



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:45 PM UTC

PDB ID : 7OG1 / pdb_00007og1
Title : AP2 clathrin adaptor core in complex with cargo peptide and FCHO2
Authors : Zaccai, N.R.; Kelly, B.T.; Evans, P.R.; Owen, D.J.
Deposited on : 2021-05-05
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:

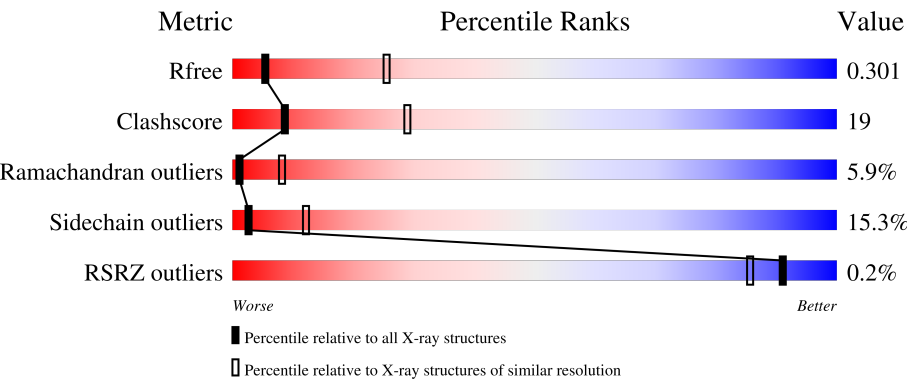
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	621	58%31%9%..
2	BBB	591	49%36%10%..
3	CCC	446	..98%
3	MMM	446	51%33%6%.9%
4	SSS	142	43%45%12%

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Mol	Chain	Length	Quality of chain
5	DDD	152	11%5%84%
5	GGG	152	13%5%79%
6	PPP	6	17%50%17%17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14391 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 AP-2 complex subunit alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	613	Total	C	N	O	S	0	0	0
			4836	3081	833	901	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	272	GLU	-	insertion	UNP P18484

- Molecule 2 is a protein called AP-2 complex subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	572	Total	C	N	O	S	0	0	0
			4527	2882	752	868	25			

- Molecule 3 is a protein called AP-2 complex subunit mu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	MMM	406	Total	C	N	O	S	0	0	0
			3254	2087	566	582	19			
3	CCC	9	Total	C	N	O	S	0	0	0
			72	45	12	14	1			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
MMM	237	MET	-	insertion	UNP P84092
MMM	238	GLU	-	insertion	UNP P84092
MMM	239	GLN	-	insertion	UNP P84092
MMM	240	LYS	-	insertion	UNP P84092
MMM	241	LEU	-	insertion	UNP P84092
MMM	242	ILE	-	insertion	UNP P84092
MMM	243	SER	-	insertion	UNP P84092

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Chain	Residue	Modelled	Actual	Comment	Reference
MMM	244	GLU	-	insertion	UNP P84092
MMM	245	GLU	-	insertion	UNP P84092
MMM	246	ASP	-	insertion	UNP P84092
MMM	247	LEU	-	insertion	UNP P84092
CCC	237	MET	-	insertion	UNP P84092
CCC	238	GLU	-	insertion	UNP P84092
CCC	239	GLN	-	insertion	UNP P84092
CCC	240	LYS	-	insertion	UNP P84092
CCC	241	LEU	-	insertion	UNP P84092
CCC	242	ILE	-	insertion	UNP P84092
CCC	243	SER	-	insertion	UNP P84092
CCC	244	GLU	-	insertion	UNP P84092
CCC	245	GLU	-	insertion	UNP P84092
CCC	246	ASP	-	insertion	UNP P84092
CCC	247	LEU	-	insertion	UNP P84092

- Molecule 4 is a protein called AP-2 complex subunit sigma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	SSS	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

- Molecule 5 is a protein called F-BAR domain only protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	GGG	32	Total	C	N	O	S	0	0	0
			245	153	43	47	2			
5	DDD	24	Total	C	N	O		0	0	0
			200	122	32	46				

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
GGG	309	GLY	-	expression tag	UNP Q0JRZ9
GGG	310	SER	-	expression tag	UNP Q0JRZ9
GGG	311	PRO	-	expression tag	UNP Q0JRZ9
GGG	312	GLU	-	expression tag	UNP Q0JRZ9
GGG	313	PHE	-	expression tag	UNP Q0JRZ9
GGG	445	GLU	-	expression tag	UNP Q0JRZ9
GGG	446	PHE	-	expression tag	UNP Q0JRZ9
GGG	447	PRO	-	expression tag	UNP Q0JRZ9
GGG	448	GLY	-	expression tag	UNP Q0JRZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
GGG	449	ARG	-	expression tag	UNP Q0JRZ9
GGG	450	PRO	-	expression tag	UNP Q0JRZ9
GGG	451	HIS	-	expression tag	UNP Q0JRZ9
GGG	452	HIS	-	expression tag	UNP Q0JRZ9
GGG	453	HIS	-	expression tag	UNP Q0JRZ9
GGG	454	HIS	-	expression tag	UNP Q0JRZ9
GGG	455	HIS	-	expression tag	UNP Q0JRZ9
GGG	456	HIS	-	expression tag	UNP Q0JRZ9
GGG	457	HIS	-	expression tag	UNP Q0JRZ9
GGG	458	HIS	-	expression tag	UNP Q0JRZ9
GGG	459	HIS	-	expression tag	UNP Q0JRZ9
GGG	460	HIS	-	expression tag	UNP Q0JRZ9
DDD	309	GLY	-	expression tag	UNP Q0JRZ9
DDD	310	SER	-	expression tag	UNP Q0JRZ9
DDD	311	PRO	-	expression tag	UNP Q0JRZ9
DDD	312	GLU	-	expression tag	UNP Q0JRZ9
DDD	313	PHE	-	expression tag	UNP Q0JRZ9
DDD	445	GLU	-	expression tag	UNP Q0JRZ9
DDD	446	PHE	-	expression tag	UNP Q0JRZ9
DDD	447	PRO	-	expression tag	UNP Q0JRZ9
DDD	448	GLY	-	expression tag	UNP Q0JRZ9
DDD	449	ARG	-	expression tag	UNP Q0JRZ9
DDD	450	PRO	-	expression tag	UNP Q0JRZ9
DDD	451	HIS	-	expression tag	UNP Q0JRZ9
DDD	452	HIS	-	expression tag	UNP Q0JRZ9
DDD	453	HIS	-	expression tag	UNP Q0JRZ9
DDD	454	HIS	-	expression tag	UNP Q0JRZ9
DDD	455	HIS	-	expression tag	UNP Q0JRZ9
DDD	456	HIS	-	expression tag	UNP Q0JRZ9
DDD	457	HIS	-	expression tag	UNP Q0JRZ9
DDD	458	HIS	-	expression tag	UNP Q0JRZ9
DDD	459	HIS	-	expression tag	UNP Q0JRZ9
DDD	460	HIS	-	expression tag	UNP Q0JRZ9

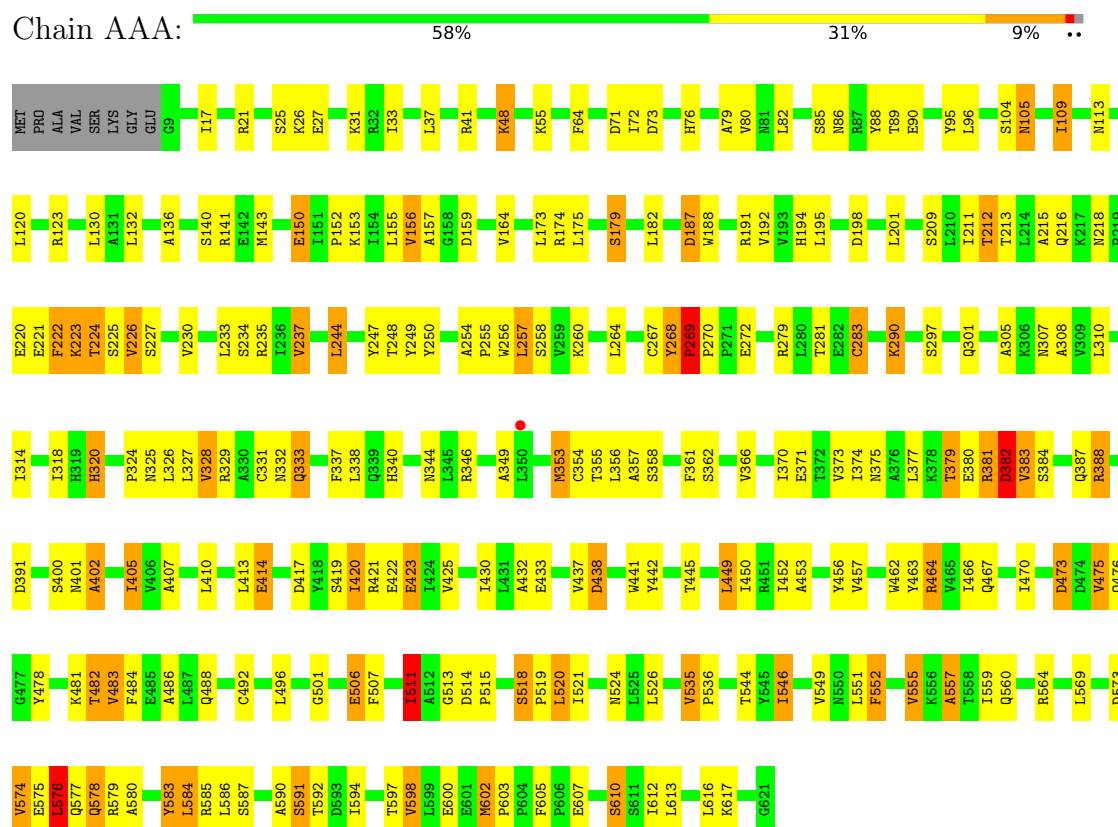
- Molecule 6 is a protein called TGN38 CARGO PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	PPP	6	Total	C	N	O	0	0	0
			57	34	11	12			

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: AP-2 complex subunit alpha-2



- Molecule 6: TGN38 CARGO PEPTIDE

Chain PPP: 17% 50% 17% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.58Å 150.07Å 96.43Å 90.00° 112.65° 90.00°	Depositor
Resolution (Å)	76.66 – 3.25 76.66 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (76.66-3.25) 99.9 (76.66-3.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX v1.19	Depositor
R, R_{free}	0.207 , 0.306 0.209 , 0.301	Depositor DCC
R_{free} test set	1881 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 114.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14391	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

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	1.09	0/4921	1.58	17/6669 (0.3%)
2	BBB	1.06	0/4597	1.59	13/6237 (0.2%)
3	CCC	1.18	0/71	1.26	0/91
3	MMM	1.08	0/3319	1.43	7/4473 (0.2%)
4	SSS	1.10	0/1224	1.48	6/1650 (0.4%)
5	DDD	1.10	0/204	1.39	0/275
5	GGG	1.20	0/250	1.75	2/339 (0.6%)
6	PPP	0.91	0/57	1.21	0/74
All	All	1.08	0/14643	1.54	45/19808 (0.2%)

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
2	BBB	0	4
5	GGG	0	1
All	All	0	5

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	GGG	360	LYS	N-CA-C	8.65	116.01	108.22
1	AAA	269	PRO	N-CA-C	8.14	120.63	110.70
2	BBB	360	GLU	N-CA-C	-7.41	103.14	111.07
3	MMM	218	ASP	CA-CB-CG	7.40	120.00	112.60
2	BBB	581	PHE	CA-C-N	6.64	130.84	120.34
2	BBB	581	PHE	C-N-CA	6.64	130.84	120.34
5	GGG	361	PRO	N-CA-CB	-6.21	96.73	103.25
3	MMM	370	ALA	CA-C-N	6.13	125.81	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	MMM	370	ALA	C-N-CA	6.13	125.81	119.92
1	AAA	400	SER	CA-C-N	6.01	128.33	120.28
1	AAA	400	SER	C-N-CA	6.01	128.33	120.28
1	AAA	150	GLU	CA-C-N	5.99	124.02	120.24
1	AAA	150	GLU	C-N-CA	5.99	124.02	120.24
3	MMM	105	PHE	CA-CB-CG	5.94	119.74	113.80
2	BBB	250	HIS	CA-CB-CG	5.61	119.41	113.80
2	BBB	430	ALA	CA-C-N	5.58	128.07	120.54
2	BBB	430	ALA	C-N-CA	5.58	128.07	120.54
3	MMM	113	ASP	CA-CB-CG	5.52	118.12	112.60
1	AAA	383	VAL	CA-C-N	5.47	127.61	120.28
1	AAA	383	VAL	C-N-CA	5.47	127.61	120.28
1	AAA	220	GLU	CA-C-N	5.44	127.83	120.65
1	AAA	220	GLU	C-N-CA	5.44	127.83	120.65
3	MMM	56	PHE	CA-C-O	-5.43	115.64	121.56
2	BBB	388	ALA	CA-C-N	5.30	127.38	120.28
2	BBB	388	ALA	C-N-CA	5.30	127.38	120.28
3	MMM	260	HIS	CA-CB-CG	5.26	119.06	113.80
1	AAA	401	ASN	CB-CA-C	-5.24	102.09	110.79
4	SSS	80	TYR	CA-C-N	5.22	127.54	120.44
4	SSS	80	TYR	C-N-CA	5.22	127.54	120.44
1	AAA	583	TYR	CB-CA-C	5.20	119.53	110.68
4	SSS	91	LEU	CA-C-N	5.18	127.22	120.28
4	SSS	91	LEU	C-N-CA	5.18	127.22	120.28
4	SSS	84	ILE	CA-C-N	5.15	127.18	120.28
4	SSS	84	ILE	C-N-CA	5.15	127.18	120.28
2	BBB	157	GLU	O-C-N	5.09	128.00	122.20
2	BBB	69	VAL	CA-C-N	5.09	127.36	120.44
2	BBB	69	VAL	C-N-CA	5.09	127.36	120.44
1	AAA	375	ASN	N-CA-C	-5.09	107.58	112.97
1	AAA	557	ALA	CA-C-N	5.09	127.51	120.29
1	AAA	557	ALA	C-N-CA	5.09	127.51	120.29
1	AAA	555	VAL	CA-C-N	5.06	127.77	120.38
1	AAA	555	VAL	C-N-CA	5.06	127.77	120.38
1	AAA	437	VAL	N-CA-C	-5.06	105.39	110.30
2	BBB	397	ASP	CA-C-N	5.01	126.99	120.28
2	BBB	397	ASP	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	158	ASP	Peptide
2	BBB	250	HIS	Peptide
2	BBB	329	ASN	Peptide
2	BBB	549	SER	Peptide
5	GGG	368	HIS	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	4836	0	4952	168	0
2	BBB	4527	0	4638	218	0
3	CCC	72	0	80	3	0
3	MMM	3254	0	3318	122	0
4	SSS	1200	0	1195	70	0
5	DDD	200	0	171	3	0
5	GGG	245	0	247	15	0
6	PPP	57	0	53	5	0
All	All	14391	0	14654	545	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 19.

All (545) 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)
2:BBB:122:LEU:O	2:BBB:125:PRO:HD2	1.66	0.96
2:BBB:249:SER:HB3	3:MMM:259:PHE:H	1.30	0.94
2:BBB:165:LEU:HD23	2:BBB:184:LEU:HD13	1.50	0.93
3:MMM:433:VAL:HG23	6:PPP:5:LEU:HD22	1.48	0.92
3:MMM:175:LEU:HD11	3:MMM:415:LEU:HD22	1.56	0.87
2:BBB:251:ALA:O	2:BBB:253:SER:N	2.08	0.87
1:AAA:218:ASN:HB2	1:AAA:221:GLU:OE1	1.77	0.85
2:BBB:461:ASN:HB2	5:GGG:360:LYS:HD2	1.57	0.83
2:BBB:477:SER:C	2:BBB:479:GLN:H	1.86	0.83
1:AAA:598:VAL:HG21	2:BBB:529:LEU:HD12	1.58	0.82
2:BBB:319:GLN:O	2:BBB:321:ILE:HG22	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SSS:6:LEU:HD13	4:SSS:8:GLN:HE21	1.44	0.79
2:BBB:322:LYS:HA	2:BBB:325:PHE:CE2	2.18	0.79
2:BBB:414:ILE:HD13	2:BBB:432:LEU:HD22	1.65	0.78
3:MMM:196:VAL:HG11	3:MMM:408:SER:HB3	1.65	0.78
1:AAA:88:TYR:CE1	4:SSS:138:LEU:HD22	2.19	0.77
4:SSS:3:ARG:HA	4:SSS:21:MET:HE3	1.66	0.76
1:AAA:307:ASN:HA	1:AAA:310:LEU:HB3	1.68	0.76
2:BBB:155:MET:HB3	2:BBB:158:ASP:HB3	1.66	0.75
4:SSS:42:ARG:NH2	4:SSS:47:THR:O	2.22	0.73
2:BBB:401:THR:OG1	2:BBB:403:VAL:HG23	1.89	0.72
3:MMM:261:GLN:OE1	3:MMM:261:GLN:HA	1.89	0.72
4:SSS:91:LEU:HD23	4:SSS:113:VAL:HG11	1.74	0.70
3:MMM:405:PHE:O	3:MMM:407:PRO:HD3	1.91	0.70
2:BBB:477:SER:O	2:BBB:479:GLN:N	2.24	0.69
3:MMM:6:PHE:CE2	3:MMM:29:VAL:HG22	2.28	0.68
3:MMM:257:CYS:HB2	3:MMM:286:MET:HE3	1.76	0.68
1:AAA:195:LEU:O	1:AAA:198:ASP:HB2	1.94	0.67
2:BBB:510:ALA:O	2:BBB:520:ARG:HA	1.95	0.67
2:BBB:157:GLU:O	2:BBB:157:GLU:HG2	1.94	0.67
4:SSS:91:LEU:CD2	4:SSS:113:VAL:HG11	2.25	0.67
2:BBB:499:THR:O	2:BBB:501:GLU:N	2.28	0.66
1:AAA:506:GLU:OE2	1:AAA:602:MET:CG	2.43	0.66
1:AAA:506:GLU:OE2	1:AAA:602:MET:HB2	1.95	0.66
2:BBB:511:THR:HG23	2:BBB:524:TYR:CZ	2.31	0.66
3:MMM:406:ALA:HB2	3:MMM:435:TYR:HD2	1.58	0.66
4:SSS:99:CYS:HB2	3:CCC:239:GLN:HA	1.77	0.66
2:BBB:155:MET:CB	2:BBB:158:ASP:HB3	2.26	0.66
2:BBB:570:LEU:HD11	3:MMM:47:VAL:HG11	1.78	0.66
3:MMM:268:PHE:CD1	3:MMM:268:PHE:O	2.49	0.66
1:AAA:486:ALA:HB1	1:AAA:496:LEU:HD21	1.76	0.65
1:AAA:575:GLU:O	1:AAA:577:GLN:N	2.29	0.65
3:MMM:263:VAL:O	3:MMM:265:LEU:HD12	1.96	0.65
3:MMM:69:THR:OG1	3:MMM:71:GLN:NE2	2.29	0.65
1:AAA:212:THR:OG1	1:AAA:264:LEU:HD13	1.96	0.65
1:AAA:535:VAL:HG12	1:AAA:576:LEU:HG	1.78	0.65
2:BBB:388:ALA:O	2:BBB:392:VAL:HG23	1.97	0.65
2:BBB:325:PHE:CD1	2:BBB:357:GLU:HG2	2.32	0.65
2:BBB:418:PHE:CE2	2:BBB:429:ILE:HD11	2.31	0.65
2:BBB:151:ILE:O	2:BBB:153:ALA:N	2.30	0.64
3:MMM:400:ASN:HA	3:MMM:439:SER:OG	1.97	0.64
4:SSS:14:THR:HG21	4:SSS:32:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:554:LEU:HD23	2:BBB:555:ILE:H	1.63	0.64
2:BBB:322:LYS:HA	2:BBB:325:PHE:CD2	2.33	0.64
1:AAA:514:ASP:OD1	1:AAA:515:PRO:HD2	1.98	0.64
3:MMM:182:ASN:HB2	3:MMM:195:HIS:CE1	2.33	0.64
1:AAA:157:ALA:HB2	1:AAA:195:LEU:HD21	1.79	0.63
2:BBB:477:SER:C	2:BBB:479:GLN:N	2.55	0.63
1:AAA:218:ASN:HD22	1:AAA:221:GLU:CD	2.06	0.63
2:BBB:165:LEU:CD2	2:BBB:184:LEU:HD13	2.26	0.63
1:AAA:187:ASP:O	1:AAA:191:ARG:NH2	2.32	0.63
3:MMM:318:ILE:HD11	3:MMM:333:VAL:HG21	1.80	0.63
4:SSS:114:VAL:HG12	4:SSS:115:ASP:N	2.13	0.63
2:BBB:482:LEU:HD21	2:BBB:519:LEU:HB2	1.80	0.63
2:BBB:249:SER:O	2:BBB:250:HIS:ND1	2.32	0.62
2:BBB:245:THR:N	2:BBB:246:PRO:HD2	2.14	0.62
2:BBB:285:ALA:HB3	2:BBB:286:PRO:HD3	1.82	0.62
3:MMM:328:ALA:HB2	3:MMM:403:VAL:HG12	1.82	0.62
2:BBB:351:ILE:HG12	2:BBB:384:VAL:HG11	1.81	0.62
2:BBB:414:ILE:CD1	2:BBB:432:LEU:HD22	2.30	0.62
1:AAA:585:ARG:HB2	2:BBB:540:VAL:HG22	1.81	0.62
2:BBB:436:LEU:HD21	2:BBB:439:LEU:HB2	1.82	0.62
3:MMM:162:ARG:HG2	3:MMM:209:MET:HE1	1.80	0.61
1:AAA:433:GLU:HB3	1:AAA:442:TYR:CE1	2.35	0.61
2:BBB:297:GLU:HB2	3:MMM:83:TYR:OH	2.00	0.61
2:BBB:474:HIS:O	2:BBB:475:ASP:HB2	2.00	0.61
1:AAA:333:GLN:O	1:AAA:333:GLN:NE2	2.34	0.61
2:BBB:240:ILE:HG21	2:BBB:266:PHE:HE2	1.66	0.61
2:BBB:250:HIS:O	2:BBB:251:ALA:C	2.44	0.61
1:AAA:569:LEU:O	1:AAA:577:GLN:NE2	2.34	0.60
1:AAA:478:TYR:CZ	1:AAA:482:THR:HG21	2.36	0.60
2:BBB:74:MET:HE2	2:BBB:109:THR:HG23	1.83	0.60
2:BBB:124:GLU:HB3	2:BBB:125:PRO:HD3	1.81	0.60
1:AAA:96:LEU:HD21	4:SSS:111:TYR:CG	2.36	0.60
2:BBB:439:LEU:HD21	2:BBB:445:ARG:HA	1.83	0.60
1:AAA:413:LEU:HD23	1:AAA:452:ILE:CG2	2.32	0.60
2:BBB:52:PRO:HD3	2:BBB:83:MET:HE1	1.84	0.60
3:MMM:298:PHE:CD2	3:MMM:399:MET:HE1	2.37	0.59
4:SSS:49:PHE:HA	4:SSS:57:ILE:O	2.01	0.59
3:MMM:328:ALA:CB	3:MMM:403:VAL:HG12	2.32	0.59
1:AAA:215:ALA:HB2	1:AAA:222:PHE:CZ	2.37	0.59
2:BBB:289:VAL:O	2:BBB:292:LEU:HD22	2.02	0.59
2:BBB:110:MET:HG2	2:BBB:122:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:541:VAL:HG12	2:BBB:542:LEU:HD23	1.85	0.58
2:BBB:34:VAL:O	2:BBB:37:VAL:N	2.37	0.58
2:BBB:68:LEU:HD21	3:MMM:106:VAL:HG22	1.85	0.58
1:AAA:153:LYS:O	1:AAA:156:VAL:HG22	2.03	0.58
1:AAA:230:VAL:HG13	1:AAA:283:CYS:SG	2.44	0.58
2:BBB:580:ALA:C	2:BBB:581:PHE:CD1	2.82	0.58
2:BBB:373:ALA:O	2:BBB:376:ALA:HB3	2.04	0.57
2:BBB:504:GLN:OE1	5:GGG:385:THR:N	2.37	0.57
2:BBB:246:PRO:O	2:BBB:248:LEU:HD23	2.05	0.57
1:AAA:64:PHE:HD1	4:SSS:107:PHE:CG	2.22	0.57
2:BBB:418:PHE:CZ	2:BBB:429:ILE:HD11	2.40	0.57
3:MMM:337:THR:HG21	3:MMM:355:TYR:CE1	2.40	0.57
1:AAA:546:ILE:HD12	1:AAA:583:TYR:HA	1.87	0.57
2:BBB:44:GLY:HA3	4:SSS:41:VAL:HG23	1.86	0.57
1:AAA:88:TYR:CD2	1:AAA:89:THR:HG23	2.40	0.56
2:BBB:433:CYS:O	5:GGG:359:ILE:HG21	2.05	0.56
2:BBB:505:GLN:O	2:BBB:506:VAL:C	2.49	0.56
1:AAA:374:ILE:O	1:AAA:377:LEU:HB3	2.05	0.56
1:AAA:473:ASP:OD1	1:AAA:473:ASP:N	2.38	0.56
2:BBB:423:ASN:OD1	2:BBB:426:GLU:HB3	2.05	0.56
1:AAA:450:ILE:HG12	1:AAA:457:VAL:HG21	1.85	0.56
2:BBB:473:PHE:CZ	2:BBB:481:GLN:HG2	2.40	0.56
4:SSS:36:HIS:CE1	4:SSS:40:THR:HG21	2.41	0.56
1:AAA:478:TYR:O	1:AAA:482:THR:OG1	2.23	0.56
2:BBB:55:VAL:HG13	2:BBB:58:MET:HE3	1.87	0.56
1:AAA:301:GLN:HG2	4:SSS:85:HIS:NE2	2.20	0.56
4:SSS:99:CYS:SG	4:SSS:101:LEU:N	2.78	0.56
1:AAA:402:ALA:O	1:AAA:405:ILE:N	2.39	0.56
3:MMM:92:TYR:O	3:MMM:135:GLN:NE2	2.38	0.56
1:AAA:379:THR:O	1:AAA:381:ARG:N	2.39	0.56
1:AAA:120:LEU:HD22	1:AAA:132:LEU:HG	1.88	0.56
3:MMM:279:PRO:HD2	3:MMM:283:PHE:CE2	2.41	0.56
1:AAA:535:VAL:HG23	1:AAA:536:PRO:CD	2.36	0.56
2:BBB:145:VAL:HG12	2:BBB:187:ILE:HD11	1.88	0.55
1:AAA:85:SER:OG	1:AAA:86:ASN:N	2.38	0.55
1:AAA:535:VAL:HG23	1:AAA:536:PRO:HD3	1.88	0.55
2:BBB:270:LEU:O	2:BBB:271:PRO:C	2.49	0.55
1:AAA:382:ASP:O	1:AAA:384:SER:N	2.39	0.55
3:MMM:165:GLY:O	3:MMM:166:ILE:C	2.50	0.55
2:BBB:249:SER:HB3	3:MMM:259:PHE:N	2.11	0.55
2:BBB:250:HIS:C	2:BBB:252:ASN:N	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:353:MET:HE2	1:AAA:366:VAL:HG13	1.90	0.54
4:SSS:6:LEU:HD13	4:SSS:8:GLN:NE2	2.18	0.54
1:AAA:590:ALA:O	1:AAA:591:SER:O	2.26	0.54
1:AAA:269:PRO:HB3	1:AAA:270:PRO:HD2	1.88	0.54
2:BBB:522:ARG:NH2	2:BBB:526:TYR:OH	2.41	0.54
3:MMM:32:PHE:CZ	3:MMM:36:VAL:HG11	2.42	0.54
1:AAA:579:ARG:CZ	2:BBB:522:ARG:HD2	2.38	0.54
2:BBB:79:SER:O	2:BBB:80:GLN:HG2	2.07	0.54
1:AAA:591:SER:HB2	1:AAA:594:ILE:HG22	1.88	0.54
3:MMM:188:GLN:HB3	3:MMM:190:GLN:HE21	1.72	0.54
3:MMM:344:VAL:HG23	3:MMM:344:VAL:O	2.08	0.54
2:BBB:114:ARG:NH2	2:BBB:150:ASP:O	2.41	0.54
1:AAA:191:ARG:O	1:AAA:194:HIS:HB3	2.09	0.53
2:BBB:556:GLU:OE1	2:BBB:559:LEU:N	2.40	0.53
3:MMM:105:PHE:HD1	3:MMM:106:VAL:N	2.05	0.53
4:SSS:62:TYR:CE2	4:SSS:88:VAL:HG21	2.43	0.53
2:BBB:473:PHE:O	2:BBB:474:HIS:C	2.51	0.53
1:AAA:344:ASN:OD1	4:SSS:47:THR:HA	2.08	0.53
2:BBB:433:CYS:HB3	5:GGG:359:ILE:CG1	2.39	0.53
2:BBB:505:GLN:O	2:BBB:508:SER:HB3	2.08	0.53
3:MMM:217:ASN:OD1	3:MMM:217:ASN:N	2.41	0.53
3:MMM:263:VAL:HA	3:MMM:276:PHE:HB3	1.89	0.53
2:BBB:511:THR:HG22	2:BBB:512:GLN:HE21	1.73	0.53
3:MMM:6:PHE:CD2	3:MMM:29:VAL:HG22	2.43	0.53
4:SSS:106:ASN:N	4:SSS:106:ASN:HD22	2.06	0.53
2:BBB:430:ALA:HB2	5:GGG:361:PRO:HB3	1.90	0.53
1:AAA:104:SER:O	1:AAA:105:ASN:ND2	2.42	0.53
1:AAA:382:ASP:OD1	1:AAA:382:ASP:N	2.41	0.53
3:MMM:208:GLY:O	3:MMM:209:MET:HE2	2.08	0.53
2:BBB:97:ASP:O	2:BBB:103:ARG:NE	2.39	0.53
2:BBB:249:SER:HB2	3:MMM:265:LEU:HD21	1.91	0.53
4:SSS:30:LYS:O	4:SSS:34:GLU:HB2	2.09	0.53
3:MMM:164:GLU:HA	3:MMM:209:MET:HE3	1.91	0.52
1:AAA:281:THR:HG23	1:AAA:326:LEU:HD11	1.90	0.52
1:AAA:506:GLU:OE2	1:AAA:602:MET:CB	2.57	0.52
3:MMM:179:GLU:OE2	3:MMM:288:TYR:OH	2.18	0.52
2:BBB:30:ARG:O	2:BBB:33:ALA:HB3	2.10	0.52
4:SSS:104:VAL:O	4:SSS:107:PHE:HB3	2.09	0.52
2:BBB:94:ASP:HB3	2:BBB:106:ALA:HB2	1.91	0.52
2:BBB:55:VAL:HG11	2:BBB:86:MET:HB3	1.90	0.52
4:SSS:114:VAL:O	4:SSS:116:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:248:LEU:HG	2:BBB:249:SER:OG	2.10	0.52
2:BBB:511:THR:CG2	2:BBB:512:GLN:HE21	2.23	0.52
3:MMM:85:MET:O	3:MMM:88:VAL:HB	2.10	0.52
4:SSS:95:PHE:CZ	4:SSS:110:VAL:HG22	2.45	0.52
5:GGG:377:LEU:HD22	5:GGG:381:ILE:HD11	1.92	0.52
3:MMM:27:ASN:OD1	3:MMM:27:ASN:N	2.43	0.52
3:MMM:403:VAL:HG21	3:MMM:405:PHE:CZ	2.45	0.52
1:AAA:483:VAL:HG12	1:AAA:484:PHE:N	2.26	0.51
1:AAA:560:GLN:OE1	1:AAA:587:SER:OG	2.28	0.51
1:AAA:579:ARG:NH2	2:BBB:482:LEU:HD13	2.26	0.51
2:BBB:529:LEU:HD23	2:BBB:537:ALA:HA	1.92	0.51
3:MMM:268:PHE:CD1	3:MMM:268:PHE:C	2.88	0.51
3:MMM:333:VAL:HG22	3:MMM:399:MET:HG2	1.93	0.51
2:BBB:151:ILE:O	2:BBB:152:ASN:C	2.53	0.51
2:BBB:430:ALA:HB2	5:GGG:361:PRO:CB	2.40	0.51
2:BBB:431:THR:O	2:BBB:434:GLU:HG2	2.11	0.51
2:BBB:582:VAL:H	3:MMM:52:ARG:HB3	1.75	0.51
1:AAA:96:LEU:HD11	4:SSS:111:TYR:HB3	1.92	0.51
3:MMM:59:LYS:O	3:MMM:60:ARG:HD3	2.10	0.51
5:GGG:366:ASN:O	5:GGG:367:SER:CB	2.58	0.51
1:AAA:433:GLU:OE1	1:AAA:464:ARG:NH1	2.44	0.51
2:BBB:436:LEU:O	2:BBB:437:ASP:HB3	2.11	0.51
1:AAA:420:ILE:O	1:AAA:422:GLU:N	2.44	0.51
1:AAA:481:LYS:HB2	1:AAA:511:ILE:HD11	1.93	0.51
2:BBB:195:ASN:O	2:BBB:197:LEU:N	2.44	0.51
3:MMM:173:LEU:C	3:MMM:173:LEU:HD12	2.35	0.51
4:SSS:98:VAL:HG13	3:CCC:241:LEU:HD12	1.93	0.51
1:AAA:71:ASP:HB3	1:AAA:73:ASP:OD1	2.11	0.51
2:BBB:392:VAL:CG1	2:BBB:428:ILE:HD11	2.41	0.51
2:BBB:408:GLN:NE2	2:BBB:440:ASP:OD1	2.44	0.51
3:MMM:6:PHE:CE2	3:MMM:29:VAL:CG2	2.94	0.51
3:MMM:6:PHE:CZ	3:MMM:29:VAL:HG22	2.46	0.51
3:MMM:356:LYS:O	3:MMM:359:GLU:HB2	2.11	0.51
2:BBB:18:LEU:O	2:BBB:21:GLU:N	2.43	0.51
2:BBB:574:TYR:CZ	3:MMM:49:ASN:HB2	2.46	0.51
2:BBB:578:PRO:O	2:BBB:580:ALA:N	2.44	0.51
2:BBB:152:ASN:CG	2:BBB:155:MET:HG3	2.36	0.50
4:SSS:49:PHE:O	4:SSS:50:VAL:HB	2.11	0.50
1:AAA:333:GLN:HE21	1:AAA:333:GLN:C	2.20	0.50
1:AAA:349:ALA:O	1:AAA:353:MET:HB2	2.11	0.50
3:MMM:406:ALA:HB2	3:MMM:435:TYR:CD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:165:LEU:O	2:BBB:166:ARG:C	2.54	0.50
5:GGG:366:ASN:O	5:GGG:367:SER:OG	2.29	0.50
1:AAA:564:ARG:HG2	1:AAA:584:LEU:HD11	1.94	0.50
2:BBB:533:ASP:OD1	2:BBB:533:ASP:C	2.53	0.50
3:MMM:81:PHE:CE2	3:MMM:116:LEU:HD13	2.46	0.50
3:MMM:419:GLU:HG3	3:MMM:422:LEU:O	2.12	0.50
4:SSS:76:ASN:HB3	4:SSS:79:ALA:HB3	1.94	0.50
1:AAA:79:ALA:HA	1:AAA:82:LEU:HD13	1.94	0.50
2:BBB:371:ARG:O	2:BBB:372:LYS:C	2.54	0.50
1:AAA:333:GLN:NE2	1:AAA:337:PHE:CE2	2.80	0.50
2:BBB:550:GLU:O	2:BBB:550:GLU:HG3	2.12	0.50
3:MMM:6:PHE:CZ	3:MMM:29:VAL:CG2	2.95	0.50
2:BBB:225:CYS:O	2:BBB:228:ASN:HB2	2.12	0.49
3:MMM:171:ASN:N	3:MMM:171:ASN:HD22	2.09	0.49
1:AAA:72:ILE:HG22	1:AAA:72:ILE:O	2.11	0.49
3:MMM:181:VAL:O	3:MMM:439:SER:O	2.30	0.49
2:BBB:524:TYR:O	2:BBB:527:TRP:N	2.44	0.49
2:BBB:154:GLN:O	2:BBB:155:MET:O	2.30	0.49
4:SSS:90:VAL:HG11	4:SSS:131:VAL:HG11	1.94	0.49
1:AAA:610:SER:O	1:AAA:610:SER:OG	2.20	0.49
3:MMM:181:VAL:N	3:MMM:439:SER:O	2.45	0.49
2:BBB:170:ALA:O	2:BBB:171:ASP:C	2.55	0.49
2:BBB:280:LEU:O	2:BBB:284:LEU:HD13	2.12	0.49
1:AAA:370:ILE:HG23	1:AAA:371:GLU:N	2.26	0.49
2:BBB:196:LEU:HD11	2:BBB:228:ASN:HD22	1.78	0.49
2:BBB:155:MET:O	2:BBB:159:GLN:N	2.46	0.49
3:MMM:419:GLU:HB3	3:MMM:424:TYR:CE1	2.47	0.49
2:BBB:208:LEU:O	2:BBB:211:LEU:HB3	2.12	0.48
3:MMM:105:PHE:CD1	3:MMM:105:PHE:C	2.91	0.48
3:MMM:349:MET:O	3:MMM:350:LYS:HB2	2.13	0.48
4:SSS:72:ASP:HB2	4:SSS:75:ASP:OD2	2.13	0.48
4:SSS:82:GLU:O	4:SSS:85:HIS:N	2.46	0.48
1:AAA:290:LYS:CE	1:AAA:290:LYS:HA	2.43	0.48
1:AAA:353:MET:CE	1:AAA:366:VAL:HG13	2.42	0.48
1:AAA:157:ALA:HB2	1:AAA:195:LEU:CD2	2.41	0.48
2:BBB:267:LEU:HD11	2:BBB:280:LEU:HD23	1.95	0.48
3:MMM:81:PHE:CZ	3:MMM:116:LEU:HD22	2.49	0.48
3:MMM:206:LEU:HD22	3:MMM:417:VAL:HG11	1.96	0.48
3:MMM:210:PRO:HB3	3:MMM:424:TYR:OH	2.13	0.48
3:MMM:298:PHE:CZ	3:MMM:331:ILE:HD13	2.48	0.48
4:SSS:31:LEU:O	4:SSS:35:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:253:SER:O	2:BBB:254:ALA:C	2.56	0.48
1:AAA:577:GLN:O	1:AAA:578:GLN:C	2.56	0.48
2:BBB:155:MET:O	2:BBB:158:ASP:N	2.47	0.48
2:BBB:155:MET:O	2:BBB:158:ASP:CA	2.61	0.48
2:BBB:244:VAL:C	2:BBB:246:PRO:HD2	2.38	0.48
3:MMM:78:VAL:O	3:MMM:81:PHE:N	2.46	0.48
2:BBB:430:ALA:CA	5:GGG:361:PRO:HB3	2.44	0.48
2:BBB:430:ALA:HA	5:GGG:361:PRO:HB3	1.96	0.48
3:MMM:152:THR:O	3:MMM:156:THR:HG22	2.14	0.48
2:BBB:526:TYR:HE1	2:BBB:541:VAL:HG22	1.78	0.48
3:MMM:182:ASN:CB	3:MMM:195:HIS:CE1	2.96	0.48
4:SSS:34:GLU:OE1	4:SSS:52:PHE:CE2	2.67	0.48
2:BBB:114:ARG:NE	2:BBB:151:ILE:HG23	2.29	0.47
3:MMM:431:LYS:O	3:MMM:432:TRP:CG	2.67	0.47
1:AAA:475:VAL:O	1:AAA:476:GLN:C	2.57	0.47
1:AAA:603:PRO:HG2	2:BBB:524:TYR:CZ	2.48	0.47
2:BBB:195:ASN:C	2:BBB:197:LEU:HD22	2.39	0.47
1:AAA:175:LEU:O	1:AAA:179:SER:N	2.44	0.47
1:AAA:188:TRP:O	1:AAA:192:VAL:HG23	2.14	0.47
2:BBB:44:GLY:O	2:BBB:45:LYS:C	2.57	0.47
4:SSS:14:THR:HG21	4:SSS:32:ILE:CD1	2.43	0.47
1:AAA:453:ALA:HB1	1:AAA:456:TYR:HB2	1.97	0.47
2:BBB:396:LEU:HD23	2:BBB:431:THR:HG21	1.96	0.47
4:SSS:102:ASP:C	4:SSS:104:VAL:H	2.21	0.47
3:MMM:201:VAL:HG12	3:MMM:201:VAL:O	2.14	0.47
1:AAA:88:TYR:OH	4:SSS:138:LEU:HD13	2.15	0.47
1:AAA:486:ALA:CB	1:AAA:496:LEU:HD21	2.42	0.47
1:AAA:573:ASP:OD1	1:AAA:573:ASP:C	2.57	0.47
2:BBB:154:GLN:O	2:BBB:155:MET:C	2.57	0.47
1:AAA:173:LEU:HD11	1:AAA:213:THR:HG21	1.96	0.47
2:BBB:139:LYS:HE2	3:MMM:122:GLN:HE21	1.80	0.47
2:BBB:142:ALA:HB2	2:BBB:168:LEU:HD13	1.95	0.47
2:BBB:173:ASN:ND2	3:MMM:156:THR:OG1	2.47	0.47
2:BBB:396:LEU:CD2	2:BBB:431:THR:HG21	2.45	0.47
2:BBB:511:THR:HG22	2:BBB:512:GLN:HG2	1.96	0.47
4:SSS:97:ASN:ND2	3:CCC:242:ILE:HD13	2.30	0.47
2:BBB:488:ILE:HD12	2:BBB:506:VAL:HG21	1.97	0.47
1:AAA:155:LEU:O	1:AAA:156:VAL:C	2.57	0.47
1:AAA:519:PRO:HB3	1:AAA:552:PHE:CD2	2.50	0.47
2:BBB:488:ILE:CD1	2:BBB:506:VAL:HG21	2.45	0.47
3:MMM:89:MET:HB3	3:MMM:93:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:MMM:172:GLU:HG3	3:MMM:430:ILE:HB	1.97	0.47
3:MMM:182:ASN:OD1	3:MMM:441:ILE:N	2.37	0.47
2:BBB:555:ILE:HG21	2:BBB:560:LEU:HD12	1.96	0.47
2:BBB:581:PHE:CD1	2:BBB:581:PHE:N	2.82	0.47
3:MMM:78:VAL:O	3:MMM:79:PHE:C	2.58	0.47
3:MMM:432:TRP:CZ2	5:DDD:333:ASP:HB2	2.49	0.47
3:MMM:433:VAL:HG23	6:PPP:5:LEU:CD2	2.32	0.47
4:SSS:12:GLY:HA2	4:SSS:36:HIS:CE1	2.50	0.47
4:SSS:90:VAL:HG23	4:SSS:128:GLN:HG2	1.97	0.47
1:AAA:212:THR:O	1:AAA:216:GLN:N	2.48	0.46
1:AAA:353:MET:HE3	1:AAA:366:VAL:HG22	1.97	0.46
2:BBB:94:ASP:C	2:BBB:96:GLU:H	2.22	0.46
2:BBB:270:LEU:HG	2:BBB:271:PRO:HD2	1.96	0.46
2:BBB:370:VAL:O	2:BBB:373:ALA:HB3	2.15	0.46
2:BBB:473:PHE:CE1	2:BBB:481:GLN:HG2	2.49	0.46
3:MMM:105:PHE:CE1	3:MMM:106:VAL:HG23	2.50	0.46
1:AAA:96:LEU:HD21	4:SSS:111:TYR:CB	2.46	0.46
2:BBB:46:ASP:C	2:BBB:48:SER:H	2.23	0.46
2:BBB:191:HIS:HA	2:BBB:195:ASN:CG	2.40	0.46
1:AAA:549:VAL:HG23	1:AAA:559:ILE:HG21	1.98	0.46
2:BBB:319:GLN:O	2:BBB:320:GLU:C	2.59	0.46
3:MMM:217:ASN:OD1	3:MMM:411:LYS:O	2.34	0.46
2:BBB:303:LEU:HD11	2:BBB:334:VAL:HG13	1.98	0.46
2:BBB:348:GLN:OE1	2:BBB:384:VAL:HG13	2.16	0.46
2:BBB:407:VAL:HG11	2:BBB:436:LEU:HA	1.97	0.46
2:BBB:418:PHE:O	2:BBB:422:PRO:HA	2.16	0.46
2:BBB:454:GLU:OE1	2:BBB:454:GLU:HA	2.15	0.46
1:AAA:109:ILE:O	1:AAA:113:ASN:ND2	2.48	0.46
1:AAA:370:ILE:O	1:AAA:373:VAL:N	2.47	0.46
1:AAA:575:GLU:C	1:AAA:577:GLN:N	2.74	0.46
2:BBB:116:ASP:OD1	2:BBB:116:ASP:N	2.48	0.46
4:SSS:74:ASN:OD1	4:SSS:74:ASN:N	2.33	0.46
2:BBB:361:TYR:HB3	2:BBB:369:PHE:CE2	2.50	0.46
3:MMM:42:GLN:HA	3:MMM:44:ARG:NH2	2.31	0.46
3:MMM:433:VAL:HG21	6:PPP:5:LEU:HD13	1.97	0.46
1:AAA:290:LYS:HA	1:AAA:290:LYS:HE2	1.98	0.46
2:BBB:18:LEU:O	2:BBB:19:LYS:C	2.58	0.46
2:BBB:393:SER:O	2:BBB:396:LEU:HB2	2.15	0.46
2:BBB:430:ALA:CB	5:GGG:361:PRO:HB3	2.46	0.46
3:MMM:295:ILE:O	3:MMM:295:ILE:HG22	2.15	0.46
1:AAA:209:SER:OG	1:AAA:260:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:89:ASN:O	2:BBB:93:LYS:HB2	2.16	0.46
3:MMM:432:TRP:CH2	5:DDD:333:ASP:HB2	2.51	0.46
1:AAA:216:GLN:HA	1:AAA:267:CYS:SG	2.56	0.45
1:AAA:333:GLN:NE2	1:AAA:333:GLN:C	2.74	0.45
1:AAA:338:LEU:O	1:AAA:346:ARG:HG2	2.17	0.45
2:BBB:514:SER:OG	2:BBB:519:LEU:HD21	2.15	0.45
3:MMM:46:PRO:HB2	3:MMM:79:PHE:CZ	2.51	0.45
3:MMM:115:ILE:CG1	3:MMM:124:SER:HA	2.46	0.45
1:AAA:430:ILE:HD13	1:AAA:613:LEU:HD23	1.98	0.45
1:AAA:88:TYR:CZ	4:SSS:138:LEU:HD22	2.51	0.45
3:MMM:88:VAL:HG21	3:MMM:115:ILE:HD11	1.98	0.45
4:SSS:114:VAL:O	4:SSS:117:MET:N	2.49	0.45
1:AAA:120:LEU:CD2	1:AAA:132:LEU:HG	2.46	0.45
3:MMM:279:PRO:HD2	3:MMM:283:PHE:CZ	2.52	0.45
1:AAA:310:LEU:O	1:AAA:314:ILE:HG13	2.15	0.45
3:MMM:92:TYR:HD2	3:MMM:107:LEU:HD21	1.81	0.45
1:AAA:88:TYR:CZ	4:SSS:138:LEU:HB3	2.51	0.45
1:AAA:156:VAL:HG23	1:AAA:156:VAL:O	2.17	0.45
3:MMM:411:LYS:HA	3:MMM:435:TYR:OH	2.15	0.45
1:AAA:211:ILE:O	1:AAA:215:ALA:HB3	2.16	0.45
1:AAA:324:PRO:HA	1:AAA:327:LEU:HB2	1.98	0.45
1:AAA:575:GLU:O	1:AAA:576:LEU:C	2.60	0.45
2:BBB:130:LEU:HG	2:BBB:141:ALA:HB1	1.99	0.45
1:AAA:462:TRP:CZ2	1:AAA:463:TYR:HE1	2.35	0.45
2:BBB:569:SER:O	2:BBB:572:SER:OG	2.33	0.45
2:BBB:577:PRO:O	2:BBB:578:PRO:C	2.60	0.45
1:AAA:270:PRO:HG3	1:AAA:320:HIS:CG	2.52	0.45
2:BBB:256:VAL:HG11	2:BBB:291:LEU:HD21	1.98	0.45
1:AAA:307:ASN:ND2	1:AAA:310:LEU:HD23	2.32	0.45
1:AAA:574:VAL:HG12	1:AAA:575:GLU:N	2.31	0.45
2:BBB:259:ALA:O	2:BBB:263:LEU:HG	2.17	0.45
2:BBB:414:ILE:HD13	2:BBB:432:LEU:CD2	2.40	0.44
1:AAA:325:ASN:O	1:AAA:329:ARG:HD2	2.17	0.44
1:AAA:387:GLN:OE1	1:AAA:388:ARG:N	2.50	0.44
1:AAA:438:ASP:OD1	1:AAA:438:ASP:C	2.61	0.44
2:BBB:155:MET:O	2:BBB:158:ASP:CB	2.64	0.44
2:BBB:582:VAL:HB	3:MMM:52:ARG:HD3	1.99	0.44
1:AAA:88:TYR:CD1	4:SSS:138:LEU:HD22	2.52	0.44
1:AAA:136:ALA:HA	1:AAA:174:ARG:HG2	1.98	0.44
1:AAA:475:VAL:O	1:AAA:478:TYR:N	2.49	0.44
2:BBB:155:MET:O	2:BBB:158:ASP:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:535:VAL:O	2:BBB:539:GLU:HG2	2.18	0.44
3:MMM:426:ASP:O	3:MMM:429:VAL:N	2.38	0.44
4:SSS:4:PHE:CZ	4:SSS:70:CYS:HB2	2.52	0.44
1:AAA:80:VAL:HG12	1:AAA:80:VAL:O	2.17	0.44
1:AAA:233:LEU:HG	1:AAA:234:SER:N	2.32	0.44
1:AAA:520:LEU:HD13	1:AAA:524:ASN:HD22	1.82	0.44
2:BBB:251:ALA:C	2:BBB:253:SER:N	2.76	0.44
2:BBB:484:LEU:O	2:BBB:485:LEU:C	2.60	0.44
1:AAA:247:TYR:HB2	1:AAA:254:ALA:HB2	1.99	0.44
3:MMM:177:VAL:HG11	3:MMM:410:LEU:HD23	1.99	0.44
3:MMM:204:SER:O	3:MMM:204:SER:OG	2.35	0.44
4:SSS:69:ILE:HG22	4:SSS:71:VAL:HG13	1.99	0.44
1:AAA:33:ILE:O	1:AAA:37:LEU:HG	2.17	0.44
1:AAA:466:ILE:O	1:AAA:467:GLN:C	2.61	0.44
2:BBB:191:HIS:N	2:BBB:192:PRO:HD3	2.32	0.44
2:BBB:220:ILE:O	2:BBB:224:ASP:HB2	2.17	0.44
3:MMM:37:ILE:HG23	3:MMM:64:TRP:CE2	2.53	0.44
3:MMM:274:ILE:O	3:MMM:274:ILE:HG22	2.18	0.44
2:BBB:59:GLN:HE22	2:BBB:90:SER:HB3	1.83	0.43
1:AAA:501:GLY:O	1:AAA:544:THR:OG1	2.24	0.43
2:BBB:449:ILE:HG13	2:BBB:469:PHE:CE2	2.53	0.43
3:MMM:108:ILE:O	3:MMM:109:TYR:C	2.61	0.43
4:SSS:106:ASN:HB3	4:SSS:109:LYS:HB2	2.00	0.43
1:AAA:605:PHE:CZ	2:BBB:520:ARG:HD3	2.53	0.43
2:BBB:304:ARG:HD2	2:BBB:337:GLU:CD	2.42	0.43
4:SSS:102:ASP:O	4:SSS:104:VAL:N	2.51	0.43
1:AAA:226:VAL:HG12	1:AAA:227:SER:N	2.33	0.43
1:AAA:590:ALA:O	1:AAA:591:SER:C	2.61	0.43
1:AAA:603:PRO:HD2	2:BBB:524:TYR:CE2	2.54	0.43
3:MMM:347:ILE:O	3:MMM:347:ILE:CG1	2.65	0.43
1:AAA:223:LYS:O	1:AAA:224:THR:C	2.62	0.43
2:BBB:563:LEU:O	2:BBB:566:HIS:N	2.52	0.43
3:MMM:32:PHE:CE1	3:MMM:36:VAL:HG11	2.53	0.43
3:MMM:259:PHE:HB3	3:MMM:263:VAL:CG1	2.49	0.43
2:BBB:267:LEU:CD1	2:BBB:280:LEU:HD23	2.48	0.43
2:BBB:343:ILE:HD11	2:BBB:376:ALA:HB1	2.01	0.43
3:MMM:105:PHE:CD1	3:MMM:106:VAL:N	2.87	0.43
1:AAA:328:VAL:O	1:AAA:332:ASN:ND2	2.52	0.43
2:BBB:145:VAL:HG11	2:BBB:165:LEU:HD22	2.00	0.43
1:AAA:318:ILE:HG21	1:AAA:355:THR:HG22	2.01	0.43
2:BBB:16:PHE:O	2:BBB:17:GLU:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:171:ASP:OD2	2:BBB:176:VAL:HG11	2.19	0.43
1:AAA:88:TYR:CE2	4:SSS:138:LEU:HB3	2.54	0.43
2:BBB:40:ALA:HB1	2:BBB:45:LYS:HD2	2.01	0.43
2:BBB:186:GLU:OE1	3:MMM:21:ARG:NH2	2.48	0.43
2:BBB:251:ALA:O	2:BBB:253:SER:C	2.62	0.43
3:MMM:168:TYR:CE2	5:DDD:324:SER:HB2	2.53	0.43
4:SSS:4:PHE:HB2	4:SSS:18:LYS:O	2.18	0.43
4:SSS:102:ASP:C	4:SSS:104:VAL:N	2.77	0.43
1:AAA:237:VAL:HG13	1:AAA:290:LYS:HE3	2.01	0.42
1:AAA:432:ALA:HA	1:AAA:441:TRP:CZ3	2.54	0.42
1:AAA:560:GLN:HG2	1:AAA:587:SER:OG	2.19	0.42
2:BBB:94:ASP:CB	2:BBB:106:ALA:HB2	2.49	0.42
2:BBB:331:PRO:O	2:BBB:332:ILE:C	2.62	0.42
2:BBB:418:PHE:HE2	2:BBB:429:ILE:HD11	1.82	0.42
3:MMM:154:GLN:HG3	3:MMM:155:VAL:N	2.34	0.42
4:SSS:34:GLU:O	4:SSS:37:ALA:N	2.52	0.42
2:BBB:204:ILE:HD11	2:BBB:229:TYR:CD1	2.54	0.42
2:BBB:392:VAL:CG1	2:BBB:428:ILE:CD1	2.97	0.42
3:MMM:336:PRO:HA	3:MMM:361:ALA:HA	2.01	0.42
4:SSS:56:LYS:NZ	4:SSS:75:ASP:O	2.49	0.42
1:AAA:55:LYS:HB3	1:AAA:82:LEU:HD11	2.01	0.42
2:BBB:114:ARG:HG3	2:BBB:151:ILE:HD12	2.00	0.42
2:BBB:560:LEU:O	2:BBB:563:LEU:N	2.52	0.42
4:SSS:4:PHE:CE2	4:SSS:70:CYS:CB	3.03	0.42
1:AAA:520:LEU:HD23	1:AAA:555:VAL:HG23	2.00	0.42
1:AAA:549:VAL:O	1:AAA:549:VAL:CG1	2.67	0.42
2:BBB:205:ASN:OD1	2:BBB:243:ARG:NH2	2.52	0.42
4:SSS:2:ILE:HD11	4:SSS:80:TYR:HE1	1.85	0.42
4:SSS:40:THR:HG22	4:SSS:66:TYR:CE2	2.54	0.42
4:SSS:137:MET:HE3	4:SSS:137:MET:HA	2.01	0.42
2:BBB:371:ARG:O	2:BBB:373:ALA:N	2.52	0.42
4:SSS:87:PHE:HA	4:SSS:117:MET:SD	2.60	0.42
1:AAA:407:ALA:HA	1:AAA:410:LEU:HD12	2.00	0.42
1:AAA:467:GLN:HA	1:AAA:605:PHE:CD2	2.55	0.42
2:BBB:151:ILE:C	2:BBB:153:ALA:N	2.78	0.42
2:BBB:174:PRO:HA	2:BBB:177:VAL:CG1	2.50	0.42
3:MMM:32:PHE:O	3:MMM:36:VAL:N	2.47	0.42
1:AAA:64:PHE:HD1	4:SSS:107:PHE:CD1	2.37	0.42
2:BBB:347:SER:O	2:BBB:351:ILE:HG13	2.18	0.42
1:AAA:17:ILE:HG22	1:AAA:64:PHE:CE2	2.55	0.42
2:BBB:325:PHE:HD1	2:BBB:357:GLU:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:MMM:9:ASN:C	3:MMM:11:LYS:H	2.28	0.42
3:MMM:108:ILE:O	3:MMM:111:LEU:N	2.53	0.42
1:AAA:192:VAL:O	1:AAA:195:LEU:HB2	2.20	0.42
2:BBB:251:ALA:O	2:BBB:254:ALA:N	2.53	0.42
2:BBB:527:TRP:O	2:BBB:531:SER:HB2	2.19	0.42
3:MMM:297:PRO:C	3:MMM:298:PHE:CD1	2.98	0.42
3:MMM:340:ASN:O	3:MMM:383:LEU:HA	2.20	0.42
3:MMM:400:ASN:OD1	3:MMM:400:ASN:N	2.53	0.42
1:AAA:513:GLY:O	1:AAA:514:ASP:C	2.63	0.41
2:BBB:307:ASN:HD22	2:BBB:341:ILE:HG13	1.84	0.41
2:BBB:332:ILE:HG23	2:BBB:333:TYR:N	2.35	0.41
2:BBB:580:ALA:O	2:BBB:581:PHE:HD1	2.03	0.41
1:AAA:598:VAL:HG21	2:BBB:529:LEU:CD1	2.39	0.41
2:BBB:482:LEU:CD2	2:BBB:519:LEU:HB2	2.48	0.41
4:SSS:56:LYS:HE2	4:SSS:71:VAL:HG23	2.01	0.41
1:AAA:470:ILE:HG22	1:AAA:507:PHE:CZ	2.55	0.41
1:AAA:506:GLU:HB3	1:AAA:507:PHE:CE2	2.55	0.41
2:BBB:516:ASN:O	2:BBB:517:PRO:C	2.61	0.41
1:AAA:95:TYR:HB2	1:AAA:130:LEU:HD22	2.01	0.41
1:AAA:211:ILE:HG23	1:AAA:222:PHE:CD2	2.55	0.41
1:AAA:268:TYR:O	1:AAA:269:PRO:O	2.38	0.41
1:AAA:519:PRO:HB3	1:AAA:552:PHE:CG	2.55	0.41
2:BBB:52:PRO:CD	2:BBB:83:MET:HE1	2.49	0.41
4:SSS:35:VAL:HG22	4:SSS:57:ILE:HD11	2.02	0.41
1:AAA:141:ARG:HH21	1:AAA:182:LEU:HD11	1.86	0.41
2:BBB:108:ARG:NH1	3:MMM:113:ASP:OD2	2.52	0.41
1:AAA:470:ILE:HG13	1:AAA:470:ILE:O	2.21	0.41
1:AAA:579:ARG:O	1:AAA:580:ALA:C	2.63	0.41
3:MMM:81:PHE:CD1	3:MMM:81:PHE:C	2.98	0.41
4:SSS:5:ILE:HG12	4:SSS:69:ILE:HG23	2.02	0.41
4:SSS:48:ASN:HD22	4:SSS:48:ASN:HA	1.65	0.41
1:AAA:249:TYR:OH	1:AAA:301:GLN:HB3	2.21	0.41
2:BBB:158:ASP:O	2:BBB:158:ASP:CG	2.63	0.41
3:MMM:163:ARG:HD3	3:MMM:166:ILE:HD12	2.03	0.41
3:MMM:173:LEU:HD11	3:MMM:415:LEU:HD23	2.02	0.41
3:MMM:215:GLY:HA3	3:MMM:414:TYR:CE1	2.55	0.41
5:GGG:381:ILE:O	5:GGG:382:GLY:C	2.63	0.41
1:AAA:152:PRO:HB3	1:AAA:188:TRP:CD1	2.56	0.41
1:AAA:215:ALA:HB2	1:AAA:222:PHE:CE1	2.55	0.41
1:AAA:301:GLN:HG2	4:SSS:85:HIS:CD2	2.56	0.41
1:AAA:305:ALA:HA	1:AAA:308:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:356:LEU:O	1:AAA:358:SER:N	2.54	0.41
1:AAA:449:LEU:HD12	1:AAA:449:LEU:HA	1.84	0.41
1:AAA:470:ILE:HG22	1:AAA:507:PHE:CE2	2.55	0.41
1:AAA:518:SER:OG	1:AAA:521:ILE:HG12	2.21	0.41
2:BBB:114:ARG:HG3	2:BBB:151:ILE:HG21	2.03	0.41
2:BBB:563:LEU:O	2:BBB:564:ILE:C	2.64	0.41
2:BBB:578:PRO:C	2:BBB:580:ALA:H	2.29	0.41
4:SSS:99:CYS:SG	4:SSS:100:GLU:N	2.93	0.41
4:SSS:127:SER:O	4:SSS:131:VAL:HG23	2.20	0.41
2:BBB:99:ASN:ND2	3:MMM:148:GLN:NE2	2.69	0.41
2:BBB:168:LEU:O	2:BBB:171:ASP:CB	2.68	0.41
2:BBB:433:CYS:HB3	5:GGG:359:ILE:HG13	2.02	0.41
2:BBB:459:ILE:C	2:BBB:461:ASN:N	2.78	0.41
3:MMM:105:PHE:CD1	3:MMM:106:VAL:HG23	2.56	0.41
2:BBB:247:ARG:HD2	2:BBB:247:ARG:N	2.36	0.40
2:BBB:504:GLN:OE1	5:GGG:385:THR:O	2.38	0.40
6:PPP:3:GLN:C	6:PPP:4:ARG:O	2.63	0.40
1:AAA:64:PHE:CD1	4:SSS:107:PHE:CG	3.07	0.40
1:AAA:82:LEU:HB3	1:AAA:90:GLU:O	2.22	0.40
1:AAA:549:VAL:O	1:AAA:549:VAL:HG12	2.20	0.40
2:BBB:17:GLU:O	2:BBB:20:ALA:HB3	2.21	0.40
2:BBB:308:LEU:HD21	2:BBB:575:HIS:CD2	2.55	0.40
2:BBB:557:PRO:O	2:BBB:561:ASP:OD1	2.38	0.40
2:BBB:563:LEU:O	2:BBB:566:HIS:HB2	2.21	0.40
3:MMM:22:ASP:C	3:MMM:24:ILE:H	2.28	0.40
3:MMM:118:PHE:CG	3:MMM:118:PHE:O	2.73	0.40
4:SSS:34:GLU:O	4:SSS:35:VAL:C	2.64	0.40
4:SSS:49:PHE:O	4:SSS:50:VAL:CB	2.70	0.40
1:AAA:254:ALA:HB1	1:AAA:257:LEU:CD1	2.51	0.40
2:BBB:268:GLU:OE2	2:BBB:269:LEU:HD13	2.22	0.40
2:BBB:385:GLU:HA	2:BBB:421:TYR:OH	2.22	0.40
2:BBB:422:PRO:O	2:BBB:423:ASN:C	2.64	0.40
3:MMM:297:PRO:HB2	3:MMM:298:PHE:CD1	2.57	0.40
3:MMM:298:PHE:CG	3:MMM:399:MET:HE1	2.56	0.40
1:AAA:223:LYS:O	1:AAA:226:VAL:HG23	2.21	0.40
1:AAA:413:LEU:O	1:AAA:414:GLU:C	2.65	0.40
1:AAA:520:LEU:HD22	1:AAA:520:LEU:HA	1.87	0.40
1:AAA:535:VAL:O	1:AAA:536:PRO:C	2.63	0.40
1:AAA:586:LEU:HG	2:BBB:540:VAL:HG21	2.04	0.40
2:BBB:485:LEU:HD22	2:BBB:526:TYR:CD2	2.57	0.40
3:MMM:406:ALA:O	3:MMM:408:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:PPP:4:ARG:NH2	6:PPP:6:ASN:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	611/621 (98%)	465 (76%)	116 (19%)	30 (5%)	1	11
2	BBB	570/591 (96%)	415 (73%)	113 (20%)	42 (7%)	1	5
3	CCC	7/446 (2%)	4 (57%)	2 (29%)	1 (14%)	0	1
3	MMM	400/446 (90%)	290 (72%)	93 (23%)	17 (4%)	2	13
4	SSS	140/142 (99%)	103 (74%)	27 (19%)	10 (7%)	1	6
5	DDD	22/152 (14%)	13 (59%)	8 (36%)	1 (4%)	2	12
5	GGG	30/152 (20%)	23 (77%)	4 (13%)	3 (10%)	0	3
6	PPP	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
All	All	1784/2556 (70%)	1316 (74%)	363 (20%)	105 (6%)	1	8

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	105	ASN
1	AAA	224	THR
1	AAA	269	PRO
1	AAA	362	SER
1	AAA	380	GLU
1	AAA	383	VAL
1	AAA	421	ARG
1	AAA	511	ILE
1	AAA	576	LEU

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Mol	Chain	Res	Type
1	AAA	591	SER
2	BBB	152	ASN
2	BBB	155	MET
2	BBB	196	LEU
2	BBB	216	GLU
2	BBB	251	ALA
2	BBB	252	ASN
2	BBB	253	SER
2	BBB	271	PRO
2	BBB	478	THR
2	BBB	500	GLN
2	BBB	566	HIS
3	MMM	23	ASP
3	MMM	27	ASN
3	MMM	202	MET
3	MMM	350	LYS
4	SSS	16	LEU
4	SSS	50	VAL
4	SSS	114	VAL
5	GGG	367	SER
3	CCC	240	LYS
6	PPP	4	ARG
1	AAA	212	THR
1	AAA	226	VAL
1	AAA	237	VAL
1	AAA	402	ALA
1	AAA	557	ALA
1	AAA	574	VAL
2	BBB	82	ASP
2	BBB	321	ILE
2	BBB	506	VAL
2	BBB	552	THR
2	BBB	553	ASP
2	BBB	564	ILE
2	BBB	579	ASN
3	MMM	157	GLY
3	MMM	166	ILE
3	MMM	296	LEU
3	MMM	358	SER
4	SSS	63	ALA
4	SSS	131	VAL
1	AAA	48	LYS

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Mol	Chain	Res	Type
1	AAA	248	THR
1	AAA	382	ASP
2	BBB	47	VAL
2	BBB	166	ARG
2	BBB	171	ASP
2	BBB	250	HIS
2	BBB	364	GLU
2	BBB	371	ARG
2	BBB	423	ASN
2	BBB	437	ASP
2	BBB	453	GLY
2	BBB	560	LEU
3	MMM	264	ARG
3	MMM	388	ASP
4	SSS	103	LEU
4	SSS	115	ASP
5	DDD	321	GLU
1	AAA	156	VAL
1	AAA	244	LEU
1	AAA	357	ALA
1	AAA	391	ASP
1	AAA	414	GLU
1	AAA	602	MET
2	BBB	17	GLU
2	BBB	95	CYS
2	BBB	165	LEU
2	BBB	320	GLU
2	BBB	473	PHE
2	BBB	505	GLN
3	MMM	165	GLY
3	MMM	204	SER
3	MMM	256	ASP
4	SSS	96	HIS
5	GGG	361	PRO
1	AAA	379	THR
1	AAA	381	ARG
1	AAA	423	GLU
1	AAA	578	GLN
2	BBB	20	ALA
2	BBB	144	CYS
3	MMM	78	VAL
3	MMM	386	THR

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Mol	Chain	Res	Type
4	SSS	97	ASN
5	GGG	368	HIS
2	BBB	149	HIS
1	AAA	255	PRO
2	BBB	80	GLN
2	BBB	370	VAL
3	MMM	108	ILE
2	BBB	294	GLY
3	MMM	404	PRO
4	SSS	35	VAL
2	BBB	525	ILE
2	BBB	557	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	AAA	537/543 (99%)	458 (85%)	79 (15%)	3	13
2	BBB	513/532 (96%)	440 (86%)	73 (14%)	3	14
3	CCC	9/398 (2%)	7 (78%)	2 (22%)	1	4
3	MMM	358/398 (90%)	297 (83%)	61 (17%)	2	9
4	SSS	131/131 (100%)	113 (86%)	18 (14%)	3	16
5	DDD	23/142 (16%)	19 (83%)	4 (17%)	2	8
5	GGG	30/142 (21%)	24 (80%)	6 (20%)	1	5
6	PPP	6/6 (100%)	3 (50%)	3 (50%)	0	0
All	All	1607/2292 (70%)	1361 (85%)	246 (15%)	3	12

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	21	ARG
1	AAA	25	SER
1	AAA	26	LYS

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Mol	Chain	Res	Type
1	AAA	27	GLU
1	AAA	31	LYS
1	AAA	41	ARG
1	AAA	48	LYS
1	AAA	76	HIS
1	AAA	109	ILE
1	AAA	123	ARG
1	AAA	140	SER
1	AAA	143	MET
1	AAA	150	GLU
1	AAA	159	ASP
1	AAA	164	VAL
1	AAA	179	SER
1	AAA	187	ASP
1	AAA	201	LEU
1	AAA	222	PHE
1	AAA	223	LYS
1	AAA	225	SER
1	AAA	235	ARG
1	AAA	244	LEU
1	AAA	250	TYR
1	AAA	256	TRP
1	AAA	257	LEU
1	AAA	258	SER
1	AAA	268	TYR
1	AAA	272	GLU
1	AAA	279	ARG
1	AAA	283	CYS
1	AAA	290	LYS
1	AAA	297	SER
1	AAA	320	HIS
1	AAA	328	VAL
1	AAA	331	CYS
1	AAA	333	GLN
1	AAA	340	HIS
1	AAA	353	MET
1	AAA	354	CYS
1	AAA	361	PHE
1	AAA	382	ASP
1	AAA	388	ARG
1	AAA	405	ILE
1	AAA	417	ASP

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Mol	Chain	Res	Type
1	AAA	419	SER
1	AAA	420	ILE
1	AAA	423	GLU
1	AAA	425	VAL
1	AAA	438	ASP
1	AAA	445	THR
1	AAA	449	LEU
1	AAA	464	ARG
1	AAA	473	ASP
1	AAA	475	VAL
1	AAA	482	THR
1	AAA	483	VAL
1	AAA	488	GLN
1	AAA	492	CYS
1	AAA	506	GLU
1	AAA	511	ILE
1	AAA	518	SER
1	AAA	520	LEU
1	AAA	526	LEU
1	AAA	535	VAL
1	AAA	546	ILE
1	AAA	551	LEU
1	AAA	552	PHE
1	AAA	576	LEU
1	AAA	584	LEU
1	AAA	592	THR
1	AAA	597	THR
1	AAA	598	VAL
1	AAA	600	GLU
1	AAA	607	GLU
1	AAA	610	SER
1	AAA	612	ILE
1	AAA	616	LEU
1	AAA	617	LYS
2	BBB	58	MET
2	BBB	59	GLN
2	BBB	73	LEU
2	BBB	82	ASP
2	BBB	108	ARG
2	BBB	116	ASP
2	BBB	118	ILE
2	BBB	119	THR

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Mol	Chain	Res	Type
2	BBB	151	ILE
2	BBB	152	ASN
2	BBB	158	ASP
2	BBB	159	GLN
2	BBB	163	ASP
2	BBB	175	MET
2	BBB	188	SER
2	BBB	193	ASN
2	BBB	196	LEU
2	BBB	198	ASP
2	BBB	206	LYS
2	BBB	219	GLN
2	BBB	228	ASN
2	BBB	245	THR
2	BBB	247	ARG
2	BBB	249	SER
2	BBB	268	GLU
2	BBB	271	PRO
2	BBB	282	LYS
2	BBB	284	LEU
2	BBB	292	LEU
2	BBB	298	VAL
2	BBB	310	VAL
2	BBB	317	LEU
2	BBB	322	LYS
2	BBB	332	ILE
2	BBB	351	ILE
2	BBB	353	GLN
2	BBB	365	VAL
2	BBB	374	VAL
2	BBB	380	CYS
2	BBB	385	GLU
2	BBB	393	SER
2	BBB	397	ASP
2	BBB	398	LEU
2	BBB	403	VAL
2	BBB	404	ASN
2	BBB	426	GLU
2	BBB	432	LEU
2	BBB	438	SER
2	BBB	448	MET
2	BBB	454	GLU

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Mol	Chain	Res	Type
2	BBB	461	ASN
2	BBB	464	GLU
2	BBB	468	SER
2	BBB	477	SER
2	BBB	485	LEU
2	BBB	489	VAL
2	BBB	515	ASP
2	BBB	518	ASP
2	BBB	519	LEU
2	BBB	531	SER
2	BBB	536	THR
2	BBB	538	LYS
2	BBB	540	VAL
2	BBB	545	LYS
2	BBB	549	SER
2	BBB	551	GLU
2	BBB	554	LEU
2	BBB	557	PRO
2	BBB	567	ILE
2	BBB	569	SER
2	BBB	570	LEU
2	BBB	579	ASN
2	BBB	581	PHE
3	MMM	5	LEU
3	MMM	8	TYR
3	MMM	22	ASP
3	MMM	24	ILE
3	MMM	27	ASN
3	MMM	47	VAL
3	MMM	48	THR
3	MMM	53	THR
3	MMM	71	GLN
3	MMM	92	TYR
3	MMM	95	LYS
3	MMM	105	PHE
3	MMM	131	THR
3	MMM	133	ILE
3	MMM	134	THR
3	MMM	144	THR
3	MMM	152	THR
3	MMM	154	GLN
3	MMM	156	THR

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Mol	Chain	Res	Type
3	MMM	161	TRP
3	MMM	163	ARG
3	MMM	167	LYS
3	MMM	169	ARG
3	MMM	171	ASN
3	MMM	174	PHE
3	MMM	196	VAL
3	MMM	204	SER
3	MMM	216	MET
3	MMM	217	ASN
3	MMM	218	ASP
3	MMM	261	GLN
3	MMM	264	ARG
3	MMM	265	LEU
3	MMM	270	SER
3	MMM	273	SER
3	MMM	275	SER
3	MMM	283	PHE
3	MMM	284	GLU
3	MMM	287	ARG
3	MMM	291	THR
3	MMM	294	ILE
3	MMM	305	ARG
3	MMM	306	GLU
3	MMM	325	SER
3	MMM	327	LEU
3	MMM	331	ILE
3	MMM	334	ARG
3	MMM	346	VAL
3	MMM	347	ILE
3	MMM	350	LYS
3	MMM	376	GLN
3	MMM	384	LEU
3	MMM	387	ASN
3	MMM	390	LYS
3	MMM	391	LYS
3	MMM	400	ASN
3	MMM	410	LEU
3	MMM	429	VAL
3	MMM	439	SER
3	MMM	444	THR
3	MMM	446	CYS

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Mol	Chain	Res	Type
4	SSS	1	MET
4	SSS	14	THR
4	SSS	21	MET
4	SSS	24	ASP
4	SSS	25	ASP
4	SSS	29	GLN
4	SSS	30	LYS
4	SSS	49	PHE
4	SSS	54	ASN
4	SSS	72	ASP
4	SSS	74	ASN
4	SSS	102	ASP
4	SSS	105	PHE
4	SSS	106	ASN
4	SSS	130	LYS
4	SSS	133	LYS
4	SSS	137	MET
4	SSS	141	LEU
5	GGG	360	LYS
5	GGG	361	PRO
5	GGG	368	HIS
5	GGG	373	SER
5	GGG	377	LEU
5	GGG	387	SER
3	CCC	235	LYS
3	CCC	238	GLU
6	PPP	1	ASP
6	PPP	3	GLN
6	PPP	4	ARG
5	DDD	326	LYS
5	DDD	332	ASN
5	DDD	339	PHE
5	DDD	340	TYR

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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	613/621 (98%)	-0.57	1 (0%) 91 85	84, 165, 244, 320	0
2	BBB	572/591 (96%)	-0.67	1 (0%) 91 85	82, 116, 165, 244	0
3	CCC	9/446 (2%)	-0.90	0 100 100	164, 179, 205, 206	0
3	MMM	406/446 (91%)	-0.64	1 (0%) 91 85	80, 123, 185, 245	0
4	SSS	142/142 (100%)	-0.57	0 100 100	134, 174, 223, 242	0
5	DDD	24/152 (15%)	-0.72	0 100 100	162, 191, 212, 215	0
5	GGG	32/152 (21%)	-0.69	0 100 100	91, 141, 168, 184	0
6	PPP	6/6 (100%)	-0.91	0 100 100	121, 141, 155, 174	0
All	All	1804/2556 (70%)	-0.63	3 (0%) 91 85	80, 134, 224, 320	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	MMM	5	LEU	2.3
1	AAA	350	LEU	2.2
2	BBB	252	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.