



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 01:19 pm BST

PDB ID : 7OG1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

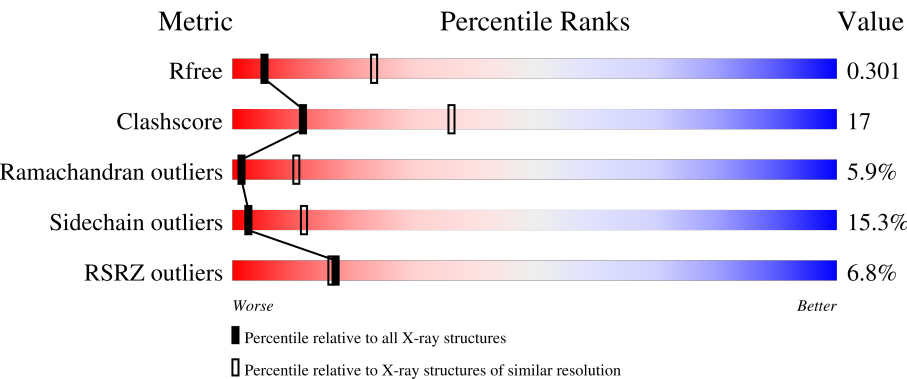
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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	<div><div>13%</div><div>60%</div><div>31%</div><div>8%</div><div>.</div></div>
2	BBB	591	<div><div>2%</div><div>51%</div><div>35%</div><div>9%</div><div>..</div></div>
3	CCC	446	<div><div>..</div><div>98%</div></div>
3	MMM	446	<div><div>%</div><div>53%</div><div>32%</div><div>6%</div><div>.</div><div>9%</div></div>
4	SSS	142	<div><div>14%</div><div>43%</div><div>47%</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
5	DDD	152	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>11%5%84%</div></div></div>
5	GGG	152	<div><div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>14%. . .79%</div></div></div>
6	PPP	6	<div><div><div></div><div></div><div></div></div><div>17%67%17%</div></div>

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			

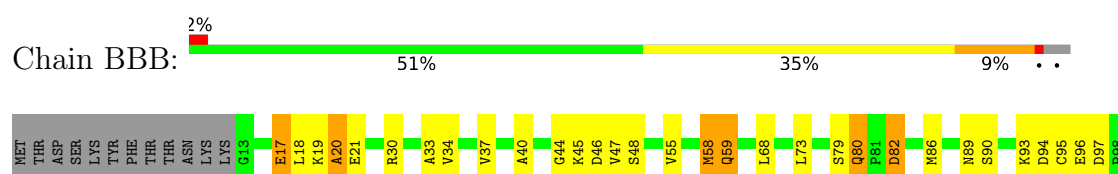
3 Residue-property plots

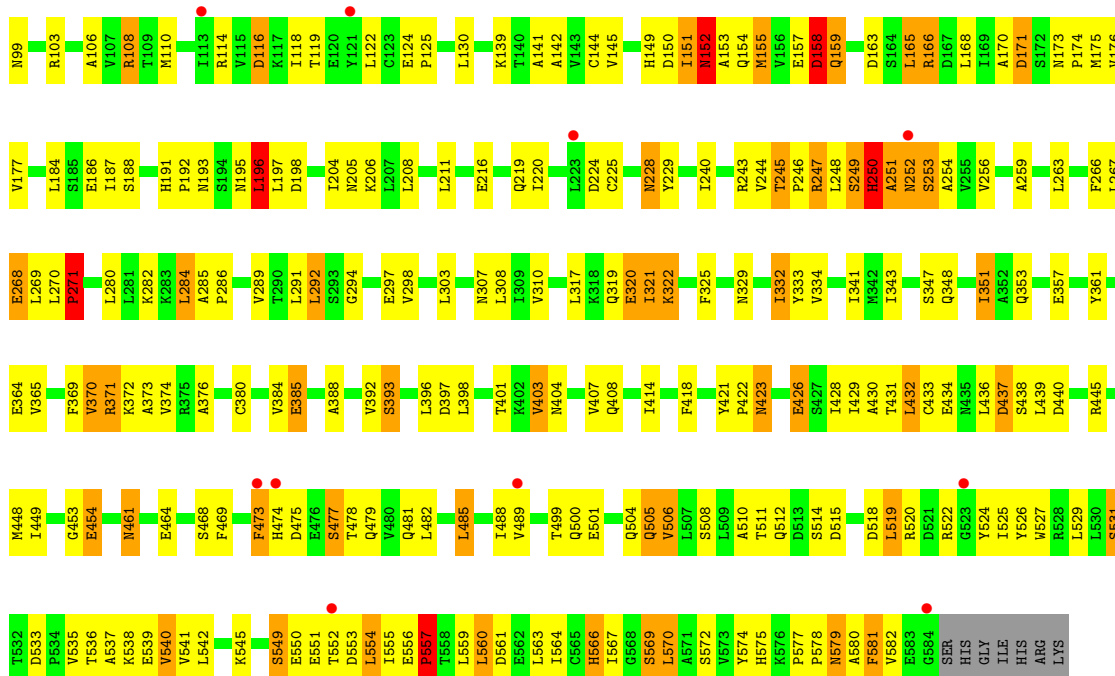
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

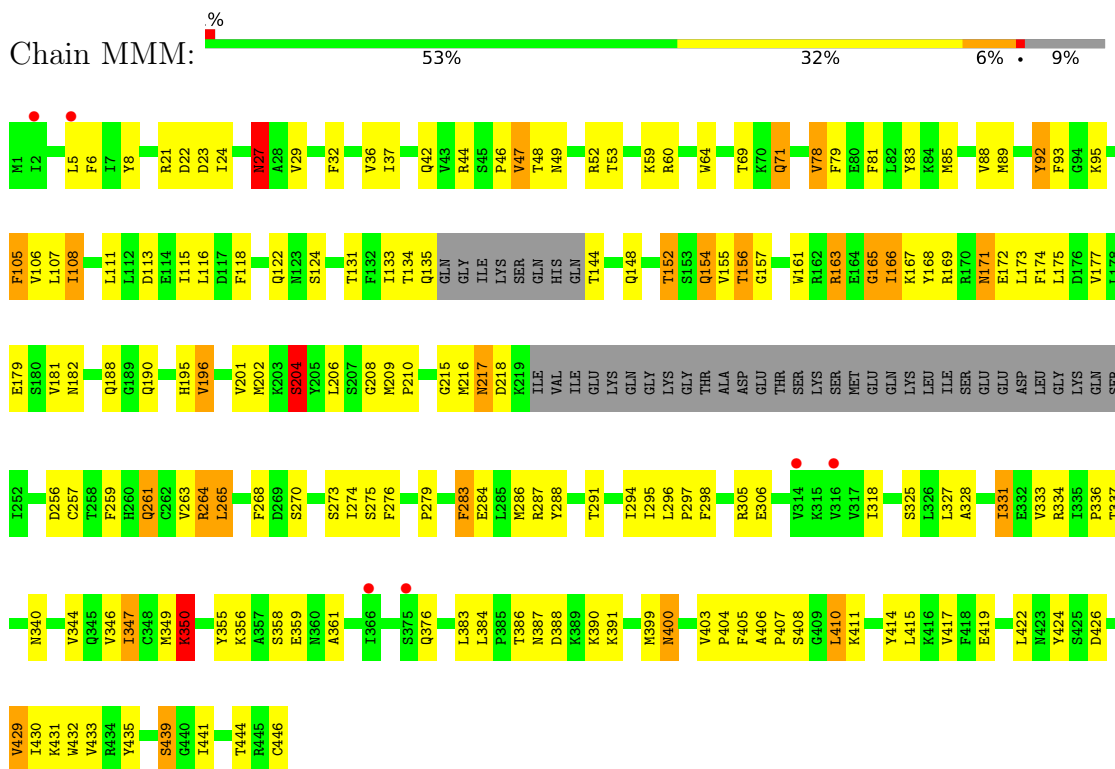


• Molecule 2: AP-2 complex subunit beta

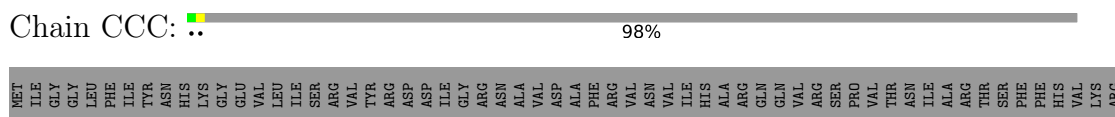




• Molecule 3: AP-2 complex subunit mu

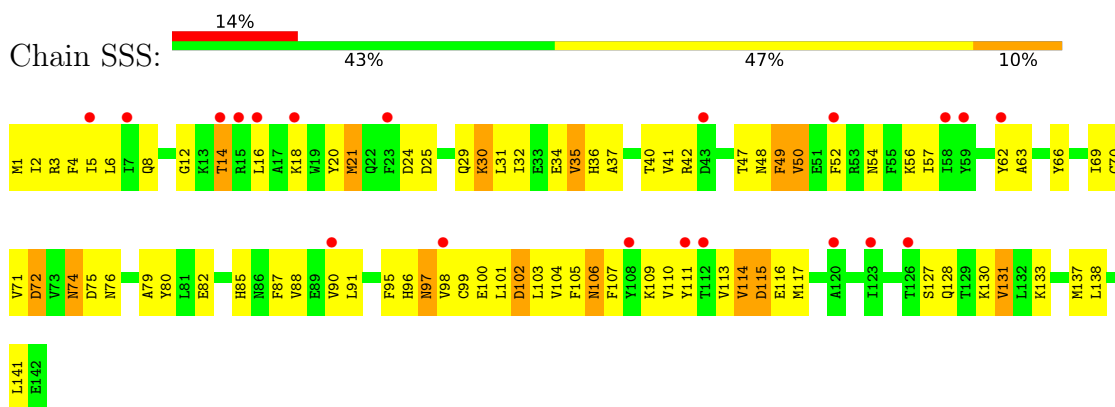


• Molecule 3: AP-2 complex subunit mu

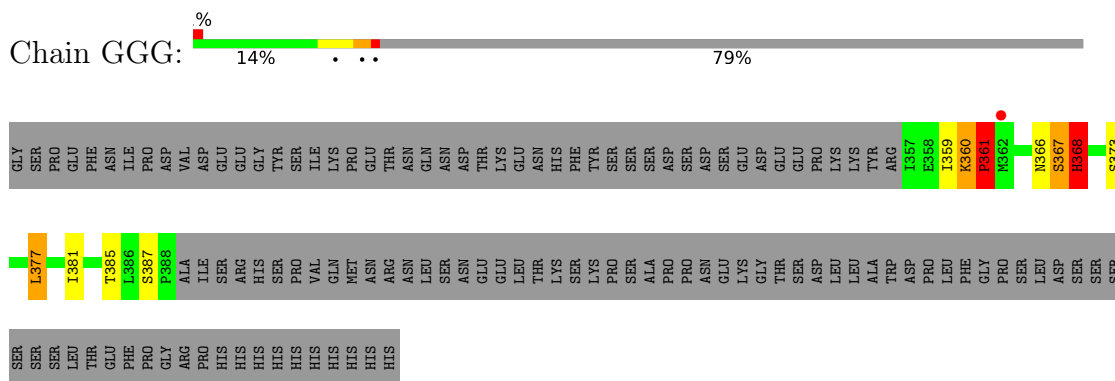


LEU	ASN	TYR	TRP	LYS	ARG	VAL	PRO	I242	VAL	PRO	SER
ASN	TRP	GLY	GLY	GLY	GLY	GLY	LEU	\$243	ASN	GLN	ASN
SER	GLY	ASP	ASP	ASP	GLY	ASP	GLU	GLU	LEU	GLY	TRP
HIS	LEU	ASP	VAL	VAL	VAL	VAL	VAL	LEU	SER	THR	ALA
ASP	VAL	ASP	GLY	ARG	GLY	GLY	GLY	GLY	PRO	ALA	VAL
VAL	MET	ASP	ARG	THR	THR	THR	LYS	LYS	GLN	ALA	VAL
ASP	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLN	GLY	VAL	THR
VAL	THR	TRP	MET	LYS	LEU	ILE	ILE	GLN	GLY	GLY	LYS
VAL	LYS	VAL	LYS	GLY	GLY	GLY	GLY	ALA	LEU	THR	ASN
ARG	GLY	VAL	GLY	VAL	VAL	ILE	ILE	ILE	SER	ILE	VAL
ASN	GLY	GLY	GLY	GLY	GLY	GLY	VAL	ASP	ALA	THR	ASN
GLY	ILE	GLY	ILE	ILE	ILE	ILE	VAL	ASP	HIS	GLN	ALA
ILE	GLY	ARG	ILE	ILE	ILE	ILE	VAL	CYS	VAL	GLY	MET
SER	GLY	SER	ALA	ALA	ALA	LYS	LYS	PHE	GLY	ILE	VAL
GLY	GLY	GLY	GLY	GLY	GLY	LYS	SER	HIS	ARG	LYS	PHE
ILE	ILE	TYR	GLY	GLY	GLY	ASN	ASN	GLN	VAL	SER	GLY
GLY	GLY	GLY	GLY	GLY	GLY	PHE	LEU	CYS	VAL	GLN	PHE
THR	THR	THR	LEU	LEU	PRO	LEU	PRO	VAL	LYS	GLN	TYR
ARG	ARG	PRO	PRO	PRO	PRO	SER	SER	ARG	SER	THR	LYS
CYS	CYS	THR	THR	THR	THR	LEU	LEU	LEU	TYR	LYS	MET
						ASN	LEU	LYS	GLY	GLY	CYS
						ASP	LEU	PHE	SER	ASP	ASP
						LYS	GLN	ASP	GLY	GLN	VAL
						LYS	LYS	SER	MET	SER	MET
						LYS	ILE	GLY	PRO	GLN	ALA
						TRP	GLY	ARG	GLY	ILE	ALA
						ALA	VAL	SER	CYS	THR	ALA
						ARG	ARG	ILE	PHE	SER	PHE
						PRO	PRO	ILE	SER	GLY	GLY
						PRO	PRO	PHE	GLY	VAL	LYS
						ILE	THR	ILE	MET	THR	ILE
						SER	PRO	PRO	ASN	GLY	SER
						THR	ASN	PRO	ASP	GLY	GLY
						ASN	ASN	ASN	LYS	ILE	GLY
						PHE	THR	GLY	ILE	ASN	TRP
						GLY	SER	GLY	VAL	TRP	ILE
						VAL	GLY	PHE	ILE	ARG	LYS
						PRO	VAL	GLY	GLY	ARG	ASN
						PHE	GLN	LEU	LYS	GLY	ASN
						ALA	VAL	MET	GLN	GLY	GLY
						PRO	PRO	ALA	ILE	ILE	VAL
						SER	PRO	ARG	GLY	LYS	LEU
						THR	GLY	THR	GLY	TYR	ILE
						LEU	TYR	ARG	THR	ARG	TYR
						LYS	LYS	LYS	ALA	GLY	GLY
						ARG	VAL	ASP	ASP	GLY	LEU
						THR	THR	THR	THR	THR	ASP
						ILE	ILE	ILE	SER	PHE	ILE
						LYS	LYS	LEU	K236	LEU	GLY
						VAL	VAL	PRO	E238	ASP	TYR
						PRO	GLY	ARG	Q239	VAL	GLY
						ASN	ASN	VAL	K240	LEU	SER
						ALA	VAL	THR	L241	GLY	THR

- Molecule 4: AP-2 complex subunit sigma

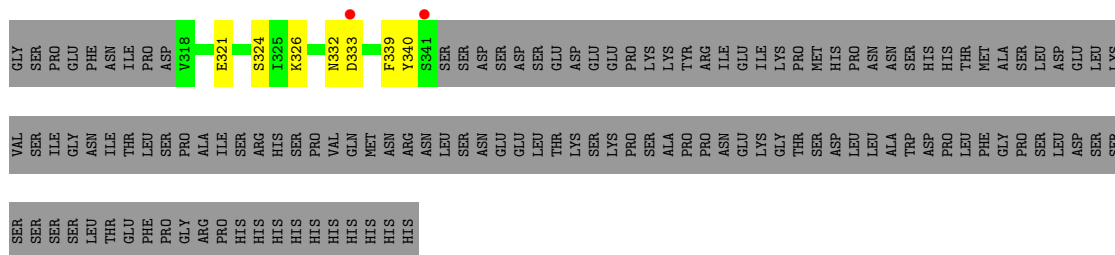


- Molecule 5: F-BAR domain only protein 2



- Molecule 5: F-BAR domain only protein 2





- Molecule 6: TGN38 CARGO PEPTIDE

Chain PPP: 17% 67% 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 76.54 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (76.66-3.25) 100.0 (76.54-3.25)	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 (4.91%)	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)	(Not available) , (Not available)	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	0.72	0/4921	0.85	0/6669
2	BBB	0.72	0/4597	0.90	0/6237
3	CCC	0.81	0/71	0.79	0/91
3	MMM	0.72	0/3319	0.89	0/4473
4	SSS	0.72	0/1224	0.83	0/1650
5	DDD	0.74	0/204	0.84	0/275
5	GGG	0.76	0/250	0.97	1/339 (0.3%)
6	PPP	0.63	0/57	0.77	0/74
All	All	0.72	0/14643	0.88	1/19808 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	BBB	0	4
5	GGG	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	GGG	361	PRO	N-CA-CB	-5.33	96.73	102.60

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

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Mol	Chain	Res	Type	Group
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	158	0
2	BBB	4527	0	4638	202	0
3	CCC	72	0	80	3	0
3	MMM	3254	0	3318	114	0
4	SSS	1200	0	1195	68	0
5	DDD	200	0	171	3	0
5	GGG	245	0	247	14	0
6	PPP	57	0	53	4	0
All	All	14391	0	14654	507	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 17.

All (507) 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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:477:SER:C	2:BBB:479:GLN:H	1.86	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:BBB:474:HIS:O	2:BBB:475:ASP:HB2	2.00	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
3:MMM:179:GLU:OE2	3:MMM:288:TYR:OH	2.18	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
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: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
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:477:SER:C	2:BBB:479:GLN:N	2.55	0.59
2:BBB:110:MET:HG2	2:BBB:122:LEU:HD13	1.85	0.58
1:AAA:218:ASN:HD22	1:AAA:221:GLU:CD	2.06	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AAA:85:SER:OG	1:AAA:86:ASN:N	2.38	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
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
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
2:BBB:250:HIS:O	2:BBB:251:ALA:C	2.44	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:535:VAL:HG23	1:AAA:536:PRO:HD3	1.88	0.55
1:AAA:382:ASP:O	1:AAA:384:SER:N	2.39	0.55
2:BBB:249:SER:HB3	3:MMM:259:PHE:N	2.11	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:SSS:3:ARG:HA	4:SSS:21:MET:HE3	1.89	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:580:ALA:C	2:BBB:581:PHE:CD1	2.82	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
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
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
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
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
2:BBB:505:GLN:O	2:BBB:506:VAL:C	2.49	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:333:VAL:HG22	3:MMM:399:MET:HG2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:270:LEU:O	2:BBB:271:PRO:C	2.49	0.50
4:SSS:49:PHE:O	4:SSS:50:VAL:HB	2.11	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
3:MMM:165:GLY:O	3:MMM:166:ILE:C	2.50	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
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
2:BBB:250:HIS:C	2:BBB:252:ASN:N	2.64	0.50
1:AAA:79:ALA:HA	1:AAA:82:LEU:HD13	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:BBB:473:PHE:O	2:BBB:474:HIS:C	2.51	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
3:MMM:208:GLY:O	3:MMM:209:MET:HE2	2.13	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
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:603:PRO:HG2	2:BBB:524:TYR:CZ	2.48	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:486:ALA:CB	1:AAA:496:LEU:HD21	2.42	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: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
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:268:PHE:CD1	3:MMM:268:PHE:C	2.88	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
2:BBB:151:ILE:O	2:BBB:152:ASN:C	2.53	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:454:GLU:OE1	2:BBB:454:GLU:HA	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
1:AAA:549:VAL:HG23	1:AAA:559:ILE:HG21	1.98	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
3:MMM:173:LEU:C	3:MMM:173:LEU:HD12	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:ASN:CG	2:BBB:155:MET:HG3	2.36	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
1:AAA:333:GLN:HE21	1:AAA:333:GLN:C	2.20	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
2:BBB:89:ASN:O	2:BBB:93:LYS:HB2	2.16	0.46
2:BBB:165:LEU:O	2:BBB:166:ARG:C	2.54	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: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
2:BBB:533:ASP:OD1	2:BBB:533:ASP:C	2.53	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
2:BBB:371:ARG:O	2:BBB:372:LYS:C	2.54	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
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
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:170:ALA:O	2:BBB:171:ASP:C	2.55	0.45
2:BBB:259:ALA:O	2:BBB:263:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:80:VAL:HG12	1:AAA:80:VAL:O	2.17	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
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: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
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
2:BBB:191:HIS:N	2:BBB:192:PRO:HD3	2.32	0.44
3:MMM:105:PHE:CD1	3:MMM:105:PHE:C	2.91	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
4:SSS:102:ASP:C	4:SSS:104:VAL:H	2.21	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
4:SSS:106:ASN:HB3	4:SSS:109:LYS:HB2	2.00	0.43
1:AAA:577:GLN:O	1:AAA:578:GLN:C	2.56	0.43
1:AAA:605:PHE:CZ	2:BBB:520:ARG:HD3	2.53	0.43
2:BBB:244:VAL:C	2:BBB:246:PRO:HD2	2.38	0.43
2:BBB:253:SER:O	2:BBB:254:ALA:C	2.56	0.43
4:SSS:20:TYR:HB2	4:SSS:21:MET:HE1	2.01	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AAA:475:VAL:O	1:AAA:476:GLN:C	2.57	0.43
2:BBB:171:ASP:OD2	2:BBB:176:VAL:HG11	2.19	0.43
2:BBB:195:ASN:C	2:BBB:197:LEU:HD22	2.39	0.43
3:MMM:257:CYS:HB2	3:MMM:286:MET:HE2	2.01	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
3:MMM:168:TYR:CE2	5:DDD:324:SER:HB2	2.53	0.43
2:BBB:44:GLY:O	2:BBB:45:LYS:C	2.57	0.43
4:SSS:4:PHE:HB2	4:SSS:18:LYS:O	2.18	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: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
1:AAA:573:ASP:OD1	1:AAA:573:ASP:C	2.57	0.42
2:BBB:114:ARG:HG3	2:BBB:151:ILE:HD12	2.00	0.42
2:BBB:154:GLN:O	2:BBB:155:MET:C	2.57	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
1:AAA:155:LEU:O	1:AAA:156:VAL:C	2.57	0.42
2:BBB:371:ARG:O	2:BBB:373:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:MMM:78:VAL:O	3:MMM:79:PHE:C	2.58	0.42
2:BBB:94:ASP:C	2:BBB:96:GLU:H	2.22	0.42
2:BBB:325:PHE:HD1	2:BBB:357:GLU:HG2	1.84	0.42
3:MMM:108:ILE:O	3:MMM:111:LEU:N	2.53	0.42
4:SSS:99:CYS:SG	4:SSS:100:GLU:N	2.93	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: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
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:46:ASP:C	2:BBB:48:SER:H	2.23	0.41
2:BBB:191:HIS:HA	2:BBB:195:ASN:CG	2.40	0.41
2:BBB:319:GLN:O	2:BBB:320:GLU:C	2.59	0.41
2:BBB:482:LEU:CD2	2:BBB:519:LEU:HB2	2.48	0.41
3:MMM:69:THR:HG1	3:MMM:71:GLN:HE21	1.66	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
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
1:AAA:575:GLU:C	1:AAA:577:GLN:N	2.74	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:18:LEU:O	2:BBB:19:LYS:C	2.58	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
4:SSS:5:ILE:HG12	4:SSS:69:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
4:SSS:127:SER:O	4:SSS:131:VAL:HG23	2.20	0.41
1:AAA:333:GLN:NE2	1:AAA:333:GLN:C	2.74	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
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
3:MMM:118:PHE:CG	3:MMM:118:PHE:O	2.73	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
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:55:VAL:HG13	2:BBB:58:MET:HE3	2.03	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
3:MMM:297:PRO:HB2	3:MMM:298:PHE:CD1	2.57	0.40
1:AAA:575:GLU:O	1:AAA:576:LEU:C	2.60	0.40
1:AAA:223:LYS:O	1:AAA:226:VAL:HG23	2.21	0.40
1:AAA:520:LEU:HD22	1:AAA:520:LEU:HA	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:577:PRO:O	2:BBB:578:PRO:C	2.60	0.40
3:MMM:406:ALA:O	3:MMM:408:SER:N	2.54	0.40
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%)	2	14
2	BBB	570/591 (96%)	415 (73%)	113 (20%)	42 (7%)	1	7
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	16
4	SSS	140/142 (99%)	103 (74%)	27 (19%)	10 (7%)	1	7
5	DDD	22/152 (14%)	13 (59%)	8 (36%)	1 (4%)	2	15
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	10

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

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Mol	Chain	Res	Type
1	AAA	511	ILE
1	AAA	576	LEU
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

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Mol	Chain	Res	Type
4	SSS	131	VAL
1	AAA	48	LYS
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

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Mol	Chain	Res	Type
3	MMM	78	VAL
3	MMM	386	THR
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	15
3	CCC	9/398 (2%)	7 (78%)	2 (22%)	1	3
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%)	2	12

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

Mol	Chain	Res	Type
1	AAA	21	ARG

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

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Mol	Chain	Res	Type
1	AAA	405	ILE
1	AAA	417	ASP
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

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Mol	Chain	Res	Type
2	BBB	118	ILE
2	BBB	119	THR
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

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Mol	Chain	Res	Type
2	BBB	448	MET
2	BBB	454	GLU
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

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Mol	Chain	Res	Type
3	MMM	154	GLN
3	MMM	156	THR
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

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Mol	Chain	Res	Type
3	MMM	444	THR
3	MMM	446	CYS
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 monosaccharides 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 ⓘ

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	613/621 (98%)	0.63	83 (13%) 3 3	84, 165, 244, 320	0
2	BBB	572/591 (96%)	0.20	10 (1%) 70 67	82, 116, 165, 244	0
3	CCC	9/446 (2%)	-0.61	0 100 100	164, 179, 205, 206	0
3	MMM	406/446 (91%)	0.14	6 (1%) 73 71	80, 123, 185, 245	0
4	SSS	142/142 (100%)	0.71	20 (14%) 2 2	134, 174, 223, 242	0
5	DDD	24/152 (15%)	0.21	2 (8%) 11 11	162, 191, 212, 215	0
5	GGG	32/152 (21%)	-0.27	1 (3%) 49 47	91, 141, 168, 184	0
6	PPP	6/6 (100%)	-0.20	0 100 100	121, 141, 155, 174	0
All	All	1804/2556 (70%)	0.36	122 (6%) 17 16	80, 134, 224, 320	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	103	ASN	7.9
1	AAA	113	ASN	7.6
1	AAA	93	ILE	6.8
1	AAA	51	ASP	6.4
1	AAA	130	LEU	5.7
1	AAA	49	ALA	5.2
4	SSS	108	TYR	5.1
1	AAA	72	ILE	4.9
4	SSS	62	TYR	4.8
1	AAA	62	LEU	4.7
4	SSS	23	PHE	4.6
1	AAA	59	VAL	4.5
1	AAA	50	LEU	4.5
1	AAA	237	VAL	4.4
1	AAA	83	LEU	4.3
1	AAA	350	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	29	GLU	4.3
1	AAA	43	LYS	4.2
1	AAA	65	ILE	4.2
1	AAA	131	ALA	4.2
1	AAA	114	ASN	4.2
1	AAA	70	HIS	4.1
1	AAA	256	TRP	4.0
1	AAA	80	VAL	3.9
1	AAA	239	SER	3.9
1	AAA	127	PHE	3.9
1	AAA	75	GLY	3.8
1	AAA	178	THR	3.7
4	SSS	14	THR	3.7
1	AAA	10	MET	3.7
1	AAA	170	LEU	3.7
1	AAA	240	ALA	3.6
2	BBB	252	ASN	3.6
1	AAA	101	LEU	3.6
1	AAA	295	PRO	3.5
4	SSS	5	ILE	3.5
1	AAA	95	TYR	3.5
1	AAA	100	VAL	3.5
1	AAA	115	ALA	3.4
1	AAA	173	LEU	3.4
1	AAA	84	SER	3.4
1	AAA	58	TYR	3.4
3	MMM	314	VAL	3.4
1	AAA	129	GLY	3.4
4	SSS	52	PHE	3.3
1	AAA	42	SER	3.3
4	SSS	15	ARG	3.2
1	AAA	90	GLU	3.2
1	AAA	248	THR	3.2
1	AAA	241	SER	3.2
1	AAA	44	PHE	3.2
1	AAA	338	LEU	3.1
1	AAA	322	SER	3.1
4	SSS	98	VAL	3.1
1	AAA	205	THR	3.0
1	AAA	108	LEU	3.0
4	SSS	123	ILE	3.0
4	SSS	90	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	385	VAL	2.9
4	SSS	58	ILE	2.9
1	AAA	61	LYS	2.9
1	AAA	109	ILE	2.9
1	AAA	92	GLN	2.9
5	DDD	333	ASP	2.8
1	AAA	271	PRO	2.8
1	AAA	66	PHE	2.8
2	BBB	473	PHE	2.8
1	AAA	77	MET	2.7
1	AAA	60	CYS	2.7
1	AAA	210	LEU	2.6
1	AAA	345	LEU	2.6
1	AAA	161	MET	2.6
4	SSS	7	ILE	2.6
2	BBB	552	THR	2.6
3	MMM	316	VAL	2.5
1	AAA	79	ALA	2.5
1	AAA	253	PRO	2.5
1	AAA	116	ILE	2.5
3	MMM	375	SER	2.5
5	DDD	341	SER	2.5
1	AAA	151	ILE	2.4
1	AAA	139	GLY	2.4
1	AAA	235	ARG	2.4
1	AAA	284	LEU	2.4
4	SSS	43	ASP	2.4
1	AAA	196	LEU	2.4
4	SSS	16	LEU	2.3
2	BBB	121	TYR	2.3
1	AAA	192	VAL	2.3
1	AAA	283	CYS	2.3
5	GGG	362	MET	2.3
2	BBB	523	GLY	2.3
3	MMM	2	ILE	2.3
1	AAA	206	ALA	2.3
1	AAA	143	MET	2.3
1	AAA	211	ILE	2.2
3	MMM	366	ILE	2.2
1	AAA	251	PHE	2.2
3	MMM	5	LEU	2.2
1	AAA	238	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	89	THR	2.2
1	AAA	134	CYS	2.2
1	AAA	175	LEU	2.2
2	BBB	223	LEU	2.2
4	SSS	18	LYS	2.2
2	BBB	584	GLY	2.2
1	AAA	327	LEU	2.2
1	AAA	242	THR	2.2
2	BBB	489	VAL	2.1
4	SSS	112	THR	2.1
1	AAA	155	LEU	2.1
4	SSS	126	THR	2.1
4	SSS	120	ALA	2.1
1	AAA	197	ASN	2.1
2	BBB	113	ILE	2.1
4	SSS	111	TYR	2.1
1	AAA	164	VAL	2.1
2	BBB	474	HIS	2.1
1	AAA	97	PHE	2.0
1	AAA	40	ILE	2.0
1	AAA	67	LEU	2.0
4	SSS	59	TYR	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 monosaccharides 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.