



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:17 PM UTC

PDB ID : 1G3N / pdb_00001g3n
Title : STRUCTURE OF A P18(INK4C)-CDK6-K-CYCLIN TERNARY COMPLEX
Authors : Jeffrey, P.D.; Tong, L.; Pavletich, N.P.
Deposited on : 2000-10-24
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

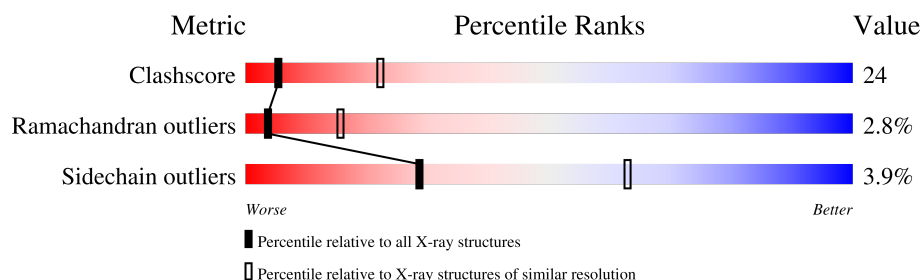
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	326	
1	E	326	
2	B	168	
2	F	168	
3	C	257	
3	G	257	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10644 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 CYCLIN-DEPENDENT KINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2341	1499	405	428	9			
1	E	293	Total	C	N	O	S	0	0	0
			2341	1499	405	428	9			

- Molecule 2 is a protein called CYCLIN-DEPENDENT KINASE 6 INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	0	0
			1181	726	227	225	3			
2	F	155	Total	C	N	O	S	0	0	0
			1181	726	227	225	3			

- Molecule 3 is a protein called V-CYCLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	233	Total	C	N	O	S	0	0	0
			1800	1156	297	339	8			
3	G	233	Total	C	N	O	S	0	0	0
			1800	1156	297	339	8			

There are 4 discrepancies between the modelled and reference sequences:

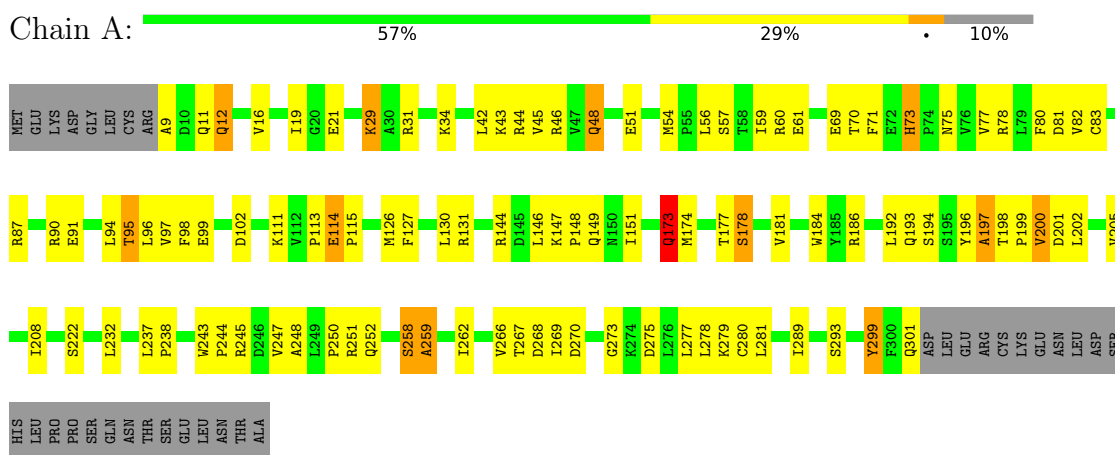
Chain	Residue	Modelled	Actual	Comment	Reference
C	163	VAL	LEU	conflict	UNP O40946
C	188	LEU	LYS	conflict	UNP O40946
G	163	VAL	LEU	conflict	UNP O40946
G	188	LEU	LYS	conflict	UNP O40946

3 Residue-property plots

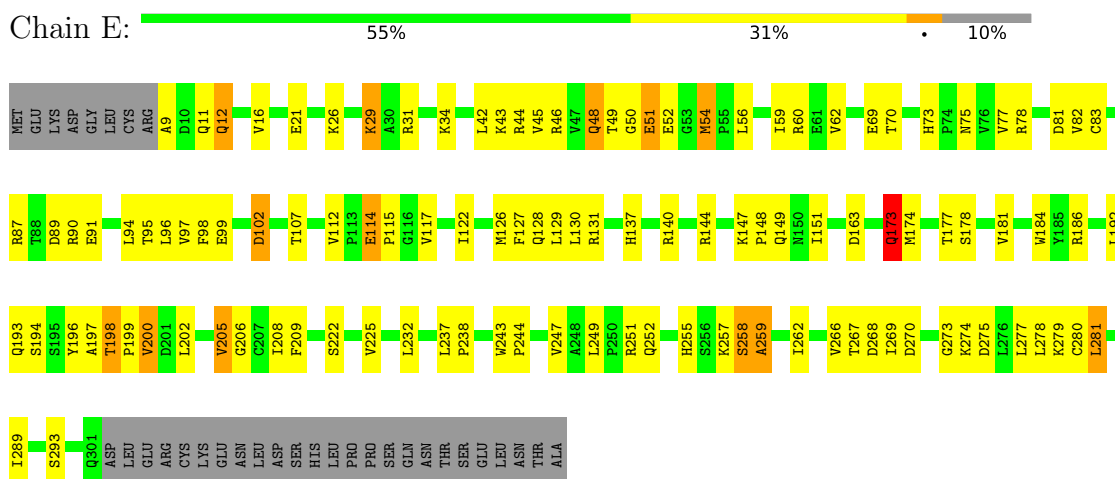
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

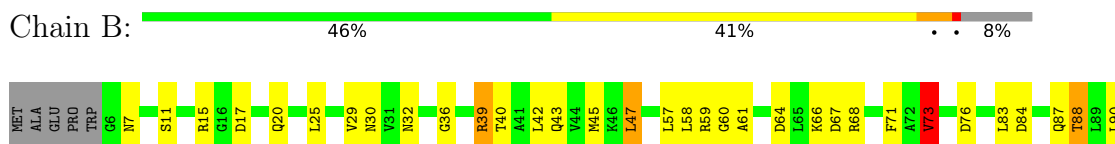
• Molecule 1: CYCLIN-DEPENDENT KINASE 6



• Molecule 1: CYCLIN-DEPENDENT KINASE 6



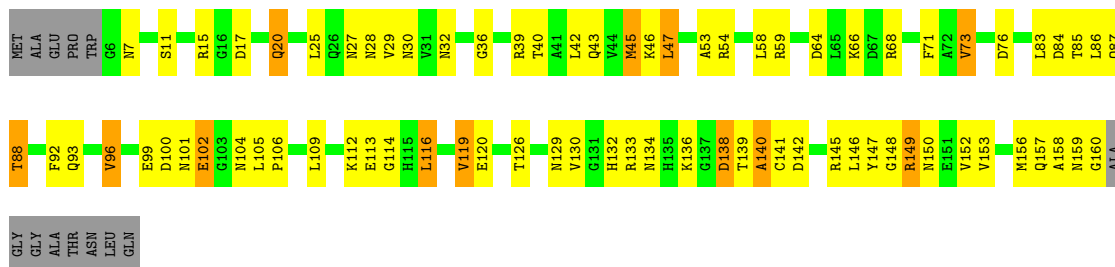
• Molecule 2: CYCLIN-DEPENDENT KINASE 6 INHIBITOR





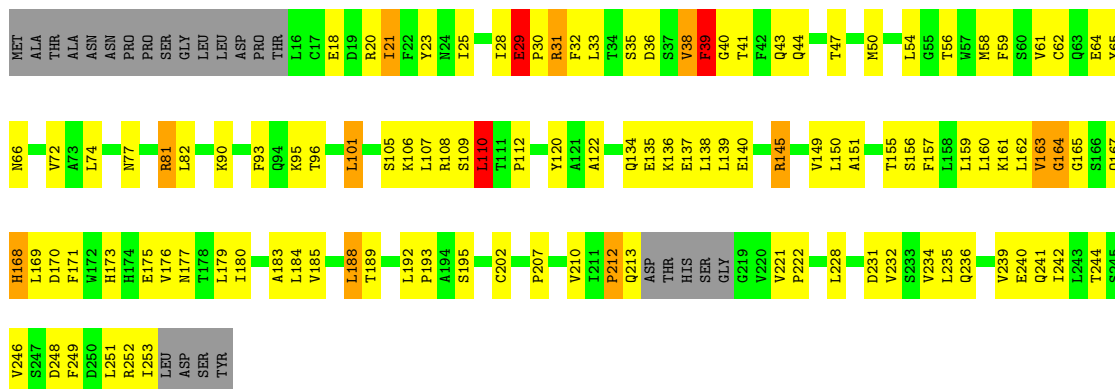
• Molecule 2: CYCLIN-DEPENDENT KINASE 6 INHIBITOR

Chain F: 46% 39% 7% 8%



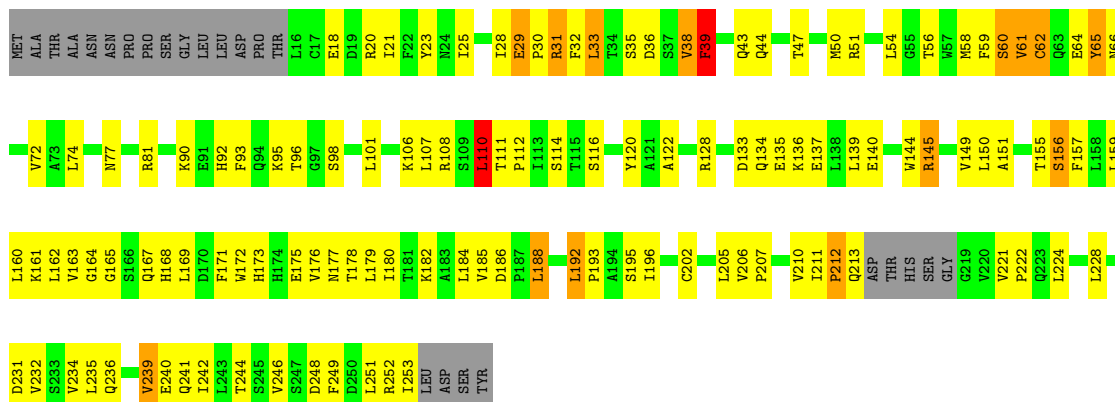
• Molecule 3: V-CYCLIN

Chain C: 47% 39% 9%



• Molecule 3: V-CYCLIN

Chain G: 43% 42% 5% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.78Å 146.95Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10644	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.81	1/2393 (0.0%)	1.20	18/3243 (0.6%)
1	E	0.77	2/2393 (0.1%)	1.22	17/3243 (0.5%)
2	B	0.75	0/1195	1.18	8/1615 (0.5%)
2	F	0.73	0/1195	1.19	9/1615 (0.6%)
3	C	0.74	0/1830	1.20	10/2489 (0.4%)
3	G	0.64	0/1830	1.17	16/2489 (0.6%)
All	All	0.75	3/10836 (0.0%)	1.20	78/14694 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	147	LYS	CG-CD	5.72	1.69	1.52
1	E	147	LYS	CD-CE	5.33	1.68	1.52
1	A	147	LYS	CG-CD	5.13	1.67	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	ALA	N-CA-C	-8.18	103.19	113.01
1	A	51	GLU	N-CA-C	-8.02	103.49	113.20
1	E	51	GLU	N-CA-C	-7.76	103.53	113.16
3	G	35	SER	N-CA-C	7.59	121.19	108.13
3	C	110	LEU	N-CA-C	-7.57	103.03	111.82
3	G	110	LEU	N-CA-C	-7.52	103.09	111.82
2	F	158	ALA	N-CA-C	-7.30	104.50	113.19
3	G	38	VAL	N-CA-C	7.30	118.07	110.62
3	C	35	SER	CA-C-N	7.11	130.51	120.28
3	C	35	SER	C-N-CA	7.11	130.51	120.28
2	B	47	LEU	N-CA-C	6.93	120.62	111.75
3	C	35	SER	N-CA-C	6.89	119.62	108.32
2	B	130	VAL	N-CA-C	6.88	117.39	110.23
2	F	119	VAL	N-CA-C	-6.78	104.16	110.53
3	G	149	VAL	N-CA-C	-6.42	101.27	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	36	ASP	N-CA-CB	-6.29	100.54	110.22
3	G	39	PHE	N-CA-C	6.25	124.12	110.80
3	C	38	VAL	N-CA-C	6.25	116.42	110.42
1	E	81	ASP	N-CA-C	6.23	117.69	108.60
1	E	12	GLN	N-CA-C	-6.19	106.27	113.88
2	F	138	ASP	N-CA-C	6.16	117.98	110.41
2	F	47	LEU	N-CA-C	6.13	119.60	111.75
3	G	151	ALA	N-CA-C	-6.11	104.70	111.36
1	A	197	ALA	N-CA-C	6.05	117.85	110.41
1	E	114	GLU	N-CA-C	6.02	121.82	113.45
1	A	114	GLU	N-CA-C	6.00	121.68	113.16
1	A	81	ASP	N-CA-C	5.90	117.22	108.60
2	B	64	ASP	N-CA-C	5.89	120.16	113.15
2	B	93	GLN	N-CA-C	5.89	120.42	113.23
1	E	225	VAL	N-CA-C	-5.83	104.13	112.35
1	A	12	GLN	N-CA-C	-5.80	106.75	113.88
1	A	280	CYS	N-CA-C	-5.80	104.33	111.40
1	E	29	LYS	N-CA-C	-5.76	99.80	109.07
1	A	147	LYS	CD-CE-NZ	5.75	130.28	111.90
3	G	205	LEU	N-CA-C	5.72	120.53	112.93
2	F	140	ALA	N-CA-C	-5.69	104.98	111.07
1	A	248	ALA	N-CA-C	5.61	118.16	111.71
3	G	35	SER	CA-C-N	5.60	128.55	120.38
3	G	35	SER	C-N-CA	5.60	128.55	120.38
3	G	192	LEU	CA-C-N	5.52	125.45	119.76
3	G	192	LEU	C-N-CA	5.52	125.45	119.76
1	A	90	ARG	N-CA-C	5.52	119.51	112.34
1	E	205	VAL	N-CA-C	-5.51	105.13	110.42
3	C	39	PHE	N-CA-C	5.50	122.52	110.80
3	G	202	CYS	N-CA-C	-5.48	104.34	111.02
1	A	29	LYS	N-CA-C	-5.48	100.25	109.07
1	A	111	LYS	N-CA-C	-5.47	107.86	114.75
1	E	114	GLU	CA-C-N	-5.46	113.02	119.84
1	E	114	GLU	C-N-CA	-5.46	113.02	119.84
3	C	149	VAL	N-CA-C	-5.45	101.64	108.84
1	E	90	ARG	N-CA-C	5.40	119.36	112.34
3	C	21	ILE	N-CA-C	-5.38	105.26	110.42
2	B	73	VAL	CB-CA-C	-5.37	104.89	112.14
1	A	73	HIS	CA-C-N	5.37	125.04	119.56
1	A	73	HIS	C-N-CA	5.37	125.04	119.56
1	A	299	TYR	N-CA-C	-5.37	105.51	111.36
3	C	81	ARG	N-CA-C	-5.36	105.48	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	45	MET	N-CA-C	5.35	117.44	110.43
1	A	147	LYS	N-CA-C	-5.34	100.87	109.58
2	F	93	GLN	N-CA-C	5.32	119.72	113.23
1	A	80	PHE	N-CA-C	5.31	117.15	111.36
3	G	239	VAL	N-CA-C	-5.29	105.16	110.30
1	E	54	MET	CA-C-N	5.29	126.12	119.98
1	E	54	MET	C-N-CA	5.29	126.12	119.98
2	B	119	VAL	N-CA-C	-5.27	105.58	110.53
2	B	123	VAL	N-CA-C	5.27	115.47	110.42
3	G	186	ASP	CA-C-N	5.25	126.40	119.84
3	G	186	ASP	C-N-CA	5.25	126.40	119.84
1	A	95	THR	N-CA-C	5.24	116.94	108.34
2	F	64	ASP	N-CA-C	5.21	119.35	113.15
1	A	273	GLY	N-CA-C	-5.20	106.19	112.49
1	E	280	CYS	N-CA-C	-5.14	104.64	112.04
3	G	36	ASP	N-CA-CB	-5.10	102.09	110.14
1	E	198	THR	N-CA-C	5.09	121.06	109.81
1	E	147	LYS	CD-CE-NZ	5.09	128.18	111.90
2	F	116	LEU	N-CA-C	5.04	116.78	111.28
1	E	249	LEU	CA-C-N	5.03	125.00	120.03
1	E	249	LEU	C-N-CA	5.03	125.00	120.03

There are no chirality outliers.

There are no planarity outliers.

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	A	2341	0	2358	100	0
1	E	2341	0	2358	118	0
2	B	1181	0	1174	65	0
2	F	1181	0	1174	75	0
3	C	1800	0	1848	92	0
3	G	1800	0	1848	101	0
All	All	10644	0	10760	514	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 24.

All (514) 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)
1:E:48:GLN:H	1:E:48:GLN:NE2	1.67	0.91
1:A:173:GLN:H	1:A:173:GLN:NE2	1.68	0.91
3:C:171:PHE:O	3:C:175:GLU:HG2	1.71	0.89
1:E:9:ALA:N	1:E:83:CYS:HG	1.70	0.89
3:G:56:THR:HG23	3:G:185:VAL:HG11	1.56	0.88
2:B:42:LEU:HG	2:B:73:VAL:HG21	1.57	0.86
2:B:25:LEU:O	2:B:59:ARG:NH1	2.09	0.86
1:E:73:HIS:HD2	1:E:75:ASN:H	1.22	0.86
1:A:9:ALA:N	1:A:83:CYS:HG	1.74	0.86
1:A:48:GLN:H	1:A:48:GLN:NE2	1.74	0.85
2:F:142:ASP:O	2:F:146:LEU:HD13	1.76	0.84
2:B:84:ASP:O	2:B:88:THR:HG22	1.79	0.83
2:B:45:MET:HE3	2:B:47:LEU:HD23	1.60	0.82
3:C:110:LEU:H	3:C:110:LEU:HD12	1.45	0.82
3:C:56:THR:HG23	3:C:185:VAL:HG11	1.62	0.82
3:G:171:PHE:O	3:G:175:GLU:HG2	1.80	0.82
3:G:157:PHE:CZ	3:G:161:LYS:HE2	2.15	0.81
3:G:110:LEU:HD12	3:G:110:LEU:H	1.46	0.80
1:E:173:GLN:H	1:E:173:GLN:NE2	1.79	0.80
2:F:25:LEU:O	2:F:59:ARG:NH1	2.14	0.79
2:F:42:LEU:HG	2:F:73:VAL:HG21	1.62	0.79
2:B:142:ASP:O	2:B:146:LEU:HD13	1.83	0.79
3:C:38:VAL:HG12	3:C:43:GLN:HG2	1.64	0.78
1:A:73:HIS:HD2	1:A:75:ASN:H	1.28	0.78
3:C:252:ARG:O	3:C:253:ILE:O	2.00	0.78
1:A:12:GLN:HG3	1:A:34:LYS:HG3	1.66	0.78
2:B:99:GLU:HA	2:B:104:ASN:O	1.83	0.78
3:C:155:THR:O	3:C:159:LEU:HB2	1.84	0.78
1:A:70:THR:HG21	3:C:28:ILE:HG23	1.64	0.77
1:E:202:LEU:HD13	1:E:289:ILE:O	1.84	0.77
3:C:145:ARG:HG2	3:C:145:ARG:HH11	1.51	0.76
3:C:50:MET:HE1	3:C:90:LYS:HG3	1.67	0.76
3:G:47:THR:OG1	3:G:50:MET:HG3	1.86	0.75
1:A:252:GLN:NE2	1:E:21:GLU:OE2	2.19	0.75
3:C:56:THR:HG22	3:C:249:PHE:CE1	2.22	0.75
1:E:69:GLU:CD	1:E:78:ARG:HH21	1.95	0.75
3:C:38:VAL:CG1	3:C:43:GLN:HG2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:VAL:HG13	3:C:235:LEU:HD23	1.68	0.74
3:G:38:VAL:CG1	3:G:43:GLN:HG2	2.17	0.74
1:A:48:GLN:H	1:A:48:GLN:CD	1.93	0.74
1:E:52:GLU:OE2	3:G:114:SER:HA	1.86	0.74
3:C:157:PHE:CZ	3:C:161:LYS:HE2	2.23	0.73
1:E:42:LEU:HD22	1:E:97:VAL:HG22	1.69	0.73
3:C:195:SER:HB2	3:C:228:LEU:HD22	1.70	0.73
2:F:84:ASP:O	2:F:88:THR:HG22	1.89	0.72
3:G:235:LEU:O	3:G:239:VAL:HG23	1.89	0.72
3:G:195:SER:HB2	3:G:228:LEU:HD22	1.70	0.72
3:G:188:LEU:HD22	3:G:241:GLN:OE1	1.90	0.72
1:E:78:ARG:H	1:E:99:GLU:HG2	1.55	0.72
1:E:12:GLN:HG3	1:E:34:LYS:HG3	1.70	0.71
3:G:155:THR:O	3:G:159:LEU:HB2	1.89	0.71
1:A:42:LEU:HD22	1:A:97:VAL:HG22	1.73	0.71
3:G:38:VAL:HG12	3:G:43:GLN:HG2	1.71	0.71
3:G:50:MET:HE1	3:G:90:LYS:HG3	1.73	0.71
1:A:70:THR:HG22	3:C:28:ILE:HD12	1.73	0.70
1:A:43:LYS:HE2	1:A:98:PHE:CE2	2.27	0.70
1:E:48:GLN:H	1:E:48:GLN:CD	2.00	0.70
1:E:131:ARG:HG3	1:E:131:ARG:HH11	1.57	0.70
1:A:199:PRO:HA	1:A:202:LEU:HD12	1.72	0.69
1:A:46:ARG:HD3	1:A:91:GLU:CD	2.18	0.69
3:C:110:LEU:HD22	3:G:111:THR:HG22	1.74	0.68
3:G:21:ILE:O	3:G:25:ILE:HG12	1.92	0.68
3:C:77:ASN:OD1	3:C:81:ARG:HD3	1.92	0.68
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.59	0.68
2:B:129:ASN:ND2	2:B:132:HIS:HB2	2.08	0.68
1:A:144:ARG:HD2	1:A:200:VAL:HG11	1.75	0.68
2:F:11:SER:O	2:F:15:ARG:HG2	1.94	0.68
3:C:21:ILE:O	3:C:25:ILE:HG12	1.94	0.68
3:G:221:VAL:HG13	3:G:235:LEU:HD23	1.76	0.68
3:G:252:ARG:O	3:G:253:ILE:O	2.12	0.68
3:C:64:GLU:C	3:C:66:ASN:H	2.02	0.67
2:F:99:GLU:HA	2:F:104:ASN:O	1.95	0.67
1:A:73:HIS:CD2	1:A:75:ASN:H	2.12	0.67
3:C:221:VAL:HG21	3:C:236:GLN:NE2	2.10	0.67
1:E:266:VAL:HG21	1:E:277:LEU:HD21	1.77	0.67
1:E:43:LYS:HE2	1:E:98:PHE:CE2	2.30	0.67
3:C:110:LEU:HD22	3:G:111:THR:CG2	2.26	0.66
3:C:188:LEU:HD22	3:C:241:GLN:OE1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:207:PRO:HG2	3:G:210:VAL:HG23	1.77	0.66
1:A:245:ARG:CZ	1:E:46:ARG:HB3	2.25	0.66
1:E:232:LEU:HD22	1:E:238:PRO:HD3	1.78	0.66
1:E:73:HIS:CD2	1:E:75:ASN:H	2.10	0.66
1:E:82:VAL:HG22	1:E:96:LEU:CD2	2.25	0.66
1:E:46:ARG:HD3	1:E:91:GLU:CD	2.21	0.66
3:G:145:ARG:HG2	3:G:145:ARG:HH11	1.61	0.66
3:G:155:THR:HG21	3:G:177:ASN:OD1	1.96	0.66
3:G:77:ASN:OD1	3:G:81:ARG:HD3	1.96	0.65
3:G:64:GLU:C	3:G:66:ASN:H	2.05	0.65
3:C:28:ILE:HG22	3:C:32:PHE:HE1	1.61	0.65
2:F:20:GLN:HA	2:F:20:GLN:HE21	1.62	0.65
1:A:197:ALA:O	1:A:200:VAL:HB	1.97	0.65
1:A:275:ASP:OD2	1:A:279:LYS:NZ	2.30	0.65
1:A:69:GLU:CD	1:A:78:ARG:HH21	2.04	0.65
3:G:62:CYS:SG	3:G:72:VAL:HG22	2.36	0.65
2:F:15:ARG:HH21	2:F:20:GLN:HG2	1.62	0.65
1:A:202:LEU:HD13	1:A:289:ILE:O	1.96	0.65
2:B:83:LEU:HG	2:B:87:GLN:HE21	1.60	0.65
1:E:70:THR:HG22	3:G:28:ILE:HD12	1.78	0.65
1:A:16:VAL:HG22	1:A:29:LYS:O	1.97	0.64
2:F:45:MET:HE3	2:F:47:LEU:HD23	1.80	0.64
2:F:29:VAL:HG22	2:F:30:ASN:H	1.63	0.64
2:F:129:ASN:ND2	2:F:132:HIS:HB2	2.13	0.64
3:G:231:ASP:HB2	3:G:234:VAL:HG23	1.80	0.64
3:C:145:ARG:HH11	3:C:145:ARG:CG	2.12	0.64
2:F:133:ARG:HA	2:F:138:ASP:O	1.99	0.63
1:E:199:PRO:HA	1:E:202:LEU:HD12	1.79	0.63
3:C:110:LEU:HD12	3:C:110:LEU:N	2.11	0.63
1:E:193:GLN:HA	1:E:196:TYR:OH	1.97	0.63
1:A:9:ALA:N	1:A:83:CYS:SG	2.72	0.63
2:B:101:ASN:C	2:B:102:GLU:OE1	2.42	0.63
1:E:114:GLU:O	1:E:115:PRO:C	2.40	0.63
1:A:12:GLN:HE21	1:A:34:LYS:HB2	1.64	0.63
2:B:139:THR:HG22	2:B:140:ALA:N	2.14	0.63
2:F:139:THR:HG22	2:F:140:ALA:N	2.14	0.63
2:B:17:ASP:CG	2:B:20:GLN:HB3	2.25	0.62
3:C:43:GLN:O	3:C:44:GLN:HB2	2.00	0.62
1:E:82:VAL:HG22	1:E:96:LEU:HD22	1.81	0.62
3:C:54:LEU:O	3:C:58:MET:HG3	2.00	0.62
3:C:167:GLN:O	3:C:168:HIS:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:PRO:HG2	1:E:149:GLN:NE2	2.14	0.62
2:F:66:LYS:HA	2:F:71:PHE:O	2.00	0.62
1:E:9:ALA:HB3	1:E:83:CYS:SG	2.39	0.62
3:G:110:LEU:HD12	3:G:110:LEU:N	2.14	0.62
1:A:21:GLU:OE2	1:E:252:GLN:NE2	2.32	0.61
1:A:258:SER:O	1:A:259:ALA:HB2	2.00	0.61
2:B:139:THR:H	2:B:142:ASP:HB2	1.63	0.61
1:A:245:ARG:NH2	1:E:46:ARG:HB3	2.15	0.61
3:G:28:ILE:O	3:G:31:ARG:HB2	2.00	0.61
1:A:177:THR:HG23	1:E:222:SER:HB2	1.83	0.61
2:B:15:ARG:HH21	2:B:20:GLN:HG2	1.64	0.61
2:B:100:ASP:OD1	2:B:104:ASN:HB2	2.01	0.61
3:G:56:THR:CG2	3:G:185:VAL:HG11	2.29	0.61
1:E:12:GLN:HE21	1:E:34:LYS:HB2	1.65	0.61
1:A:77:VAL:HG23	1:A:99:GLU:HG3	1.83	0.60
1:A:173:GLN:H	1:A:173:GLN:CD	2.06	0.60
3:C:47:THR:OG1	3:C:50:MET:HG3	2.00	0.60
3:C:39:PHE:HA	3:C:43:GLN:HB2	1.84	0.60
3:C:180:ILE:O	3:C:184:LEU:HG	2.02	0.60
1:E:144:ARG:HD2	1:E:200:VAL:HG11	1.82	0.60
1:E:197:ALA:O	1:E:200:VAL:HB	2.00	0.60
1:A:130:LEU:HD21	1:A:205:VAL:HG11	1.84	0.60
3:C:231:ASP:HB2	3:C:234:VAL:HG23	1.83	0.60
1:E:16:VAL:HG22	1:E:29:LYS:O	2.01	0.60
3:G:145:ARG:HH11	3:G:145:ARG:CG	2.15	0.60
1:E:77:VAL:HG23	1:E:99:GLU:HG3	1.83	0.60
2:F:17:ASP:CG	2:F:20:GLN:HB3	2.27	0.60
3:G:20:ARG:NH1	3:G:23:TYR:CD2	2.69	0.60
1:A:232:LEU:HD22	1:A:238:PRO:HD3	1.82	0.59
3:G:242:ILE:O	3:G:246:VAL:HG23	2.02	0.59
3:G:43:GLN:O	3:G:44:GLN:HB2	2.01	0.59
1:E:70:THR:HG21	3:G:28:ILE:HG23	1.83	0.59
2:F:29:VAL:HG22	2:F:30:ASN:N	2.17	0.59
3:G:28:ILE:HG22	3:G:32:PHE:HE1	1.67	0.59
3:G:162:LEU:O	3:G:212:PRO:HD2	2.03	0.58
2:B:30:ASN:ND2	2:B:32:ASN:H	2.02	0.58
3:C:235:LEU:O	3:C:239:VAL:HG23	2.03	0.58
3:G:221:VAL:HG21	3:G:236:GLN:NE2	2.19	0.58
3:C:155:THR:HG21	3:C:177:ASN:OD1	2.03	0.58
3:C:221:VAL:HG21	3:C:236:GLN:HE21	1.69	0.58
1:E:78:ARG:N	1:E:99:GLU:HG2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:PHE:O	1:E:131:ARG:HG2	2.02	0.58
1:A:148:PRO:HG2	1:A:149:GLN:NE2	2.18	0.58
3:C:56:THR:CG2	3:C:185:VAL:HG11	2.33	0.58
1:E:186:ARG:HG3	1:E:186:ARG:HH11	1.69	0.57
3:G:180:ILE:O	3:G:184:LEU:HG	2.03	0.57
3:C:110:LEU:H	3:C:110:LEU:CD1	2.17	0.57
1:A:222:SER:HB2	1:E:177:THR:HG23	1.87	0.57
3:C:95:LYS:HG2	3:C:134:GLN:HG3	1.86	0.57
2:F:83:LEU:CD1	2:F:87:GLN:HE21	2.17	0.57
1:A:198:THR:CG2	1:A:199:PRO:HD3	2.35	0.57
1:A:177:THR:CG2	1:E:222:SER:HB2	2.35	0.56
3:C:74:LEU:HB2	3:C:150:LEU:HD11	1.86	0.56
2:B:66:LYS:HA	2:B:71:PHE:O	2.06	0.56
1:E:51:GLU:HB2	3:G:128:ARG:NH1	2.20	0.56
3:G:107:LEU:O	3:G:108:ARG:HD3	2.05	0.56
3:G:167:GLN:O	3:G:168:HIS:HB2	2.04	0.56
1:A:19:ILE:HD11	1:A:29:LYS:HB2	1.87	0.56
2:B:40:THR:OG1	2:B:43:GLN:HG3	2.04	0.56
1:A:126:MET:HE1	1:A:205:VAL:HG12	1.86	0.56
2:F:148:GLY:O	2:F:150:ASN:N	2.36	0.56
2:B:133:ARG:HA	2:B:138:ASP:O	2.06	0.56
1:A:44:ARG:HD2	1:A:95:THR:OG1	2.05	0.56
1:E:9:ALA:CB	1:E:83:CYS:SG	2.94	0.56
1:E:48:GLN:CD	1:E:48:GLN:N	2.63	0.56
1:A:173:GLN:H	1:A:173:GLN:HE21	1.54	0.55
3:C:64:GLU:O	3:C:66:ASN:N	2.39	0.55
3:G:93:PHE:O	3:G:96:THR:HB	2.06	0.55
1:A:193:GLN:HA	1:A:196:TYR:OH	2.06	0.55
1:A:201:ASP:O	1:A:205:VAL:HG23	2.05	0.55
2:B:157:GLN:C	2:B:159:ASN:N	2.63	0.55
3:C:242:ILE:O	3:C:246:VAL:HG23	2.06	0.55
3:G:54:LEU:O	3:G:58:MET:HG3	2.07	0.55
3:C:56:THR:HG22	3:C:249:PHE:HE1	1.68	0.55
1:E:46:ARG:CZ	1:E:48:GLN:HG3	2.36	0.55
1:E:258:SER:O	1:E:259:ALA:HB2	2.05	0.55
3:C:20:ARG:NH1	3:C:23:TYR:CD2	2.75	0.55
2:F:139:THR:H	2:F:142:ASP:HB2	1.70	0.55
3:G:110:LEU:H	3:G:110:LEU:CD1	2.19	0.55
2:B:11:SER:O	2:B:15:ARG:HG2	2.07	0.55
3:G:244:THR:O	3:G:248:ASP:OD1	2.25	0.54
2:B:29:VAL:HG22	2:B:30:ASN:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:LEU:HD23	1:E:60:ARG:HH21	1.72	0.54
2:F:58:LEU:HD13	2:F:92:PHE:CE2	2.42	0.54
1:A:70:THR:CG2	3:C:28:ILE:HD12	2.35	0.54
1:A:78:ARG:H	1:A:99:GLU:HG2	1.72	0.54
2:B:96:VAL:HG11	2:B:126:THR:HB	1.88	0.54
2:B:157:GLN:C	2:B:159:ASN:H	2.15	0.54
3:C:207:PRO:HG2	3:C:210:VAL:HG23	1.89	0.54
2:F:139:THR:HB	2:F:142:ASP:OD1	2.08	0.54
3:C:162:LEU:O	3:C:212:PRO:HD2	2.07	0.54
2:B:29:VAL:HG22	2:B:30:ASN:H	1.73	0.54
1:A:127:PHE:O	1:A:131:ARG:HG2	2.07	0.54
3:G:196:ILE:HD13	3:G:228:LEU:HD13	1.89	0.54
3:G:221:VAL:HG12	3:G:232:VAL:HG13	1.90	0.54
1:E:173:GLN:HG2	1:E:174:MET:H	1.72	0.54
1:E:177:THR:HG22	1:E:178:SER:N	2.23	0.54
3:G:64:GLU:O	3:G:66:ASN:N	2.40	0.54
1:A:127:PHE:CE1	1:A:131:ARG:HD3	2.43	0.53
2:F:153:VAL:O	2:F:157:GLN:HG2	2.07	0.53
1:A:48:GLN:CD	1:A:48:GLN:N	2.64	0.53
3:C:62:CYS:SG	3:C:72:VAL:HG22	2.48	0.53
1:A:70:THR:OG1	3:C:145:ARG:NH2	2.41	0.53
3:C:29:GLU:HB3	3:C:30:PRO:CD	2.38	0.53
1:E:70:THR:CG2	3:G:28:ILE:HD12	2.37	0.53
1:E:173:GLN:H	1:E:173:GLN:CD	2.16	0.53
2:B:30:ASN:C	2:B:30:ASN:HD22	2.16	0.53
3:G:136:LYS:O	3:G:140:GLU:HG3	2.08	0.53
3:C:93:PHE:O	3:C:96:THR:HB	2.08	0.53
2:F:96:VAL:HG11	2:F:126:THR:HB	1.90	0.53
2:B:152:VAL:HG12	2:B:156:MET:CE	2.39	0.53
1:E:46:ARG:NH2	1:E:48:GLN:HG3	2.23	0.53
3:C:195:SER:HB2	3:C:228:LEU:CD2	2.38	0.52
1:A:56:LEU:HD23	1:A:60:ARG:HH21	1.74	0.52
3:C:145:ARG:CG	3:C:145:ARG:NH1	2.72	0.52
3:C:82:LEU:HD22	3:C:138:LEU:HD13	1.92	0.52
3:G:159:LEU:CD2	3:G:173:HIS:HA	2.39	0.52
3:C:18:GLU:HA	3:C:18:GLU:OE1	2.10	0.52
1:E:269:ILE:HG12	1:E:270:ASP:N	2.25	0.52
1:A:78:ARG:N	1:A:99:GLU:HG2	2.24	0.51
1:A:177:THR:HG22	1:A:178:SER:N	2.25	0.51
1:E:177:THR:HG22	1:E:178:SER:H	1.74	0.51
3:G:95:LYS:HG2	3:G:134:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:VAL:N	3:C:222:PRO:HD2	2.26	0.51
1:A:181:VAL:HG13	1:A:184:TRP:CE3	2.46	0.51
3:G:120:TYR:C	3:G:122:ALA:H	2.18	0.51
1:A:177:THR:HG22	1:A:178:SER:H	1.76	0.51
2:F:40:THR:OG1	2:F:43:GLN:HG3	2.11	0.51
1:A:31:ARG:NH2	2:B:76:ASP:OD1	2.43	0.51
1:A:9:ALA:HB3	1:A:83:CYS:SG	2.51	0.50
3:C:136:LYS:O	3:C:140:GLU:HG3	2.11	0.50
1:E:60:ARG:CZ	3:G:106:LYS:O	2.59	0.50
1:A:71:PHE:HA	3:C:28:ILE:HD11	1.93	0.50
1:E:9:ALA:N	1:E:83:CYS:SG	2.79	0.50
1:E:87:ARG:HD3	1:E:91:GLU:OE1	2.11	0.50
1:E:181:VAL:HG13	1:E:184:TRP:CE3	2.46	0.50
1:E:269:ILE:HD11	1:E:273:GLY:C	2.36	0.50
1:A:198:THR:HG22	1:A:199:PRO:HD3	1.93	0.50
1:E:56:LEU:HD21	3:G:112:PRO:HG3	1.94	0.50
1:E:131:ARG:HG3	1:E:131:ARG:NH1	2.24	0.50
3:G:56:THR:HG22	3:G:249:PHE:CE1	2.47	0.50
2:F:15:ARG:NH2	2:F:20:GLN:HG2	2.26	0.50
2:F:54:ARG:O	2:F:58:LEU:HB2	2.11	0.50
2:F:30:ASN:C	2:F:30:ASN:HD22	2.19	0.50
3:G:74:LEU:HB2	3:G:150:LEU:HD11	1.92	0.50
2:B:139:THR:CG2	2:B:140:ALA:N	2.75	0.50
1:A:266:VAL:HG21	1:A:277:LEU:HD21	1.94	0.50
3:C:176:VAL:O	3:C:180:ILE:HG12	2.11	0.50
3:G:61:VAL:O	3:G:65:TYR:HB2	2.12	0.50
3:G:162:LEU:HD11	3:G:224:LEU:HD21	1.94	0.50
3:G:195:SER:HB2	3:G:228:LEU:CD2	2.41	0.50
1:A:114:GLU:CD	1:A:114:GLU:O	2.55	0.49
1:A:173:GLN:HG2	1:A:174:MET:H	1.76	0.49
2:F:139:THR:CG2	2:F:140:ALA:N	2.75	0.49
2:B:116:LEU:CD1	2:B:152:VAL:HA	2.42	0.49
1:A:222:SER:HB2	1:E:177:THR:CG2	2.42	0.49
1:E:262:ILE:HG22	1:E:274:LYS:HE3	1.93	0.49
2:F:30:ASN:C	2:F:30:ASN:ND2	2.70	0.49
1:A:9:ALA:CB	1:A:83:CYS:SG	3.00	0.49
2:B:145:ARG:HB2	2:B:145:ARG:NH1	2.28	0.49
2:F:112:LYS:HE3	2:F:147:TYR:CZ	2.47	0.49
3:G:29:GLU:HB3	3:G:30:PRO:CD	2.43	0.49
1:A:245:ARG:HH21	1:E:46:ARG:H	1.60	0.49
2:B:148:GLY:O	2:B:150:ASN:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ASN:ND2	2:B:30:ASN:C	2.70	0.49
3:C:212:PRO:O	3:C:213:GLN:HB2	2.12	0.49
1:E:126:MET:HE1	1:E:205:VAL:HG12	1.95	0.49
1:E:275:ASP:OD2	1:E:279:LYS:NZ	2.45	0.49
3:G:221:VAL:N	3:G:222:PRO:HD2	2.28	0.49
2:F:20:GLN:HE21	2:F:20:GLN:CA	2.22	0.49
2:F:45:MET:SD	2:F:53:ALA:HB2	2.53	0.49
2:F:83:LEU:HD11	2:F:87:GLN:HE21	1.78	0.49
2:F:114:GLY:HA2	2:F:149:ARG:HG2	1.95	0.49
3:G:120:TYR:C	3:G:122:ALA:N	2.71	0.48
2:B:156:MET:O	2:B:160:GLY:N	2.37	0.48
2:B:39:ARG:HD3	2:B:67:ASP:HB2	1.95	0.48
3:C:110:LEU:O	3:C:112:PRO:HD2	2.12	0.48
3:G:135:GLU:O	3:G:139:LEU:HG	2.13	0.48
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.28	0.48
1:A:245:ARG:NH2	1:E:46:ARG:H	2.12	0.48
2:F:157:GLN:C	2:F:159:ASN:H	2.21	0.48
1:A:258:SER:O	1:A:259:ALA:CB	2.61	0.48
3:G:221:VAL:HG21	3:G:236:GLN:HE21	1.77	0.48
1:A:57:SER:O	1:A:61:GLU:HG3	2.13	0.48
1:A:267:THR:O	1:A:268:ASP:HB3	2.13	0.48
2:F:114:GLY:CA	2:F:149:ARG:HG2	2.44	0.48
2:F:134:ASN:ND2	2:F:136:LYS:H	2.11	0.48
2:F:148:GLY:C	2:F:150:ASN:H	2.19	0.48
2:F:83:LEU:HG	2:F:87:GLN:HE21	1.79	0.48
1:A:45:VAL:HG12	1:A:46:ARG:N	2.29	0.48
1:E:31:ARG:NH2	2:F:76:ASP:OD1	2.47	0.48
1:A:245:ARG:NH2	1:E:46:ARG:CB	2.77	0.47
1:A:252:GLN:NE2	1:E:21:GLU:HG2	2.28	0.47
3:G:145:ARG:CG	3:G:145:ARG:NH1	2.73	0.47
3:G:116:SER:HB3	3:G:128:ARG:NH2	2.29	0.47
3:G:176:VAL:O	3:G:180:ILE:HG12	2.13	0.47
1:E:107:THR:HG21	2:F:46:LYS:HZ3	1.79	0.47
2:F:42:LEU:O	2:F:45:MET:HG2	2.13	0.47
2:B:45:MET:HE2	2:B:73:VAL:HG11	1.96	0.47
2:B:114:GLY:HA2	2:B:152:VAL:HG21	1.96	0.47
2:B:153:VAL:O	2:B:157:GLN:HG2	2.15	0.47
3:G:62:CYS:C	3:G:64:GLU:N	2.73	0.47
3:G:212:PRO:O	3:G:213:GLN:HB2	2.14	0.47
3:C:39:PHE:O	3:C:41:THR:N	2.47	0.47
2:B:139:THR:HB	2:B:142:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:179:LEU:HD23	3:G:179:LEU:C	2.40	0.47
1:A:46:ARG:NH2	1:A:48:GLN:HG3	2.30	0.46
2:B:83:LEU:CG	2:B:87:GLN:HE21	2.26	0.46
2:B:84:ASP:O	2:B:88:THR:CG2	2.59	0.46
2:B:112:LYS:HE3	2:B:147:TYR:CZ	2.50	0.46
2:F:58:LEU:HD13	2:F:92:PHE:CZ	2.50	0.46
1:A:151:ILE:HD11	1:A:208:ILE:HD13	1.96	0.46
2:B:20:GLN:HE21	2:B:20:GLN:HA	1.79	0.46
1:A:289:ILE:HG12	1:A:293:SER:HB2	1.97	0.46
3:G:196:ILE:HD13	3:G:228:LEU:CD1	2.44	0.46
1:A:54:MET:HB3	1:A:59:ILE:HD11	1.97	0.46
3:C:62:CYS:C	3:C:64:GLU:N	2.72	0.46
1:E:192:LEU:O	1:E:193:GLN:C	2.56	0.46
1:E:262:ILE:HB	1:E:278:LEU:HD21	1.98	0.46
3:C:179:LEU:C	3:C:179:LEU:HD23	2.40	0.46
1:E:194:SER:O	1:E:196:TYR:CE1	2.69	0.46
2:F:85:THR:HA	2:F:88:THR:HG23	1.97	0.46
2:F:139:THR:HG22	2:F:141:CYS:H	1.80	0.46
1:E:151:ILE:HD11	1:E:208:ILE:HD13	1.98	0.46
3:G:39:PHE:HA	3:G:43:GLN:HB2	1.98	0.46
1:E:69:GLU:CD	1:E:78:ARG:NH2	2.70	0.46
2:F:101:ASN:C	2:F:102:GLU:OE1	2.59	0.46
3:G:116:SER:HB3	3:G:128:ARG:HH21	1.80	0.46
3:G:50:MET:CE	3:G:90:LYS:HG3	2.46	0.46
3:G:59:PHE:C	3:G:59:PHE:CD2	2.94	0.46
1:E:130:LEU:HD21	1:E:205:VAL:HG11	1.98	0.45
1:E:173:GLN:H	1:E:173:GLN:HE21	1.62	0.45
2:F:116:LEU:CD1	2:F:152:VAL:HA	2.46	0.45
1:A:87:ARG:HD3	1:A:91:GLU:OE1	2.17	0.45
2:B:15:ARG:NH2	2:B:20:GLN:HG2	2.31	0.45
2:B:45:MET:HE3	2:B:47:LEU:CD2	2.40	0.45
2:B:100:ASP:CG	2:B:104:ASN:HB2	2.41	0.45
2:B:114:GLY:HA2	2:B:149:ARG:HG2	1.97	0.45
3:C:59:PHE:C	3:C:59:PHE:CD2	2.94	0.45
1:E:243:TRP:CD1	1:E:244:PRO:HD2	2.51	0.45
2:F:147:TYR:HB3	2:F:149:ARG:HH11	1.81	0.45
2:F:152:VAL:O	2:F:156:MET:HB2	2.16	0.45
3:G:30:PRO:HA	3:G:33:LEU:HD22	1.97	0.45
3:G:64:GLU:C	3:G:66:ASN:N	2.72	0.45
1:A:46:ARG:CZ	1:A:48:GLN:HG3	2.46	0.45
2:F:84:ASP:O	2:F:88:THR:CG2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ASP:OD1	2:F:46:LYS:HD2	2.17	0.45
1:A:194:SER:O	1:A:196:TYR:CE1	2.70	0.45
2:B:148:GLY:C	2:B:150:ASN:H	2.22	0.45
1:E:46:ARG:HD3	1:E:91:GLU:CG	2.47	0.45
3:C:151:ALA:O	3:C:155:THR:HG23	2.17	0.45
2:B:58:LEU:HD13	2:B:92:PHE:CZ	2.52	0.45
3:C:120:TYR:CD1	3:C:120:TYR:C	2.95	0.45
1:E:206:GLY:HA3	1:E:281:LEU:HD13	1.99	0.45
2:B:152:VAL:HG12	2:B:156:MET:HE2	1.99	0.45
3:G:156:SER:HB2	3:G:173:HIS:NE2	2.32	0.45
2:B:83:LEU:CD1	2:B:87:GLN:HE21	2.30	0.44
3:G:120:TYR:C	3:G:120:TYR:CD1	2.94	0.44
3:G:159:LEU:HD21	3:G:172:TRP:C	2.42	0.44
3:C:167:GLN:O	3:C:168:HIS:CB	2.65	0.44
1:E:62:VAL:HG11	3:G:144:TRP:CB	2.47	0.44
2:B:45:MET:O	2:B:45:MET:HG3	2.17	0.44
2:B:57:LEU:HB3	2:B:92:PHE:CD2	2.52	0.44
2:B:105:LEU:O	2:B:106:PRO:C	2.59	0.44
2:B:114:GLY:CA	2:B:149:ARG:HG2	2.47	0.44
2:F:157:GLN:C	2:F:159:ASN:N	2.74	0.44
3:C:156:SER:HB2	3:C:173:HIS:NE2	2.33	0.44
3:C:159:LEU:CD2	3:C:173:HIS:HA	2.47	0.44
1:E:50:GLY:C	1:E:52:GLU:H	2.25	0.44
1:E:267:THR:O	1:E:268:ASP:HB3	2.17	0.44
1:E:31:ARG:HH22	2:F:76:ASP:CG	2.25	0.44
1:E:122:ILE:O	1:E:126:MET:HB2	2.17	0.44
2:F:134:ASN:OD1	2:F:138:ASP:HB2	2.17	0.44
3:C:39:PHE:C	3:C:41:THR:H	2.26	0.44
1:E:42:LEU:CD2	1:E:97:VAL:HG22	2.43	0.44
1:E:77:VAL:HG23	1:E:99:GLU:CG	2.47	0.44
1:A:173:GLN:NE2	1:A:173:GLN:N	2.50	0.44
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.83	0.44
3:C:163:VAL:O	3:C:164:GLY:C	2.60	0.44
1:E:128:GLN:O	1:E:131:ARG:HB2	2.18	0.44
2:F:109:LEU:O	2:F:113:GLU:HG2	2.17	0.44
1:A:243:TRP:CD1	1:A:244:PRO:HD2	2.53	0.44
2:B:7:ASN:HD21	2:B:36:GLY:H	1.66	0.44
2:B:60:GLY:O	2:B:61:ALA:C	2.60	0.44
1:E:151:ILE:CD1	1:E:208:ILE:HD13	2.48	0.44
2:F:86:LEU:HD23	2:F:86:LEU:C	2.43	0.44
3:G:192:LEU:HA	3:G:193:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:LEU:HD21	3:C:246:VAL:HG21	2.00	0.43
3:C:244:THR:O	3:C:248:ASP:OD1	2.36	0.43
1:E:12:GLN:NE2	1:E:34:LYS:HB2	2.31	0.43
1:E:258:SER:O	1:E:259:ALA:CB	2.66	0.43
3:G:157:PHE:CE1	3:G:161:LYS:HE2	2.52	0.43
3:C:107:LEU:O	3:C:108:ARG:HD3	2.19	0.43
2:F:30:ASN:ND2	2:F:32:ASN:H	2.16	0.43
3:G:56:THR:HG22	3:G:249:PHE:HE1	1.82	0.43
3:G:206:VAL:HG12	3:G:211:ILE:HD11	2.00	0.43
2:F:114:GLY:HA2	2:F:149:ARG:CG	2.48	0.43
3:G:92:HIS:O	3:G:93:PHE:C	2.61	0.43
1:A:46:ARG:HD3	1:A:91:GLU:CG	2.48	0.43
2:B:147:TYR:HB3	2:B:149:ARG:HH11	1.82	0.43
1:E:46:ARG:HD3	1:E:91:GLU:OE2	2.18	0.43
2:B:109:LEU:O	2:B:113:GLU:HG2	2.19	0.43
3:C:210:VAL:HG12	3:C:210:VAL:O	2.19	0.43
1:E:198:THR:CG2	1:E:199:PRO:HD3	2.48	0.43
3:C:135:GLU:O	3:C:139:LEU:HG	2.19	0.43
1:E:107:THR:HG21	2:F:46:LYS:NZ	2.33	0.43
1:E:126:MET:HE1	1:E:209:PHE:HB2	1.99	0.43
1:E:237:LEU:HG	1:E:251:ARG:HH11	1.84	0.43
3:C:20:ARG:HA	3:C:20:ARG:HD3	1.71	0.43
3:C:192:LEU:HA	3:C:193:PRO:HD3	1.89	0.43
1:A:114:GLU:O	1:A:114:GLU:OE2	2.37	0.43
1:A:192:LEU:O	1:A:193:GLN:C	2.62	0.43
3:C:106:LYS:HE3	3:C:135:GLU:OE1	2.19	0.43
2:F:100:ASP:CG	2:F:104:ASN:HB2	2.43	0.43
1:A:250:PRO:HB3	1:E:21:GLU:HG3	2.01	0.42
3:C:101:LEU:HD12	3:C:101:LEU:HA	1.89	0.42
1:A:46:ARG:NH1	1:A:91:GLU:HG2	2.34	0.42
1:A:114:GLU:O	1:A:115:PRO:C	2.62	0.42
3:C:109:SER:O	3:C:112:PRO:HD3	2.19	0.42
3:C:159:LEU:HD13	3:C:202:CYS:SG	2.60	0.42
1:E:54:MET:HB3	1:E:59:ILE:HD11	2.02	0.42
1:A:46:ARG:HH11	1:A:91:GLU:HG2	1.83	0.42
1:A:299:TYR:C	1:A:301:GLN:H	2.28	0.42
2:F:43:GLN:HA	2:F:73:VAL:HG22	2.00	0.42
1:A:151:ILE:CD1	1:A:208:ILE:HD13	2.49	0.42
1:E:21:GLU:HB3	1:E:26:LYS:HG2	2.00	0.42
2:F:130:VAL:HG11	2:F:160:GLY:O	2.19	0.42
1:A:70:THR:CG2	3:C:28:ILE:HG23	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:HIS:CD2	1:A:75:ASN:HB2	2.55	0.42
3:C:105:SER:HB2	3:C:109:SER:OG	2.19	0.42
2:F:7:ASN:HD21	2:F:36:GLY:H	1.65	0.42
2:F:27:ASN:O	2:F:28:ASN:C	2.63	0.42
2:F:148:GLY:C	2:F:150:ASN:N	2.77	0.42
3:G:51:ARG:HG3	3:G:51:ARG:HH11	1.84	0.42
1:E:44:ARG:HD2	1:E:95:THR:OG1	2.18	0.42
1:E:262:ILE:HG21	1:E:274:LYS:HG3	2.01	0.42
1:A:262:ILE:HB	1:A:278:LEU:HD21	2.01	0.42
1:E:45:VAL:HG12	1:E:46:ARG:N	2.34	0.42
1:E:129:LEU:HD11	1:E:151:ILE:HD13	2.01	0.42
1:A:78:ARG:HB2	1:A:99:GLU:HG2	2.02	0.42
2:B:90:LEU:HD21	2:B:96:VAL:HG13	2.01	0.42
3:C:163:VAL:O	3:C:163:VAL:HG12	2.19	0.42
1:E:51:GLU:HB2	3:G:128:ARG:HH11	1.84	0.42
1:A:269:ILE:HG12	1:A:270:ASP:N	2.35	0.41
3:C:120:TYR:C	3:C:122:ALA:N	2.77	0.41
2:F:152:VAL:HG12	2:F:156:MET:CE	2.50	0.41
1:E:137:HIS:O	1:E:140:ARG:N	2.49	0.41
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.90	0.41
1:A:237:LEU:HG	1:A:251:ARG:HH11	1.86	0.41
2:B:124:LYS:HE2	2:B:125:HIS:HE1	1.84	0.41
2:F:100:ASP:OD1	2:F:104:ASN:HB2	2.19	0.41
3:C:168:HIS:O	3:C:170:ASP:N	2.52	0.41
2:F:119:VAL:O	2:F:120:GLU:C	2.63	0.41
2:F:145:ARG:NH1	2:F:145:ARG:HB2	2.35	0.41
3:G:156:SER:HA	3:G:173:HIS:HD2	1.85	0.41
3:C:183:ALA:O	3:C:189:THR:OG1	2.33	0.41
1:E:62:VAL:HG11	3:G:144:TRP:HB3	2.02	0.41
1:E:186:ARG:HG3	1:E:186:ARG:NH1	2.33	0.41
3:G:50:MET:HE1	3:G:90:LYS:HE2	2.02	0.41
3:G:120:TYR:O	3:G:122:ALA:N	2.53	0.41
3:G:156:SER:O	3:G:157:PHE:C	2.63	0.41
1:A:238:PRO:O	1:A:251:ARG:HD2	2.21	0.41
2:B:134:ASN:ND2	2:B:136:LYS:H	2.19	0.41
3:C:156:SER:O	3:C:157:PHE:C	2.62	0.41
3:G:133:ASP:O	3:G:137:GLU:HB2	2.21	0.41
3:G:18:GLU:OE1	3:G:18:GLU:HA	2.19	0.41
1:E:49:THR:OG1	1:E:89:ASP:O	2.37	0.41
1:A:114:GLU:OE2	1:A:114:GLU:CA	2.68	0.41
2:B:100:ASP:OD2	2:B:100:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:HG11	2:B:160:GLY:O	2.21	0.41
3:C:156:SER:HA	3:C:173:HIS:HD2	1.86	0.41
1:E:112:VAL:HG11	1:E:117:VAL:HG22	2.02	0.41
1:E:262:ILE:CG2	1:E:274:LYS:HG3	2.51	0.41
2:F:45:MET:HE1	2:F:53:ALA:HB2	2.03	0.41
2:F:83:LEU:CG	2:F:87:GLN:HE21	2.34	0.41
2:F:114:GLY:HA2	2:F:152:VAL:HG21	2.02	0.41
3:G:110:LEU:O	3:G:112:PRO:HD2	2.21	0.41
3:G:178:THR:O	3:G:182:LYS:HG3	2.21	0.41
1:E:52:GLU:OE1	1:E:52:GLU:HA	2.20	0.41
1:E:46:ARG:C	1:E:46:ARG:HD2	2.45	0.40
3:G:95:LYS:O	3:G:98:SER:HB2	2.21	0.40
1:A:82:VAL:HG22	1:A:96:LEU:HD22	2.03	0.40
1:E:289:ILE:HG12	1:E:293:SER:HB2	2.02	0.40
2:F:58:LEU:HD13	2:F:92:PHE:HE2	1.86	0.40
3:G:60:SER:O	3:G:61:VAL:C	2.64	0.40
2:B:42:LEU:O	2:B:45:MET:HG2	2.21	0.40
1:E:48:GLN:NE2	1:E:48:GLN:N	2.50	0.40
1:E:237:LEU:H	1:E:257:LYS:HB2	1.86	0.40
3:C:28:ILE:O	3:C:31:ARG:HB2	2.21	0.40
2:F:105:LEU:O	2:F:106:PRO:C	2.63	0.40
2:F:136:LYS:HD3	2:F:136:LYS:HA	1.92	0.40
2:B:102:GLU:O	2:B:134:ASN:HB2	2.21	0.40
3:C:221:VAL:HG12	3:C:232:VAL:HG13	2.04	0.40
1:E:255:HIS:O	1:E:257:LYS:HG2	2.22	0.40
3:G:159:LEU:HD12	3:G:159:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

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	291/326 (89%)	259 (89%)	27 (9%)	5 (2%)	7	26
1	E	291/326 (89%)	258 (89%)	28 (10%)	5 (2%)	7	26
2	B	153/168 (91%)	134 (88%)	17 (11%)	2 (1%)	9	32
2	F	153/168 (91%)	136 (89%)	16 (10%)	1 (1%)	18	48
3	C	229/257 (89%)	198 (86%)	19 (8%)	12 (5%)	1	5
3	G	229/257 (89%)	189 (82%)	27 (12%)	13 (6%)	1	4
All	All	1346/1502 (90%)	1174 (87%)	134 (10%)	38 (3%)	4	15

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	SER
1	A	259	ALA
3	C	39	PHE
3	C	65	TYR
3	C	212	PRO
1	E	258	SER
1	E	259	ALA
3	G	39	PHE
3	G	65	TYR
3	G	212	PRO
1	A	11	GLN
1	A	173	GLN
3	C	164	GLY
3	C	169	LEU
1	E	11	GLN
1	E	173	GLN
3	G	164	GLY
3	C	29	GLU
3	C	40	GLY
3	C	251	LEU
3	G	169	LEU
3	G	251	LEU
2	F	149	ARG
2	B	149	ARG
2	B	154	SER
3	C	61	VAL
3	C	168	HIS
1	E	163	ASP
3	G	60	SER
3	G	61	VAL

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Mol	Chain	Res	Type
3	G	62	CYS
3	G	156	SER
3	C	163	VAL
3	G	29	GLU
3	G	163	VAL
1	A	113	PRO
3	C	165	GLY
3	G	165	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	A	258/289 (89%)	250 (97%)	8 (3%)	35	69
1	E	258/289 (89%)	251 (97%)	7 (3%)	39	73
2	B	122/130 (94%)	116 (95%)	6 (5%)	22	54
2	F	122/130 (94%)	115 (94%)	7 (6%)	18	49
3	C	205/225 (91%)	195 (95%)	10 (5%)	22	54
3	G	205/225 (91%)	197 (96%)	8 (4%)	28	63
All	All	1170/1288 (91%)	1124 (96%)	46 (4%)	28	63

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	94	LEU
1	A	102	ASP
1	A	173	GLN
1	A	178	SER
1	A	200	VAL
1	A	247	VAL
1	A	281	LEU
2	B	39	ARG
2	B	68	ARG

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Mol	Chain	Res	Type
2	B	73	VAL
2	B	88	THR
2	B	96	VAL
2	B	102	GLU
3	C	29	GLU
3	C	31	ARG
3	C	33	LEU
3	C	101	LEU
3	C	110	LEU
3	C	137	GLU
3	C	145	ARG
3	C	160	LEU
3	C	188	LEU
3	C	240	GLU
1	E	48	GLN
1	E	94	LEU
1	E	102	ASP
1	E	173	GLN
1	E	200	VAL
1	E	247	VAL
1	E	281	LEU
2	F	20	GLN
2	F	39	ARG
2	F	68	ARG
2	F	73	VAL
2	F	88	THR
2	F	96	VAL
2	F	102	GLU
3	G	31	ARG
3	G	33	LEU
3	G	101	LEU
3	G	110	LEU
3	G	145	ARG
3	G	160	LEU
3	G	188	LEU
3	G	240	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	48	GLN

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Mol	Chain	Res	Type
1	A	73	HIS
1	A	75	ASN
1	A	137	HIS
1	A	149	GLN
1	A	173	GLN
1	A	260	GLN
1	A	301	GLN
2	B	7	ASN
2	B	20	GLN
2	B	26	GLN
2	B	30	ASN
2	B	34	GLN
2	B	87	GLN
2	B	101	ASN
2	B	104	ASN
2	B	108	HIS
2	B	129	ASN
2	B	132	HIS
2	B	134	ASN
3	C	94	GLN
3	C	134	GLN
3	C	167	GLN
3	C	173	HIS
3	C	223	GLN
3	C	236	GLN
1	E	12	GLN
1	E	48	GLN
1	E	73	HIS
1	E	75	ASN
1	E	137	HIS
1	E	149	GLN
1	E	173	GLN
1	E	301	GLN
2	F	7	ASN
2	F	20	GLN
2	F	26	GLN
2	F	30	ASN
2	F	34	GLN
2	F	87	GLN
2	F	104	ASN
2	F	129	ASN
2	F	134	ASN

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Mol	Chain	Res	Type
3	G	92	HIS
3	G	94	GLN
3	G	167	GLN
3	G	173	HIS
3	G	223	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.