



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:20 AM UTC

PDB ID : 7Q9B / pdb_00007q9b
Title : MHC Class I A02 Allele presenting EAAGIGILTV, in complex with Mel8 TCR
Authors : Rizkallah, P.J.; Sewell, A.K.; Wall, A.; Fuller, A.
Deposited on : 2021-11-12
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

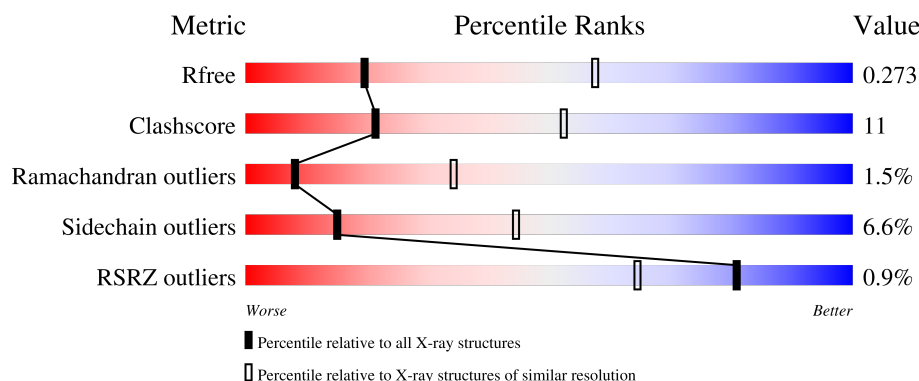
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	275	
1	FFF	275	
2	BBB	100	
2	GGG	100	
3	CCC	10	

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Mol	Chain	Length	Quality of chain
3	HHH	10	 70% 10% 20%
4	DDD	193	 % 73% 23% •
4	III	193	 4% 67% 29% • •
5	EEE	245	 67% 30% •
5	JJJ	245	 69% 29% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13221 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			
1	FFF	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	GGG	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	MET	-	initiating methionine	UNP P61769
GGG	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called GLU-ALA-ALA-GLY-ILE-GLY-ILE-LEU-THR-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	10	Total	C	N	O	0	0	0
			66	42	10	14			
3	HHH	10	Total	C	N	O	0	0	0
			66	42	10	14			

- Molecule 4 is a protein called Human T Cell Receptor Mel8, Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	193	Total	C	N	O	S	0	0	0
			1501	932	251	310	8			

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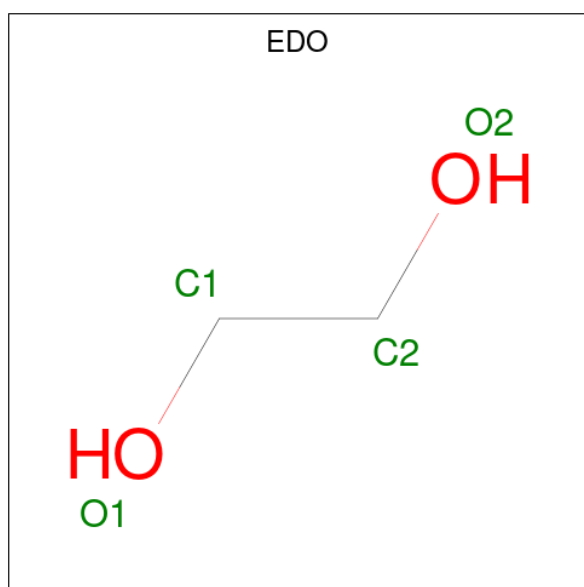
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	III	190	Total	C	N	O	S	0	0	0
			1475	915	248	304	8			

- Molecule 5 is a protein called Human T Cell Receptor Mel8, Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	EEE	245	Total	C	N	O	S	0	0	0
			1942	1221	332	380	9			
5	JJJ	245	Total	C	N	O	S	0	0	0
			1942	1221	332	380	9			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			4	2	2		
6	GGG	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	11	Total	O	0	0
			11	11		
7	BBB	7	Total	O	0	0
			7	7		

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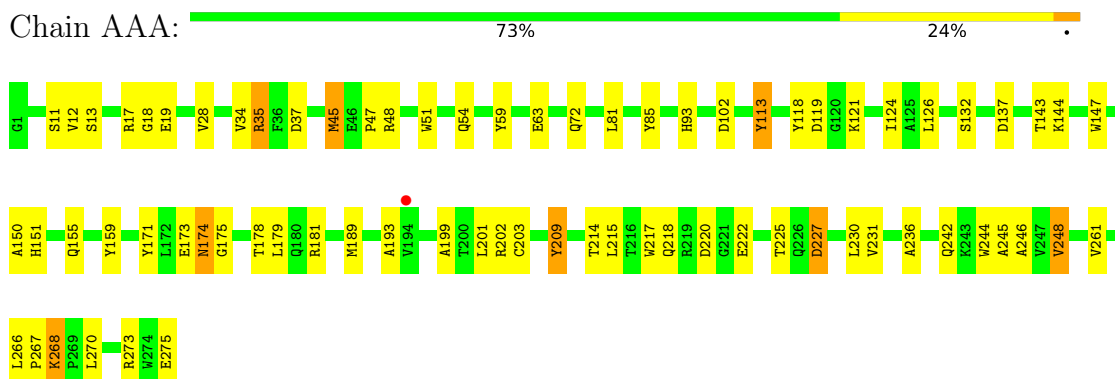
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total 1	O 1	0	0
7	DDD	11	Total 11	O 11	0	0
7	EEE	5	Total 5	O 5	0	0
7	FFF	7	Total 7	O 7	0	0
7	GGG	6	Total 6	O 6	0	0
7	III	2	Total 2	O 2	0	0
7	JJJ	3	Total 3	O 3	0	0

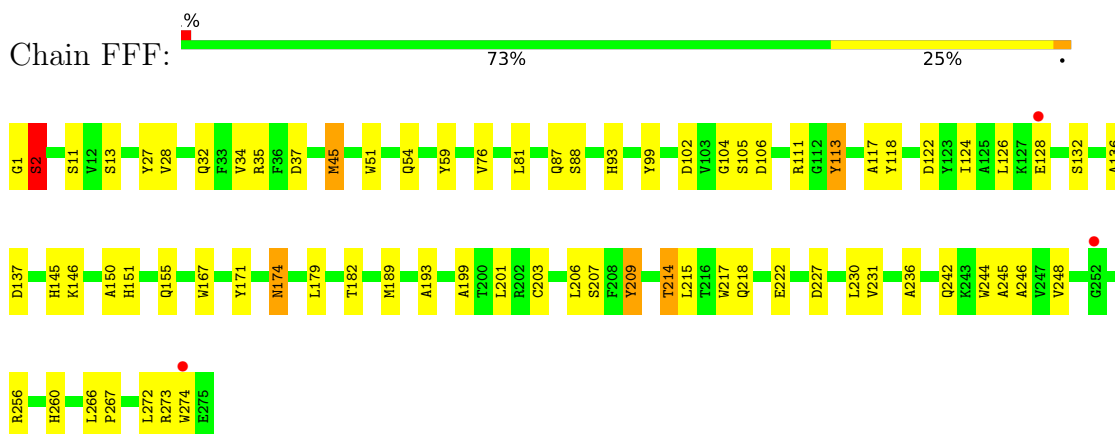
3 Residue-property plots

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.

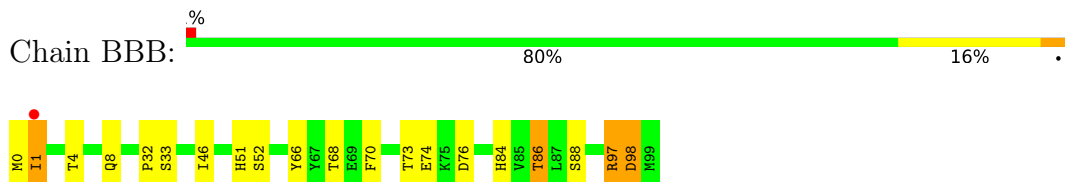
- Molecule 1: MHC class I antigen



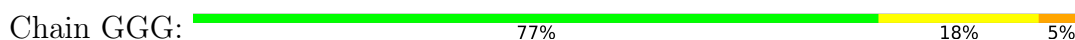
- Molecule 1: MHC class I antigen



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin

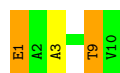




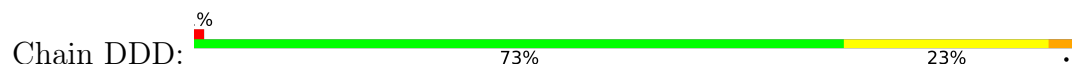
- Molecule 3: GLU-ALA-ALA-GLY-ILE-GLY-ILE-LEU-THR-VAL



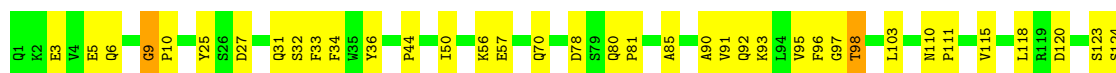
- Molecule 3: GLU-ALA-ALA-GLY-ILE-GLY-ILE-LEU-THR-VAL



- Molecule 4: Human T Cell Receptor Mel8, Alpha Chain

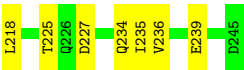


- Molecule 4: Human T Cell Receptor Mel8, Alpha Chain

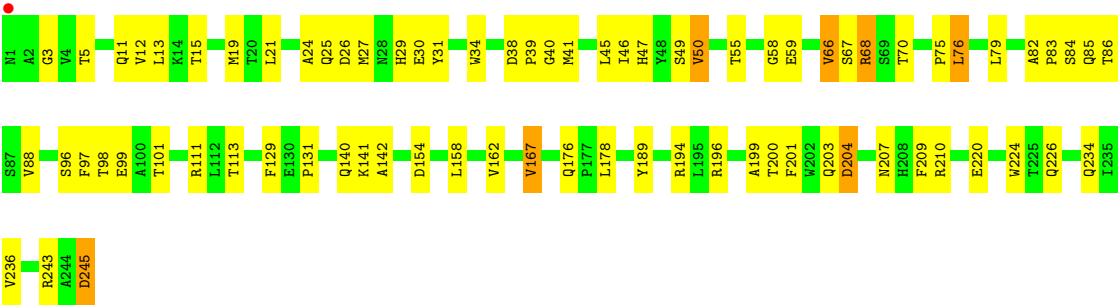


- Molecule 5: Human T Cell Receptor Mel8, Beta Chain





● Molecule 5: Human T Cell Receptor Mel8, Beta Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.97Å 53.65Å 203.51Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	99.69 – 3.24 99.69 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.69-3.24) 99.9 (99.69-3.24)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.226 , 0.277 0.227 , 0.273	Depositor DCC
R_{free} test set	1743 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	1.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13221	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.17	1/2312 (0.0%)	1.41	0/3137
1	FFF	1.15	1/2312 (0.0%)	1.41	2/3137 (0.1%)
2	BBB	1.19	1/860 (0.1%)	1.29	0/1162
2	GGG	1.17	1/860 (0.1%)	1.31	0/1162
3	CCC	1.46	1/65 (1.5%)	1.61	0/86
3	HHH	1.40	0/65	1.62	0/86
4	DDD	1.21	2/1530 (0.1%)	1.39	0/2072
4	III	1.21	2/1503 (0.1%)	1.41	2/2035 (0.1%)
5	EEE	1.16	1/1996 (0.1%)	1.35	3/2721 (0.1%)
5	JJJ	1.16	2/1996 (0.1%)	1.33	2/2721 (0.1%)
All	All	1.18	12/13499 (0.1%)	1.37	9/18319 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	FFF	0	1
4	DDD	0	1
5	EEE	0	1
5	JJJ	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	1	ILE	C-O	6.78	1.31	1.24
2	GGG	21	ASN	C-O	5.57	1.28	1.24
4	III	44	PRO	C-O	-5.40	1.17	1.23
5	JJJ	68	ARG	C-O	5.32	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	6	GLY	C-O	5.31	1.32	1.24
4	DDD	111	PRO	C-O	-5.31	1.17	1.23
1	FFF	88	SER	C-O	5.25	1.30	1.23
4	DDD	179	CYS	C-O	5.22	1.30	1.24
1	AAA	268	LYS	N-CA	5.15	1.50	1.45
4	III	111	PRO	C-O	-5.14	1.18	1.23
5	JJJ	30	GLU	C-O	5.11	1.29	1.24
5	EEE	4	VAL	N-CA	5.06	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	JJJ	204	ASP	CB-CA-C	6.79	119.16	109.38
4	III	27	ASP	CA-C-N	6.09	128.72	120.38
4	III	27	ASP	C-N-CA	6.09	128.72	120.38
5	EEE	155	HIS	CA-C-N	5.69	132.21	121.97
5	EEE	155	HIS	C-N-CA	5.69	132.21	121.97
1	FFF	87	GLN	CA-C-N	5.28	128.21	120.71
1	FFF	87	GLN	C-N-CA	5.28	128.21	120.71
5	JJJ	50	VAL	N-CA-C	-5.21	107.40	112.29
5	EEE	50	VAL	N-CA-C	-5.14	107.46	112.29

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	DDD	29	GLY	Peptide
5	EEE	96	SER	Peptide
1	FFF	274	TRP	Peptide
5	JJJ	96	SER	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	2247	0	2096	48	0
1	FFF	2247	0	2096	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	837	0	803	16	0
2	GGG	837	0	803	14	0
3	CCC	66	0	73	7	0
3	HHH	66	0	73	4	0
4	DDD	1501	0	1429	32	0
4	III	1475	0	1409	36	0
5	EEE	1942	0	1826	58	0
5	JJJ	1942	0	1826	54	0
6	AAA	4	0	6	0	0
6	GGG	4	0	6	0	0
7	AAA	11	0	0	0	0
7	BBB	7	0	0	1	0
7	CCC	1	0	0	0	0
7	DDD	11	0	0	1	0
7	EEE	5	0	0	0	0
7	FFF	7	0	0	1	0
7	GGG	6	0	0	0	0
7	III	2	0	0	0	0
7	JJJ	3	0	0	0	0
All	All	13221	0	12446	278	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 11.

All (278) 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)
5:EEE:25:GLN:HE21	5:EEE:32:MET:HE2	1.21	1.06
4:DDD:187:ILE:O	4:DDD:188:ILE:HG23	1.61	1.01
4:DDD:151:THR:HG22	4:DDD:152:ASP:O	1.85	0.76
5:JJJ:66:VAL:HG11	5:JJJ:76:LEU:HD12	1.68	0.75
5:EEE:13:LEU:HD12	5:EEE:112:LEU:HD11	1.69	0.75
1:AAA:35:ARG:HD3	1:AAA:48:ARG:NH1	2.01	0.75
2:BBB:97:ARG:O	2:BBB:98:ASP:HB2	1.86	0.75
5:JJJ:66:VAL:HB	5:JJJ:76:LEU:HA	1.67	0.74
5:EEE:25:GLN:NE2	5:EEE:32:MET:HE2	2.00	0.73
5:EEE:8:PRO:HG3	5:EEE:11:GLN:HG3	1.70	0.72
4:DDD:189:PRO:HG3	5:EEE:138:HIS:CE1	2.25	0.71
4:III:184:ASN:HD21	4:III:188:ILE:HD12	1.56	0.71
1:FFF:150:ALA:HA	5:JJJ:101:THR:HG21	1.75	0.68
4:DDD:188:ILE:HD12	4:DDD:190:GLU:OE2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:III:115:VAL:O	4:III:115:VAL:HG13	1.96	0.66
5:EEE:32:MET:HE3	5:EEE:68:ARG:NH2	2.11	0.64
5:EEE:47:HIS:HE1	5:EEE:64:TYR:O	1.81	0.62
5:JJJ:86:THR:HG23	5:JJJ:113:THR:HA	1.82	0.62
5:JJJ:66:VAL:HG23	5:JJJ:75:PRO:O	2.00	0.61
5:EEE:86:THR:HG23	5:EEE:113:THR:HA	1.83	0.60
1:AAA:121:LYS:HE3	2:BBB:1:ILE:HB	1.84	0.60
5:EEE:32:MET:HE3	5:EEE:68:ARG:HH22	1.66	0.60
5:JJJ:82:ALA:N	5:JJJ:85:GLN:OE1	2.34	0.60
5:JJJ:88:VAL:HG22	5:JJJ:111:ARG:CD	2.32	0.60
5:EEE:8:PRO:HG3	5:EEE:11:GLN:CG	2.33	0.59
5:EEE:62:ASN:N	5:EEE:62:ASN:HD22	2.01	0.58
4:III:143:SER:HA	4:III:150:ILE:HD12	1.86	0.58
5:JJJ:243:ARG:HG2	5:JJJ:245:ASP:HB3	1.86	0.58
2:BBB:51:HIS:HB3	2:BBB:66:TYR:CD2	2.39	0.57
4:III:6:GLN:HE21	4:III:97:GLY:HA3	1.69	0.57
5:EEE:21:LEU:N	5:EEE:21:LEU:HD12	2.19	0.57
4:DDD:6:GLN:HE21	4:DDD:97:GLY:HA3	1.70	0.57
4:DDD:187:ILE:O	4:DDD:188:ILE:CG2	2.47	0.56
1:FFF:59:TYR:OH	1:FFF:171:TYR:OH	2.22	0.56
5:EEE:131:PRO:HG2	5:EEE:142:ALA:HB1	1.86	0.56
2:GGG:73:THR:HB	2:GGG:76:ASP:HB2	1.87	0.56
4:III:33:PHE:CD1	4:III:91:VAL:HG12	2.41	0.56
4:III:120:ASP:HB3	5:JJJ:129:PHE:CE2	2.41	0.56
1:AAA:59:TYR:HH	1:AAA:171:TYR:HH	1.53	0.56
1:AAA:159:TYR:HD1	4:DDD:31:GLN:HE22	1.53	0.56
2:BBB:46:ILE:HG21	2:BBB:68:THR:HG21	1.88	0.55
4:III:103:LEU:HD21	4:III:153:LYS:NZ	2.21	0.55
2:GGG:51:HIS:HB3	2:GGG:66:TYR:CD2	2.41	0.55
1:FFF:34:VAL:HG21	1:FFF:45:MET:HE3	1.87	0.55
5:JJJ:50:VAL:HG12	5:JJJ:50:VAL:O	2.07	0.55
2:GGG:46:ILE:HG21	2:GGG:68:THR:HG21	1.88	0.55
4:III:103:LEU:HD21	4:III:153:LYS:CE	2.37	0.55
2:GGG:84:HIS:ND1	2:GGG:86:THR:OG1	2.40	0.54
1:AAA:147:TRP:CD1	3:CCC:8:LEU:HD21	2.43	0.54
5:JJJ:13:LEU:HD21	5:JJJ:19:MET:HB2	1.90	0.54
5:EEE:198:SER:OG	1:FFF:106:ASP:OD2	2.14	0.54
5:JJJ:88:VAL:HG22	5:JJJ:111:ARG:HD2	1.90	0.54
5:JJJ:3:GLY:HA2	5:JJJ:27:MET:HE3	1.90	0.54
2:BBB:97:ARG:O	2:BBB:98:ASP:CB	2.56	0.54
1:FFF:81:LEU:HD13	1:FFF:118:TYR:CD1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:102:ASP:OD1	1:FFF:113:TYR:OH	2.18	0.53
1:AAA:85:TYR:CE2	1:AAA:137:ASP:OD2	2.61	0.53
5:EEE:5:THR:OG1	5:EEE:24:ALA:HB3	2.09	0.53
4:DDD:175:SER:C	4:DDD:177:PHE:H	2.17	0.53
5:JJJ:131:PRO:HG2	5:JJJ:142:ALA:HB1	1.90	0.53
1:AAA:102:ASP:OD1	1:AAA:113:TYR:OH	2.20	0.53
1:FFF:1:GLY:O	1:FFF:2:SER:HB2	2.08	0.53
4:III:184:ASN:ND2	4:III:188:ILE:HD12	2.22	0.53
5:JJJ:11:GLN:HG3	5:JJJ:12:VAL:O	2.08	0.52
5:EEE:70:THR:HG22	5:EEE:72:GLU:H	1.75	0.52
2:GGG:4:THR:HB	2:GGG:86:THR:HG21	1.91	0.52
1:AAA:81:LEU:HD13	1:AAA:118:TYR:CD1	2.45	0.52
2:BBB:84:HIS:HD1	2:BBB:86:THR:HG1	1.58	0.52
5:JJJ:68:ARG:HB2	5:JJJ:75:PRO:HD2	1.91	0.52
5:EEE:235:ILE:N	5:EEE:235:ILE:HD12	2.25	0.52
4:III:163:PHE:CE2	5:JJJ:141:LYS:HE3	2.45	0.52
1:AAA:34:VAL:HG21	1:AAA:45:MET:HE3	1.92	0.52
5:EEE:50:VAL:HG12	5:EEE:50:VAL:O	2.10	0.52
5:JJJ:162:VAL:HG12	5:JJJ:167:VAL:CG2	2.40	0.52
1:AAA:189:MET:HE2	1:AAA:273:ARG:C	2.35	0.51
5:EEE:38:ASP:O	5:EEE:39:PRO:C	2.54	0.51
4:III:175:SER:C	4:III:177:PHE:H	2.18	0.51
1:AAA:150:ALA:HA	5:EEE:101:THR:HG21	1.91	0.51
1:FFF:28:VAL:HG11	1:FFF:179:LEU:HD13	1.91	0.51
1:FFF:34:VAL:CG2	1:FFF:45:MET:HE3	2.40	0.51
1:FFF:99:TYR:CZ	3:HHH:3:ALA:HB3	2.45	0.51
1:FFF:126:LEU:HD12	1:FFF:132:SER:O	2.11	0.51
5:EEE:156:VAL:HG12	5:EEE:215:PHE:HA	1.92	0.51
3:CCC:6:GLY:C	3:CCC:7:ILE:HD13	2.36	0.51
4:III:184:ASN:HD21	4:III:188:ILE:CD1	2.23	0.51
5:JJJ:25:GLN:NE2	5:JJJ:29:HIS:HB2	2.26	0.51
5:JJJ:88:VAL:HG22	5:JJJ:111:ARG:HD3	1.91	0.51
4:DDD:7:ASN:HB2	4:DDD:100:THR:CG2	2.41	0.51
1:FFF:167:TRP:CE2	3:HHH:1:GLU:HG3	2.46	0.50
4:DDD:90:ALA:HB2	4:DDD:96:PHE:CD2	2.46	0.50
5:JJJ:79:LEU:HD12	5:JJJ:79:LEU:H	1.77	0.50
1:AAA:202:ARG:NH2	2:BBB:98:ASP:O	2.45	0.50
5:JJJ:200:THR:HA	5:JJJ:203:GLN:HG3	1.93	0.50
5:JJJ:34:TRP:CG	5:JJJ:76:LEU:HD13	2.47	0.50
5:EEE:234:GLN:HE21	5:EEE:236:VAL:CG2	2.24	0.50
4:DDD:189:PRO:O	4:DDD:191:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:189:MET:HE2	1:FFF:273:ARG:C	2.36	0.49
5:EEE:166:GLU:O	1:FFF:111:ARG:HD3	2.12	0.49
1:FFF:218:GLN:HA	1:FFF:222:GLU:O	2.13	0.49
5:JJJ:45:LEU:CD1	5:JJJ:58:GLY:HA3	2.42	0.49
4:III:50:ILE:HD12	4:III:56:LYS:HB2	1.94	0.49
5:JJJ:178:LEU:HD12	5:JJJ:178:LEU:C	2.36	0.49
4:DDD:81:PRO:HA	4:DDD:104:VAL:HB	1.92	0.49
1:AAA:209:TYR:CD1	1:AAA:209:TYR:C	2.91	0.49
1:AAA:218:GLN:HA	1:AAA:222:GLU:O	2.13	0.49
5:EEE:155:HIS:C	5:EEE:156:VAL:HG13	2.38	0.49
1:FFF:236:ALA:HB2	1:FFF:242:GLN:HE21	1.77	0.49
5:JJJ:13:LEU:HD21	5:JJJ:19:MET:CB	2.43	0.49
5:JJJ:15:THR:CG2	5:JJJ:83:PRO:HD3	2.43	0.49
1:AAA:231:VAL:HB	2:BBB:8:GLN:OE1	2.13	0.49
1:AAA:12:VAL:HG21	2:BBB:33:SER:OG	2.13	0.49
1:AAA:155:GLN:CG	3:CCC:5:ILE:HB	2.43	0.49
1:FFF:209:TYR:CD1	1:FFF:209:TYR:C	2.90	0.49
1:FFF:272:LEU:HA	7:FFF:307:HOH:O	2.13	0.48
1:FFF:13:SER:HG	1:FFF:93:HIS:H	1.60	0.48
1:FFF:27:TYR:HD1	1:FFF:32:GLN:HA	1.77	0.48
1:AAA:230:LEU:HD12	1:AAA:245:ALA:HB2	1.96	0.48
5:EEE:178:LEU:HD12	5:EEE:178:LEU:C	2.37	0.48
2:BBB:97:ARG:HA	7:BBB:101:HOH:O	2.14	0.48
1:AAA:178:THR:O	1:AAA:181:ARG:HG3	2.14	0.48
5:EEE:154:ASP:HB3	5:EEE:189:TYR:CZ	2.49	0.48
1:AAA:34:VAL:CG2	1:AAA:45:MET:HE3	2.44	0.48
5:EEE:4:VAL:HG22	5:EEE:25:GLN:HB3	1.95	0.48
4:III:90:ALA:HB2	4:III:96:PHE:CD2	2.49	0.48
5:JJJ:15:THR:HG22	5:JJJ:83:PRO:HD3	1.94	0.48
5:JJJ:162:VAL:HG12	5:JJJ:167:VAL:HG21	1.95	0.48
1:AAA:13:SER:HG	1:AAA:93:HIS:H	1.62	0.48
5:JJJ:19:MET:HE3	5:JJJ:21:LEU:CD2	2.44	0.48
1:FFF:76:VAL:HG11	3:HHH:9:THR:HG21	1.96	0.48
2:GGG:97:ARG:O	2:GGG:99:MET:HE2	2.13	0.48
4:III:91:VAL:HG22	4:III:95:VAL:HG23	1.95	0.48
1:AAA:230:LEU:CD1	1:AAA:245:ALA:HB2	2.44	0.47
5:JJJ:38:ASP:O	5:JJJ:39:PRO:C	2.55	0.47
4:DDD:33:PHE:CD1	4:DDD:91:VAL:HG12	2.49	0.47
5:JJJ:234:GLN:HE21	5:JJJ:236:VAL:CG2	2.27	0.47
1:AAA:126:LEU:HD12	1:AAA:132:SER:O	2.14	0.47
1:AAA:143:THR:HG23	3:CCC:10:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:227:ASP:HB3	1:AAA:248:VAL:CG2	2.44	0.47
1:AAA:28:VAL:HG11	1:AAA:179:LEU:HD13	1.97	0.47
5:EEE:13:LEU:CD1	5:EEE:112:LEU:HD11	2.42	0.47
5:EEE:97:PHE:O	5:EEE:99:GLU:N	2.48	0.47
4:III:33:PHE:CE1	4:III:91:VAL:HG12	2.50	0.47
2:BBB:84:HIS:ND1	2:BBB:86:THR:OG1	2.45	0.47
5:EEE:158:LEU:C	5:EEE:158:LEU:HD23	2.40	0.47
5:JJJ:25:GLN:HG3	5:JJJ:27:MET:H	1.79	0.47
4:DDD:33:PHE:CE1	4:DDD:91:VAL:HG12	2.50	0.47
1:AAA:51:TRP:O	1:AAA:54:GLN:HG2	2.15	0.46
1:AAA:193:ALA:HA	1:AAA:199:ALA:HA	1.98	0.46
5:EEE:65:ASN:HB2	5:EEE:77:ARG:HG3	1.97	0.46
5:JJJ:31:TYR:CD1	5:JJJ:31:TYR:C	2.93	0.46
1:AAA:236:ALA:HB2	1:AAA:242:GLN:HE21	1.80	0.46
5:EEE:15:THR:HG22	5:EEE:83:PRO:HD3	1.97	0.46
4:III:123:SER:OG	4:III:124:SER:N	2.48	0.46
5:EEE:201:PHE:CE2	1:FFF:104:GLY:HA3	2.50	0.46
1:FFF:203:CYS:HB2	1:FFF:217:TRP:CZ2	2.51	0.46
5:JJJ:45:LEU:HD12	5:JJJ:58:GLY:HA3	1.97	0.46
4:DDD:80:GLN:HB3	4:DDD:81:PRO:HD2	1.98	0.46
4:DDD:156:LEU:N	4:DDD:156:LEU:HD12	2.31	0.46
5:EEE:155:HIS:O	5:EEE:156:VAL:HG13	2.16	0.46
4:III:141:SER:OG	4:III:183:PHE:HB2	2.16	0.46
2:BBB:0:MET:HE1	2:BBB:32:PRO:HB3	1.97	0.45
4:DDD:7:ASN:HB2	4:DDD:100:THR:HG23	1.97	0.45
4:DDD:158:MET:HE2	4:DDD:161:MET:HE2	1.97	0.45
1:AAA:203:CYS:HB2	1:AAA:217:TRP:CZ2	2.51	0.45
5:EEE:2:ALA:HB2	1:FFF:136:ALA:O	2.15	0.45
5:JJJ:46:ILE:HG22	5:JJJ:47:HIS:CD2	2.52	0.45
3:CCC:7:ILE:HB	5:EEE:98:THR:OG1	2.17	0.45
1:FFF:230:LEU:HD12	1:FFF:245:ALA:HB2	1.97	0.45
2:BBB:73:THR:O	2:BBB:74:GLU:C	2.59	0.45
5:EEE:199:ALA:O	5:EEE:203:GLN:HG2	2.16	0.45
1:FFF:193:ALA:HA	1:FFF:199:ALA:HA	1.98	0.45
5:JJJ:47:HIS:CD2	5:JJJ:66:VAL:HG13	2.52	0.45
1:AAA:35:ARG:HD3	1:AAA:48:ARG:CZ	2.46	0.45
2:GGG:41:LYS:HE3	2:GGG:78:TYR:OH	2.17	0.45
1:FFF:99:TYR:OH	3:HHH:3:ALA:HB3	2.16	0.45
4:III:135:ASP:O	4:III:138:THR:OG1	2.33	0.45
4:III:175:SER:C	4:III:177:PHE:N	2.75	0.45
4:DDD:188:ILE:O	4:DDD:190:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:JJJ:158:LEU:HD23	5:JJJ:158:LEU:C	2.42	0.44
5:JJJ:162:VAL:O	5:JJJ:162:VAL:HG13	2.17	0.44
4:DDD:138:THR:HG23	4:DDD:184:ASN:HD22	1.81	0.44
4:III:143:SER:O	4:III:144:LYS:HB3	2.16	0.44
5:EEE:27:MET:HB2	5:EEE:29:HIS:CD2	2.52	0.44
2:GGG:51:HIS:HB3	2:GGG:66:TYR:CE2	2.53	0.44
1:AAA:72:GLN:HG3	5:EEE:51:GLY:HA3	1.99	0.44
4:DDD:91:VAL:HG22	4:DDD:95:VAL:HG23	1.99	0.44
2:GGG:73:THR:O	2:GGG:74:GLU:C	2.61	0.44
1:AAA:119:ASP:HB3	2:BBB:0:MET:HG3	2.00	0.44
5:EEE:105:TYR:OH	1:FFF:145:HIS:HE1	2.00	0.44
4:III:156:LEU:HD12	4:III:156:LEU:N	2.33	0.44
1:AAA:261:VAL:HB	1:AAA:270:LEU:HB2	2.00	0.44
5:EEE:1:ASN:HA	1:FFF:137:ASP:HA	2.00	0.44
5:EEE:208:HIS:NE2	5:EEE:239:GLU:CD	2.75	0.44
4:DDD:84:SER:HB3	4:DDD:104:VAL:H	1.83	0.44
4:III:90:ALA:HB2	4:III:96:PHE:CE2	2.53	0.44
4:DDD:175:SER:C	4:DDD:177:PHE:N	2.75	0.44
5:EEE:15:THR:CG2	5:EEE:83:PRO:HD3	2.47	0.44
5:EEE:31:TYR:CD1	5:EEE:31:TYR:C	2.95	0.44
1:FFF:230:LEU:CD1	1:FFF:245:ALA:HB2	2.48	0.44
4:III:80:GLN:HB3	4:III:81:PRO:HD2	1.98	0.44
4:DDD:34:PHE:HB3	4:DDD:36:TYR:CE1	2.53	0.43
1:FFF:51:TRP:CZ2	1:FFF:179:LEU:HD11	2.53	0.43
4:III:32:SER:OG	4:III:92:GLN:HA	2.18	0.43
4:DDD:167:SER:O	4:DDD:168:ALA:HB2	2.19	0.43
4:III:115:VAL:O	4:III:115:VAL:CG1	2.64	0.43
1:FFF:215:LEU:HD12	1:FFF:215:LEU:N	2.33	0.43
1:AAA:37:ASP:C	1:AAA:37:ASP:OD1	2.60	0.43
5:EEE:36:ARG:NH1	5:EEE:38:ASP:OD1	2.51	0.43
4:III:95:VAL:HG12	5:JJJ:59:GLU:OE2	2.18	0.43
5:JJJ:5:THR:OG1	5:JJJ:24:ALA:HB3	2.19	0.43
5:EEE:162:VAL:O	5:EEE:162:VAL:HG13	2.18	0.43
2:GGG:79:ALA:HB2	2:GGG:94:LYS:HA	2.00	0.43
5:JJJ:162:VAL:HG23	5:JJJ:209:PHE:CD1	2.54	0.43
5:EEE:121:VAL:HG11	5:EEE:218:LEU:CD2	2.48	0.42
1:FFF:37:ASP:C	1:FFF:37:ASP:OD1	2.61	0.42
1:AAA:51:TRP:CZ2	1:AAA:179:LEU:HD11	2.55	0.42
3:CCC:7:ILE:HD13	3:CCC:7:ILE:N	2.33	0.42
2:GGG:73:THR:HG22	2:GGG:76:ASP:H	1.85	0.42
1:AAA:201:LEU:O	1:AAA:246:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:17:ARG:C	1:AAA:19:GLU:H	2.27	0.42
1:FFF:214:THR:C	1:FFF:215:LEU:HD12	2.45	0.42
2:BBB:51:HIS:HB3	2:BBB:66:TYR:CE2	2.54	0.42
4:DDD:159:ARG:O	4:DDD:160:SER:C	2.63	0.42
5:EEE:78:LEU:HD23	5:EEE:85:GLN:NE2	2.34	0.42
5:JJJ:97:PHE:O	5:JJJ:99:GLU:N	2.53	0.42
5:JJJ:142:ALA:O	5:JJJ:196:ARG:HA	2.20	0.42
4:DDD:25:TYR:CZ	4:DDD:70:GLN:HA	2.55	0.42
1:FFF:124:ILE:O	1:FFF:124:ILE:HG23	2.20	0.42
5:EEE:21:LEU:N	5:EEE:21:LEU:CD1	2.82	0.42
1:AAA:47:PRO:O	1:AAA:48:ARG:HD3	2.20	0.42
1:FFF:151:HIS:O	1:FFF:155:GLN:HB2	2.19	0.42
4:III:167:SER:O	4:III:168:ALA:HB2	2.20	0.42
1:AAA:63:GLU:OE1	3:CCC:1:GLU:OE2	2.38	0.41
1:FFF:266:LEU:HA	1:FFF:267:PRO:HD2	1.93	0.41
4:III:93:LYS:NZ	5:JJJ:99:GLU:O	2.52	0.41
5:JJJ:11:GLN:HG2	5:JJJ:19:MET:SD	2.60	0.41
1:AAA:203:CYS:O	1:AAA:244:TRP:HA	2.20	0.41
4:III:118:LEU:HD22	5:JJJ:131:PRO:HA	2.01	0.41
5:JJJ:154:ASP:HB3	5:JJJ:189:TYR:CD2	2.55	0.41
5:JJJ:83:PRO:C	5:JJJ:85:GLN:H	2.29	0.41
1:AAA:143:THR:O	1:AAA:144:LYS:C	2.63	0.41
2:BBB:73:THR:HG22	2:BBB:76:ASP:H	1.85	0.41
4:DDD:90:ALA:HB2	4:DDD:96:PHE:CE2	2.55	0.41
5:EEE:168:HIS:CG	1:FFF:128:GLU:HB2	2.54	0.41
5:EEE:68:ARG:HG3	5:EEE:68:ARG:O	2.20	0.41
4:DDD:184:ASN:O	4:DDD:185:ASN:CB	2.68	0.41
5:EEE:142:ALA:O	5:EEE:196:ARG:HA	2.21	0.41
5:JJJ:224:TRP:CZ2	5:JJJ:226:GLN:HG3	2.55	0.41
1:AAA:124:ILE:O	1:AAA:124:ILE:HG23	2.21	0.41
1:FFF:117:ALA:HB2	2:GGG:60:TRP:CE2	2.56	0.41
1:FFF:231:VAL:HG13	1:FFF:244:TRP:CZ2	2.56	0.41
2:GGG:79:ALA:CB	2:GGG:94:LYS:HA	2.51	0.41
1:AAA:266:LEU:HA	1:AAA:267:PRO:HD2	1.92	0.41
5:EEE:25:GLN:NE2	5:EEE:29:HIS:HB2	2.36	0.41
5:EEE:146:CYS:HB2	5:EEE:160:TRP:CZ2	2.56	0.41
5:EEE:200:THR:HA	5:EEE:203:GLN:CG	2.51	0.41
1:FFF:51:TRP:O	1:FFF:54:GLN:HG2	2.21	0.41
1:FFF:203:CYS:O	1:FFF:244:TRP:HA	2.21	0.41
4:III:120:ASP:HA	5:JJJ:129:PHE:HA	2.03	0.41
1:AAA:227:ASP:HB3	1:AAA:248:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GGG:16:GLU:CB	2:GGG:19:LYS:HD3	2.51	0.40
4:III:25:TYR:CZ	4:III:70:GLN:HA	2.57	0.40
5:JJJ:140:GLN:C	5:JJJ:199:ALA:HB2	2.45	0.40
4:DDD:28:ARG:HD2	7:DDD:205:HOH:O	2.20	0.40
5:EEE:163:ASN:HD21	5:EEE:207:ASN:ND2	2.19	0.40
4:III:9:GLY:HA3	4:III:10:PRO:C	2.46	0.40
4:III:34:PHE:HB3	4:III:36:TYR:CE1	2.57	0.40
4:III:159:ARG:O	4:III:160:SER:C	2.64	0.40
1:AAA:275:GLU:OE1	1:AAA:275:GLU:N	2.54	0.40
4:III:98:THR:HG23	5:JJJ:40:GLY:O	2.21	0.40
1:AAA:173:GLU:O	1:AAA:175:GLY:N	2.54	0.40
1:AAA:214:THR:C	1:AAA:215:LEU:HD12	2.47	0.40
5:JJJ:39:PRO:HB3	5:JJJ:176:GLN:HE22	1.86	0.40
4:DDD:54:GLY:O	4:DDD:64:GLN:HA	2.22	0.40
4:DDD:158:MET:SD	4:DDD:161:MET:CE	3.09	0.40
5:EEE:97:PHE:O	5:EEE:98:THR:C	2.64	0.40
5:EEE:140:GLN:C	5:EEE:199:ALA:HB2	2.47	0.40
1:FFF:201:LEU:O	1:FFF:246:ALA:HA	2.22	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	273/275 (99%)	247 (90%)	23 (8%)	3 (1%)	11	40
1	FFF	273/275 (99%)	246 (90%)	25 (9%)	2 (1%)	18	50
2	BBB	98/100 (98%)	89 (91%)	7 (7%)	2 (2%)	6	28
2	GGG	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
3	CCC	8/10 (80%)	7 (88%)	0	1 (12%)	0	1
3	HHH	8/10 (80%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	DDD	191/193 (99%)	160 (84%)	24 (13%)	7 (4%)	2	16
4	III	188/193 (97%)	156 (83%)	27 (14%)	5 (3%)	4	22
5	EEE	243/245 (99%)	219 (90%)	21 (9%)	3 (1%)	10	38
5	JJJ	243/245 (99%)	222 (91%)	20 (8%)	1 (0%)	30	60
All	All	1623/1646 (99%)	1440 (89%)	159 (10%)	24 (2%)	8	34

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	CCC	9	THR
4	DDD	176	ASP
4	DDD	185	ASN
4	DDD	190	GLU
1	FFF	2	SER
4	III	176	ASP
2	BBB	98	ASP
4	DDD	168	ALA
4	III	85	ALA
4	III	168	ALA
5	JJJ	98	THR
1	AAA	174	ASN
4	DDD	160	SER
5	EEE	98	THR
1	FFF	174	ASN
4	III	9	GLY
4	III	144	LYS
2	BBB	52	SER
4	DDD	85	ALA
4	DDD	189	PRO
5	EEE	2	ALA
5	EEE	84	SER
1	AAA	151	HIS
1	AAA	18	GLY

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	231/231 (100%)	220 (95%)	11 (5%)	23	53
1	FFF	231/231 (100%)	213 (92%)	18 (8%)	11	38
2	BBB	95/95 (100%)	90 (95%)	5 (5%)	20	51
2	GGG	95/95 (100%)	87 (92%)	8 (8%)	10	35
3	CCC	6/6 (100%)	6 (100%)	0	100	100
3	HHH	6/6 (100%)	4 (67%)	2 (33%)	0	1
4	DDD	173/173 (100%)	164 (95%)	9 (5%)	21	51
4	III	170/173 (98%)	157 (92%)	13 (8%)	12	39
5	EEE	212/212 (100%)	200 (94%)	12 (6%)	18	49
5	JJJ	212/212 (100%)	195 (92%)	17 (8%)	11	37
All	All	1431/1434 (100%)	1336 (93%)	95 (7%)	15	44

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	11	SER
1	AAA	35	ARG
1	AAA	45	MET
1	AAA	113	TYR
1	AAA	174	ASN
1	AAA	209	TYR
1	AAA	220	ASP
1	AAA	225	THR
1	AAA	227	ASP
1	AAA	248	VAL
1	AAA	268	LYS
2	BBB	4	THR
2	BBB	70	PHE
2	BBB	86	THR
2	BBB	88	SER
2	BBB	97	ARG
4	DDD	4	VAL
4	DDD	31	GLN
4	DDD	77	ARG
4	DDD	135	ASP
4	DDD	137	GLN
4	DDD	141	SER
4	DDD	165	SER

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Mol	Chain	Res	Type
4	DDD	173	ASN
4	DDD	177	PHE
5	EEE	19	MET
5	EEE	49	SER
5	EEE	54	ILE
5	EEE	62	ASN
5	EEE	66	VAL
5	EEE	67	SER
5	EEE	71	THR
5	EEE	84	SER
5	EEE	98	THR
5	EEE	176	GLN
5	EEE	225	THR
5	EEE	227	ASP
1	FFF	2	SER
1	FFF	11	SER
1	FFF	35	ARG
1	FFF	45	MET
1	FFF	105	SER
1	FFF	113	TYR
1	FFF	122	ASP
1	FFF	146	LYS
1	FFF	174	ASN
1	FFF	182	THR
1	FFF	206	LEU
1	FFF	207	SER
1	FFF	209	TYR
1	FFF	214	THR
1	FFF	227	ASP
1	FFF	248	VAL
1	FFF	256	ARG
1	FFF	260	HIS
2	GGG	19	LYS
2	GGG	74	GLU
2	GGG	75	LYS
2	GGG	76	ASP
2	GGG	86	THR
2	GGG	87	LEU
2	GGG	94	LYS
2	GGG	98	ASP
3	HHH	1	GLU
3	HHH	9	THR

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Mol	Chain	Res	Type
4	III	3	GLU
4	III	5	GLU
4	III	31	GLN
4	III	57	GLU
4	III	78	ASP
4	III	98	THR
4	III	110	ASN
4	III	125	ASP
4	III	127	SER
4	III	129	CYS
4	III	135	ASP
4	III	137	GLN
4	III	165	SER
5	JJJ	26	ASP
5	JJJ	41	MET
5	JJJ	49	SER
5	JJJ	55	THR
5	JJJ	66	VAL
5	JJJ	67	SER
5	JJJ	70	THR
5	JJJ	76	LEU
5	JJJ	84	SER
5	JJJ	167	VAL
5	JJJ	194	ARG
5	JJJ	201	PHE
5	JJJ	204	ASP
5	JJJ	207	ASN
5	JJJ	210	ARG
5	JJJ	220	GLU
5	JJJ	245	ASP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EDO	AAA	301	-	3,3,3	0.23	0	2,2,2	0.21	0
6	EDO	GGG	101	-	3,3,3	0.09	0	2,2,2	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	AAA	301	-	-	0/1/1/1	-
6	EDO	GGG	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	275/275 (100%)	-0.08	1 (0%) 88 79	34, 51, 89, 126	0
1	FFF	275/275 (100%)	0.14	3 (1%) 78 61	35, 55, 122, 145	0
2	BBB	100/100 (100%)	-0.31	1 (1%) 79 63	30, 44, 59, 69	0
2	GGG	100/100 (100%)	-0.22	0 100 100	37, 46, 55, 62	0
3	CCC	10/10 (100%)	-0.17	0 100 100	34, 37, 44, 46	0
3	HHH	10/10 (100%)	-0.28	0 100 100	37, 39, 46, 48	0
4	DDD	193/193 (100%)	0.19	1 (0%) 87 76	38, 51, 87, 99	0
4	III	190/193 (98%)	0.57	7 (3%) 45 29	47, 73, 115, 132	0
5	EEE	245/245 (100%)	0.02	0 100 100	35, 58, 83, 102	0
5	JJJ	245/245 (100%)	0.40	1 (0%) 88 79	45, 71, 96, 110	0
All	All	1643/1646 (99%)	0.13	14 (0%) 81 64	30, 56, 102, 145	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	III	188	ILE	3.4
4	DDD	180	ALA	3.0
4	III	184	ASN	2.9
4	III	187	ILE	2.7
4	III	182	ALA	2.7
4	III	177	PHE	2.5
1	FFF	128	GLU	2.5
4	III	183	PHE	2.4
1	AAA	194	VAL	2.1
1	FFF	252	GLY	2.1
1	FFF	274	TRP	2.1
4	III	129	CYS	2.1
5	JJJ	1	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	BBB	1	ILE	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	AAA	301	4/4	0.94	0.09	39,39,40,40	0
6	EDO	GGG	101	4/4	0.94	0.09	37,37,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.