:CCC:176:PRO:HD2	1.81	0.63
2:HHH:125:ALA:HB1	2:HHH:214:LYS:HZ2	1.63	0.63
3:NNN:172:LYS:HA	3:NNN:172:LYS:HZ3	1.63	0.63
1:CCC:239:ILE:HG22	1:CCC:244:ARG:HG3	1.81	0.62
1:CCC:119:ASP:CG	1:CCC:121:SER:OG	2.41	0.62
1:CCC:194:VAL:HG23	1:CCC:238:LEU:HD21	1.80	0.62
2:III:146:PHE:CE2	2:III:174:GLY:O	2.52	0.62
1:AAA:152:LEU:HD11	1:CCC:338:PRO:CB	2.28	0.62
1:BBB:35:GLN:HE21	1:BBB:39:ARG:CG	2.01	0.62
1:BBB:298:ASN:OD1	1:BBB:301:LEU:HD23	2.00	0.62
2:III:117:LYS:HE3	2:III:144:ASP:O	1.99	0.61
2:JJJ:141:LEU:HA	2:JJJ:179:SER:OG	2.00	0.61
2:HHH:203:SER:OG	2:HHH:205:THR:OG1	2.16	0.61
1:BBB:84:ASN:H	1:BBB:84:ASN:ND2	1.98	0.61
1:AAA:151:PRO:HG2	1:AAA:176:PRO:CG	2.31	0.61
1:BBB:117:GLY:HA3	1:BBB:295:VAL:HG12	1.82	0.61
2:III:11:LEU:C	2:III:11:LEU:HD23	2.25	0.61
2:HHH:99:LEU:HB3	3:LLL:50:ASP:OD2	1.99	0.61
2:JJJ:143:LYS:HD3	2:JJJ:144:ASP:HB2	1.82	0.61
3:LLL:47:LEU:HD23	3:LLL:58:ILE:HD13	1.82	0.61
3:MMM:54:ARG:HD3	3:MMM:62:PHE:O	2.01	0.61
3:NNN:171:ASN:ND2	3:NNN:173:TYR:CE2	2.69	0.61
1:BBB:150:THR:C	1:BBB:162:GLN:NE2	2.57	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:39:ARG:CZ	1:CCC:160:HIS:CE1	2.84	0.61
1:AAA:82:TYR:HB2	2:HHH:100(A):LEU:HD11	1.83	0.61
1:AAA:120:HIS:NE2	1:AAA:141:TRP:CZ2	2.68	0.61
3:NNN:137:ILE:HG22	3:NNN:140:PHE:CE2	2.35	0.61
1:AAA:152:LEU:HD11	1:CCC:338:PRO:HB2	1.82	0.61
1:BBB:159:LEU:C	1:BBB:162:GLN:H	2.09	0.61
3:LLL:80:THR:HA	3:LLL:106:VAL:HG21	1.82	0.60
1:AAA:85:LEU:HB3	2:HHH:97:ALA:CB	2.31	0.60
1:BBB:159:LEU:HA	1:BBB:162:GLN:CB	2.29	0.60
3:NNN:137:ILE:HG12	3:NNN:196:VAL:HG11	1.83	0.60
3:NNN:195:GLN:NE2	3:NNN:204:GLU:OE2	2.34	0.60
1:BBB:149:ASN:CG	1:BBB:154:THR:HG21	2.24	0.60
2:III:126:PRO:CG	2:III:213:PRO:HA	2.31	0.60
2:JJJ:94:ARG:HE	2:JJJ:101:ASP:CG	2.08	0.60
3:MMM:105:THR:HG21	3:MMM:142:PRO:HB3	1.83	0.60
1:AAA:256:ASP:HB2	1:AAA:270:GLY:O	2.01	0.60
1:CCC:81:LEU:HB3	3:NNN:91:TRP:CZ2	2.36	0.60
2:JJJ:119:PRO:HD3	2:JJJ:200:HIS:ND1	2.17	0.60
3:MMM:111:LYS:O	3:MMM:111:LYS:HD3	2.01	0.60
1:CCC:149:ASN:HD22	1:CCC:149:ASN:H	1.49	0.60
1:AAA:149:ASN:ND2	1:AAA:205:GLU:CD	2.60	0.60
1:AAA:42:VAL:HG11	1:AAA:118:GLY:C	2.27	0.60
1:AAA:337:LEU:N	1:AAA:338:PRO:HD3	2.17	0.60
1:BBB:32:PRO:O	1:BBB:43:GLU:HG2	2.02	0.60
2:HHH:178:LEU:HD12	2:HHH:178:LEU:C	2.27	0.60
2:HHH:204:ASN:CG	2:HHH:204:ASN:O	2.43	0.59
2:III:30:SER:HB3	2:III:73:ASN:HB3	1.84	0.59
2:III:178:LEU:C	2:III:178:LEU:HD12	2.27	0.59
2:JJJ:94:ARG:NE	2:JJJ:101:ASP:OD1	2.31	0.59
3:NNN:39:LEU:HD22	3:NNN:39:LEU:N	2.18	0.59
3:NNN:193:SER:OG	3:NNN:205:LYS:O	2.10	0.59
2:HHH:99:LEU:HD23	2:HHH:99:LEU:C	2.27	0.59
3:MMM:163:THR:HG1	3:MMM:176:SER:HG	1.51	0.59
3:LLL:109:GLN:N	3:LLL:110:PRO:HD3	2.17	0.59
1:AAA:203:PRO:HG2	1:AAA:204:PRO:HD3	1.85	0.59
3:MMM:162:THR:HG1	3:MMM:177:SER:CB	2.16	0.59
1:CCC:277:MET:HE2	1:CCC:277:MET:HA	1.84	0.59
2:JJJ:4:LEU:HD12	2:JJJ:102:LEU:HG	1.84	0.59
2:JJJ:178:LEU:HD12	2:JJJ:178:LEU:C	2.28	0.59
3:NNN:145:VAL:HG12	3:NNN:198:HIS:HD2	1.68	0.59
1:CCC:32:PRO:HB3	1:CCC:43:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:298:ASN:HD21	1:CCC:300:GLN:HB2	1.67	0.59
2:III:14:PRO:HG3	2:III:113:SER:HB2	1.84	0.59
3:LLL:27(A):SER:O	3:LLL:31:HIS:CE1	2.56	0.58
1:CCC:85:LEU:HB3	2:JJJ:97:ALA:HB2	1.84	0.58
2:JJJ:13:GLN:HE21	2:JJJ:14:PRO:HD2	1.68	0.58
1:AAA:327:ARG:HB3	1:BBB:199:ARG:HA	1.86	0.58
3:NNN:5:LEU:HD11	3:NNN:90:THR:HG22	1.84	0.58
1:AAA:252:ILE:HB	1:AAA:297:VAL:HG22	1.84	0.58
1:BBB:30:GLY:O	1:BBB:71:LEU:CD2	2.50	0.58
2:JJJ:166:PHE:CE1	3:NNN:136:LEU:HD13	2.38	0.58
3:NNN:27(B):ASN:N	3:NNN:27(B):ASN:OD1	2.37	0.58
3:NNN:150:LYS:CD	3:NNN:195:GLN:NE2	2.66	0.58
1:AAA:153:THR:O	1:AAA:153:THR:OG1	2.22	0.58
1:BBB:82:TYR:O	1:BBB:84:ASN:ND2	2.37	0.58
1:CCC:85:LEU:N	1:CCC:85:LEU:HD22	2.19	0.57
1:CCC:149:ASN:HB2	1:CCC:162:GLN:HB2	1.87	0.57
3:NNN:116:VAL:HG21	3:NNN:196:VAL:HG21	1.86	0.57
3:LLL:140:PHE:HD2	3:LLL:198:HIS:CD2	2.20	0.57
2:HHH:138:LEU:HD13	2:HHH:138:LEU:C	2.29	0.57
2:III:126:PRO:CB	2:III:213:PRO:HA	2.34	0.57
2:HHH:4:LEU:HD21	2:HHH:34:MET:HE1	1.85	0.57
2:JJJ:201:LYS:HB3	2:JJJ:202:PRO:HD3	1.85	0.57
1:BBB:178:LEU:CG	1:BBB:179:PRO:HD2	2.35	0.57
3:NNN:140:PHE:HE2	3:NNN:174:ALA:HA	1.65	0.57
3:NNN:179:LEU:HD11	3:NNN:181:LEU:HD21	1.87	0.57
1:CCC:88:ASN:OD1	1:CCC:89:PRO:CD	2.34	0.57
3:LLL:27(A):SER:O	3:LLL:31:HIS:HE1	1.88	0.57
1:AAA:150:THR:HG1	1:AAA:153:THR:HG22	1.68	0.56
1:CCC:122:LEU:HD21	1:CCC:295:VAL:HG12	1.86	0.56
3:NNN:46:LEU:HD23	3:NNN:55:PRO:HG3	1.86	0.56
1:AAA:117:GLY:HA3	1:AAA:295:VAL:HG12	1.86	0.56
1:AAA:151:PRO:CG	1:AAA:176:PRO:HD2	2.34	0.56
3:MMM:105:THR:HG21	3:MMM:142:PRO:CB	2.35	0.56
3:NNN:149:TRP:HE3	3:NNN:194:CYS:HA	1.63	0.56
3:NNN:172:LYS:HA	3:NNN:172:LYS:NZ	2.20	0.56
1:AAA:42:VAL:HG11	1:AAA:119:ASP:N	2.20	0.56
1:AAA:187:CYS:HB2	1:AAA:188:ILE:HG23	1.87	0.56
3:NNN:28:ILE:HG23	3:NNN:66:LYS:HE2	1.88	0.56
1:AAA:150:THR:CB	1:AAA:153:THR:CG2	2.83	0.56
1:BBB:99:LEU:HD21	1:BBB:126:THR:CG2	2.35	0.56
2:JJJ:116:THR:OG1	2:JJJ:147:PRO:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:NNN:116:VAL:HG13	3:NNN:137:ILE:HG13	1.86	0.56
1:AAA:251:ASP:OD1	1:AAA:296:GLU:HB2	2.06	0.56
2:HHH:126:PRO:HG3	2:HHH:138:LEU:HD23	1.87	0.56
2:HHH:144:ASP:CA	2:HHH:175:LEU:HD11	2.19	0.56
3:MMM:4:VAL:HG21	3:MMM:97:VAL:HG12	1.87	0.56
1:AAA:35:GLN:HB2	1:AAA:158:ASN:HB2	1.88	0.56
1:CCC:162:GLN:H	1:CCC:163:PRO:HD3	1.70	0.56
2:III:192:GLN:HG3	2:III:194:TYR:CZ	2.41	0.56
1:CCC:99:LEU:HD21	1:CCC:126:THR:CG2	2.37	0.55
3:NNN:167:LYS:HB3	3:NNN:173:TYR:CD1	2.41	0.55
3:NNN:182:THR:N	3:NNN:185:GLN:OE1	2.26	0.55
1:CCC:86:ILE:O	1:CCC:86:ILE:HD12	2.06	0.55
2:HHH:214:LYS:H	2:HHH:214:LYS:HE3	1.69	0.55
1:CCC:73:PHE:CG	1:CCC:73:PHE:O	2.58	0.55
1:CCC:171:LEU:O	1:CCC:171:LEU:HG	2.06	0.55
1:AAA:99:LEU:HD21	1:AAA:126:THR:CG2	2.36	0.55
1:AAA:251:ASP:OD2	1:AAA:296:GLU:HG3	2.07	0.55
1:BBB:187:CYS:HB2	1:BBB:188:ILE:HG23	1.88	0.55
1:CCC:44:HIS:CD2	1:CCC:44:HIS:H	2.25	0.55
1:AAA:159:LEU:CD2	1:AAA:162:GLN:CD	2.74	0.55
2:JJJ:89:VAL:HG11	2:JJJ:91:TYR:CZ	2.42	0.55
3:LLL:36:TYR:CE1	3:LLL:98:PHE:HE2	2.24	0.55
1:CCC:42:VAL:HG22	1:CCC:118:GLY:CA	2.37	0.55
1:CCC:162:GLN:HG2	1:CCC:162:GLN:O	2.06	0.55
1:AAA:327:ARG:HD3	1:AAA:327:ARG:N	2.22	0.54
1:BBB:172:GLN:HA	1:BBB:175:VAL:CG2	2.37	0.54
2:JJJ:147:PRO:HG2	2:JJJ:200:HIS:NE2	2.22	0.54
3:NNN:139:ASP:HA	3:NNN:172:LYS:HB3	1.90	0.54
1:AAA:35:GLN:CB	1:AAA:39:ARG:HD2	2.37	0.54
2:JJJ:89:VAL:CG1	2:JJJ:91:TYR:CZ	2.90	0.54
3:MMM:80:THR:O	3:MMM:83:GLU:HB3	2.07	0.54
3:NNN:5:LEU:N	3:NNN:5:LEU:HD23	2.22	0.54
3:NNN:167:LYS:HB3	3:NNN:173:TYR:CE1	2.43	0.54
1:AAA:172:GLN:HA	1:AAA:175:VAL:CG2	2.37	0.54
1:BBB:39:ARG:HG3	1:BBB:39:ARG:O	2.06	0.54
1:CCC:42:VAL:O	1:CCC:45:GLY:N	2.39	0.54
2:HHH:143:LYS:HE2	3:LLL:132:THR:OG1	2.07	0.54
3:LLL:35:TRP:CH2	3:LLL:88:CYS:HB2	2.43	0.54
1:AAA:276:GLY:HA2	1:AAA:279:ILE:HD12	1.89	0.54
2:JJJ:30:SER:HB2	2:JJJ:73:ASN:ND2	2.23	0.54
1:BBB:162:GLN:N	1:BBB:163:PRO:CD	2.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:194:VAL:HG23	1:BBB:238:LEU:HD21	1.89	0.54
3:MMM:35:TRP:CZ3	3:MMM:88:CYS:HB2	2.42	0.54
1:CCC:307:GLU:O	1:CCC:310:THR:HG22	2.08	0.54
3:LLL:35:TRP:CZ3	3:LLL:88:CYS:HB2	2.43	0.54
3:NNN:112:ALA:HB3	3:NNN:141:TYR:N	2.23	0.54
1:AAA:251:ASP:OD1	1:AAA:296:GLU:HG3	2.08	0.53
2:HHH:101:ASP:HA	3:LLL:46:LEU:HD22	1.90	0.53
1:AAA:152:LEU:HD21	1:CCC:338:PRO:HB2	1.89	0.53
2:III:135:THR:HB	2:III:183:THR:HG21	1.91	0.53
3:NNN:133:LEU:HB2	3:NNN:179:LEU:HB3	1.90	0.53
1:AAA:339:THR:OG1	1:AAA:340:PRO:HD2	2.09	0.53
1:BBB:151:PRO:HG2	1:BBB:176:PRO:HD2	1.90	0.53
1:BBB:203:PRO:N	1:BBB:204:PRO:HD2	2.24	0.53
2:HHH:99:LEU:CD2	3:LLL:32:TYR:CE2	2.91	0.53
1:BBB:162:GLN:HG3	1:BBB:162:GLN:O	2.08	0.53
1:BBB:166:PHE:N	1:BBB:166:PHE:HD2	2.06	0.53
3:LLL:190:ARG:HA	3:LLL:190:ARG:NE	2.23	0.53
1:CCC:82:TYR:C	1:CCC:82:TYR:CD2	2.87	0.53
2:HHH:50:ALA:C	2:HHH:69:ILE:HD13	2.33	0.53
1:CCC:35:GLN:NE2	1:CCC:159:LEU:CD1	2.72	0.53
1:CCC:151:PRO:HD2	1:CCC:176:PRO:HD2	1.90	0.53
2:III:52:SER:O	2:III:71:ARG:NH1	2.41	0.53
3:NNN:109:GLN:HB3	3:NNN:110:PRO:HD2	1.91	0.53
1:CCC:239:ILE:HG22	1:CCC:244:ARG:CG	2.39	0.53
3:MMM:35:TRP:CH2	3:MMM:88:CYS:HB2	2.43	0.53
1:BBB:35:GLN:NE2	1:BBB:39:ARG:HE	2.07	0.53
1:AAA:203:PRO:CG	1:AAA:204:PRO:HD3	2.39	0.52
1:AAA:252:ILE:CB	1:AAA:297:VAL:HG22	2.39	0.52
1:BBB:41:GLY:HA3	1:BBB:300:GLN:HG3	1.90	0.52
2:HHH:127:SER:OG	2:HHH:130:SER:N	2.36	0.52
2:JJJ:51:ILE:CG2	2:JJJ:69:ILE:HD13	2.40	0.52
1:AAA:224:ARG:HB3	1:AAA:225:LEU:HG	1.92	0.52
1:BBB:39:ARG:HD2	1:BBB:42:VAL:HG11	1.92	0.52
1:BBB:166:PHE:N	1:BBB:166:PHE:CD2	2.77	0.52
1:CCC:84:ASN:HA	1:CCC:88:ASN:HD21	1.75	0.52
2:HHH:189:LEU:HD11	2:HHH:213:PRO:HD3	1.91	0.52
2:III:126:PRO:HG3	2:III:213:PRO:HA	1.90	0.52
3:NNN:28:ILE:O	3:NNN:66:LYS:NZ	2.39	0.52
1:AAA:42:VAL:HA	1:AAA:298:ASN:HB2	1.92	0.52
1:BBB:81:LEU:HD12	3:MMM:95(A):SER:CB	2.39	0.52
1:BBB:89:PRO:O	1:BBB:92:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JJJ:154:TRP:CZ3	2:JJJ:196:CYS:HB3	2.45	0.52
3:NNN:38:GLN:HG3	3:NNN:44:PRO:HD3	1.91	0.52
3:NNN:124:GLU:OE2	3:NNN:124:GLU:N	2.37	0.52
3:NNN:129:ASN:HA	3:NNN:183:PRO:CG	2.40	0.52
1:BBB:151:PRO:HA	1:BBB:162:GLN:CD	2.36	0.51
1:AAA:147:ASP:HA	1:AAA:161:GLY:HA2	1.91	0.51
3:NNN:78:LEU:HG	3:NNN:106:VAL:HG21	1.93	0.51
1:AAA:105:ARG:HG3	1:AAA:106:ALA:H	1.74	0.51
1:BBB:99:LEU:HD21	1:BBB:126:THR:HG23	1.93	0.51
1:AAA:35:GLN:HG2	1:AAA:39:ARG:NE	2.25	0.51
2:JJJ:28:THR:HB	2:JJJ:31:SER:HB2	1.93	0.51
3:NNN:133:LEU:N	3:NNN:133:LEU:HD23	2.26	0.51
1:BBB:32:PRO:C	1:BBB:43:GLU:HG2	2.36	0.51
2:HHH:144:ASP:C	2:HHH:175:LEU:HD21	2.36	0.51
2:III:145:TYR:N	2:III:175:LEU:HD13	2.26	0.51
3:NNN:31:HIS:NE2	3:NNN:93:SER:OG	2.44	0.51
1:AAA:151:PRO:HA	1:AAA:162:GLN:NE2	2.25	0.51
1:AAA:206:HIS:CE1	1:AAA:210:LYS:HG3	2.46	0.51
1:AAA:43:GLU:HB3	1:AAA:73:PHE:CZ	2.46	0.51
3:NNN:4:VAL:HG21	3:NNN:97:VAL:CG1	2.39	0.51
1:BBB:85:LEU:HD22	1:BBB:85:LEU:N	2.20	0.51
2:HHH:99:LEU:HD21	3:LLL:32:TYR:CZ	2.45	0.51
2:III:59:TYR:O	2:III:64:LYS:HE3	2.11	0.51
2:JJJ:4:LEU:HD23	2:JJJ:24:ALA:HB2	1.93	0.51
3:NNN:35:TRP:CH2	3:NNN:88:CYS:HB2	2.46	0.51
3:NNN:149:TRP:CE3	3:NNN:194:CYS:CA	2.66	0.51
1:AAA:32:PRO:O	1:AAA:43:GLU:HG3	2.11	0.50
1:AAA:120:HIS:CE1	1:AAA:251:ASP:HB2	2.46	0.50
1:BBB:149:ASN:CG	1:BBB:154:THR:CG2	2.83	0.50
1:CCC:78:LYS:HB3	1:CCC:81:LEU:CD2	2.40	0.50
1:CCC:199:ARG:HB3	1:CCC:267:VAL:HG11	1.93	0.50
2:JJJ:51:ILE:HB	2:JJJ:69:ILE:HG21	1.91	0.50
1:BBB:37:GLN:HB2	2:III:56:SER:OG	2.10	0.50
1:BBB:42:VAL:HA	1:BBB:298:ASN:HA	1.92	0.50
1:CCC:35:GLN:NE2	1:CCC:159:LEU:HD11	2.26	0.50
1:AAA:150:THR:CG2	1:AAA:153:THR:HG22	2.40	0.50
1:CCC:152:LEU:HD21	1:CCC:176:PRO:HD3	1.93	0.50
2:HHH:175:LEU:C	2:HHH:175:LEU:CD1	2.75	0.50
1:AAA:220:ARG:HG2	1:CCC:327:ARG:NH2	2.25	0.50
2:JJJ:184:VAL:HB	2:JJJ:194:TYR:OH	2.11	0.50
3:NNN:129:ASN:HA	3:NNN:183:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:122:LEU:C	1:BBB:122:LEU:HD12	2.37	0.50
1:CCC:44:HIS:CD2	1:CCC:44:HIS:N	2.78	0.50
2:III:29:PHE:CD2	2:III:76:ASN:HA	2.46	0.50
1:AAA:122:LEU:HD12	1:AAA:122:LEU:C	2.36	0.50
1:BBB:75:PRO:HB2	1:BBB:78:LYS:HE2	1.93	0.50
3:NNN:118:LEU:HD23	3:NNN:118:LEU:O	2.11	0.50
1:AAA:159:LEU:HD23	1:AAA:162:GLN:OE1	2.11	0.50
1:CCC:122:LEU:C	1:CCC:122:LEU:HD12	2.37	0.49
1:CCC:159:LEU:HA	1:CCC:162:GLN:NE2	2.23	0.49
2:JJJ:145:TYR:HB2	2:JJJ:200:HIS:HE1	1.76	0.49
2:JJJ:166:PHE:CZ	3:NNN:136:LEU:HB3	2.46	0.49
3:MMM:5:LEU:HD11	3:MMM:90:THR:HG22	1.93	0.49
2:III:184:VAL:CG2	2:III:185:PRO:HD2	2.42	0.49
1:AAA:194:VAL:HG23	1:AAA:238:LEU:HD21	1.94	0.49
2:JJJ:51:ILE:HG22	2:JJJ:69:ILE:HD13	1.92	0.49
2:JJJ:145:TYR:HB2	2:JJJ:200:HIS:CE1	2.47	0.49
3:NNN:167:LYS:CD	3:NNN:173:TYR:CE1	2.93	0.49
3:LLL:55:PRO:HD2	3:LLL:58:ILE:HD12	1.94	0.49
1:AAA:32:PRO:HB3	1:AAA:43:GLU:HA	1.94	0.49
1:BBB:154:THR:HG23	1:BBB:162:GLN:NE2	2.27	0.49
1:BBB:154:THR:O	1:BBB:154:THR:OG1	2.31	0.49
1:CCC:120:HIS:CE1	1:CCC:141:TRP:CZ2	3.00	0.49
1:CCC:206:HIS:CE1	1:CCC:210:LYS:HG3	2.47	0.49
3:MMM:197:THR:HG1	3:MMM:202:THR:HG1	1.54	0.49
3:NNN:137:ILE:HD11	3:NNN:196:VAL:HG21	1.94	0.49
1:AAA:147:ASP:CB	1:AAA:161:GLY:HA2	2.43	0.49
2:III:115:SER:O	2:III:146:PHE:HB3	2.13	0.49
2:III:144:ASP:C	2:III:175:LEU:HD11	2.35	0.49
2:JJJ:87:THR:OG1	2:JJJ:111:VAL:HG13	2.13	0.49
1:BBB:159:LEU:CB	1:BBB:162:GLN:HG2	2.42	0.49
1:AAA:99:LEU:HD21	1:AAA:126:THR:HG23	1.95	0.49
1:AAA:105:ARG:HG3	1:AAA:106:ALA:N	2.28	0.49
1:AAA:297:VAL:HG12	1:AAA:297:VAL:O	2.13	0.49
1:BBB:151:PRO:HA	1:BBB:162:GLN:NE2	2.28	0.49
1:BBB:181:PHE:HB3	1:BBB:184:ILE:HD12	1.94	0.49
2:III:124:LEU:N	2:III:124:LEU:HD23	2.28	0.49
2:JJJ:51:ILE:HB	2:JJJ:69:ILE:CG2	2.43	0.49
1:BBB:71:LEU:O	1:BBB:71:LEU:HG	2.12	0.48
1:BBB:251:ASP:OD1	1:BBB:296:GLU:HB2	2.13	0.48
3:MMM:61:ARG:HB3	3:MMM:76:THR:O	2.13	0.48
3:MMM:105:THR:CG2	3:MMM:142:PRO:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:94:LEU:HD12	1:AAA:95:ALA:N	2.28	0.48
1:AAA:220:ARG:NH2	5:AAA:404:SO4:O3	2.47	0.48
2:HHH:100(B):TYR:CG	3:LLL:49:TYR:HB2	2.49	0.48
2:III:35:SER:HB2	2:III:95:LEU:CD2	2.43	0.48
3:LLL:80:THR:O	3:LLL:83:GLU:HB2	2.13	0.48
1:AAA:337:LEU:HD21	1:BBB:174:LYS:HZ1	1.78	0.48
3:NNN:28:ILE:CG2	3:NNN:66:LYS:HE2	2.44	0.48
3:NNN:60:ASP:OD1	3:NNN:60:ASP:N	2.44	0.48
1:AAA:42:VAL:HG12	1:AAA:118:GLY:N	2.28	0.48
1:AAA:124:ILE:HA	1:AAA:167:LEU:HD11	1.95	0.48
3:MMM:60:ASP:OD1	3:MMM:60:ASP:N	2.47	0.48
1:BBB:307:GLU:O	1:BBB:310:THR:HG22	2.13	0.48
2:III:86:ASP:O	2:III:90:TYR:OH	2.31	0.48
3:LLL:27(B):ASN:HA	3:LLL:91:TRP:O	2.13	0.48
3:NNN:35:TRP:CZ3	3:NNN:88:CYS:HB2	2.48	0.48
3:MMM:170:ASN:HD21	3:MMM:172:LYS:HB2	1.78	0.48
2:JJJ:51:ILE:HB	2:JJJ:69:ILE:HD13	1.96	0.47
1:AAA:147:ASP:HA	1:AAA:161:GLY:CA	2.44	0.47
2:III:184:VAL:HG11	2:III:194:TYR:CZ	2.49	0.47
2:JJJ:2:VAL:N	2:JJJ:25:SER:O	2.47	0.47
3:NNN:144:ALA:CB	3:NNN:165:PRO:HG3	2.43	0.47
1:AAA:282:GLU:OE1	1:AAA:282:GLU:HA	2.14	0.47
1:CCC:148:ILE:HG12	1:CCC:148:ILE:O	2.15	0.47
3:LLL:140:PHE:CD1	3:LLL:140:PHE:N	2.81	0.47
3:NNN:78:LEU:CG	3:NNN:106:VAL:CG2	2.92	0.47
1:BBB:74:THR:N	1:BBB:75:PRO:HD2	2.29	0.47
1:CCC:42:VAL:HG22	1:CCC:118:GLY:N	2.29	0.47
1:CCC:149:ASN:HD22	1:CCC:149:ASN:N	2.11	0.47
3:NNN:135:CYS:HB3	3:NNN:149:TRP:CZ2	2.44	0.47
1:BBB:178:LEU:CD1	1:BBB:179:PRO:HD2	2.44	0.47
1:CCC:120:HIS:CE1	1:CCC:251:ASP:HB2	2.49	0.47
2:HHH:200:HIS:CD2	2:HHH:202:PRO:HD2	2.50	0.47
1:AAA:151:PRO:CG	1:AAA:176:PRO:HG2	2.45	0.47
1:AAA:255:PHE:CD2	1:AAA:314:LEU:HD21	2.49	0.47
1:CCC:148:ILE:O	1:CCC:148:ILE:HG23	2.14	0.47
2:III:184:VAL:HG23	2:III:185:PRO:HD2	1.95	0.47
2:JJJ:83:ARG:C	2:JJJ:111:VAL:HG21	2.40	0.47
3:LLL:5:LEU:HD11	3:LLL:90:THR:HG22	1.97	0.47
3:NNN:133:LEU:HG	3:NNN:179:LEU:HG	1.97	0.47
1:CCC:35:GLN:CD	1:CCC:159:LEU:CD1	2.88	0.47
1:CCC:39:ARG:HE	1:CCC:160:HIS:CE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JJJ:138:LEU:C	2:JJJ:138:LEU:HD12	2.40	0.47
3:MMM:62:PHE:CD2	3:MMM:75:ILE:HG12	2.50	0.47
3:MMM:114:PRO:HD3	3:MMM:198:HIS:HD2	1.80	0.47
3:NNN:39:LEU:N	3:NNN:39:LEU:CD2	2.78	0.47
3:NNN:78:LEU:HD21	3:NNN:106:VAL:HG23	1.97	0.47
3:NNN:121:PRO:HD2	3:NNN:186:TRP:CZ2	2.50	0.47
1:AAA:147:ASP:HB3	1:AAA:163:PRO:HD2	1.96	0.47
2:HHH:201:LYS:HB3	2:HHH:202:PRO:HD3	1.96	0.47
2:JJJ:29:PHE:CD2	2:JJJ:76:ASN:HA	2.50	0.47
3:LLL:83:GLU:CG	3:LLL:106:VAL:CG2	2.93	0.47
1:AAA:147:ASP:OD1	1:AAA:147:ASP:N	2.46	0.46
1:AAA:307:GLU:O	1:AAA:310:THR:HG22	2.14	0.46
1:CCC:151:PRO:CG	1:CCC:176:PRO:HD2	2.44	0.46
2:JJJ:169:VAL:HB	3:NNN:163:THR:HG22	1.96	0.46
1:AAA:38:LYS:HD2	1:AAA:39:ARG:CZ	2.45	0.46
1:AAA:159:LEU:HD22	1:AAA:162:GLN:NE2	2.26	0.46
1:CCC:137:LEU:HA	1:CCC:245:PRO:HG2	1.97	0.46
1:CCC:199:ARG:NH1	1:CCC:267:VAL:HG12	2.30	0.46
2:JJJ:139:GLY:HA2	2:JJJ:154:TRP:HH2	1.80	0.46
3:NNN:137:ILE:HD11	3:NNN:196:VAL:CG2	2.45	0.46
2:JJJ:83:ARG:O	2:JJJ:111:VAL:HG11	2.15	0.46
3:LLL:47:LEU:HA	3:LLL:58:ILE:CD1	2.45	0.46
3:NNN:167:LYS:HB3	3:NNN:173:TYR:CZ	2.49	0.46
1:AAA:219:MET:HE1	1:AAA:271:LEU:HD23	1.97	0.46
1:BBB:252:ILE:HG21	1:BBB:297:VAL:HG22	1.97	0.46
2:HHH:99:LEU:HB3	3:LLL:50:ASP:CG	2.40	0.46
2:HHH:165:THR:HG23	2:HHH:180:SER:HB2	1.98	0.46
2:HHH:171:GLN:HG2	2:HHH:175:LEU:O	2.16	0.46
2:HHH:189:LEU:HD12	2:HHH:189:LEU:O	2.15	0.46
1:AAA:151:PRO:HG2	1:AAA:176:PRO:HG2	1.97	0.46
1:BBB:147:ASP:HB3	1:BBB:160:HIS:O	2.15	0.46
1:AAA:284:HIS:CD2	1:AAA:324:GLY:HA2	2.51	0.46
1:BBB:219:MET:HG3	1:BBB:269:GLY:O	2.15	0.46
3:LLL:140:PHE:N	3:LLL:140:PHE:HD1	2.14	0.46
1:AAA:76:VAL:HG12	1:AAA:77:PRO:HD3	1.97	0.46
1:AAA:120:HIS:CD2	1:AAA:141:TRP:CZ2	3.03	0.46
1:BBB:224:ARG:HB3	1:BBB:225:LEU:HG	1.97	0.46
3:NNN:37:GLN:HG3	3:NNN:37:GLN:O	2.15	0.46
1:BBB:120:HIS:CE1	1:BBB:251:ASP:HB2	2.49	0.46
1:BBB:122:LEU:HD21	1:BBB:295:VAL:CG1	2.46	0.46
1:BBB:147:ASP:OD1	1:BBB:161:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:255:PHE:CD2	1:CCC:314:LEU:HD21	2.50	0.46
2:HHH:189:LEU:HD11	2:HHH:213:PRO:CD	2.45	0.46
3:NNN:167:LYS:HB3	3:NNN:173:TYR:CG	2.51	0.46
3:NNN:184:GLU:OE2	3:NNN:184:GLU:N	2.38	0.46
1:CCC:81:LEU:HD12	3:NNN:91:TRP:HH2	1.81	0.46
1:CCC:335:ASP:OD1	1:CCC:335:ASP:N	2.42	0.45
2:HHH:166:PHE:CZ	3:LLL:136:LEU:HB3	2.51	0.45
2:III:61:ASP:HA	2:III:64:LYS:HD2	1.98	0.45
2:III:127:SER:O	2:III:127:SER:OG	2.29	0.45
3:NNN:120:PRO:HB2	3:NNN:121:PRO:CD	2.41	0.45
1:AAA:42:VAL:CG1	1:AAA:118:GLY:N	2.79	0.45
1:AAA:274:ARG:HB3	1:BBB:223:ASP:OD2	2.17	0.45
1:AAA:289:LEU:HD23	1:AAA:323:PHE:CE1	2.51	0.45
1:BBB:122:LEU:HD21	1:BBB:295:VAL:HG12	1.97	0.45
1:BBB:255:PHE:CD2	1:BBB:314:LEU:HD21	2.52	0.45
2:III:212:GLU:O	2:III:212:GLU:HG3	2.16	0.45
3:LLL:78:LEU:HD11	3:LLL:104:LEU:HD21	1.97	0.45
1:BBB:145:HIS:ND1	1:BBB:145:HIS:N	2.65	0.45
1:BBB:159:LEU:O	1:BBB:163:PRO:CD	2.65	0.45
2:JJJ:34:MET:HG2	2:JJJ:71:ARG:HH12	1.80	0.45
1:AAA:199:ARG:CZ	1:AAA:199:ARG:HB2	2.46	0.45
1:AAA:219:MET:HE1	1:AAA:271:LEU:CD2	2.46	0.45
3:NNN:167:LYS:HB2	3:NNN:171:ASN:HA	1.98	0.45
1:BBB:251:ASP:CG	1:BBB:296:GLU:OE1	2.60	0.45
1:BBB:284:HIS:CD2	1:BBB:324:GLY:HA2	2.52	0.45
1:CCC:80:ASP:HA	2:JJJ:58:TYR:CE1	2.51	0.45
2:HHH:166:PHE:CE1	3:LLL:136:LEU:HB3	2.51	0.45
2:JJJ:139:GLY:HA2	2:JJJ:154:TRP:CH2	2.52	0.45
3:MMM:27(B):ASN:HA	3:MMM:91:TRP:O	2.17	0.45
1:AAA:248:LEU:O	1:AAA:292:LEU:HA	2.17	0.45
1:BBB:30:GLY:HA3	1:BBB:70:ASP:OD1	2.17	0.45
1:BBB:124:ILE:HA	1:BBB:167:LEU:HD11	1.97	0.45
1:CCC:42:VAL:CG2	1:CCC:118:GLY:C	2.90	0.45
1:CCC:99:LEU:HD21	1:CCC:126:THR:HG23	1.98	0.45
1:CCC:152:LEU:H	1:CCC:152:LEU:HG	1.51	0.45
2:III:137:ALA:HB2	2:III:183:THR:CG2	2.47	0.45
2:JJJ:89:VAL:HB	2:JJJ:91:TYR:CE2	2.52	0.45
3:LLL:27(B):ASN:O	3:LLL:31:HIS:ND1	2.26	0.45
3:NNN:107:LEU:CD1	3:NNN:142:PRO:HG3	2.44	0.45
3:MMM:109:GLN:OE1	3:MMM:141:TYR:CE1	2.69	0.45
1:AAA:227:ILE:HD11	1:AAA:279:ILE:CG1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:178:LEU:HD12	1:BBB:179:PRO:HD2	1.98	0.45
1:CCC:297:VAL:HG12	1:CCC:297:VAL:O	2.17	0.45
2:HHH:99:LEU:HD23	2:HHH:99:LEU:O	2.16	0.45
2:JJJ:89:VAL:CG1	2:JJJ:91:TYR:CE2	3.00	0.45
1:AAA:85:LEU:HB3	2:HHH:97:ALA:HB3	1.98	0.45
1:AAA:149:ASN:HD21	1:AAA:205:GLU:CD	2.24	0.45
1:BBB:153:THR:O	2:III:31:SER:OG	2.32	0.45
1:CCC:282:GLU:OE1	1:CCC:282:GLU:HA	2.17	0.45
3:LLL:83:GLU:HG3	3:LLL:106:VAL:HG22	1.99	0.45
1:CCC:298:ASN:OD1	1:CCC:301:LEU:HB2	2.17	0.44
2:HHH:137:ALA:CB	3:LLL:117:THR:HG21	2.46	0.44
2:III:184:VAL:HG11	2:III:194:TYR:CE1	2.52	0.44
3:MMM:47:LEU:HD23	3:MMM:47:LEU:HA	1.84	0.44
1:CCC:167:LEU:HB3	1:CCC:187:CYS:SG	2.58	0.44
3:LLL:140:PHE:HE1	3:LLL:174:ALA:HA	1.81	0.44
3:NNN:103:LYS:HE2	3:NNN:105:THR:HG23	1.99	0.44
3:NNN:140:PHE:CE2	3:NNN:173:TYR:O	2.70	0.44
1:BBB:142:VAL:HG11	1:BBB:250:PHE:CE2	2.53	0.44
2:HHH:147:PRO:HD2	2:HHH:202:PRO:HB3	2.00	0.44
2:HHH:168:ALA:HA	2:HHH:178:LEU:HB3	1.98	0.44
2:JJJ:168:ALA:HB2	2:JJJ:178:LEU:HB3	1.99	0.44
1:AAA:338:PRO:HB2	1:BBB:152:LEU:HD11	1.98	0.44
1:BBB:200:ASP:CB	1:BBB:267:VAL:HG21	2.48	0.44
1:BBB:248:LEU:O	1:BBB:292:LEU:HA	2.17	0.44
2:HHH:30:SER:HB3	2:HHH:73:ASN:ND2	2.33	0.44
2:JJJ:57:THR:HG23	2:JJJ:59:TYR:CE2	2.53	0.44
2:JJJ:57:THR:OG1	2:JJJ:69:ILE:HG22	2.17	0.44
2:JJJ:89:VAL:HG12	2:JJJ:91:TYR:CE2	2.52	0.44
3:LLL:46:LEU:O	3:LLL:58:ILE:CD1	2.63	0.44
3:NNN:18:LYS:HA	3:NNN:75:ILE:O	2.18	0.44
2:HHH:100(B):TYR:CD1	3:LLL:49:TYR:CB	3.01	0.44
3:LLL:173:TYR:N	3:LLL:173:TYR:CD2	2.86	0.44
3:MMM:18:LYS:HA	3:MMM:75:ILE:O	2.18	0.44
3:MMM:170:ASN:ND2	3:MMM:172:LYS:HB2	2.31	0.44
3:NNN:120:PRO:CB	3:NNN:121:PRO:HD2	2.39	0.44
3:NNN:135:CYS:SG	3:NNN:149:TRP:CH2	3.11	0.44
3:NNN:167:LYS:HA	3:NNN:173:TYR:HA	2.00	0.44
1:AAA:35:GLN:HB3	1:AAA:39:ARG:HB2	1.99	0.44
1:AAA:172:GLN:HG3	1:AAA:186:PRO:HG2	2.00	0.44
1:AAA:228:GLN:NE2	1:AAA:232:GLU:OE2	2.51	0.44
1:BBB:75:PRO:HB2	1:BBB:78:LYS:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:151:PRO:CD	1:CCC:176:PRO:HD2	2.47	0.44
2:HHH:100(A):LEU:HD23	2:HHH:100(A):LEU:HA	1.79	0.44
2:JJJ:165:THR:OG1	2:JJJ:180:SER:HB2	2.15	0.44
1:BBB:162:GLN:H	1:BBB:163:PRO:HD3	1.80	0.44
1:BBB:298:ASN:HD22	1:BBB:298:ASN:C	2.26	0.44
1:CCC:149:ASN:N	1:CCC:149:ASN:ND2	2.65	0.44
1:CCC:206:HIS:CE1	1:CCC:210:LYS:HE3	2.53	0.44
1:CCC:219:MET:HG3	1:CCC:269:GLY:O	2.17	0.44
2:III:100(C):MET:HE1	3:MMM:98:PHE:HZ	1.83	0.44
2:JJJ:170:LEU:HD23	2:JJJ:176:TYR:CD2	2.53	0.44
1:BBB:37:GLN:HG3	1:BBB:80:ASP:OD1	2.18	0.44
1:BBB:82:TYR:CE1	1:BBB:86:ILE:HG21	2.53	0.44
2:HHH:124:LEU:HD21	2:HHH:141:LEU:HB2	2.00	0.44
2:JJJ:166:PHE:CE1	3:NNN:136:LEU:HD22	2.53	0.44
1:AAA:43:GLU:O	1:AAA:46:PRO:HD2	2.18	0.43
1:AAA:131:ALA:HA	1:AAA:137:LEU:HD23	1.99	0.43
1:CCC:42:VAL:HG22	1:CCC:118:GLY:H	1.82	0.43
2:HHH:84:ALA:HA	2:HHH:111:VAL:HB	1.99	0.43
2:III:168:ALA:HA	2:III:178:LEU:HB3	2.00	0.43
3:LLL:4:VAL:HG21	3:LLL:97:VAL:CG1	2.43	0.43
3:LLL:140:PHE:CD2	3:LLL:198:HIS:HD2	2.28	0.43
1:AAA:142:VAL:HG11	1:AAA:250:PHE:CE2	2.53	0.43
3:NNN:59:PRO:HB2	3:NNN:61:ARG:HG3	2.00	0.43
1:BBB:155:SER:HB3	2:III:31:SER:HA	2.00	0.43
1:CCC:71:LEU:HD23	1:CCC:71:LEU:HA	1.87	0.43
1:CCC:248:LEU:O	1:CCC:292:LEU:HA	2.17	0.43
1:CCC:284:HIS:CD2	1:CCC:324:GLY:HA2	2.54	0.43
2:III:84:ALA:O	2:III:87:THR:OG1	2.34	0.43
3:NNN:38:GLN:CG	3:NNN:44:PRO:HD3	2.48	0.43
3:NNN:121:PRO:CD	3:NNN:186:TRP:CH2	3.01	0.43
3:NNN:136:LEU:HD23	3:NNN:176:SER:HB2	2.00	0.43
1:AAA:61:LEU:HD21	1:AAA:325:GLN:HB2	2.00	0.43
1:AAA:84:ASN:O	1:AAA:85:LEU:HB2	2.17	0.43
1:CCC:142:VAL:HG11	1:CCC:250:PHE:CZ	2.54	0.43
2:III:4:LEU:HB3	2:III:92:CYS:SG	2.58	0.43
3:MMM:114:PRO:HD3	3:MMM:198:HIS:CD2	2.53	0.43
1:AAA:268:VAL:HG23	1:CCC:273:TYR:CZ	2.53	0.43
1:AAA:272:THR:OG1	1:AAA:275:GLU:HG3	2.18	0.43
1:AAA:298:ASN:ND2	1:AAA:298:ASN:C	2.77	0.43
1:BBB:298:ASN:O	1:BBB:301:LEU:HB2	2.18	0.43
2:HHH:214:LYS:HE2	2:HHH:214:LYS:N	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:18:LYS:HA	3:LLL:75:ILE:O	2.17	0.43
1:BBB:81:LEU:O	1:BBB:81:LEU:CD2	2.61	0.43
3:LLL:83:GLU:HB2	3:LLL:106:VAL:CG2	2.49	0.43
3:LLL:83:GLU:CG	3:LLL:106:VAL:HG22	2.48	0.43
1:BBB:159:LEU:N	1:BBB:159:LEU:CD1	2.78	0.43
1:CCC:155:SER:O	2:JJJ:53:SER:N	2.51	0.43
1:CCC:277:MET:HE2	1:CCC:277:MET:CA	2.48	0.43
2:JJJ:146:PHE:CD1	2:JJJ:146:PHE:C	2.96	0.43
2:JJJ:170:LEU:HD23	2:JJJ:176:TYR:CE2	2.53	0.43
1:AAA:30:GLY:O	1:AAA:71:LEU:N	2.44	0.43
1:AAA:121:SER:HA	1:AAA:163:PRO:HG3	2.00	0.43
1:CCC:252:ILE:HD13	1:CCC:252:ILE:HA	1.82	0.43
1:BBB:76:VAL:HB	1:BBB:77:PRO:CD	2.49	0.43
1:BBB:172:GLN:HG3	1:BBB:186:PRO:HG2	2.01	0.43
1:CCC:263:THR:HG23	1:CCC:266:PRO:HB3	2.01	0.43
2:III:98:ASP:N	2:III:98:ASP:OD1	2.50	0.43
3:NNN:14:ALA:O	3:NNN:17:GLN:HB2	2.19	0.43
1:CCC:85:LEU:HD22	1:CCC:85:LEU:H	1.84	0.43
1:CCC:218:SER:O	1:CCC:222:ILE:HG13	2.19	0.43
1:CCC:255:PHE:CZ	1:CCC:276:GLY:HA3	2.54	0.43
2:HHH:127:SER:O	2:HHH:131:THR:HG23	2.19	0.43
2:III:87:THR:HG23	2:III:110:THR:HA	1.88	0.43
2:III:165:THR:HG23	2:III:180:SER:HB2	1.99	0.43
2:JJJ:13:GLN:HE21	2:JJJ:14:PRO:CD	2.31	0.43
3:NNN:125:GLU:HA	3:NNN:128:ALA:HB3	2.01	0.43
1:AAA:82:TYR:CD1	1:AAA:82:TYR:C	2.95	0.42
1:BBB:32:PRO:CB	1:BBB:43:GLU:HB3	2.46	0.42
1:BBB:142:VAL:HG11	1:BBB:250:PHE:CZ	2.54	0.42
1:BBB:145:HIS:HD1	1:BBB:145:HIS:H	1.66	0.42
3:LLL:79:GLN:HG3	3:LLL:80:THR:N	2.34	0.42
1:CCC:43:GLU:O	1:CCC:46:PRO:HD2	2.19	0.42
3:LLL:35:TRP:HB2	3:LLL:48:ILE:HB	2.01	0.42
2:JJJ:91:TYR:CD2	2:JJJ:91:TYR:N	2.88	0.42
2:JJJ:147:PRO:HB2	2:JJJ:202:PRO:HB2	2.01	0.42
3:LLL:83:GLU:CD	3:LLL:106:VAL:CG2	2.89	0.42
3:NNN:47:LEU:HD23	3:NNN:47:LEU:HA	1.88	0.42
1:AAA:142:VAL:HG11	1:AAA:250:PHE:CZ	2.54	0.42
1:CCC:86:ILE:C	1:CCC:89:PRO:HD2	2.44	0.42
1:CCC:152:LEU:CD2	1:CCC:176:PRO:HD3	2.48	0.42
2:JJJ:178:LEU:HD12	2:JJJ:179:SER:N	2.35	0.42
1:AAA:39:ARG:O	1:AAA:42:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:44:HIS:ND1	1:AAA:44:HIS:N	2.64	0.42
1:AAA:171:LEU:O	1:AAA:175:VAL:HG22	2.20	0.42
1:BBB:298:ASN:C	1:BBB:298:ASN:ND2	2.76	0.42
2:III:192:GLN:CG	2:III:194:TYR:CZ	3.02	0.42
3:LLL:66:LYS:HA	3:LLL:71:ALA:HA	2.01	0.42
3:MMM:27:SER:HA	3:MMM:29:GLY:HA3	2.01	0.42
3:NNN:27:SER:HA	3:NNN:29:GLY:HA3	2.02	0.42
1:AAA:42:VAL:HG12	1:AAA:118:GLY:H	1.85	0.42
1:BBB:39:ARG:NH2	1:BBB:160:HIS:CE1	2.88	0.42
2:JJJ:34:MET:HG2	2:JJJ:71:ARG:NH1	2.34	0.42
2:JJJ:147:PRO:HG2	2:JJJ:200:HIS:CE1	2.53	0.42
1:AAA:42:VAL:CA	1:AAA:298:ASN:HB2	2.49	0.42
1:CCC:142:VAL:HG11	1:CCC:250:PHE:CE2	2.55	0.42
2:JJJ:142:VAL:HG12	2:JJJ:145:TYR:CD2	2.55	0.42
3:NNN:136:LEU:CD2	3:NNN:176:SER:HB2	2.49	0.42
3:NNN:167:LYS:HB3	3:NNN:173:TYR:CE2	2.54	0.42
1:AAA:142:VAL:HA	1:AAA:196:ILE:O	2.19	0.42
1:AAA:195:TYR:HB2	1:AAA:216:TYR:HB2	2.01	0.42
2:JJJ:143:LYS:HD3	2:JJJ:144:ASP:CB	2.50	0.42
3:NNN:167:LYS:CD	3:NNN:173:TYR:OH	2.63	0.42
1:AAA:145:HIS:ND1	1:AAA:145:HIS:N	2.66	0.42
2:III:138:LEU:HD12	2:III:211:VAL:HB	2.02	0.42
3:LLL:31:HIS:CD2	3:LLL:91:TRP:HD1	2.37	0.42
3:NNN:121:PRO:HD2	3:NNN:186:TRP:CH2	2.53	0.42
1:BBB:159:LEU:O	1:BBB:163:PRO:HD3	2.19	0.42
3:NNN:146:THR:N	3:NNN:197:THR:O	2.53	0.42
1:BBB:119:ASP:OD1	1:BBB:119:ASP:C	2.62	0.41
1:BBB:255:PHE:CZ	1:BBB:276:GLY:HA3	2.56	0.41
2:HHH:99:LEU:HD21	3:LLL:32:TYR:CE2	2.55	0.41
2:III:124:LEU:N	2:III:124:LEU:CD2	2.83	0.41
1:CCC:44:HIS:H	1:CCC:44:HIS:HD2	1.65	0.41
2:III:144:ASP:CB	2:III:175:LEU:CD1	2.86	0.41
3:MMM:168:GLN:HE21	3:MMM:168:GLN:HB3	1.69	0.41
3:NNN:66:LYS:HA	3:NNN:71:ALA:HA	2.02	0.41
3:NNN:141:TYR:HA	3:NNN:142:PRO:HA	1.89	0.41
1:AAA:327:ARG:HD3	1:AAA:327:ARG:H	1.84	0.41
1:BBB:90:ARG:HG3	1:BBB:179:PRO:C	2.44	0.41
1:BBB:131:ALA:HA	1:BBB:137:LEU:HD23	2.01	0.41
1:CCC:81:LEU:HD11	3:NNN:95(A):SER:OG	2.21	0.41
2:III:35:SER:HB2	2:III:95:LEU:HD23	2.02	0.41
2:III:143:LYS:HE3	3:MMM:132:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JJJ:184:VAL:HG11	2:JJJ:194:TYR:CE1	2.55	0.41
3:NNN:167:LYS:HB3	3:NNN:173:TYR:CD2	2.55	0.41
1:BBB:171:LEU:O	1:BBB:175:VAL:HG22	2.21	0.41
1:CCC:233:ARG:NH1	5:CCC:407:SO4:O3	2.54	0.41
2:JJJ:116:THR:HA	2:JJJ:147:PRO:HD3	2.00	0.41
3:NNN:26:SER:O	3:NNN:27(B):ASN:OD1	2.39	0.41
3:NNN:192:TYR:HB2	3:NNN:207:VAL:HG23	2.02	0.41
1:CCC:84:ASN:ND2	2:JJJ:58:TYR:OH	2.39	0.41
2:III:184:VAL:CG2	2:III:185:PRO:CD	2.99	0.41
2:III:137:ALA:HA	2:III:183:THR:HA	2.03	0.41
2:JJJ:82:MET:HB3	2:JJJ:82(C):LEU:HD21	2.02	0.41
3:LLL:186:TRP:CZ2	3:LLL:209:PRO:HA	2.55	0.41
1:AAA:35:GLN:HA	1:AAA:158:ASN:CG	2.46	0.41
1:BBB:74:THR:N	1:BBB:75:PRO:CD	2.83	0.41
3:NNN:133:LEU:HD13	3:NNN:186:TRP:HZ3	1.86	0.41
1:AAA:147:ASP:HB3	1:AAA:161:GLY:HA2	2.03	0.41
1:AAA:151:PRO:HG2	1:AAA:176:PRO:CD	2.50	0.41
1:CCC:263:THR:CG2	1:CCC:266:PRO:HB3	2.51	0.41
2:III:129:LYS:O	2:III:129:LYS:HG2	2.21	0.41
2:JJJ:52(A):GLY:O	2:JJJ:73:ASN:ND2	2.40	0.41
2:JJJ:98:ASP:OD1	2:JJJ:98:ASP:N	2.53	0.41
3:NNN:133:LEU:CD1	3:NNN:186:TRP:HZ3	2.34	0.41
1:AAA:35:GLN:HA	1:AAA:158:ASN:ND2	2.36	0.41
1:AAA:80:ASP:HB3	2:HHH:58:TYR:CE1	2.55	0.41
1:AAA:117:GLY:HA2	1:AAA:118:GLY:HA3	1.92	0.41
1:AAA:328:GLU:HG2	1:AAA:328:GLU:O	2.21	0.41
1:BBB:137:LEU:C	1:BBB:137:LEU:HD12	2.45	0.41
1:BBB:162:GLN:O	1:BBB:162:GLN:CG	2.69	0.41
1:BBB:166:PHE:HD2	1:BBB:166:PHE:H	1.67	0.41
1:BBB:200:ASP:HB3	1:BBB:267:VAL:HG21	2.03	0.41
1:CCC:142:VAL:HA	1:CCC:196:ILE:O	2.21	0.41
1:CCC:183:TRP:CE2	1:CCC:184:ILE:HG13	2.56	0.41
2:HHH:86:ASP:O	2:HHH:90:TYR:OH	2.32	0.41
2:JJJ:150:VAL:HG12	2:JJJ:200:HIS:CD2	2.56	0.41
1:AAA:263:THR:O	1:AAA:301:LEU:HD12	2.21	0.41
1:AAA:337:LEU:HD21	1:BBB:174:LYS:CE	2.50	0.41
1:CCC:181:PHE:HB3	1:CCC:184:ILE:HD12	2.02	0.41
2:III:201:LYS:N	2:III:202:PRO:CD	2.84	0.41
3:MMM:199:GLU:OE2	3:MMM:199:GLU:HA	2.20	0.41
1:AAA:326:THR:OG1	1:AAA:327:ARG:N	2.54	0.40
1:AAA:337:LEU:O	1:AAA:337:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:252:ILE:HG12	1:BBB:297:VAL:HG22	2.03	0.40
1:CCC:149:ASN:ND2	1:CCC:161:GLY:O	2.54	0.40
2:III:38:ARG:HD3	2:III:48:VAL:HG22	2.02	0.40
1:BBB:151:PRO:HA	1:BBB:162:GLN:OE1	2.22	0.40
2:III:38:ARG:HD3	2:III:48:VAL:CG2	2.51	0.40
2:III:148:GLU:HG3	2:III:176:TYR:CD2	2.56	0.40
2:JJJ:165:THR:HG1	2:JJJ:180:SER:HG	1.66	0.40
1:AAA:32:PRO:HB3	1:AAA:43:GLU:CB	2.51	0.40
1:AAA:58:LEU:HA	1:AAA:61:LEU:HD12	2.03	0.40
1:CCC:172:GLN:HA	1:CCC:175:VAL:HG22	2.03	0.40
2:HHH:82:MET:HB3	2:HHH:82(C):LEU:HD21	2.03	0.40
2:HHH:127:SER:HB3	2:HHH:130:SER:HB3	2.03	0.40
2:JJJ:171:GLN:HA	3:NNN:161:GLU:HG3	2.04	0.40
3:MMM:105:THR:CB	3:MMM:142:PRO:HB3	2.52	0.40
1:AAA:200:ASP:CB	1:AAA:267:VAL:HG21	2.52	0.40
1:CCC:85:LEU:N	1:CCC:85:LEU:CD2	2.85	0.40
2:JJJ:147:PRO:C	2:JJJ:200:HIS:HE2	2.29	0.40
2:JJJ:14:PRO:HD3	2:JJJ:112:SER:O	2.22	0.40
2:JJJ:145:TYR:O	2:JJJ:176:TYR:N	2.55	0.40
2:JJJ:165:THR:HG23	2:JJJ:178:LEU:HD13	2.03	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:76:VAL:HG12	3:NNN:95(A):SER:HG[8_555]	0.79	0.81
1:AAA:300:GLN:OE1	1:AAA:300:GLN:OE1[8_555]	1.48	0.72
1:AAA:40:LYS:HZ3	1:AAA:40:LYS:HZ3[8_555]	1.17	0.43
1:AAA:40:LYS:HZ2	1:AAA:40:LYS:HZ2[8_555]	1.20	0.40
3:LLL:188:SER:HG	3:NNN:26:SER:OG[8_545]	1.35	0.25
1:BBB:76:VAL:CG1	3:NNN:95(A):SER:HG[8_555]	1.39	0.21
3:LLL:188:SER:OG	3:NNN:26:SER:HG[8_545]	1.43	0.17
2:HHH:204:ASN:ND2	2:III:105:ARG:O[8_555]	2.10	0.10
1:BBB:76:VAL:HG12	3:NNN:95(A):SER:OG[8_555]	1.51	0.09
1:BBB:76:VAL:CG1	3:NNN:95(A):SER:OG[8_555]	2.14	0.06
3:LLL:188:SER:OG	3:NNN:26:SER:OG[8_545]	2.15	0.05
1:AAA:40:LYS:NZ	1:AAA:40:LYS:NZ[8_555]	2.16	0.04

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	AAA	316/346 (91%)	287 (91%)	27 (8%)	2 (1%)	21	51
1	BBB	306/346 (88%)	278 (91%)	25 (8%)	3 (1%)	12	40
1	CCC	315/346 (91%)	282 (90%)	28 (9%)	5 (2%)	7	30
2	HHH	220/233 (94%)	206 (94%)	13 (6%)	1 (0%)	24	55
2	III	220/233 (94%)	205 (93%)	13 (6%)	2 (1%)	14	42
2	JJJ	216/233 (93%)	206 (95%)	9 (4%)	1 (0%)	24	55
3	LLL	212/220 (96%)	198 (93%)	13 (6%)	1 (0%)	24	55
3	MMM	211/220 (96%)	195 (92%)	16 (8%)	0	100	100
3	NNN	209/220 (95%)	189 (90%)	19 (9%)	1 (0%)	24	55
All	All	2225/2397 (93%)	2046 (92%)	163 (7%)	16 (1%)	18	48

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	77	PRO
1	CCC	77	PRO
1	CCC	162	GLN
2	III	56	SER
2	III	213	PRO
1	BBB	163	PRO
2	HHH	127	SER
1	CCC	75	PRO
2	JJJ	115	SER
1	BBB	164	VAL
1	AAA	162	GLN
1	BBB	162	GLN
1	CCC	186	PRO
3	NNN	39	LEU
1	CCC	297	VAL
3	LLL	106	VAL

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	AAA	268/292 (92%)	219 (82%)	49 (18%)	2	7
1	BBB	258/292 (88%)	221 (86%)	37 (14%)	3	14
1	CCC	267/292 (91%)	219 (82%)	48 (18%)	2	7
2	HHH	183/190 (96%)	157 (86%)	26 (14%)	3	14
2	III	183/190 (96%)	156 (85%)	27 (15%)	3	13
2	JJJ	179/190 (94%)	158 (88%)	21 (12%)	5	21
3	LLL	179/184 (97%)	155 (87%)	24 (13%)	4	16
3	MMM	178/184 (97%)	149 (84%)	29 (16%)	2	10
3	NNN	176/184 (96%)	140 (80%)	36 (20%)	1	5
All	All	1871/1998 (94%)	1574 (84%)	297 (16%)	2	11

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	39	ARG
1	AAA	40	LYS
1	AAA	44	HIS
1	AAA	59	SER
1	AAA	73	PHE
1	AAA	76	VAL
1	AAA	78	LYS
1	AAA	80	ASP
1	AAA	82	TYR
1	AAA	84	ASN
1	AAA	85	LEU
1	AAA	88	ASN
1	AAA	105	ARG
1	AAA	113	CYS
1	AAA	115	THR
1	AAA	120	HIS
1	AAA	145	HIS
1	AAA	147	ASP

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Mol	Chain	Res	Type
1	AAA	150	THR
1	AAA	152	LEU
1	AAA	153	THR
1	AAA	158	ASN
1	AAA	171	LEU
1	AAA	175	VAL
1	AAA	182	SER
1	AAA	185	LYS
1	AAA	187	CYS
1	AAA	199	ARG
1	AAA	218	SER
1	AAA	219	MET
1	AAA	221	ASP
1	AAA	222	ILE
1	AAA	225	LEU
1	AAA	228	GLN
1	AAA	229	LYS
1	AAA	242	ARG
1	AAA	249	SER
1	AAA	252	ILE
1	AAA	253	ASP
1	AAA	263	THR
1	AAA	272	THR
1	AAA	294	LEU
1	AAA	298	ASN
1	AAA	301	LEU
1	AAA	321	SER
1	AAA	327	ARG
1	AAA	331	HIS
1	AAA	336	GLN
1	AAA	339	THR
1	BBB	39	ARG
1	BBB	40	LYS
1	BBB	46	PRO
1	BBB	74	THR
1	BBB	80	ASP
1	BBB	81	LEU
1	BBB	82	TYR
1	BBB	84	ASN
1	BBB	85	LEU
1	BBB	86	ILE
1	BBB	88	ASN

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Mol	Chain	Res	Type
1	BBB	91	SER
1	BBB	113	CYS
1	BBB	115	THR
1	BBB	145	HIS
1	BBB	150	THR
1	BBB	154	THR
1	BBB	156	SER
1	BBB	159	LEU
1	BBB	162	GLN
1	BBB	166	PHE
1	BBB	171	LEU
1	BBB	175	VAL
1	BBB	182	SER
1	BBB	185	LYS
1	BBB	187	CYS
1	BBB	199	ARG
1	BBB	201	VAL
1	BBB	221	ASP
1	BBB	224	ARG
1	BBB	225	LEU
1	BBB	252	ILE
1	BBB	253	ASP
1	BBB	294	LEU
1	BBB	298	ASN
1	BBB	301	LEU
1	BBB	328	GLU
1	CCC	24	HIS
1	CCC	25	SER
1	CCC	35	GLN
1	CCC	39	ARG
1	CCC	40	LYS
1	CCC	63	CYS
1	CCC	71	LEU
1	CCC	76	VAL
1	CCC	77	PRO
1	CCC	78	LYS
1	CCC	80	ASP
1	CCC	81	LEU
1	CCC	82	TYR
1	CCC	83	ASN
1	CCC	112	SER
1	CCC	115	THR

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Mol	Chain	Res	Type
1	CCC	137	LEU
1	CCC	145	HIS
1	CCC	149	ASN
1	CCC	152	LEU
1	CCC	153	THR
1	CCC	155	SER
1	CCC	156	SER
1	CCC	158	ASN
1	CCC	159	LEU
1	CCC	160	HIS
1	CCC	162	GLN
1	CCC	168	LEU
1	CCC	169	ARG
1	CCC	172	GLN
1	CCC	182	SER
1	CCC	185	LYS
1	CCC	187	CYS
1	CCC	188	ILE
1	CCC	205	GLU
1	CCC	233	ARG
1	CCC	244	ARG
1	CCC	252	ILE
1	CCC	253	ASP
1	CCC	267	VAL
1	CCC	268	VAL
1	CCC	294	LEU
1	CCC	301	LEU
1	CCC	326	THR
1	CCC	332	ILE
1	CCC	335	ASP
1	CCC	336	GLN
1	CCC	337	LEU
2	HHH	4	LEU
2	HHH	12	VAL
2	HHH	19	ARG
2	HHH	30	SER
2	HHH	46	GLU
2	HHH	53	SER
2	HHH	56	SER
2	HHH	61	ASP
2	HHH	77	THR
2	HHH	83	ARG

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Mol	Chain	Res	Type
2	HHH	101	ASP
2	HHH	105	ARG
2	HHH	111	VAL
2	HHH	116	THR
2	HHH	129	LYS
2	HHH	138	LEU
2	HHH	148	GLU
2	HHH	171	GLN
2	HHH	175	LEU
2	HHH	188	SER
2	HHH	199	ASN
2	HHH	204	ASN
2	HHH	205	THR
2	HHH	210	ARG
2	HHH	211	VAL
2	HHH	214	LYS
2	III	2	VAL
2	III	3	GLN
2	III	19	ARG
2	III	53	SER
2	III	77	THR
2	III	83	ARG
2	III	87	THR
2	III	95	LEU
2	III	96	ARG
2	III	98	ASP
2	III	99	LEU
2	III	101	ASP
2	III	124	LEU
2	III	127	SER
2	III	135	THR
2	III	138	LEU
2	III	146	PHE
2	III	163	VAL
2	III	173	SER
2	III	175	LEU
2	III	182	VAL
2	III	183	THR
2	III	186	SER
2	III	189	LEU
2	III	210	ARG
2	III	211	VAL

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Mol	Chain	Res	Type
2	III	214	LYS
2	JJJ	11	LEU
2	JJJ	12	VAL
2	JJJ	13	GLN
2	JJJ	19	ARG
2	JJJ	31	SER
2	JJJ	57	THR
2	JJJ	61	ASP
2	JJJ	69	ILE
2	JJJ	77	THR
2	JJJ	83	ARG
2	JJJ	95	LEU
2	JJJ	98	ASP
2	JJJ	100(A)	LEU
2	JJJ	105	ARG
2	JJJ	111	VAL
2	JJJ	148	GLU
2	JJJ	166	PHE
2	JJJ	170	LEU
2	JJJ	179	SER
2	JJJ	197	ASN
2	JJJ	198	VAL
3	LLL	4	VAL
3	LLL	12	SER
3	LLL	26	SER
3	LLL	27	SER
3	LLL	27(B)	ASN
3	LLL	31	HIS
3	LLL	47	LEU
3	LLL	54	ARG
3	LLL	60	ASP
3	LLL	66	LYS
3	LLL	85	ASP
3	LLL	88	CYS
3	LLL	105	THR
3	LLL	106	VAL
3	LLL	109	GLN
3	LLL	111	LYS
3	LLL	115	SER
3	LLL	127	GLN
3	LLL	134	VAL
3	LLL	140	PHE

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Mol	Chain	Res	Type
3	LLL	145	VAL
3	LLL	190	ARG
3	LLL	191	SER
3	LLL	210	THR
3	MMM	4	VAL
3	MMM	12	SER
3	MMM	27(B)	ASN
3	MMM	30	ASN
3	MMM	47	LEU
3	MMM	60	ASP
3	MMM	61	ARG
3	MMM	78	LEU
3	MMM	80	THR
3	MMM	85	ASP
3	MMM	88	CYS
3	MMM	103	LYS
3	MMM	105	THR
3	MMM	109	GLN
3	MMM	111	LYS
3	MMM	115	SER
3	MMM	127	GLN
3	MMM	152	ASP
3	MMM	157	LYS
3	MMM	162	THR
3	MMM	163	THR
3	MMM	167	LYS
3	MMM	168	GLN
3	MMM	170	ASN
3	MMM	171	ASN
3	MMM	190	ARG
3	MMM	197	THR
3	MMM	199	GLU
3	MMM	210	THR
3	NNN	4	VAL
3	NNN	5	LEU
3	NNN	12	SER
3	NNN	27(B)	ASN
3	NNN	30	ASN
3	NNN	37	GLN
3	NNN	38	GLN
3	NNN	42	THR
3	NNN	45	LYS

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Mol	Chain	Res	Type
3	NNN	47	LEU
3	NNN	79	GLN
3	NNN	85	ASP
3	NNN	88	CYS
3	NNN	94	SER
3	NNN	105	THR
3	NNN	106	VAL
3	NNN	107	LEU
3	NNN	115	SER
3	NNN	118	LEU
3	NNN	120	PRO
3	NNN	127	GLN
3	NNN	135	CYS
3	NNN	145	VAL
3	NNN	152	ASP
3	NNN	153	SER
3	NNN	154	SER
3	NNN	156	VAL
3	NNN	163	THR
3	NNN	167	LYS
3	NNN	171	ASN
3	NNN	172	LYS
3	NNN	187	LYS
3	NNN	189	HIS
3	NNN	193	SER
3	NNN	197	THR
3	NNN	204	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 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	$\# Z > 2$
5	SO4	III	302	-	4,4,4	0.33	0	6,6,6	0.06	0
5	SO4	HHH	302	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	BBB	405	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	AAA	405	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	LLL	301	-	4,4,4	0.34	0	6,6,6	0.06	0
5	SO4	CCC	408	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	LLL	302	-	4,4,4	0.35	0	6,6,6	0.08	0
5	SO4	JJJ	301	-	4,4,4	0.33	0	6,6,6	0.09	0
5	SO4	CCC	405	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	MMM	302	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	AAA	404	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	MMM	303	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	III	303	-	4,4,4	0.35	0	6,6,6	0.10	0
5	SO4	CCC	406	-	4,4,4	0.35	0	6,6,6	0.08	0
5	SO4	MMM	301	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	CCC	404	-	4,4,4	0.34	0	6,6,6	0.05	0
5	SO4	HHH	301	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	AAA	403	-	4,4,4	0.31	0	6,6,6	0.11	0
5	SO4	BBB	404	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	HHH	305	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	BBB	403	-	4,4,4	0.34	0	6,6,6	0.07	0
5	SO4	CCC	403	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	III	304	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	CCC	407	-	4,4,4	0.34	0	6,6,6	0.06	0
5	SO4	III	301	-	4,4,4	0.34	0	6,6,6	0.06	0
5	SO4	HHH	303	-	4,4,4	0.34	0	6,6,6	0.07	0
5	SO4	HHH	304	-	4,4,4	0.33	0	6,6,6	0.06	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	404	SO4	1	0
5	CCC	407	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	AAA	318/346 (91%)	0.42	10 (3%)	51	34	43, 89, 125, 200	0
1	BBB	308/346 (89%)	0.22	5 (1%)	70	52	47, 91, 125, 146	0
1	CCC	317/346 (91%)	0.36	9 (2%)	55	36	59, 92, 133, 213	0
2	HHH	222/233 (95%)	0.20	0	100	100	53, 87, 147, 173	0
2	III	222/233 (95%)	0.31	7 (3%)	50	34	45, 99, 170, 203	0
2	JJJ	218/233 (93%)	0.29	6 (2%)	55	36	71, 115, 208, 234	0
3	LLL	214/220 (97%)	0.12	3 (1%)	73	54	71, 102, 123, 163	0
3	MMM	213/220 (96%)	0.17	9 (4%)	40	26	35, 107, 143, 165	0
3	NNN	211/220 (95%)	0.13	4 (1%)	66	48	79, 136, 182, 203	0
All	All	2243/2397 (93%)	0.26	53 (2%)	59	40	35, 99, 170, 234	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	III	97	ALA	5.2
2	III	137	ALA	4.2
1	CCC	190	SER	4.1
1	BBB	85	LEU	4.0
1	CCC	76	VAL	3.8
3	MMM	95(B)	ALA	3.8
2	III	53	SER	3.7
3	MMM	92	ASP	3.6
2	III	100(A)	LEU	3.4
2	III	47	TRP	3.3
1	BBB	86	ILE	3.3
1	CCC	75	PRO	3.3
1	BBB	82	TYR	3.1
2	III	54	GLY	3.0
1	CCC	114	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	JJJ	152	VAL	2.9
1	AAA	227	ILE	2.8
3	LLL	147	VAL	2.7
1	AAA	79	ASP	2.7
1	CCC	124	ILE	2.7
1	AAA	113	CYS	2.7
3	MMM	91	TRP	2.6
1	AAA	279	ILE	2.5
3	LLL	211	GLU	2.5
2	JJJ	146	PHE	2.5
1	CCC	301	LEU	2.5
2	JJJ	167	PRO	2.5
3	LLL	190	ARG	2.5
1	AAA	218	SER	2.5
1	BBB	124	ILE	2.4
3	NNN	132	THR	2.4
3	MMM	95	LEU	2.4
3	MMM	179	LEU	2.3
1	AAA	117	GLY	2.3
3	MMM	165	PRO	2.3
1	CCC	294	LEU	2.2
3	MMM	149	TRP	2.2
2	JJJ	149	PRO	2.2
3	NNN	4	VAL	2.2
1	CCC	276	GLY	2.2
2	JJJ	124	LEU	2.2
2	III	198	VAL	2.2
3	MMM	2	GLN	2.2
1	AAA	297	VAL	2.2
1	AAA	255	PHE	2.1
3	NNN	133	LEU	2.1
3	MMM	135	CYS	2.1
1	AAA	221	ASP	2.1
2	JJJ	185	PRO	2.1
3	NNN	138	SER	2.1
1	BBB	116	LEU	2.0
1	CCC	85	LEU	2.0
1	AAA	319	ILE	2.0

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

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

6.3 Carbohydrates [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(Å ²)	Q<0.9
5	SO4	III	304	5/5	0.46	0.10	175,175,182,186	0
5	SO4	HHH	303	5/5	0.50	0.08	177,184,188,189	0
5	SO4	JJJ	301	5/5	0.52	0.08	171,176,180,185	0
5	SO4	CCC	405	5/5	0.53	0.08	161,163,168,170	0
5	SO4	III	301	5/5	0.55	0.07	181,182,187,189	0
5	SO4	CCC	407	5/5	0.56	0.12	138,141,146,155	0
5	SO4	CCC	406	5/5	0.57	0.10	170,174,176,180	0
5	SO4	MMM	303	5/5	0.57	0.18	132,133,137,138	0
5	SO4	III	303	5/5	0.58	0.10	140,142,146,148	0
5	SO4	HHH	304	5/5	0.58	0.16	152,160,162,162	0
5	SO4	HHH	305	5/5	0.59	0.10	178,183,184,185	0
5	SO4	AAA	405	5/5	0.59	0.08	186,188,190,191	0
5	SO4	CCC	404	5/5	0.67	0.13	141,145,148,156	0
5	SO4	BBB	405	5/5	0.67	0.08	175,175,179,180	0
5	SO4	BBB	404	5/5	0.69	0.09	152,155,156,156	0
5	SO4	BBB	403	5/5	0.71	0.07	155,161,163,166	0
5	SO4	LLL	302	5/5	0.71	0.15	135,136,138,140	0
5	SO4	MMM	302	5/5	0.71	0.09	145,147,149,150	0
5	SO4	CCC	408	5/5	0.71	0.08	162,164,169,169	0
5	SO4	LLL	301	5/5	0.72	0.09	157,157,159,161	0
5	SO4	AAA	404	5/5	0.73	0.19	111,115,116,121	0
5	SO4	III	302	5/5	0.74	0.21	129,130,132,135	0
5	SO4	MMM	301	5/5	0.74	0.10	129,133,136,136	0
5	SO4	AAA	403	5/5	0.75	0.09	117,119,122,124	0
5	SO4	CCC	403	5/5	0.75	0.15	111,111,113,117	0
5	SO4	HHH	301	5/5	0.86	0.11	103,104,107,108	0
5	SO4	HHH	302	5/5	0.87	0.11	102,103,106,107	0
4	MN	CCC	402	1/1	0.93	0.06	121,121,121,121	0
4	MN	AAA	402	1/1	0.95	0.06	100,100,100,100	0
4	MN	BBB	401	1/1	0.95	0.05	87,87,87,87	0
4	MN	BBB	402	1/1	0.98	0.04	98,98,98,98	0
4	MN	CCC	401	1/1	0.98	0.04	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MN	AAA	401	1/1	0.98	0.05	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.