



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:44 PM UTC

PDB ID : 2IAE / pdb_00002iae
Title : Crystal structure of a protein phosphatase 2A (PP2A) holoenzyme.
Authors : Cho, U.S.; Xu, W.
Deposited on : 2006-09-07
Resolution : 3.50 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)
Xtrriage (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

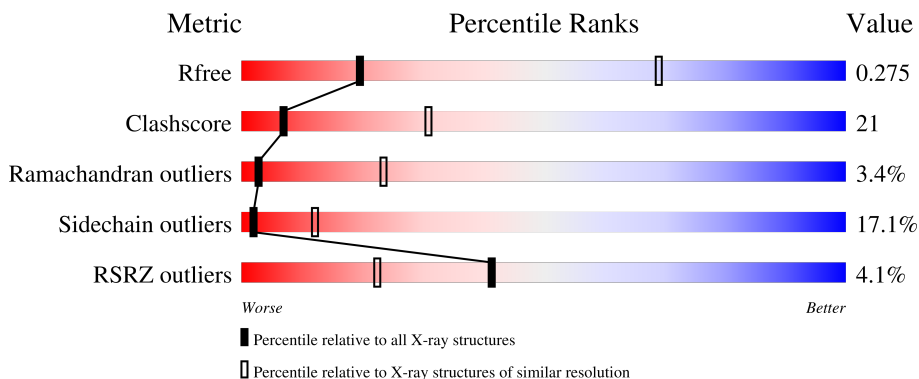
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



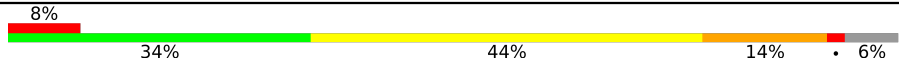


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	A	589	 5% 59% 34% 5% ..
1	D	589	 2% 61% 31% 6% .
2	B	407	 2% 49% 35% 8% . 8%
2	E	407	 3% 44% 37% 11% 7%
3	C	309	 5% 50% 38% 10% ..

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Mol	Chain	Length	Quality of chain
3	F	309	
4	M	7	
4	N	7	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLL	C	309	-	X	-	-
4	DAM	M	7	-	-	X	-
4	ACB	N	3	-	-	X	-
4	DAM	N	7	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19955 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	Total	C	N	O	S	0	0	0
			4541	2885	765	864	27			
1	D	583	Total	C	N	O	S	0	0	0
			4541	2885	765	864	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	376	Total	C	N	O	S	0	0	0
			2974	1945	486	533	10			
2	E	377	Total	C	N	O	S	0	0	0
			2987	1958	487	531	11			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	306	Total	C	N	O	S	0	0	0
			2430	1538	415	462	15			
3	F	291	Total	C	N	O	S	0	0	0
			2336	1479	402	440	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	ASN	ASP	engineered mutation	UNP P67775
F	88	ASN	ASP	engineered mutation	UNP P67775

- Molecule 4 is a protein called microcystin-LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	N	7	Total	C	N	O	0	0	0
			71	49	10	12			

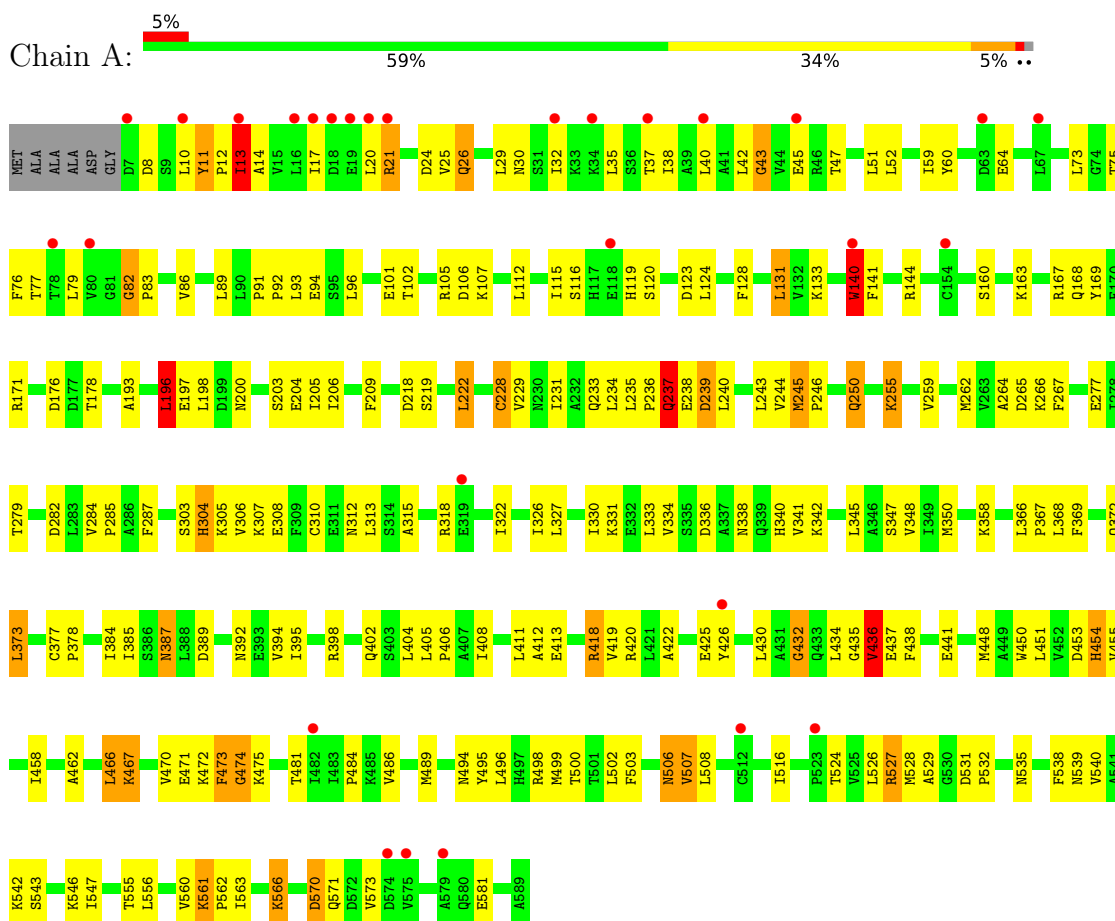
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		

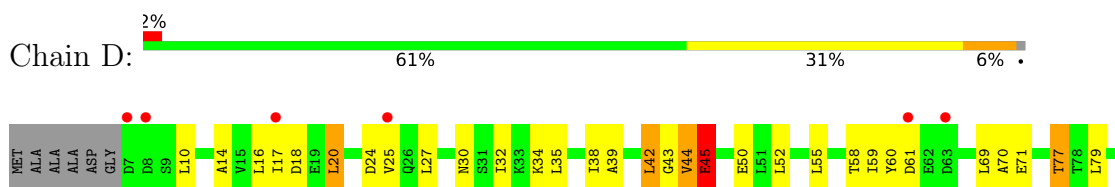
3 Residue-property plots [i](#)

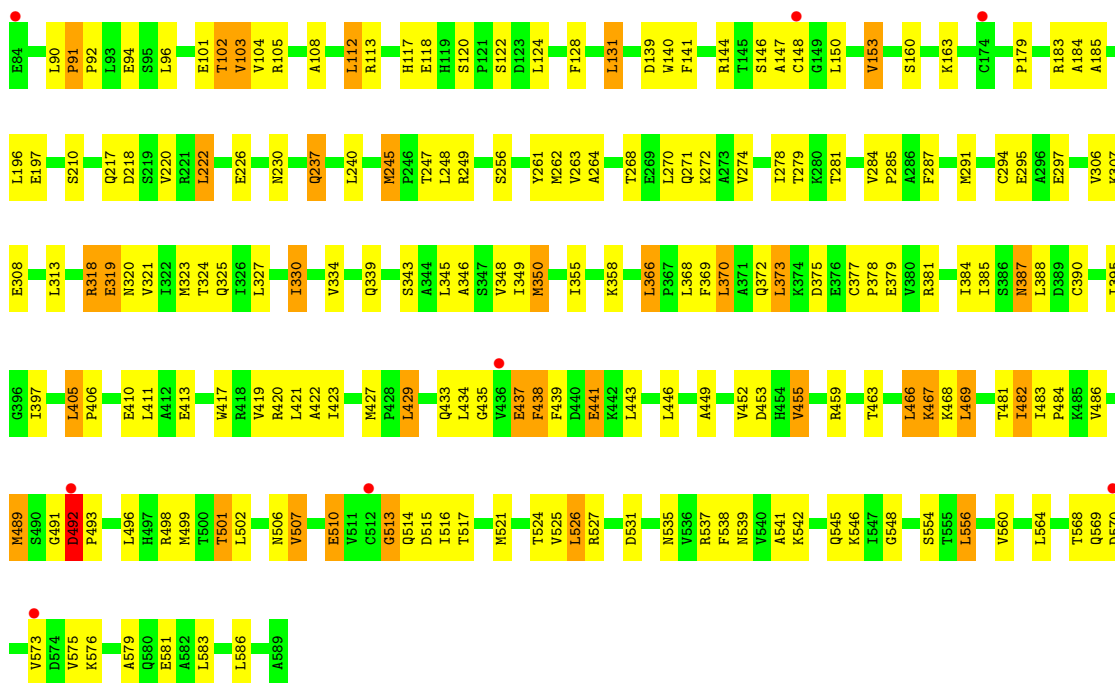
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

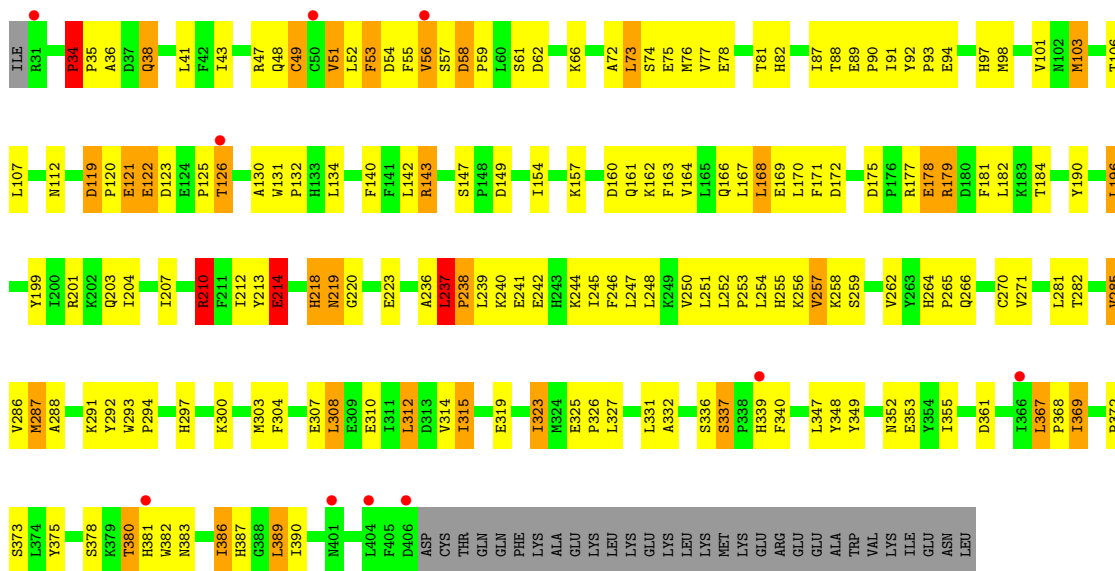


- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

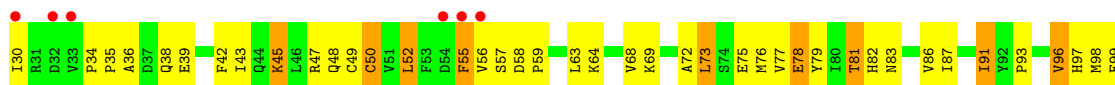
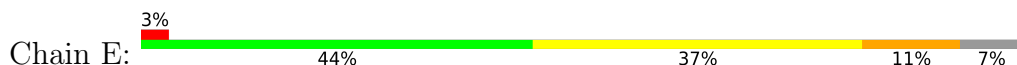


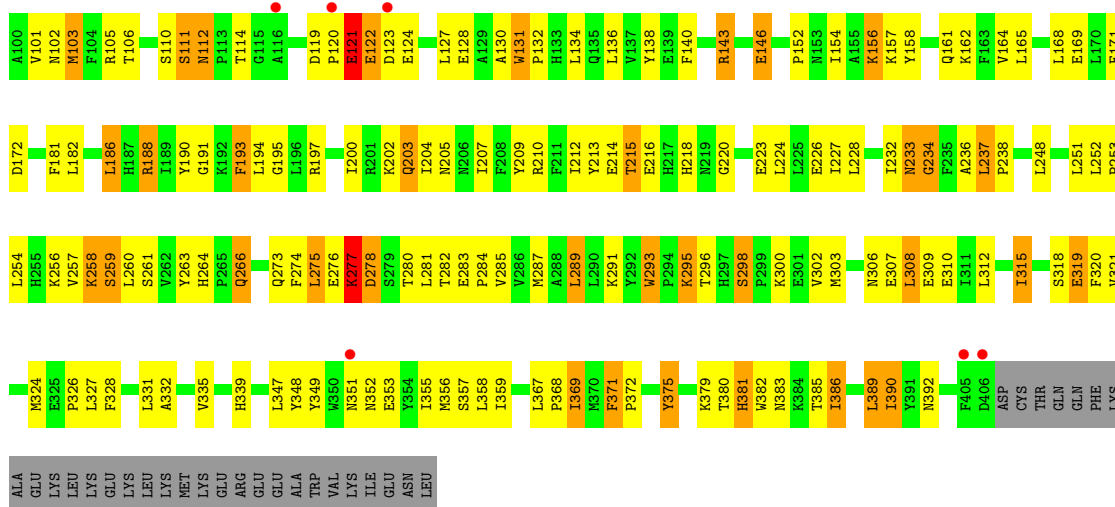


• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

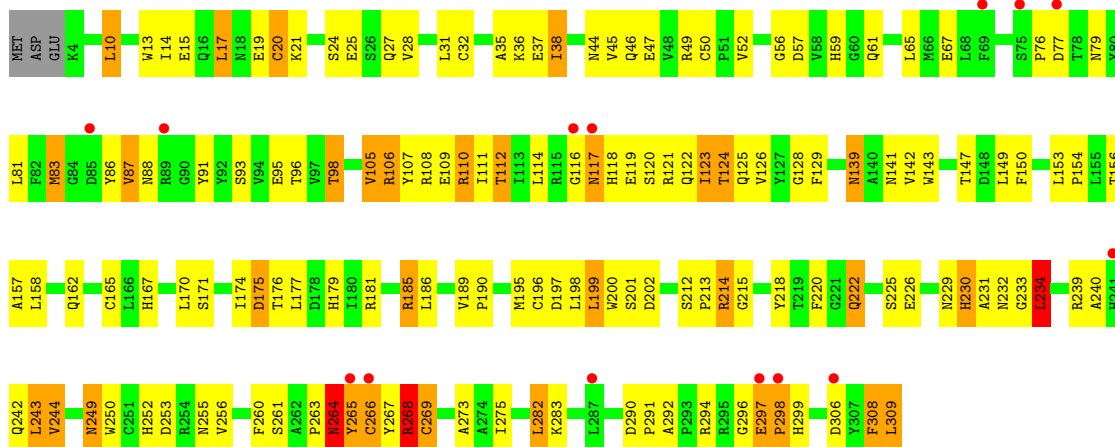


• Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

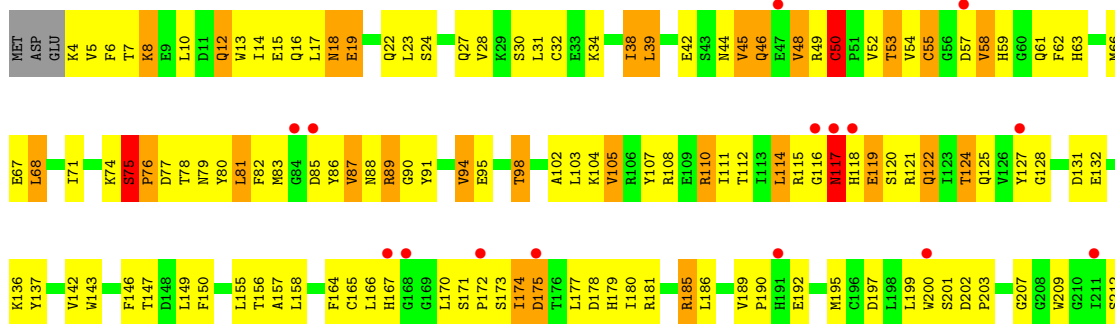


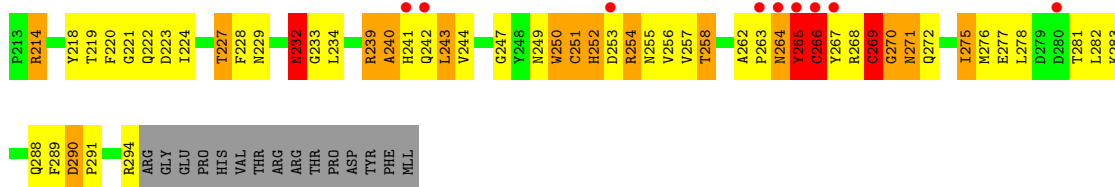


• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform



• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform





- Molecule 4: microcystin-LR



- Molecule 4: microcystin-LR



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	265.30Å 265.30Å 265.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.50) 96.9 (20.00-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.316 0.233 , 0.275	Depositor DCC
R_{free} test set	3853 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	111.3	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 169.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.037 for l,-k,h	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19955	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1ZN, DAM, MLL, MN, FGA, DAL, ACB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/4615	0.95	8/6266 (0.1%)
1	D	0.54	0/4615	0.96	6/6266 (0.1%)
2	B	0.57	0/3056	1.00	10/4170 (0.2%)
2	E	0.57	0/3073	0.99	9/4195 (0.2%)
3	C	0.56	0/2480	0.98	7/3371 (0.2%)
3	F	0.66	0/2393	1.04	6/3247 (0.2%)
4	M	0.67	0/17	1.03	0/19
4	N	1.56	0/17	1.27	0/19
All	All	0.57	0/20266	0.98	46/27553 (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
1	A	0	1
1	D	0	2
2	B	0	1
2	E	0	2
3	C	0	4
3	F	0	2
4	M	0	4
4	N	0	1
All	All	0	17

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	87	VAL	N-CA-C	9.29	119.20	110.74
2	B	49	CYS	N-CA-C	-7.77	104.32	113.88
2	B	34	PRO	N-CA-CB	7.47	110.33	103.08
3	C	298	PRO	N-CA-CB	7.41	111.03	103.25
3	C	234	LEU	N-CA-C	7.34	124.19	113.40
2	E	293	TRP	CA-C-N	7.12	127.16	119.90
2	E	293	TRP	C-N-CA	7.12	127.16	119.90
2	E	353	GLU	N-CA-C	6.86	118.45	110.97
2	B	66	LYS	N-CA-C	-6.85	104.49	112.92
2	E	352	ASN	N-CA-C	6.68	120.42	109.06
1	A	140	TRP	N-CA-C	6.66	118.25	108.86
2	B	337	SER	CA-C-N	6.66	128.16	119.84
2	B	337	SER	C-N-CA	6.66	128.16	119.84
1	D	438	PHE	N-CA-C	-6.24	106.20	113.88
3	C	297	GLU	N-CA-C	6.21	118.61	109.42
1	A	17	ILE	N-CA-C	6.14	117.86	108.71
1	A	527	ARG	N-CA-C	-6.09	106.39	113.88
3	C	88	ASN	N-CA-C	6.07	123.73	110.80
2	E	193	PHE	N-CA-C	5.95	117.98	108.41
1	D	319	GLU	N-CA-C	-5.93	104.82	111.28
3	C	87	VAL	N-CA-C	5.92	120.50	113.22
3	F	50	CYS	N-CA-C	5.91	122.86	109.81
1	A	235	LEU	N-CA-C	5.88	122.80	109.81
1	A	82	GLY	CA-C-N	5.71	126.98	119.84
1	A	82	GLY	C-N-CA	5.71	126.98	119.84
3	F	253	ASP	N-CA-C	-5.61	98.85	110.80
2	B	236	ALA	N-CA-C	5.56	118.32	109.65
2	B	361	ASP	N-CA-C	-5.55	105.87	113.30
2	E	298	SER	N-CA-C	5.54	120.45	113.25
1	A	470	VAL	N-CA-C	-5.50	108.14	113.53
3	C	264	ASN	N-CA-C	5.47	117.61	107.99
1	A	259	VAL	N-CA-C	-5.46	106.37	111.45
3	F	90	GLY	N-CA-C	-5.45	100.25	113.18
2	E	112	ASN	CA-C-N	5.29	125.59	119.93
2	E	112	ASN	C-N-CA	5.29	125.59	119.93
2	E	215	THR	CB-CA-C	-5.28	102.91	110.62
3	F	50	CYS	CA-C-N	-5.23	113.91	119.98
3	F	50	CYS	C-N-CA	-5.23	113.91	119.98
2	B	210	ARG	N-CA-C	-5.23	105.47	111.07
1	D	516	ILE	N-CA-C	-5.23	105.44	110.72
1	D	91	PRO	N-CA-C	5.14	116.97	110.70
1	D	570	ASP	N-CA-C	5.14	117.67	109.65
3	C	50	CYS	N-CA-C	5.06	119.38	112.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	ASP	CA-C-N	5.05	124.77	119.82
2	B	119	ASP	C-N-CA	5.05	124.77	119.82
1	D	230	ASN	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	LEU	Peptide
2	B	214	GLU	Peptide
3	C	233	GLY	Peptide
3	C	266	CYS	Peptide
3	C	296	GLY	Peptide
3	C	308	PHE	Peptide
1	D	492	ASP	Peptide
1	D	59	ILE	Peptide
2	E	234	GLY	Peptide
2	E	277	LYS	Peptide
3	F	266	CYS	Peptide
3	F	75	SER	Peptide
4	M	2	LEU	Mainchain
4	M	4	ARG	Peptide
4	M	5	1ZN	Peptide,Mainchain
4	N	5	1ZN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4541	0	4641	142	0
1	D	4541	0	4641	133	0
2	B	2974	0	2849	127	0
2	E	2987	0	2858	137	0
3	C	2430	0	2273	112	2
3	F	2336	0	2229	188	4
4	M	71	0	62	16	2
4	N	71	0	63	29	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	19955	0	19616	835	6

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 21.

All (835) 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)
4:N:2:LEU:HA	4:N:3:ACB:C4	1.12	1.53
4:N:2:LEU:CA	4:N:3:ACB:H43	1.04	1.51
4:N:2:LEU:O	4:N:3:ACB:N	1.74	1.18
4:N:2:LEU:CA	4:N:3:ACB:C4	1.86	1.17
4:N:2:LEU:HA	4:N:3:ACB:H42	1.29	1.12
4:N:2:LEU:N	4:N:3:ACB:C4	2.09	1.12
3:F:171:SER:HB2	3:F:197:ASP:HB3	1.33	1.08
3:C:269:CYS:SG	4:M:7:DAM:HB2	1.95	1.07
3:F:88:ASN:HB2	3:F:118:HIS:HD2	1.20	1.05
1:D:245:MET:HE3	1:D:245:MET:HA	1.38	1.03
1:D:437:GLU:OE1	1:D:437:GLU:HA	1.52	1.03
4:N:2:LEU:C	4:N:3:ACB:H43	1.84	1.03
3:F:46:GLN:HE21	3:F:46:GLN:HA	1.22	1.01
1:D:492:ASP:HA	1:D:498:ARG:HD3	1.38	1.00
4:N:2:LEU:N	4:N:3:ACB:H41	1.76	0.99
3:C:269:CYS:SG	4:M:7:DAM:CB	2.51	0.99
3:F:45:VAL:HG23	3:F:156:THR:HG23	1.43	0.98
3:F:79:ASN:HD21	3:F:110:ARG:HE	1.12	0.97
3:C:185:ARG:HH21	3:C:185:ARG:HG3	1.28	0.95
2:E:237:LEU:HB3	2:E:238:PRO:HD2	1.49	0.94
3:C:124:THR:CG2	3:C:143:TRP:HE1	1.82	0.93
2:E:57:SER:HB2	2:E:59:PRO:HD2	1.52	0.92
2:E:103:MET:HE3	2:E:103:MET:HA	1.50	0.91
2:B:352:ASN:HB2	2:B:355:ILE:HD12	1.53	0.91
3:F:244:VAL:HG11	3:F:249:ASN:HB2	1.51	0.91
3:F:243:LEU:CD2	4:N:7:DAM:HB1	2.00	0.90
4:N:2:LEU:N	4:N:3:ACB:H43	1.77	0.90
3:F:171:SER:HB2	3:F:197:ASP:CB	2.02	0.89
3:F:88:ASN:HB2	3:F:118:HIS:CD2	2.06	0.89
2:E:120:PRO:C	2:E:122:GLU:H	1.79	0.88
3:F:214:ARG:HG2	3:F:214:ARG:HH11	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:214:ARG:NE	3:F:241:HIS:HE1	1.70	0.88
1:D:499:MET:HE2	1:D:539:ASN:HD22	1.37	0.88
4:N:2:LEU:H	4:N:3:ACB:H41	1.37	0.88
3:F:243:LEU:HD21	4:N:7:DAM:HB1	1.55	0.87
3:F:124:THR:HG21	3:F:143:TRP:HE1	1.38	0.87
2:B:87:ILE:HA	2:B:91:ILE:HD11	1.56	0.87
3:F:214:ARG:O	4:N:4:ARG:NH1	2.08	0.87
3:F:276:MET:HE3	3:F:278:LEU:HD21	1.55	0.86
1:D:417:TRP:HZ3	1:D:421:LEU:HD12	1.41	0.85
1:D:245:MET:HA	1:D:245:MET:CE	2.06	0.85
3:F:124:THR:CG2	3:F:143:TRP:HE1	1.91	0.84
3:F:269:CYS:SG	4:N:7:DAM:CB	2.66	0.83
3:C:185:ARG:HH21	3:C:185:ARG:CG	1.92	0.82
2:B:367:LEU:H	2:B:368:PRO:HD2	1.44	0.82
3:C:171:SER:HB2	3:C:197:ASP:HB2	1.62	0.81
3:F:8:LYS:HE3	3:F:8:LYS:HA	1.61	0.81
3:F:98:THR:HB	3:F:146:PHE:HZ	1.45	0.81
1:D:492:ASP:HA	1:D:498:ARG:CD	2.10	0.80
3:F:229:ASN:HD22	3:F:255:ASN:HD22	1.29	0.80
3:F:79:ASN:ND2	3:F:110:ARG:HE	1.79	0.80
3:F:116:GLY:H	3:F:119:GLU:HG2	1.47	0.80
1:D:548:GLY:HA3	1:D:586:LEU:HD21	1.62	0.80
3:F:269:CYS:CB	4:N:7:DAM:HB2	2.12	0.79
2:B:256:LYS:HB2	3:C:309:MLL:HD22	1.64	0.79
3:C:17:LEU:HD12	3:C:98:THR:HG23	1.65	0.79
1:A:115:ILE:O	1:A:119:HIS:HD2	1.65	0.78
3:C:124:THR:HG23	3:C:143:TRP:HE1	1.46	0.78
1:D:499:MET:HE2	1:D:539:ASN:ND2	1.98	0.78
3:F:171:SER:HB3	3:F:174:ILE:HD11	1.63	0.78
3:F:201:SER:HB2	3:F:218:TYR:O	1.83	0.78
2:E:190:TYR:CZ	2:E:197:ARG:HG3	2.19	0.78
3:C:201:SER:HB2	3:C:218:TYR:O	1.85	0.77
3:F:264:ASN:HA	3:F:267:TYR:O	1.85	0.77
3:C:243:LEU:HD21	4:M:7:DAM:HB1	1.65	0.77
2:B:237:LEU:HB2	2:B:238:PRO:HD2	1.67	0.77
3:F:269:CYS:SG	4:N:7:DAM:HB2	2.26	0.76
1:D:268:THR:HG21	1:D:308:GLU:HG2	1.68	0.75
1:D:435:GLY:HA2	1:D:438:PHE:HB3	1.68	0.75
3:F:24:SER:H	3:F:27:GLN:HE21	1.35	0.75
1:A:237:GLN:H	1:A:239:ASP:HB3	1.51	0.75
3:C:265:TYR:O	3:C:268:ARG:HB3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:201:SER:HB3	3:C:218:TYR:H	1.52	0.74
3:F:147:THR:HA	3:F:150:PHE:CD1	2.22	0.74
2:B:52:LEU:HD11	2:B:97:HIS:CD2	2.22	0.74
2:B:121:GLU:OE1	4:M:2:LEU:CD1	2.36	0.74
3:F:88:ASN:CB	3:F:118:HIS:HD2	1.99	0.74
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.69	0.73
3:C:120:SER:O	3:C:124:THR:HB	1.87	0.73
3:F:38:ILE:HD12	3:F:108:ARG:HD3	1.70	0.73
1:A:418:ARG:CG	1:A:418:ARG:HH21	2.02	0.73
1:A:303:SER:C	1:A:305:LYS:H	1.95	0.73
3:F:214:ARG:HH11	3:F:214:ARG:CG	2.01	0.73
1:A:244:VAL:O	1:A:244:VAL:HG22	1.87	0.72
1:A:500:THR:HA	1:A:503:PHE:HB2	1.70	0.72
3:F:45:VAL:HG11	3:F:181:ARG:NH1	2.03	0.72
3:F:45:VAL:HG23	3:F:156:THR:CG2	2.19	0.72
1:A:101:GLU:HG2	2:B:256:LYS:HE2	1.70	0.72
1:D:268:THR:HG21	1:D:308:GLU:CG	2.20	0.72
3:F:46:GLN:HE21	3:F:46:GLN:CA	2.01	0.72
1:A:418:ARG:HH21	1:A:418:ARG:HG3	1.54	0.71
1:D:455:VAL:HG23	3:F:71:ILE:HA	1.73	0.71
3:F:68:LEU:HD13	3:F:275:ILE:HG21	1.73	0.71
3:F:214:ARG:NE	3:F:241:HIS:CE1	2.56	0.71
1:A:11:TYR:N	1:A:12:PRO:HD3	2.06	0.71
2:B:252:LEU:HD22	2:B:288:ALA:HB3	1.73	0.71
2:B:332:ALA:HB1	2:B:372:PRO:HG2	1.73	0.71
2:B:168:LEU:HD21	2:B:204:ILE:HG22	1.73	0.71
3:F:24:SER:H	3:F:27:GLN:NE2	1.88	0.71
3:F:75:SER:O	3:F:77:ASP:N	2.23	0.71
4:M:3:ACB:O	4:M:6:FGA:HB3	1.91	0.71
1:D:324:THR:HG23	1:D:325:GLN:HG3	1.72	0.70
2:E:321:VAL:HA	2:E:324:MET:HE3	1.73	0.70
3:F:76:PRO:HG3	3:F:107:TYR:CE2	2.25	0.70
3:F:53:THR:HB	3:F:277:GLU:HG2	1.72	0.70
3:C:107:TYR:HB3	3:C:110:ARG:HB2	1.72	0.70
2:B:58:ASP:H	2:B:59:PRO:HD3	1.57	0.70
1:A:133:LYS:HE2	1:A:169:TYR:HE1	1.57	0.69
2:B:287:MET:O	2:B:291:LYS:HG2	1.93	0.69
2:B:52:LEU:HD11	2:B:97:HIS:HD2	1.55	0.69
1:D:499:MET:CE	1:D:539:ASN:HD22	2.06	0.69
2:B:74:SER:O	2:B:77:VAL:HG12	1.92	0.69
3:C:76:PRO:HB3	3:C:107:TYR:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:381:HIS:CG	2:E:386:ILE:HD11	2.28	0.69
1:D:43:GLY:C	1:D:45:GLU:H	1.97	0.68
3:F:232:ASN:HB3	3:F:234:LEU:HG	1.75	0.68
1:D:222:LEU:HD23	1:D:262:MET:HG3	1.75	0.68
2:E:212:ILE:HD11	2:E:254:LEU:HG	1.75	0.68
3:F:17:LEU:HD13	3:F:23:LEU:HD23	1.75	0.68
3:C:65:LEU:HD22	3:C:96:THR:HG23	1.75	0.68
3:C:124:THR:HG21	3:C:143:TRP:HE1	1.59	0.68
3:C:150:PHE:HA	3:C:153:LEU:HD12	1.76	0.68
1:A:494:ASN:HD21	1:A:496:LEU:HD23	1.59	0.67
4:N:2:LEU:C	4:N:3:ACB:H2	2.02	0.67
2:B:38:GLN:HA	2:B:38:GLN:HE21	1.59	0.67
1:D:274:VAL:CG1	1:D:278:ILE:HB	2.25	0.67
3:F:269:CYS:HB3	4:N:7:DAM:HB2	1.75	0.67
1:A:494:ASN:HD22	1:A:495:TYR:N	1.92	0.67
2:B:51:VAL:HG21	2:B:73:LEU:HB3	1.76	0.67
2:B:81:THR:HG21	2:B:143:ARG:HG2	1.76	0.67
2:E:228:LEU:O	2:E:232:ILE:HG12	1.95	0.67
3:F:247:GLY:HA2	3:F:272:GLN:O	1.95	0.67
2:E:248:LEU:HA	2:E:252:LEU:HD12	1.76	0.67
1:A:128:PHE:O	1:A:131:LEU:HB3	1.96	0.66
1:D:535:ASN:HA	1:D:538:PHE:CE1	2.30	0.66
3:F:243:LEU:HD23	4:N:7:DAM:HB1	1.77	0.66
2:B:81:THR:CG2	2:B:143:ARG:HG2	2.26	0.66
1:D:417:TRP:CZ3	1:D:421:LEU:HD12	2.28	0.66
3:F:264:ASN:HB2	3:F:270:GLY:HA2	1.78	0.66
4:N:2:LEU:H	4:N:3:ACB:C4	1.94	0.66
1:A:306:VAL:HG11	1:A:330:ILE:HD11	1.78	0.66
2:E:57:SER:CB	2:E:59:PRO:HD2	2.25	0.66
1:A:561:LYS:H	1:A:562:PRO:HD2	1.61	0.65
2:E:320:PHE:CE2	2:E:324:MET:HG3	2.31	0.65
2:E:112:ASN:HD21	2:E:124:GLU:H	1.42	0.65
2:E:204:ILE:HA	2:E:207:ILE:HG12	1.77	0.65
2:B:160:ASP:HB3	2:B:163:PHE:H	1.60	0.65
1:A:529:ALA:HB2	1:A:540:VAL:HG11	1.79	0.65
3:F:31:LEU:HD11	3:F:102:ALA:HA	1.78	0.65
3:F:214:ARG:CZ	3:F:241:HIS:HE1	2.09	0.65
3:F:18:ASN:HD22	3:F:66:MET:HE1	1.61	0.65
3:F:39:LEU:HD23	3:F:149:LEU:HD11	1.79	0.65
2:B:300:LYS:HA	2:B:303:MET:HE3	1.79	0.64
2:B:34:PRO:N	2:B:35:PRO:CD	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:237:LEU:HB3	2:E:238:PRO:CD	2.26	0.64
3:F:174:ILE:HG22	3:F:179:HIS:HB3	1.79	0.64
3:C:264:ASN:HA	3:C:267:TYR:O	1.97	0.64
4:M:3:ACB:O	4:M:6:FGA:CB	2.46	0.63
3:F:24:SER:HB3	3:F:27:GLN:HB2	1.80	0.63
3:C:243:LEU:CD2	4:M:7:DAM:HB1	2.29	0.63
1:D:496:LEU:CD2	3:F:78:THR:HG22	2.29	0.63
2:E:146:GLU:OE1	2:E:146:GLU:HA	1.97	0.63
3:F:46:GLN:HA	3:F:46:GLN:NE2	2.06	0.63
1:A:341:VAL:HG23	1:A:342:LYS:N	2.14	0.63
1:D:256:SER:HB3	2:E:106:THR:HG21	1.81	0.63
2:E:223:GLU:O	2:E:226:GLU:HB3	1.99	0.63
2:B:34:PRO:N	2:B:35:PRO:HD3	2.14	0.62
3:F:88:ASN:HD21	3:F:124:THR:HA	1.63	0.62
3:F:239:ARG:HG3	3:F:258:THR:HA	1.81	0.62
2:B:130:ALA:O	2:B:134:LEU:HG	1.99	0.62
1:A:176:ASP:OD2	1:A:178:THR:HG22	1.99	0.62
2:E:278:ASP:OD1	2:E:280:THR:HG22	2.00	0.62
3:F:164:PHE:HE2	3:F:166:LEU:HD21	1.64	0.62
2:B:218:HIS:HD2	2:B:220:GLY:H	1.48	0.62
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.80	0.62
1:D:140:TRP:HZ3	2:E:209:TYR:HH	1.48	0.62
3:F:75:SER:HB3	3:F:76:PRO:CD	2.30	0.62
4:M:3:ACB:O	4:M:6:FGA:N	2.32	0.62
1:D:372:GLN:HB3	1:D:384:ILE:HG13	1.82	0.62
1:D:346:ALA:HA	1:D:372:GLN:OE1	1.99	0.62
3:C:215:GLY:HA3	4:M:5:1ZN:H16	1.82	0.61
2:B:48:GLN:HA	2:B:51:VAL:HG12	1.83	0.61
1:A:338:ASN:HD22	1:A:340:HIS:H	1.49	0.61
1:D:538:PHE:HB3	1:D:575:VAL:HA	1.81	0.61
1:A:133:LYS:HG2	1:A:169:TYR:CE1	2.36	0.61
2:B:383:ASN:O	2:B:386:ILE:HD13	2.00	0.61
2:E:83:ASN:HB3	2:E:86:VAL:HG21	1.82	0.61
2:B:121:GLU:OE1	4:M:2:LEU:HD13	2.00	0.60
1:A:115:ILE:O	1:A:119:HIS:CD2	2.52	0.60
4:N:5:1ZN:H19	4:N:5:1ZN:H6	1.83	0.60
3:F:120:SER:O	3:F:124:THR:HB	2.01	0.60
3:C:117:ASN:H	3:C:117:ASN:HD22	1.46	0.60
2:B:347:LEU:HB3	2:B:389:LEU:HD22	1.83	0.60
2:B:58:ASP:N	2:B:59:PRO:CD	2.64	0.60
2:E:332:ALA:HB2	2:E:369:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:383:ASN:O	2:E:386:ILE:HD13	2.02	0.60
1:D:467:LYS:HB2	1:D:507:VAL:HG13	1.83	0.60
2:E:110:SER:C	2:E:112:ASN:H	2.09	0.60
3:F:45:VAL:CG1	3:F:181:ARG:HH11	2.15	0.60
1:A:539:ASN:O	1:A:543:SER:HB2	2.02	0.60
2:B:52:LEU:HD21	2:B:101:VAL:HG21	1.84	0.60
2:B:72:ALA:O	2:B:75:GLU:HG2	2.02	0.60
2:E:168:LEU:HD21	2:E:204:ILE:HG22	1.82	0.60
3:C:24:SER:H	3:C:27:GLN:HE21	1.50	0.59
2:E:291:LYS:C	2:E:293:TRP:H	2.10	0.59
3:F:8:LYS:HA	3:F:8:LYS:CE	2.29	0.59
1:D:350:MET:HG2	1:D:387:ASN:O	2.00	0.59
2:E:263:TYR:O	2:E:266:GLN:HG2	2.02	0.59
2:B:281:LEU:O	2:B:285:VAL:HG13	2.02	0.59
1:A:13:ILE:HD12	1:A:14:ALA:H	1.66	0.59
2:E:332:ALA:HB1	2:E:372:PRO:HG2	1.83	0.59
3:C:222:GLN:O	3:C:226:GLU:HB2	2.02	0.59
3:F:209:TRP:CZ3	3:F:220:PHE:HB3	2.36	0.59
3:C:202:ASP:HB3	3:C:242:GLN:OE1	2.03	0.59
1:D:334:VAL:HG21	1:D:368:LEU:HD22	1.84	0.59
3:C:17:LEU:CD1	3:C:98:THR:HG23	2.32	0.59
2:E:58:ASP:N	2:E:59:PRO:HD2	2.18	0.59
3:F:155:LEU:HD21	3:F:195:MET:HE3	1.84	0.59
1:A:120:SER:HB2	1:A:123:ASP:HB2	1.85	0.58
1:A:366:LEU:C	1:A:368:LEU:H	2.11	0.58
2:B:171:PHE:CE1	2:B:182:LEU:HB3	2.36	0.58
3:F:57:ASP:HB3	3:F:59:HIS:HD2	1.67	0.58
3:F:104:LYS:HA	3:F:111:ILE:HD11	1.85	0.58
1:A:140:TRP:CD1	1:A:141:PHE:H	2.21	0.58
1:A:451:LEU:HD12	1:A:462:ALA:HB1	1.85	0.58
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.37	0.58
1:A:307:LYS:HB3	1:A:348:VAL:HB	1.84	0.58
3:C:176:THR:H	3:C:179:HIS:HD2	1.49	0.58
2:E:355:ILE:HD12	2:E:355:ILE:H	1.69	0.58
3:F:104:LYS:CA	3:F:111:ILE:HD11	2.32	0.58
1:A:200:ASN:HA	1:A:203:SER:HB3	1.85	0.58
3:F:76:PRO:HG3	3:F:107:TYR:CZ	2.38	0.58
2:E:119:ASP:CG	2:E:120:PRO:HD2	2.29	0.58
3:F:91:TYR:HB2	3:F:265:TYR:OH	2.03	0.58
3:F:266:CYS:HA	3:F:268:ARG:HB2	1.86	0.58
1:D:307:LYS:HB3	1:D:348:VAL:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:250:TRP:CD1	3:F:257:VAL:HG22	2.39	0.58
2:B:304:PHE:O	2:B:308:LEU:HB2	2.03	0.57
3:C:244:VAL:HG21	3:C:249:ASN:HB2	1.86	0.57
3:F:16:GLN:O	3:F:19:GLU:HG3	2.03	0.57
3:F:98:THR:HB	3:F:146:PHE:CZ	2.33	0.57
1:A:543:SER:O	1:A:547:ILE:HG12	2.04	0.57
2:B:77:VAL:HG23	2:B:140:PHE:HA	1.86	0.57
2:E:120:PRO:C	2:E:122:GLU:N	2.54	0.57
2:B:168:LEU:C	2:B:170:LEU:H	2.13	0.57
1:D:39:ALA:O	1:D:43:GLY:HA3	2.04	0.57
2:E:112:ASN:ND2	2:E:123:ASP:HA	2.19	0.57
3:C:76:PRO:HB3	3:C:107:TYR:CZ	2.39	0.57
2:B:286:VAL:HG11	2:B:323:ILE:HG13	1.85	0.57
3:C:230:HIS:HA	3:C:234:LEU:HD13	1.87	0.57
2:E:146:GLU:HG2	2:E:188:ARG:HH21	1.68	0.57
2:B:120:PRO:O	2:B:122:GLU:N	2.32	0.57
2:B:282:THR:HB	2:B:319:GLU:HG2	1.86	0.57
3:C:121:ARG:O	3:C:124:THR:HG22	2.05	0.57
1:D:366:LEU:HD12	1:D:369:PHE:HD2	1.69	0.57
2:E:335:VAL:HG22	2:E:347:LEU:HG	1.86	0.57
2:E:283:GLU:HB3	2:E:284:PRO:HD3	1.87	0.57
1:A:467:LYS:HB2	1:A:507:VAL:HG12	1.86	0.56
3:F:57:ASP:HB3	3:F:59:HIS:CD2	2.40	0.56
2:B:168:LEU:HG	2:B:207:ILE:HD11	1.86	0.56
2:B:339:HIS:CD2	3:C:125:GLN:HB2	2.40	0.56
3:C:116:GLY:HA2	3:C:167:HIS:CG	2.41	0.56
3:F:214:ARG:CZ	3:F:241:HIS:CE1	2.88	0.56
2:B:97:HIS:O	2:B:101:VAL:HG23	2.05	0.56
1:A:412:ALA:HB1	1:A:450:TRP:HZ2	1.71	0.56
1:D:284:VAL:HB	1:D:285:PRO:HD3	1.87	0.56
3:F:62:PHE:HD1	3:F:63:HIS:HD2	1.53	0.56
3:C:185:ARG:HG3	3:C:185:ARG:NH2	2.08	0.56
3:C:201:SER:CB	3:C:218:TYR:H	2.18	0.56
3:F:167:HIS:CD2	3:F:241:HIS:HB2	2.40	0.56
3:C:149:LEU:HD23	3:C:149:LEU:O	2.06	0.56
1:D:369:PHE:O	1:D:373:LEU:HB2	2.06	0.56
2:B:212:ILE:CD1	2:B:253:PRO:HB2	2.36	0.56
1:D:483:ILE:N	1:D:484:PRO:HD2	2.20	0.56
2:E:103:MET:HA	2:E:103:MET:CE	2.30	0.56
3:F:265:TYR:O	3:F:268:ARG:HG3	2.06	0.56
3:F:13:TRP:CG	3:F:23:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:290:ASP:OD2	3:F:290:ASP:N	2.38	0.55
1:A:91:PRO:HB2	1:A:92:PRO:HD3	1.88	0.55
2:E:381:HIS:ND1	2:E:386:ILE:HD11	2.22	0.55
1:A:494:ASN:HD22	1:A:494:ASN:C	2.14	0.55
3:F:212:SER:HA	3:F:219:THR:HG23	1.88	0.55
1:A:524:THR:O	1:A:528:MET:HG3	2.07	0.55
2:E:78:GLU:HA	2:E:81:THR:OG1	2.07	0.55
1:A:366:LEU:HB3	1:A:367:PRO:HD3	1.88	0.55
1:A:435:GLY:HA2	1:A:438:PHE:HB3	1.89	0.55
2:E:143:ARG:HH11	2:E:143:ARG:HB2	1.72	0.55
3:F:79:ASN:HD21	3:F:110:ARG:NE	1.94	0.55
3:F:95:GLU:OE2	3:F:136:LYS:HE3	2.07	0.55
1:A:24:ASP:CG	1:A:25:VAL:H	2.15	0.55
1:D:222:LEU:HD23	1:D:262:MET:CG	2.37	0.55
2:E:58:ASP:N	2:E:59:PRO:CD	2.70	0.55
1:A:303:SER:O	1:A:305:LYS:N	2.39	0.54
3:C:117:ASN:HB3	3:C:199:LEU:O	2.07	0.54
1:A:140:TRP:HD1	1:A:141:PHE:H	1.55	0.54
2:B:179:ARG:HB2	2:B:223:GLU:HG2	1.88	0.54
2:E:264:HIS:HE1	2:E:307:GLU:OE2	1.91	0.54
3:F:172:PRO:HG3	3:F:209:TRP:CD2	2.42	0.54
3:C:171:SER:HB2	3:C:197:ASP:CB	2.36	0.54
3:C:297:GLU:C	3:C:299:HIS:H	2.15	0.54
1:D:94:GLU:HB2	1:D:131:LEU:HD21	1.90	0.54
2:E:328:PHE:HA	2:E:331:LEU:HB2	1.90	0.54
3:F:91:TYR:N	3:F:265:TYR:OH	2.39	0.54
3:C:19:GLU:O	3:C:21:LYS:N	2.41	0.54
3:F:214:ARG:HE	3:F:241:HIS:CE1	2.26	0.54
1:D:306:VAL:HG11	1:D:330:ILE:HD11	1.90	0.54
2:E:164:VAL:HG21	2:E:200:ILE:HG12	1.89	0.54
2:B:246:PHE:O	2:B:250:VAL:HB	2.08	0.54
3:C:265:TYR:CD1	3:C:266:CYS:N	2.76	0.54
2:E:72:ALA:O	2:E:76:MET:HG3	2.07	0.54
2:E:253:PRO:O	2:E:256:LYS:HG2	2.07	0.54
2:B:121:GLU:OE1	4:M:2:LEU:HD11	2.07	0.54
1:D:237:GLN:HA	1:D:240:LEU:HD12	1.89	0.54
4:M:5:1ZN:H6	4:M:5:1ZN:H19	1.90	0.54
3:C:185:ARG:CG	3:C:185:ARG:NH2	2.60	0.54
3:C:114:LEU:HD23	3:C:154:PRO:HG2	1.89	0.53
2:E:260:LEU:HG	2:E:264:HIS:HB2	1.89	0.53
1:A:338:ASN:ND2	1:A:340:HIS:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ASN:O	1:D:324:THR:HG22	2.09	0.53
2:B:120:PRO:C	2:B:122:GLU:N	2.67	0.53
1:D:397:ILE:HG21	1:D:434:LEU:HB2	1.90	0.53
3:F:157:ALA:HB3	3:F:165:CYS:HB2	1.90	0.53
1:D:531:ASP:O	1:D:537:ARG:HD3	2.09	0.53
2:E:194:LEU:O	2:E:197:ARG:HB3	2.08	0.53
3:F:58:VAL:HG12	3:F:86:TYR:HA	1.89	0.53
3:F:171:SER:HB3	3:F:174:ILE:CD1	2.35	0.53
3:F:264:ASN:O	3:F:265:TYR:HB3	2.08	0.53
3:C:229:ASN:O	3:C:234:LEU:HB3	2.09	0.53
3:C:252:HIS:O	3:C:253:ASP:C	2.52	0.53
3:F:132:GLU:OE1	3:F:136:LYS:HE2	2.09	0.53
3:F:174:ILE:HG21	3:F:180:ILE:HG22	1.91	0.53
3:F:75:SER:HB3	3:F:76:PRO:HD2	1.91	0.53
3:C:117:ASN:HD22	3:C:117:ASN:N	2.06	0.53
2:E:55:PHE:CD1	2:E:55:PHE:N	2.77	0.53
3:F:170:LEU:HD11	3:F:228:PHE:CD2	2.44	0.53
3:F:174:ILE:HG21	3:F:180:ILE:CG2	2.40	0.52
1:A:163:LYS:O	1:A:167:ARG:HG3	2.09	0.52
3:C:121:ARG:O	3:C:125:GLN:HG2	2.10	0.52
2:B:212:ILE:HD11	2:B:213:TYR:CZ	2.44	0.52
3:C:265:TYR:O	3:C:268:ARG:CB	2.57	0.52
1:A:93:LEU:HA	1:A:96:LEU:HB2	1.90	0.52
1:A:236:PRO:HB2	1:A:240:LEU:HG	1.91	0.52
1:A:303:SER:OG	1:A:333:LEU:HD13	2.10	0.52
3:F:45:VAL:HG11	3:F:181:ARG:HH11	1.70	0.52
3:F:240:ALA:O	3:F:242:GLN:N	2.42	0.52
2:E:79:TYR:CE2	2:E:86:VAL:HG11	2.44	0.52
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.91	0.52
1:A:418:ARG:CG	1:A:418:ARG:NH2	2.68	0.51
3:C:44:ASN:HB2	3:C:181:ARG:HA	1.92	0.51
3:C:212:SER:OG	3:C:214:ARG:HB2	2.10	0.51
1:D:43:GLY:C	1:D:45:GLU:N	2.68	0.51
2:E:152:PRO:O	2:E:156:LYS:HB3	2.10	0.51
2:E:273:GLN:O	2:E:276:GLU:HB2	2.09	0.51
3:F:229:ASN:ND2	3:F:255:ASN:HD22	2.04	0.51
2:B:89:GLU:HG2	2:B:154:ILE:HD13	1.92	0.51
3:F:45:VAL:CG1	3:F:181:ARG:NH1	2.72	0.51
3:F:50:CYS:SG	3:F:282:LEU:HD13	2.50	0.51
2:E:97:HIS:O	2:E:101:VAL:HG23	2.10	0.51
1:D:506:ASN:HB2	1:D:546:LYS:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:193:PHE:CE2	2:E:195:GLY:HA3	2.46	0.51
2:E:300:LYS:HA	2:E:303:MET:HE3	1.91	0.51
1:A:322:ILE:HA	1:A:326:ILE:HB	1.93	0.51
3:C:110:ARG:HA	3:C:110:ARG:HH21	1.75	0.51
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.93	0.51
3:F:232:ASN:C	3:F:234:LEU:H	2.17	0.51
3:F:243:LEU:C	3:F:243:LEU:HD12	2.35	0.51
2:B:52:LEU:CD1	2:B:98:MET:HA	2.40	0.51
2:B:297:HIS:C	2:B:297:HIS:CD2	2.89	0.51
1:D:278:ILE:HA	1:D:281:THR:HG22	1.93	0.51
2:E:232:ILE:HD12	2:E:274:PHE:CE1	2.46	0.51
2:E:386:ILE:O	2:E:390:ILE:HG22	2.11	0.51
3:C:215:GLY:HA3	4:M:5:1ZN:H14	1.92	0.50
1:A:264:ALA:HA	1:A:267:PHE:HB2	1.92	0.50
4:N:3:ACB:OXT	4:N:4:ARG:NE	2.44	0.50
2:E:347:LEU:C	2:E:349:TYR:N	2.70	0.50
3:F:239:ARG:NH2	3:F:242:GLN:OE1	2.44	0.50
3:C:35:ALA:HA	3:C:38:ILE:HG22	1.93	0.50
3:C:81:LEU:HA	3:C:112:THR:O	2.11	0.50
1:D:69:LEU:HD23	1:D:96:LEU:HD11	1.94	0.50
2:B:58:ASP:N	2:B:59:PRO:HD3	2.24	0.50
3:C:195:MET:O	3:C:198:LEU:HB2	2.10	0.50
3:C:266:CYS:HA	3:C:268:ARG:HG2	1.93	0.50
3:F:10:LEU:HD11	3:F:105:VAL:HG22	1.94	0.50
3:F:265:TYR:CD2	3:F:266:CYS:N	2.79	0.50
2:B:121:GLU:OE1	4:M:2:LEU:CD2	2.60	0.50
2:B:170:LEU:C	2:B:172:ASP:H	2.19	0.50
3:F:68:LEU:CD1	3:F:275:ILE:HG21	2.40	0.50
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.94	0.50
2:B:52:LEU:CD1	2:B:97:HIS:HD2	2.21	0.50
1:A:466:LEU:HD23	1:A:508:LEU:HD11	1.94	0.50
1:A:11:TYR:H	1:A:12:PRO:HD3	1.76	0.50
1:A:229:VAL:O	1:A:233:GLN:HB2	2.11	0.50
1:A:369:PHE:O	1:A:373:LEU:HB2	2.12	0.50
1:D:439:PHE:CZ	1:D:469:LEU:HD11	2.47	0.50
2:E:52:LEU:HD12	2:E:98:MET:HB3	1.94	0.50
2:E:277:LYS:HA	2:E:277:LYS:CE	2.42	0.50
1:D:222:LEU:CD2	1:D:262:MET:HG3	2.42	0.49
2:B:103:MET:HE3	2:B:103:MET:HA	1.94	0.49
1:D:319:GLU:O	1:D:323:MET:HB2	2.13	0.49
1:D:419:VAL:O	1:D:420:ARG:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:ASP:H	3:F:116:GLY:HA3	1.77	0.49
1:A:102:THR:O	1:A:106:ASP:HB2	2.12	0.49
3:C:24:SER:H	3:C:27:GLN:NE2	2.10	0.49
3:C:240:ALA:O	3:C:242:GLN:N	2.43	0.49
3:F:67:GLU:O	3:F:71:ILE:HG12	2.12	0.49
2:B:219:ASN:ND2	2:B:219:ASN:H	2.09	0.49
2:B:367:LEU:H	2:B:368:PRO:CD	2.20	0.49
3:F:244:VAL:CG1	3:F:249:ASN:HB2	2.35	0.49
1:A:404:LEU:O	1:A:408:ILE:HG12	2.12	0.49
2:B:52:LEU:HD12	2:B:98:MET:HA	1.95	0.49
1:D:108:ALA:O	1:D:112:LEU:HB2	2.12	0.49
1:A:37:THR:HG22	1:A:40:LEU:HD21	1.94	0.49
1:A:246:PRO:O	1:A:250:GLN:HB2	2.13	0.49
1:A:535:ASN:HD21	3:C:79:ASN:ND2	2.10	0.49
1:D:339:GLN:NE2	1:D:377:CYS:HB2	2.28	0.49
1:D:556:LEU:HA	1:D:560:VAL:HB	1.95	0.49
3:F:115:ARG:HD2	3:F:119:GLU:HB2	1.93	0.49
1:D:438:PHE:HA	1:D:441:GLU:OE2	2.13	0.49
2:E:99:PHE:CZ	2:E:103:MET:HG2	2.48	0.49
2:B:219:ASN:H	2:B:219:ASN:HD22	1.60	0.49
3:C:147:THR:HA	3:C:150:PHE:CD1	2.48	0.48
2:B:251:LEU:O	2:B:254:LEU:HB2	2.13	0.48
1:D:429:LEU:O	1:D:433:GLN:HG2	2.12	0.48
3:F:89:ARG:HG3	3:F:128:GLY:CA	2.42	0.48
4:N:1:DAL:O	4:N:2:LEU:HG	2.13	0.48
3:C:20:CYS:O	3:C:95:GLU:HG2	2.13	0.48
1:D:128:PHE:O	1:D:131:LEU:HB3	2.13	0.48
1:D:513:GLY:O	1:D:515:ASP:N	2.46	0.48
1:D:541:ALA:HB1	1:D:579:ALA:HA	1.94	0.48
2:E:287:MET:HE1	2:E:326:PRO:HG2	1.96	0.48
1:A:234:LEU:C	1:A:236:PRO:HD3	2.39	0.48
1:A:240:LEU:HD23	1:A:244:VAL:HG13	1.96	0.48
1:D:318:ARG:HA	1:D:321:VAL:HG12	1.95	0.48
2:E:52:LEU:HD12	2:E:98:MET:CB	2.43	0.48
2:E:119:ASP:HB3	2:E:121:GLU:CD	2.38	0.48
1:A:43:GLY:C	1:A:45:GLU:H	2.22	0.48
1:D:44:VAL:O	1:D:45:GLU:HB2	2.13	0.48
3:F:48:VAL:HG21	3:F:81:LEU:HD22	1.94	0.48
3:F:251:CYS:HB3	3:F:256:VAL:O	2.13	0.48
3:C:14:ILE:HA	3:C:17:LEU:CD2	2.44	0.48
3:C:229:ASN:O	3:C:231:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:548:GLY:HA3	1:D:586:LEU:CD2	2.39	0.48
2:E:371:PHE:CG	2:E:372:PRO:HD3	2.49	0.48
3:F:34:LYS:O	3:F:38:ILE:HG23	2.13	0.48
1:A:240:LEU:HD23	1:A:244:VAL:CG1	2.44	0.48
1:A:436:VAL:HG13	1:A:437:GLU:H	1.79	0.48
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.44	0.48
2:E:347:LEU:C	2:E:349:TYR:H	2.21	0.48
1:A:495:TYR:HA	1:A:498:ARG:HG2	1.95	0.48
2:B:92:TYR:N	2:B:93:PRO:HD2	2.29	0.48
2:E:320:PHE:O	2:E:324:MET:HB2	2.12	0.48
3:F:265:TYR:CG	3:F:266:CYS:N	2.82	0.48
1:A:101:GLU:CG	2:B:256:LYS:HE2	2.43	0.48
1:A:307:LYS:HG3	1:A:308:GLU:N	2.28	0.48
2:B:55:PHE:O	2:B:57:SER:N	2.47	0.48
3:C:139:ASN:ND2	3:C:141:ASN:HB2	2.28	0.48
3:F:124:THR:HG21	3:F:143:TRP:NE1	2.19	0.48
1:A:341:VAL:HG23	1:A:342:LYS:H	1.79	0.47
2:B:255:HIS:CE1	2:B:271:VAL:HG21	2.49	0.47
1:A:10:LEU:HB3	1:A:12:PRO:HD3	1.96	0.47
1:A:481:THR:C	1:A:484:PRO:HD2	2.39	0.47
2:E:218:HIS:CD2	2:E:220:GLY:H	2.32	0.47
3:F:74:LYS:HG3	3:F:75:SER:H	1.79	0.47
3:F:82:PHE:HB3	3:F:86:TYR:HE1	1.80	0.47
3:F:170:LEU:HB3	3:F:209:TRP:HH2	1.78	0.47
2:B:256:LYS:CB	3:C:309:MLL:HD22	2.41	0.47
3:C:91:TYR:HD2	3:C:91:TYR:O	1.97	0.47
1:D:449:ALA:O	1:D:452:VAL:HG12	2.14	0.47
2:E:49:CYS:O	2:E:52:LEU:HD22	2.14	0.47
3:F:50:CYS:O	3:F:52:VAL:HG12	2.14	0.47
3:F:114:LEU:HD21	3:F:157:ALA:HB2	1.96	0.47
2:B:120:PRO:C	2:B:122:GLU:H	2.17	0.47
2:B:123:ASP:OD1	4:M:2:LEU:HD21	2.14	0.47
1:D:52:LEU:HD12	1:D:92:PRO:HG3	1.96	0.47
2:E:257:VAL:HG12	2:E:259:SER:H	1.79	0.47
2:E:356:MET:HA	2:E:359:ILE:HD12	1.97	0.47
2:E:371:PHE:CD2	2:E:372:PRO:HD3	2.49	0.47
3:F:45:VAL:CG2	3:F:156:THR:HG23	2.29	0.47
4:N:2:LEU:HA	4:N:3:ACB:H43	0.61	0.47
1:A:244:VAL:O	1:A:244:VAL:CG2	2.58	0.47
1:A:560:VAL:HG12	1:A:560:VAL:O	2.14	0.47
3:C:45:VAL:HA	3:C:156:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:ASP:HB2	3:C:260:PHE:CE2	2.49	0.47
3:C:123:ILE:HA	3:C:126:VAL:HG12	1.96	0.47
3:C:265:TYR:CG	3:C:266:CYS:N	2.82	0.47
3:F:201:SER:HB3	3:F:218:TYR:H	1.79	0.47
2:B:218:HIS:HD2	2:B:220:GLY:N	2.09	0.47
3:F:78:THR:OG1	3:F:80:TYR:HE2	1.97	0.47
1:A:116:SER:HB3	1:A:128:PHE:CE1	2.49	0.47
1:A:262:MET:HE1	1:A:266:LYS:HD3	1.96	0.47
1:A:336:ASP:OD2	1:A:341:VAL:HG21	2.15	0.47
2:B:212:ILE:HD13	2:B:253:PRO:HB2	1.97	0.47
2:B:378:SER:O	2:B:387:HIS:HE1	1.98	0.47
1:D:14:ALA:HA	1:D:17:ILE:HG12	1.96	0.47
1:D:245:MET:O	1:D:249:ARG:HB2	2.13	0.47
2:E:382:TRP:HB2	3:F:121:ARG:HD3	1.97	0.47
3:F:251:CYS:SG	3:F:252:HIS:N	2.88	0.47
2:B:325:GLU:HB2	2:B:326:PRO:HD3	1.96	0.47
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.95	0.47
2:E:172:ASP:HB2	2:E:218:HIS:CE1	2.49	0.47
3:F:170:LEU:HD11	3:F:228:PHE:CE2	2.49	0.47
3:F:214:ARG:HG2	3:F:214:ARG:NH1	2.19	0.47
1:A:420:ARG:NH1	1:A:458:ILE:HG13	2.30	0.47
1:A:267:PHE:CE1	1:A:287:PHE:HB2	2.50	0.47
1:A:341:VAL:CG2	1:A:342:LYS:N	2.78	0.47
2:B:237:LEU:CB	2:B:238:PRO:HD2	2.41	0.47
1:D:245:MET:HE2	1:D:248:LEU:HD22	1.97	0.47
3:F:83:MET:HE3	3:F:240:ALA:HB2	1.96	0.47
2:B:47:ARG:O	2:B:51:VAL:N	2.45	0.46
3:C:195:MET:HA	3:C:198:LEU:HD12	1.97	0.46
2:E:103:MET:HE1	2:E:134:LEU:HB3	1.96	0.46
3:F:281:THR:HG23	3:F:283:LYS:HG3	1.96	0.46
1:A:563:ILE:O	1:A:566:LYS:HG3	2.15	0.46
3:C:174:ILE:C	3:C:174:ILE:HD12	2.40	0.46
1:D:105:ARG:HD2	1:D:146:SER:OG	2.15	0.46
2:B:175:ASP:O	2:B:178:GLU:HB2	2.16	0.46
2:E:168:LEU:HD22	2:E:203:GLN:HG3	1.97	0.46
3:F:6:PHE:CZ	3:F:10:LEU:HD12	2.50	0.46
3:C:230:HIS:CG	3:C:230:HIS:O	2.68	0.46
1:D:489:MET:HB3	1:D:501:THR:OG1	2.16	0.46
2:E:77:VAL:HG23	2:E:140:PHE:HA	1.96	0.46
2:E:282:THR:HB	2:E:319:GLU:HG2	1.96	0.46
3:F:276:MET:CE	3:F:278:LEU:HD21	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:O	1:A:334:VAL:HG23	2.16	0.46
3:C:32:CYS:O	3:C:36:LYS:HB2	2.16	0.46
3:C:308:PHE:O	3:C:309:MLL:HD13	2.16	0.46
1:D:526:LEU:HD12	1:D:526:LEU:HA	1.83	0.46
2:E:295:LYS:HD3	2:E:295:LYS:H	1.80	0.46
3:F:137:TYR:CD1	3:F:142:VAL:HG11	2.51	0.46
1:A:20:LEU:HB2	1:A:21:ARG:HH11	1.81	0.46
2:B:81:THR:O	2:B:82:HIS:CD2	2.68	0.46
2:B:292:TYR:HA	3:C:309:MLL:HG	1.98	0.46
3:C:267:TYR:C	3:C:269:CYS:H	2.24	0.46
1:D:568:THR:O	1:D:576:LYS:HG3	2.15	0.46
2:E:110:SER:C	2:E:112:ASN:N	2.74	0.46
1:A:47:THR:HG23	1:A:51:LEU:HD23	1.98	0.46
1:A:245:MET:O	1:A:246:PRO:C	2.57	0.46
2:B:131:TRP:N	2:B:132:PRO:CD	2.78	0.46
2:B:237:LEU:O	2:B:238:PRO:C	2.58	0.46
3:C:157:ALA:HB3	3:C:165:CYS:HB2	1.98	0.46
1:D:373:LEU:HD13	1:D:384:ILE:CG2	2.46	0.46
3:F:240:ALA:C	3:F:242:GLN:H	2.23	0.46
1:A:160:SER:HA	1:A:163:LYS:HB2	1.98	0.46
2:B:168:LEU:HD21	2:B:204:ILE:CG2	2.44	0.46
2:B:247:LEU:HD21	2:B:285:VAL:HG11	1.98	0.46
2:B:307:GLU:HA	2:B:310:GLU:HB2	1.97	0.46
2:E:356:MET:C	2:E:358:LEU:H	2.24	0.46
2:B:51:VAL:HG13	2:B:51:VAL:O	2.16	0.46
2:B:119:ASP:HA	2:B:120:PRO:HD3	1.83	0.46
1:D:245:MET:HE3	1:D:245:MET:CA	2.27	0.46
2:E:171:PHE:CE1	2:E:182:LEU:HB3	2.50	0.46
1:A:11:TYR:N	1:A:12:PRO:CD	2.77	0.45
1:A:368:LEU:O	1:A:372:GLN:HB2	2.16	0.45
1:A:573:VAL:HG11	3:C:108:ARG:HH12	1.80	0.45
2:E:98:MET:O	2:E:102:ASN:ND2	2.47	0.45
2:E:191:GLY:HA2	2:E:197:ARG:HH11	1.80	0.45
2:E:291:LYS:C	2:E:293:TRP:N	2.74	0.45
3:F:232:ASN:O	3:F:234:LEU:N	2.49	0.45
3:F:288:GLN:O	3:F:289:PHE:HB3	2.16	0.45
3:C:157:ALA:N	3:C:165:CYS:O	2.45	0.45
1:D:306:VAL:CG1	1:D:330:ILE:HD11	2.45	0.45
2:E:202:LYS:O	2:E:205:ASN:HB2	2.16	0.45
1:A:102:THR:HG23	2:B:213:TYR:HB3	1.98	0.45
1:A:219:SER:HB2	2:B:210:ARG:HH22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LYS:O	1:A:471:GLU:HB2	2.16	0.45
1:D:248:LEU:HD11	1:D:270:LEU:HD13	1.98	0.45
1:D:274:VAL:HG13	1:D:278:ILE:HB	1.98	0.45
1:D:427:MET:HE1	1:D:443:LEU:HD23	1.98	0.45
2:B:201:ARG:NE	2:B:242:GLU:OE1	2.49	0.45
3:C:118:HIS:HA	3:C:123:ILE:HG21	1.97	0.45
1:D:486:VAL:O	1:D:489:MET:HB2	2.15	0.45
1:D:535:ASN:O	1:D:539:ASN:HB2	2.16	0.45
3:F:271:ASN:CG	3:F:272:GLN:N	2.73	0.45
1:A:310:CYS:HA	1:A:313:LEU:HD11	1.99	0.45
2:B:352:ASN:CB	2:B:355:ILE:HD12	2.35	0.45
3:F:209:TRP:CE2	3:F:224:ILE:HD13	2.51	0.45
4:N:2:LEU:C	4:N:3:ACB:N	2.64	0.45
1:A:193:ALA:HB2	1:A:205:ILE:HG21	1.97	0.45
2:E:47:ARG:HA	2:E:50:CYS:HB2	1.97	0.45
2:E:87:ILE:HG22	2:E:87:ILE:O	2.15	0.45
3:C:124:THR:HG21	3:C:143:TRP:NE1	2.29	0.45
2:E:132:PRO:O	2:E:136:LEU:HD12	2.16	0.45
3:F:116:GLY:H	3:F:119:GLU:CG	2.24	0.45
2:B:47:ARG:HH11	2:B:72:ALA:HB2	1.82	0.45
2:B:54:ASP:OD1	2:B:54:ASP:N	2.50	0.45
2:E:49:CYS:HA	2:E:52:LEU:HD13	1.99	0.45
2:E:200:ILE:O	2:E:204:ILE:HG23	2.16	0.45
1:D:349:ILE:HG21	1:D:372:GLN:OE1	2.17	0.45
1:D:564:LEU:O	1:D:568:THR:HG23	2.16	0.45
2:E:45:LYS:HE3	2:E:45:LYS:H	1.80	0.45
2:E:52:LEU:HB3	2:E:98:MET:HB2	1.98	0.45
2:E:120:PRO:O	2:E:122:GLU:N	2.49	0.45
2:B:88:THR:C	2:B:90:PRO:HD2	2.42	0.45
2:B:248:LEU:HA	2:B:252:LEU:HD12	1.99	0.45
1:D:517:THR:HA	1:D:521:MET:HE3	1.98	0.45
3:F:116:GLY:N	3:F:119:GLU:HG2	2.25	0.45
1:D:122:SER:C	1:D:124:LEU:H	2.25	0.44
3:F:55:CYS:SG	3:F:68:LEU:HD21	2.57	0.44
2:E:96:VAL:HG21	2:E:158:TYR:HB3	2.00	0.44
3:F:207:GLY:HA2	3:F:221:GLY:HA3	2.00	0.44
4:N:2:LEU:CA	4:N:3:ACB:H2	2.30	0.44
1:A:231:ILE:HA	1:A:234:LEU:HD12	1.98	0.44
1:A:419:VAL:O	1:A:422:ALA:HB3	2.17	0.44
1:D:101:GLU:HG3	1:D:103:VAL:HG23	1.99	0.44
1:D:141:PHE:CE2	2:E:209:TYR:CD2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:MET:HE1	2:E:134:LEU:HD22	1.99	0.44
3:F:167:HIS:CD2	3:F:241:HIS:CD2	3.06	0.44
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.99	0.44
2:B:251:LEU:HD11	2:B:270:CYS:HB3	1.98	0.44
1:D:112:LEU:HB3	1:D:150:LEU:HD21	2.00	0.44
1:A:209:PHE:CE1	1:A:228:CYS:HB2	2.53	0.44
2:B:41:LEU:HD21	2:B:90:PRO:HG2	2.00	0.44
3:C:261:SER:HA	3:C:273:ALA:HB1	2.00	0.44
3:F:94:VAL:O	3:F:95:GLU:C	2.60	0.44
3:F:223:ASP:OD1	3:F:224:ILE:N	2.51	0.44
1:A:222:LEU:HD23	1:A:262:MET:CG	2.47	0.44
3:C:86:TYR:CD2	3:C:119:GLU:OE2	2.71	0.44
1:D:261:TYR:C	1:D:261:TYR:CD2	2.95	0.44
1:D:378:PRO:O	1:D:379:GLU:C	2.60	0.44
1:D:466:LEU:HG	1:D:482:ILE:HD13	1.99	0.44
3:F:263:PRO:HB2	3:F:291:PRO:HB3	1.99	0.44
1:A:206:ILE:HG13	1:A:243:LEU:HD23	2.00	0.44
1:D:18:ASP:C	1:D:20:LEU:H	2.25	0.44
1:D:496:LEU:HD21	3:F:78:THR:HG22	2.00	0.44
1:A:197:GLU:O	1:A:198:LEU:C	2.61	0.44
1:D:545:GLN:HA	1:D:586:LEU:HD11	2.00	0.44
3:F:202:ASP:O	3:F:219:THR:HA	2.18	0.44
1:D:535:ASN:ND2	3:F:76:PRO:O	2.51	0.44
1:A:82:GLY:HA3	1:A:83:PRO:HD2	1.77	0.43
3:C:139:ASN:C	3:C:139:ASN:HD22	2.26	0.43
1:D:271:GLN:HG3	1:D:279:THR:HG21	1.99	0.43
1:A:330:ILE:HG23	1:A:345:LEU:HD11	2.00	0.43
2:B:252:LEU:HD22	2:B:288:ALA:CB	2.47	0.43
2:B:372:PRO:HA	2:B:375:TYR:CE1	2.53	0.43
2:E:275:LEU:HD11	2:E:282:THR:HA	2.00	0.43
3:F:214:ARG:CG	3:F:214:ARG:NH1	2.67	0.43
1:D:313:LEU:HD13	1:D:321:VAL:HG13	2.01	0.43
1:D:370:LEU:HD12	1:D:370:LEU:HA	1.87	0.43
1:D:498:ARG:NE	1:D:531:ASP:OD2	2.45	0.43
2:E:131:TRP:O	2:E:132:PRO:C	2.59	0.43
3:F:203:PRO:HG3	3:F:256:VAL:HG11	1.99	0.43
1:A:411:LEU:C	1:A:413:GLU:H	2.27	0.43
2:B:170:LEU:C	2:B:172:ASP:N	2.75	0.43
2:B:252:LEU:HB2	2:B:253:PRO:HD3	2.01	0.43
2:B:369:ILE:HG22	2:B:369:ILE:O	2.18	0.43
2:E:252:LEU:HD11	2:E:285:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD13	1:A:384:ILE:HG21	2.00	0.43
2:B:336:SER:O	2:B:337:SER:C	2.62	0.43
3:C:189:VAL:HG11	3:C:199:LEU:HD21	2.00	0.43
3:C:196:CYS:O	3:C:200:TRP:HB2	2.18	0.43
1:D:420:ARG:NH1	1:D:453:ASP:OD1	2.50	0.43
2:E:204:ILE:HA	2:E:207:ILE:CG1	2.46	0.43
3:F:117:ASN:N	3:F:117:ASN:HD22	2.17	0.43
3:F:222:GLN:HB2	3:F:252:HIS:CD2	2.53	0.43
3:C:170:LEU:HD12	3:C:220:PHE:CE2	2.54	0.43
2:E:55:PHE:HB2	2:E:56:VAL:H	1.56	0.43
2:E:156:LYS:HD2	2:E:193:PHE:CZ	2.53	0.43
3:F:223:ASP:O	3:F:227:THR:HB	2.18	0.43
1:A:140:TRP:HA	1:A:144:ARG:NH1	2.33	0.43
1:A:350:MET:HG2	1:A:387:ASN:O	2.18	0.43
2:B:131:TRP:CZ3	2:B:178:GLU:HG2	2.53	0.43
2:B:293:TRP:HA	2:B:294:PRO:HD3	1.86	0.43
3:C:10:LEU:HD22	3:C:106:ARG:HB2	2.00	0.43
1:D:466:LEU:HA	1:D:469:LEU:CD2	2.48	0.43
2:E:121:GLU:CB	4:N:2:LEU:HD12	2.48	0.43
2:E:258:LYS:HG3	2:E:259:SER:N	2.33	0.43
2:E:382:TRP:CB	3:F:121:ARG:HD3	2.48	0.43
3:F:49:ARG:HG2	3:F:49:ARG:HH21	1.83	0.43
1:A:102:THR:HG22	1:A:105:ARG:CZ	2.49	0.43
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.54	0.43
2:E:81:THR:HB	2:E:82:HIS:CD2	2.53	0.43
1:A:171:ARG:HH12	1:A:204:GLU:HG2	1.83	0.43
2:B:164:VAL:HG21	2:B:196:LEU:HG	2.00	0.43
3:C:56:GLY:HA2	3:C:83:MET:HB2	2.00	0.43
1:D:70:ALA:HB2	1:D:96:LEU:HD12	2.01	0.43
1:D:256:SER:CB	2:E:106:THR:HG21	2.47	0.43
1:D:350:MET:HE2	1:D:388:LEU:HA	2.01	0.43
1:D:387:ASN:ND2	1:D:390:CYS:HB2	2.33	0.43
3:F:88:ASN:ND2	3:F:124:THR:HA	2.32	0.43
3:F:290:ASP:HB2	3:F:291:PRO:CD	2.49	0.43
1:A:222:LEU:HD23	1:A:262:MET:HG3	2.00	0.43
1:A:336:ASP:HB3	1:A:341:VAL:HG21	1.99	0.43
1:A:426:TYR:HE1	1:A:430:LEU:HD12	1.84	0.43
2:B:380:THR:OG1	2:B:381:HIS:N	2.50	0.43
1:D:183:ARG:HG3	1:D:220:VAL:HG22	2.01	0.43
3:F:254:ARG:HD3	3:F:254:ARG:N	2.33	0.43
1:D:179:PRO:HB3	1:D:217:GLN:HG3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:367:LEU:N	2:E:368:PRO:CD	2.82	0.42
2:B:125:PRO:O	2:B:126:THR:C	2.62	0.42
2:B:212:ILE:CD1	2:B:253:PRO:CB	2.96	0.42
3:C:252:HIS:O	3:C:255:ASN:HB2	2.19	0.42
1:D:419:VAL:O	1:D:422:ALA:N	2.52	0.42
2:E:45:LYS:HE2	2:E:91:ILE:HG22	2.02	0.42
1:A:473:PHE:HD2	1:A:474:GLY:H	1.66	0.42
1:A:506:ASN:HB2	1:A:546:LYS:HG2	2.00	0.42
1:A:555:THR:HG22	1:A:555:THR:O	2.19	0.42
2:B:190:TYR:CD1	2:B:190:TYR:C	2.96	0.42
3:C:264:ASN:H	3:C:264:ASN:ND2	2.17	0.42
2:E:48:GLN:HE21	2:E:98:MET:HG2	1.84	0.42
3:F:232:ASN:HD22	3:F:232:ASN:HA	1.51	0.42
1:A:197:GLU:O	1:A:200:ASN:N	2.52	0.42
3:C:252:HIS:O	3:C:255:ASN:N	2.48	0.42
1:D:117:HIS:CE1	1:D:153:VAL:HG12	2.54	0.42
2:E:210:ARG:HG2	2:E:214:GLU:HB3	2.01	0.42
3:F:28:VAL:HG11	3:F:142:VAL:HG23	2.01	0.42
3:F:167:HIS:CD2	3:F:241:HIS:HD2	2.37	0.42
1:A:338:ASN:HD21	1:A:340:HIS:HB2	1.84	0.42
2:B:53:PHE:HD2	2:B:53:PHE:HA	1.75	0.42
2:B:257:VAL:HG23	2:B:259:SER:H	1.84	0.42
3:C:13:TRP:O	3:C:17:LEU:HD22	2.20	0.42
3:F:85:ASP:HB2	3:F:167:HIS:HE1	1.85	0.42
3:F:132:GLU:CD	3:F:136:LYS:HE2	2.45	0.42
3:F:177:LEU:O	3:F:180:ILE:HG12	2.19	0.42
1:A:73:LEU:HD23	1:A:89:LEU:HD22	2.02	0.42
1:A:466:LEU:HB3	1:A:508:LEU:HD21	2.01	0.42
2:B:238:PRO:HD3	2:E:42:PHE:CZ	2.55	0.42
2:B:264:HIS:N	2:B:265:PRO:HD2	2.35	0.42
3:C:91:TYR:C	3:C:91:TYR:CD2	2.98	0.42
3:C:171:SER:O	3:C:174:ILE:HG13	2.20	0.42
1:D:218:ASP:O	1:D:222:LEU:HD12	2.19	0.42
1:D:538:PHE:CD2	1:D:538:PHE:C	2.98	0.42
3:F:52:VAL:HG13	3:F:52:VAL:O	2.19	0.42
1:D:366:LEU:HD12	1:D:369:PHE:CD2	2.52	0.42
1:D:375:ASP:O	1:D:381:ARG:HD3	2.19	0.42
2:E:93:PRO:HB3	2:E:158:TYR:CE1	2.55	0.42
2:E:131:TRP:N	2:E:132:PRO:CD	2.82	0.42
3:F:4:LYS:C	3:F:6:PHE:H	2.28	0.42
3:F:189:VAL:HA	3:F:190:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:262:ALA:HA	3:F:263:PRO:HD3	1.84	0.42
1:A:377:CYS:HA	1:A:378:PRO:HD2	1.86	0.42
3:C:239:ARG:HH12	3:C:242:GLN:HB2	1.85	0.42
1:D:184:ALA:O	1:D:185:ALA:C	2.63	0.42
1:D:405:LEU:N	1:D:406:PRO:CD	2.83	0.42
1:D:482:ILE:HG22	1:D:483:ILE:N	2.35	0.42
3:F:12:GLN:CD	3:F:12:GLN:C	2.88	0.42
3:F:178:ASP:OD2	3:F:178:ASP:N	2.51	0.42
3:F:290:ASP:CB	3:F:291:PRO:CD	2.97	0.42
1:A:453:ASP:OD2	1:A:454:HIS:N	2.53	0.42
2:B:241:GLU:O	2:B:245:ILE:HG12	2.20	0.42
2:B:253:PRO:O	2:B:256:LYS:HG2	2.20	0.42
1:D:287:PHE:CD2	1:D:291:MET:HE2	2.55	0.42
2:E:36:ALA:C	2:E:38:GLN:H	2.27	0.42
2:E:130:ALA:O	2:E:134:LEU:HG	2.20	0.42
2:E:282:THR:HG21	2:E:315:ILE:HD11	2.02	0.42
3:F:119:GLU:OE1	3:F:119:GLU:N	2.53	0.42
1:A:119:HIS:HB3	1:A:120:SER:H	1.58	0.42
2:B:48:GLN:HB3	2:B:76:MET:HE1	2.02	0.42
2:B:52:LEU:HD23	2:B:52:LEU:O	2.20	0.42
1:A:489:MET:HE3	1:A:489:MET:HB2	1.88	0.41
2:B:219:ASN:HD22	2:B:219:ASN:N	2.17	0.41
1:D:16:LEU:HB3	1:D:38:ILE:HD11	2.01	0.41
2:E:171:PHE:CD2	2:E:224:LEU:HG	2.54	0.41
3:F:200:TRP:HE3	3:F:214:ARG:HD3	1.83	0.41
1:D:263:VAL:O	1:D:264:ALA:C	2.63	0.41
2:E:339:HIS:CD2	3:F:125:GLN:HB3	2.55	0.41
2:E:390:ILE:C	2:E:392:ASN:H	2.28	0.41
3:C:114:LEU:HD21	3:C:157:ALA:HB2	2.03	0.41
3:C:212:SER:HA	3:C:213:PRO:HD3	1.94	0.41
3:C:215:GLY:HA3	4:M:5:1ZN:C12	2.50	0.41
1:D:32:ILE:O	1:D:35:LEU:HB2	2.20	0.41
1:D:217:GLN:HB2	1:D:220:VAL:HG23	2.01	0.41
1:D:385:ILE:HD12	1:D:423:ILE:HD11	2.02	0.41
3:F:171:SER:C	3:F:173:SER:H	2.28	0.41
3:C:91:TYR:HD2	3:C:91:TYR:C	2.28	0.41
1:D:343:SER:HB2	1:D:379:GLU:HG3	2.02	0.41
1:A:75:THR:C	1:A:77:THR:H	2.28	0.41
1:A:538:PHE:O	1:A:542:LYS:HB2	2.20	0.41
2:B:340:PHE:CE1	3:C:122:GLN:HG3	2.55	0.41
1:D:160:SER:HA	1:D:163:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:ILE:N	2:E:34:PRO:HG3	2.34	0.41
2:E:379:LYS:O	2:E:381:HIS:N	2.54	0.41
3:F:147:THR:HA	3:F:150:PHE:HD1	1.77	0.41
3:F:222:GLN:O	3:F:223:ASP:C	2.63	0.41
3:F:224:ILE:O	3:F:227:THR:N	2.54	0.41
1:A:570:ASP:HB3	1:A:571:GLN:H	1.51	0.41
2:B:308:LEU:HB3	2:B:349:TYR:OH	2.21	0.41
2:B:308:LEU:HD11	2:B:327:LEU:HD11	2.02	0.41
1:A:222:LEU:C	1:A:222:LEU:HD22	2.45	0.41
2:B:352:ASN:HB2	2:B:355:ILE:CD1	2.37	0.41
2:B:367:LEU:N	2:B:368:PRO:HD2	2.24	0.41
1:D:24:ASP:HB3	1:D:27:LEU:HD23	2.02	0.41
1:A:26:GLN:HA	1:A:29:LEU:HB3	2.03	0.41
1:A:35:LEU:HD12	1:A:38:ILE:HD12	2.03	0.41
1:A:279:THR:O	1:A:284:VAL:HG23	2.20	0.41
1:A:341:VAL:CG2	1:A:342:LYS:H	2.34	0.41
1:A:539:ASN:ND2	1:A:542:LYS:HD3	2.36	0.41
2:B:76:MET:HE2	2:B:76:MET:HB3	1.95	0.41
2:B:161:GLN:HG2	2:B:199:TYR:CG	2.56	0.41
2:B:312:LEU:HA	2:B:315:ILE:HB	2.03	0.41
3:C:114:LEU:HD13	3:C:156:THR:HA	2.03	0.41
3:C:117:ASN:HB2	3:C:200:TRP:CE2	2.56	0.41
1:D:467:LYS:NZ	1:D:510:GLU:OE2	2.48	0.41
1:D:564:LEU:HB3	1:D:583:LEU:HD21	2.03	0.41
2:E:69:LYS:O	2:E:73:LEU:HD22	2.21	0.41
2:E:128:GLU:O	2:E:131:TRP:HB2	2.21	0.41
3:F:155:LEU:HD23	3:F:155:LEU:HA	1.87	0.41
3:F:185:ARG:O	3:F:195:MET:HE1	2.21	0.41
3:C:10:LEU:HD11	3:C:105:VAL:HG22	2.03	0.41
3:C:240:ALA:C	3:C:242:GLN:H	2.29	0.41
1:D:141:PHE:HZ	2:E:213:TYR:CD1	2.38	0.41
2:E:55:PHE:HD1	2:E:56:VAL:O	2.03	0.41
2:E:99:PHE:O	2:E:103:MET:HB2	2.20	0.41
2:E:138:TYR:CD2	2:E:181:PHE:HB3	2.56	0.41
2:E:186:LEU:HD12	2:E:227:ILE:HD13	2.02	0.41
3:F:117:ASN:HD22	3:F:117:ASN:H	1.68	0.41
3:F:122:GLN:OE1	4:N:5:1ZN:H7	2.21	0.41
1:A:338:ASN:ND2	1:A:340:HIS:HB2	2.36	0.40
2:B:38:GLN:HA	2:B:38:GLN:NE2	2.31	0.40
3:C:189:VAL:HA	3:C:190:PRO:HD3	1.89	0.40
2:E:190:TYR:CE2	2:E:197:ARG:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:HB3	1:A:238:GLU:H	1.80	0.40
1:A:432:GLY:HA3	1:A:472:LYS:HE2	2.02	0.40
1:D:38:ILE:O	1:D:42:LEU:HB3	2.22	0.40
1:D:147:ALA:O	1:D:148:CYS:C	2.64	0.40
2:E:295:LYS:HG2	2:E:296:THR:N	2.37	0.40
2:E:386:ILE:HA	2:E:389:LEU:HB2	2.03	0.40
3:F:14:ILE:HD13	3:F:103:LEU:HD23	2.02	0.40
1:A:255:LYS:O	2:B:106:THR:HG21	2.21	0.40
1:A:265:ASP:O	1:A:266:LYS:HD2	2.21	0.40
1:A:310:CYS:HA	1:A:313:LEU:CD1	2.51	0.40
1:A:373:LEU:HD11	1:A:385:ILE:HD11	2.03	0.40
1:D:524:THR:O	1:D:525:VAL:C	2.64	0.40
2:E:251:LEU:O	2:E:254:LEU:HB2	2.21	0.40
1:D:52:LEU:CD1	1:D:92:PRO:HG3	2.50	0.40
1:D:210:SER:HA	1:D:247:THR:HG21	2.04	0.40
2:E:289:LEU:HD23	2:E:308:LEU:CD2	2.52	0.40
2:E:375:TYR:C	2:E:375:TYR:CD2	3.00	0.40
3:F:59:HIS:CD2	3:F:267:TYR:HE2	2.40	0.40
1:A:94:GLU:HB2	1:A:131:LEU:CD2	2.51	0.40
1:A:499:MET:HE2	1:A:503:PHE:HE1	1.87	0.40
1:A:531:ASP:HA	1:A:532:PRO:HD2	1.89	0.40
1:A:539:ASN:ND2	3:C:77:ASP:OD2	2.55	0.40
1:D:90:LEU:N	1:D:91:PRO:HD2	2.37	0.40
2:E:121:GLU:HB3	4:N:2:LEU:HD12	2.02	0.40
3:F:214:ARG:NH2	3:F:241:HIS:CE1	2.89	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ASP:OD1	4:M:4:ARG:NE[11_466]	1.57	0.63
3:F:175:ASP:OD2	4:N:4:ARG:NE[12_664]	1.61	0.59
3:F:175:ASP:OD2	4:N:3:ACB:OXT[12_664]	1.65	0.55
3:C:175:ASP:CG	4:M:4:ARG:NE[11_466]	2.01	0.19
3:F:175:ASP:CG	4:N:4:ARG:NE[12_664]	2.05	0.15
3:F:175:ASP:OD1	4:N:4:ARG:NE[12_664]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/589 (99%)	502 (86%)	63 (11%)	16 (3%)	4	26
1	D	581/589 (99%)	505 (87%)	65 (11%)	11 (2%)	6	33
2	B	374/407 (92%)	300 (80%)	60 (16%)	14 (4%)	2	21
2	E	375/407 (92%)	307 (82%)	53 (14%)	15 (4%)	2	19
3	C	304/309 (98%)	253 (83%)	40 (13%)	11 (4%)	2	22
3	F	289/309 (94%)	231 (80%)	41 (14%)	17 (6%)	1	12
4	M	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2505/2617 (96%)	2099 (84%)	322 (13%)	84 (3%)	3	23

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	304	HIS
2	B	34	PRO
2	B	56	VAL
2	B	121	GLU
2	B	382	TRP
3	C	269	CYS
3	C	298	PRO
1	D	493	PRO
1	D	514	GLN
2	E	121	GLU
2	E	161	GLN
2	E	380	THR
3	F	75	SER
3	F	76	PRO
3	F	94	VAL
3	F	252	HIS
3	F	265	TYR

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Mol	Chain	Res	Type
1	A	239	ASP
2	B	238	PRO
2	B	380	THR
3	C	20	CYS
3	C	232	ASN
3	C	282	LEU
1	D	102	THR
1	D	491	GLY
1	D	510	GLU
1	D	513	GLY
1	D	573	VAL
2	E	234	GLY
3	F	232	ASN
3	F	233	GLY
3	F	251	CYS
1	A	43	GLY
1	A	237	GLN
1	A	315	ALA
1	A	475	LYS
2	B	61	SER
2	B	218	HIS
3	C	230	HIS
3	C	268	ARG
1	D	45	GLU
1	D	61	ASP
2	E	64	LYS
2	E	111	SER
2	E	237	LEU
2	E	348	TYR
3	F	240	ALA
3	F	271	ASN
1	A	76	PHE
1	A	196	LEU
1	A	245	MET
2	B	214	GLU
2	B	367	LEU
2	E	122	GLU
2	E	233	ASN
2	E	236	ALA
2	E	278	ASP
2	E	357	SER
1	A	79	LEU

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Mol	Chain	Res	Type
1	A	432	GLY
1	A	561	LYS
2	B	36	ALA
3	C	263	PRO
1	D	492	ASP
3	F	89	ARG
3	F	127	TYR
3	F	269	CYS
3	F	270	GLY
1	A	474	GLY
3	C	59	HIS
3	C	129	PHE
2	E	35	PRO
2	E	371	PHE
3	F	117	ASN
1	A	11	TYR
1	A	436	VAL
2	B	58	ASP
1	D	44	VAL
2	B	51	VAL
2	B	237	LEU
3	C	128	GLY
3	F	50	CYS
3	F	5	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	509/512 (99%)	445 (87%)	64 (13%)	4 21
1	D	509/512 (99%)	434 (85%)	75 (15%)	3 17
2	B	310/379 (82%)	253 (82%)	57 (18%)	1 9
2	E	311/379 (82%)	248 (80%)	63 (20%)	1 7
3	C	257/273 (94%)	207 (80%)	50 (20%)	1 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	253/273 (93%)	196 (78%)	57 (22%)	1	5
4	M	2/2 (100%)	0	2 (100%)	0	0
4	N	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	2153/2332 (92%)	1784 (83%)	369 (17%)	2	12

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	13	ILE
1	A	21	ARG
1	A	26	GLN
1	A	30	ASN
1	A	32	ILE
1	A	42	LEU
1	A	52	LEU
1	A	59	ILE
1	A	60	TYR
1	A	64	GLU
1	A	86	VAL
1	A	107	LYS
1	A	112	LEU
1	A	124	LEU
1	A	131	LEU
1	A	140	TRP
1	A	168	GLN
1	A	196	LEU
1	A	218	ASP
1	A	222	LEU
1	A	228	CYS
1	A	237	GLN
1	A	250	GLN
1	A	255	LYS
1	A	277	GLU
1	A	282	ASP
1	A	304	HIS
1	A	312	ASN
1	A	318	ARG
1	A	327	LEU
1	A	331	LYS
1	A	347	SER

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Mol	Chain	Res	Type
1	A	358	LYS
1	A	373	LEU
1	A	387	ASN
1	A	389	ASP
1	A	392	ASN
1	A	394	VAL
1	A	395	ILE
1	A	398	ARG
1	A	402	GLN
1	A	418	ARG
1	A	425	GLU
1	A	434	LEU
1	A	436	VAL
1	A	441	GLU
1	A	448	MET
1	A	454	HIS
1	A	455	VAL
1	A	466	LEU
1	A	467	LYS
1	A	473	PHE
1	A	486	VAL
1	A	502	LEU
1	A	506	ASN
1	A	507	VAL
1	A	516	ILE
1	A	526	LEU
1	A	527	ARG
1	A	556	LEU
1	A	566	LYS
1	A	570	ASP
1	A	581	GLU
2	B	38	GLN
2	B	43	ILE
2	B	49	CYS
2	B	53	PHE
2	B	56	VAL
2	B	62	ASP
2	B	73	LEU
2	B	78	GLU
2	B	94	GLU
2	B	103	MET
2	B	107	LEU

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Mol	Chain	Res	Type
2	B	112	ASN
2	B	122	GLU
2	B	126	THR
2	B	142	LEU
2	B	143	ARG
2	B	147	SER
2	B	149	ASP
2	B	157	LYS
2	B	162	LYS
2	B	166	GLN
2	B	167	LEU
2	B	168	LEU
2	B	169	GLU
2	B	177	ARG
2	B	178	GLU
2	B	179	ARG
2	B	181	PHE
2	B	184	THR
2	B	196	LEU
2	B	203	GLN
2	B	210	ARG
2	B	214	GLU
2	B	219	ASN
2	B	237	LEU
2	B	239	LEU
2	B	240	LYS
2	B	244	LYS
2	B	257	VAL
2	B	258	LYS
2	B	262	VAL
2	B	266	GLN
2	B	285	VAL
2	B	287	MET
2	B	308	LEU
2	B	312	LEU
2	B	314	VAL
2	B	315	ILE
2	B	323	ILE
2	B	331	LEU
2	B	348	TYR
2	B	353	GLU
2	B	369	ILE

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Mol	Chain	Res	Type
2	B	373	SER
2	B	386	ILE
2	B	389	LEU
2	B	390	ILE
3	C	10	LEU
3	C	15	GLU
3	C	17	LEU
3	C	25	GLU
3	C	31	LEU
3	C	37	GLU
3	C	38	ILE
3	C	46	GLN
3	C	47	GLU
3	C	49	ARG
3	C	52	VAL
3	C	61	GLN
3	C	83	MET
3	C	87	VAL
3	C	93	SER
3	C	98	THR
3	C	105	VAL
3	C	106	ARG
3	C	109	GLU
3	C	110	ARG
3	C	111	ILE
3	C	112	THR
3	C	117	ASN
3	C	123	ILE
3	C	124	THR
3	C	139	ASN
3	C	158	LEU
3	C	162	GLN
3	C	175	ASP
3	C	177	LEU
3	C	185	ARG
3	C	186	LEU
3	C	199	LEU
3	C	214	ARG
3	C	222	GLN
3	C	225	SER
3	C	234	LEU
3	C	243	LEU

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Mol	Chain	Res	Type
3	C	244	VAL
3	C	249	ASN
3	C	250	TRP
3	C	256	VAL
3	C	264	ASN
3	C	265	TYR
3	C	268	ARG
3	C	275	ILE
3	C	282	LEU
3	C	283	LYS
3	C	294	ARG
3	C	306	ASP
1	D	10	LEU
1	D	20	LEU
1	D	25	VAL
1	D	30	ASN
1	D	34	LYS
1	D	42	LEU
1	D	45	GLU
1	D	50	GLU
1	D	55	LEU
1	D	58	THR
1	D	60	TYR
1	D	71	GLU
1	D	77	THR
1	D	79	LEU
1	D	102	THR
1	D	103	VAL
1	D	104	VAL
1	D	112	LEU
1	D	113	ARG
1	D	120	SER
1	D	131	LEU
1	D	139	ASP
1	D	144	ARG
1	D	153	VAL
1	D	196	LEU
1	D	197	GLU
1	D	222	LEU
1	D	226	GLU
1	D	237	GLN
1	D	245	MET

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Mol	Chain	Res	Type
1	D	272	LYS
1	D	294	CYS
1	D	295	GLU
1	D	297	GLU
1	D	318	ARG
1	D	327	LEU
1	D	330	ILE
1	D	345	LEU
1	D	350	MET
1	D	355	ILE
1	D	358	LYS
1	D	366	LEU
1	D	370	LEU
1	D	373	LEU
1	D	387	ASN
1	D	395	ILE
1	D	405	LEU
1	D	410	GLU
1	D	411	LEU
1	D	413	GLU
1	D	429	LEU
1	D	437	GLU
1	D	441	GLU
1	D	446	LEU
1	D	455	VAL
1	D	459	ARG
1	D	463	THR
1	D	466	LEU
1	D	467	LYS
1	D	468	LYS
1	D	469	LEU
1	D	481	THR
1	D	482	ILE
1	D	489	MET
1	D	492	ASP
1	D	501	THR
1	D	502	LEU
1	D	507	VAL
1	D	526	LEU
1	D	527	ARG
1	D	542	LYS
1	D	554	SER

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Mol	Chain	Res	Type
1	D	556	LEU
1	D	569	GLN
1	D	581	GLU
2	E	39	GLU
2	E	43	ILE
2	E	45	LYS
2	E	50	CYS
2	E	52	LEU
2	E	55	PHE
2	E	63	LEU
2	E	68	VAL
2	E	73	LEU
2	E	75	GLU
2	E	78	GLU
2	E	81	THR
2	E	91	ILE
2	E	96	VAL
2	E	103	MET
2	E	105	ARG
2	E	111	SER
2	E	114	THR
2	E	121	GLU
2	E	127	LEU
2	E	131	TRP
2	E	143	ARG
2	E	146	GLU
2	E	154	ILE
2	E	156	LYS
2	E	157	LYS
2	E	162	LYS
2	E	165	LEU
2	E	169	GLU
2	E	186	LEU
2	E	188	ARG
2	E	203	GLN
2	E	215	THR
2	E	216	GLU
2	E	233	ASN
2	E	258	LYS
2	E	259	SER
2	E	261	SER
2	E	266	GLN

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Mol	Chain	Res	Type
2	E	275	LEU
2	E	277	LYS
2	E	281	LEU
2	E	289	LEU
2	E	295	LYS
2	E	298	SER
2	E	302	VAL
2	E	306	ASN
2	E	308	LEU
2	E	309	GLU
2	E	310	GLU
2	E	312	LEU
2	E	315	ILE
2	E	318	SER
2	E	319	GLU
2	E	327	LEU
2	E	351	ASN
2	E	369	ILE
2	E	375	TYR
2	E	381	HIS
2	E	385	THR
2	E	386	ILE
2	E	389	LEU
2	E	390	ILE
3	F	7	THR
3	F	8	LYS
3	F	12	GLN
3	F	15	GLU
3	F	18	ASN
3	F	19	GLU
3	F	22	GLN
3	F	30	SER
3	F	32	CYS
3	F	38	ILE
3	F	39	LEU
3	F	42	GLU
3	F	44	ASN
3	F	45	VAL
3	F	46	GLN
3	F	48	VAL
3	F	53	THR
3	F	54	VAL

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Mol	Chain	Res	Type
3	F	55	CYS
3	F	58	VAL
3	F	61	GLN
3	F	68	LEU
3	F	75	SER
3	F	81	LEU
3	F	87	VAL
3	F	98	THR
3	F	105	VAL
3	F	110	ARG
3	F	112	THR
3	F	114	LEU
3	F	117	ASN
3	F	119	GLU
3	F	122	GLN
3	F	124	THR
3	F	131	ASP
3	F	158	LEU
3	F	174	ILE
3	F	175	ASP
3	F	185	ARG
3	F	186	LEU
3	F	192	GLU
3	F	199	LEU
3	F	214	ARG
3	F	227	THR
3	F	232	ASN
3	F	239	ARG
3	F	243	LEU
3	F	250	TRP
3	F	254	ARG
3	F	258	THR
3	F	264	ASN
3	F	265	TYR
3	F	266	CYS
3	F	269	CYS
3	F	275	ILE
3	F	290	ASP
3	F	294	ARG
4	M	2	LEU
4	M	4	ARG
4	N	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	119	HIS
1	A	172	ASN
1	A	200	ASN
1	A	211	ASN
1	A	217	GLN
1	A	288	GLN
1	A	289	ASN
1	A	338	ASN
1	A	360	ASN
1	A	364	HIS
1	A	387	ASN
1	A	465	ASN
1	A	494	ASN
1	A	506	ASN
1	A	520	HIS
1	A	539	ASN
1	A	545	GLN
1	A	553	ASN
2	B	38	GLN
2	B	44	GLN
2	B	82	HIS
2	B	97	HIS
2	B	135	GLN
2	B	203	GLN
2	B	218	HIS
2	B	219	ASN
2	B	243	HIS
2	B	264	HIS
2	B	273	GLN
2	B	297	HIS
2	B	351	ASN
2	B	352	ASN
2	B	383	ASN
2	B	387	HIS
3	C	12	GLN
3	C	27	GLN
3	C	59	HIS
3	C	61	GLN
3	C	79	ASN
3	C	139	ASN

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Mol	Chain	Res	Type
3	C	179	HIS
3	C	187	GLN
3	C	222	GLN
3	C	264	ASN
3	C	271	ASN
3	C	288	GLN
1	D	30	ASN
1	D	87	HIS
1	D	117	HIS
1	D	127	HIS
1	D	172	ASN
1	D	200	ASN
1	D	233	GLN
1	D	250	GLN
1	D	288	GLN
1	D	325	GLN
1	D	339	GLN
1	D	387	ASN
1	D	402	GLN
1	D	514	GLN
1	D	539	ASN
1	D	571	GLN
2	E	44	GLN
2	E	82	HIS
2	E	97	HIS
2	E	112	ASN
2	E	218	HIS
2	E	233	ASN
2	E	264	HIS
2	E	297	HIS
2	E	362	ASN
3	F	16	GLN
3	F	18	ASN
3	F	27	GLN
3	F	46	GLN
3	F	63	HIS
3	F	79	ASN
3	F	118	HIS
3	F	162	GLN
3	F	191	HIS
3	F	232	ASN
3	F	241	HIS

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Mol	Chain	Res	Type
3	F	255	ASN
3	F	288	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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
4	FGA	N	6	4	7,8,9	1.58	1 (14%)	6,9,11	1.37	0
4	FGA	M	6	4	7,8,9	1.54	1 (14%)	6,9,11	1.08	0
4	DAM	N	7	4	4,5,6	1.74	1 (25%)	3,5,7	5.11	3 (100%)
4	ACB	M	3	4	7,8,9	1.70	2 (28%)	8,10,12	1.87	2 (25%)
4	DAM	M	7	4	4,5,6	1.72	1 (25%)	3,5,7	3.66	3 (100%)
4	1ZN	M	5	4	21,23,24	1.96	1 (4%)	25,29,31	3.19	5 (20%)
4	ACB	N	3	4	7,8,9	1.99	2 (28%)	8,10,12	1.51	1 (12%)
3	MLL	C	309	3	8,9,9	3.53	2 (25%)	9,11,11	2.45	2 (22%)
4	1ZN	N	5	4	21,23,24	2.18	2 (9%)	25,29,31	4.09	10 (40%)

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
4	FGA	N	6	4	-	3/8/8/9	-
4	FGA	M	6	4	-	2/8/8/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DAM	N	7	4	-	0/0/4/6	-
4	ACB	M	3	4	-	2/10/10/12	-
4	DAM	M	7	4	-	0/0/4/6	-
4	1ZN	M	5	4	-	4/23/25/27	0/1/1/1
4	ACB	N	3	4	-	3/10/10/12	-
3	MLL	C	309	3	-	8/10/10/10	-
4	1ZN	N	5	4	-	3/23/25/27	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	5	1ZN	C15-C13	-9.24	1.26	1.46
3	C	309	MLL	O-C	9.01	1.44	1.21
4	M	5	1ZN	C15-C13	-8.60	1.27	1.46
4	N	3	ACB	O-C	4.27	1.34	1.22
3	C	309	MLL	OXT-C	4.14	1.43	1.33
4	M	3	ACB	O-C	3.68	1.33	1.22
4	M	6	FGA	OE2-CD	-3.53	1.24	1.42
4	N	6	FGA	OE2-CD	-3.49	1.24	1.42
4	N	7	DAM	C-CA	3.09	1.50	1.45
4	M	7	DAM	C-CA	2.83	1.49	1.45
4	N	5	1ZN	C15-C16	-2.24	1.27	1.32
4	M	3	ACB	OD1-CG	2.10	1.27	1.20
4	N	3	ACB	OD1-CG	2.04	1.27	1.20

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	5	1ZN	C16-C15-C13	17.64	164.26	126.32
4	M	5	1ZN	C16-C15-C13	13.73	155.86	126.32
3	C	309	MLL	OXT-C-O	-6.58	111.04	123.85
4	N	7	DAM	O-C-CA	-6.52	116.85	125.33
4	N	7	DAM	CM-N-CA	-4.95	116.47	123.98
4	M	7	DAM	O-C-CA	-4.76	119.14	125.33
4	N	5	1ZN	C18-CA-C16	-4.75	106.17	112.98
4	M	3	ACB	OD1-CG-CB	-3.74	115.44	124.96
4	N	5	1ZN	CA-C16-C15	3.64	129.57	123.62
4	N	5	1ZN	CA-C18-C	3.54	115.17	110.67
4	N	3	ACB	CA-CB-CG	-3.41	106.29	110.69
4	M	7	DAM	CM-N-CA	-3.40	118.82	123.98
4	M	5	1ZN	C15-C13-C12	3.40	127.94	118.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	7	DAM	CB-CA-N	-3.36	117.57	125.84
4	M	5	1ZN	C14-C13-C15	-3.35	112.97	118.09
4	N	5	1ZN	C14-C13-C15	-3.30	113.05	118.09
4	N	5	1ZN	C11-C10-C2	-3.26	107.02	111.78
4	N	5	1ZN	C15-C13-C12	3.06	127.02	118.82
4	M	5	1ZN	C10-C12-C13	-2.98	117.46	126.72
3	C	309	MLL	O-C-CA	-2.88	110.93	120.62
4	M	5	1ZN	C18-CA-C16	-2.85	108.89	112.98
4	N	5	1ZN	C10-C12-C13	-2.77	118.11	126.72
4	M	3	ACB	CA-CB-CG	-2.69	107.21	110.69
4	N	5	1ZN	C2-C10-C12	2.55	114.95	110.33
4	M	7	DAM	CB-CA-N	-2.45	119.81	125.84
4	N	5	1ZN	C16-CA-N	-2.04	105.27	109.92

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	309	MLL	O-C-CA-CB
4	M	3	ACB	C4-CB-CG-OD1
4	N	3	ACB	CA-CB-CG-OD1
4	N	5	1ZN	C12-C13-C15-C16
4	N	5	1ZN	C14-C13-C15-C16
3	C	309	MLL	CA-C-OXT-C10
4	M	5	1ZN	C14-C13-C15-C16
4	M	5	1ZN	C12-C13-C15-C16
4	N	6	FGA	OE2-CD-CG-CB
4	N	3	ACB	OXT-C-CA-CB
3	C	309	MLL	CA-CB-CG-CD2
3	C	309	MLL	CA-CB-CG-CD1
4	N	6	FGA	OXT-C-CA-N
4	N	6	FGA	CA-CB-CG-CD
4	M	6	FGA	OXT-C-CA-N
3	C	309	MLL	O-C-CA-N
4	M	6	FGA	OE2-CD-CG-CB
4	M	3	ACB	CA-CB-CG-OD1
4	M	5	1ZN	O-C-C18-CA
4	M	5	1ZN	C10-C2-C3-C4
3	C	309	MLL	OXT-C-CA-CB
3	C	309	MLL	N-CA-CB-CG
4	N	3	ACB	O-C-CA-CB
4	N	5	1ZN	C10-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	C	309	MLL	C-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	6	FGA	3	0
4	N	7	DAM	7	0
4	M	3	ACB	3	0
4	M	7	DAM	4	0
4	M	5	1ZN	4	0
4	N	3	ACB	16	1
3	C	309	MLL	4	0
4	N	5	1ZN	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	2:LEU	C	3:ACB	N	2.64

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	583/589 (98%)	0.63	29 (4%)	34	19	85, 114, 172, 203	0
1	D	583/589 (98%)	0.34	14 (2%)	59	35	96, 113, 129, 144	0
2	B	376/407 (92%)	0.16	10 (2%)	56	33	77, 90, 126, 152	0
2	E	377/407 (92%)	0.13	12 (3%)	50	29	63, 76, 103, 139	0
3	C	305/309 (98%)	0.34	14 (4%)	37	20	81, 93, 112, 139	0
3	F	291/309 (94%)	0.71	24 (8%)	17	11	131, 149, 159, 166	0
4	M	2/7 (28%)	1.80	0	100	100	86, 86, 86, 91	0
4	N	2/7 (28%)	1.75	0	100	100	80, 80, 80, 85	0
All	All	2519/2624 (95%)	0.39	103 (4%)	41	22	63, 106, 153, 203	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	241	HIS	6.0
3	F	117	ASN	4.9
2	E	406	ASP	4.7
1	D	8	ASP	4.7
3	C	241	HIS	4.4
3	F	85	ASP	4.3
2	B	406	ASP	4.2
1	D	570	ASP	4.1
1	A	17	ILE	4.0
3	C	266	CYS	4.0
3	F	266	CYS	4.0
3	F	175	ASP	3.9
3	C	85	ASP	3.9
2	B	56	VAL	3.8
1	A	16	LEU	3.6
1	D	7	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
3	F	172	PRO	3.5
3	F	167	HIS	3.5
1	A	7	ASP	3.4
2	E	56	VAL	3.4
3	F	265	TYR	3.4
3	F	200	TRP	3.3
1	D	61	ASP	3.1
3	C	298	PRO	3.1
2	B	339	HIS	3.1
1	A	319	GLU	3.1
3	C	265	TYR	3.0
3	F	168	GLY	3.0
1	D	492	ASP	3.0
1	A	13	ILE	3.0
1	A	80	VAL	3.0
2	E	32	ASP	3.0
3	C	117	ASN	2.9
2	B	401	ASN	2.9
1	A	20	LEU	2.9
1	D	436	VAL	2.8
3	F	242	GLN	2.8
1	A	34	LYS	2.8
1	D	174	CYS	2.8
3	F	118	HIS	2.8
3	F	267	TYR	2.8
3	F	264	ASN	2.8
2	B	381	HIS	2.7
1	A	140	TRP	2.7
1	A	523	PRO	2.7
1	A	63	ASP	2.7
3	C	75	SER	2.7
1	D	573	VAL	2.6
1	A	18	ASP	2.6
2	E	55	PHE	2.6
1	A	32	ILE	2.6
2	E	33	VAL	2.6
3	C	116	GLY	2.6
2	E	54	ASP	2.5
3	F	211	ILE	2.5
1	A	482	ILE	2.5
2	E	30	ILE	2.5
1	D	25	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	F	127	TYR	2.5
1	A	579	ALA	2.5
3	C	89	ARG	2.4
1	A	512	CYS	2.4
1	D	148	CYS	2.4
1	A	118	GLU	2.4
2	B	366	ILE	2.4
1	A	10	LEU	2.4
2	E	351	ASN	2.4
3	F	263	PRO	2.4
1	A	575	VAL	2.4
3	F	47	GLU	2.4
2	B	126	THR	2.3
1	A	426	TYR	2.3
1	A	21	ARG	2.3
3	C	306	ASP	2.3
3	F	84	GLY	2.3
3	F	116	GLY	2.3
1	A	154	CYS	2.3
1	A	45	GLU	2.3
1	A	19	GLU	2.2
2	B	31	ARG	2.2
2	E	116	ALA	2.2
1	A	37	THR	2.2
3	F	280	ASP	2.2
3	C	297	GLU	2.2
1	D	63	ASP	2.2
2	B	50	CYS	2.2
2	B	404	LEU	2.2
2	E	120	PRO	2.1
3	C	69	PHE	2.1
3	C	77	ASP	2.1
3	F	191	HIS	2.1
1	A	78	THR	2.1
1	D	512	CYS	2.1
3	F	253	ASP	2.1
2	E	123	ASP	2.0
1	D	84	GLU	2.0
3	C	287	LEU	2.0
1	A	574	ASP	2.0
3	F	57	ASP	2.0
1	A	40	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	17	ILE	2.0
1	A	67	LEU	2.0
2	E	405	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	DAM	M	7	6/7	0.31	0.31	93,93,93,93	0
4	DAL	N	1	5/6	0.51	0.24	84,84,84,84	0
4	ACB	M	3	9/10	0.52	0.23	87,88,90,90	0
4	ACB	N	3	9/10	0.56	0.26	82,83,85,86	0
4	DAL	M	1	5/6	0.59	0.23	91,91,91,91	0
4	FGA	N	6	9/10	0.66	0.29	78,82,83,84	0
4	DAM	N	7	6/7	0.66	0.24	84,84,84,85	0
4	FGA	M	6	9/10	0.68	0.27	87,90,91,92	0
4	1ZN	M	5	23/24	0.74	0.23	85,85,89,90	0
3	MLL	C	309	10/10	0.77	0.30	139,139,139,140	0
4	1ZN	N	5	23/24	0.80	0.23	63,66,76,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MN	F	310	1/1	0.97	0.20	86,86,86,86	0
5	MN	C	310	1/1	0.98	0.20	119,119,119,119	0
5	MN	C	311	1/1	0.99	0.26	63,63,63,63	0
5	MN	F	311	1/1	0.99	0.27	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.