



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 AM UTC

PDB ID : 1O6O / pdb_00001o6o
Title : Importin Beta aa1-442 bound to five FxFG repeats from yeast Nsp1p. Second crystal form
Authors : Bayliss, R.; Stewart, M.
Deposited on : 2002-10-10
Resolution : 2.80 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

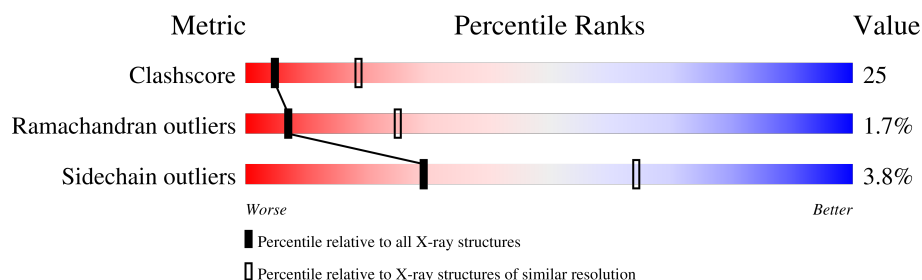
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	442	
1	B	442	
1	C	442	
2	D	119	
2	E	119	
2	F	119	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10433 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 IMPORTIN BETA-1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	1
			3433	2164	576	669	24			
1	B	440	Total	C	N	O	S	0	0	1
			3433	2164	576	669	24			
1	C	440	Total	C	N	O	S	0	0	1
			3433	2164	576	669	24			

- Molecule 2 is a protein called NUCLEOPORIN NSP1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	0	0	1
			38	26	6	6			
2	E	7	Total	C	N	O	0	0	1
			45	31	7	7			
2	F	6	Total	C	N	O	0	0	1
			38	26	6	6			

- Molecule 3 is water.

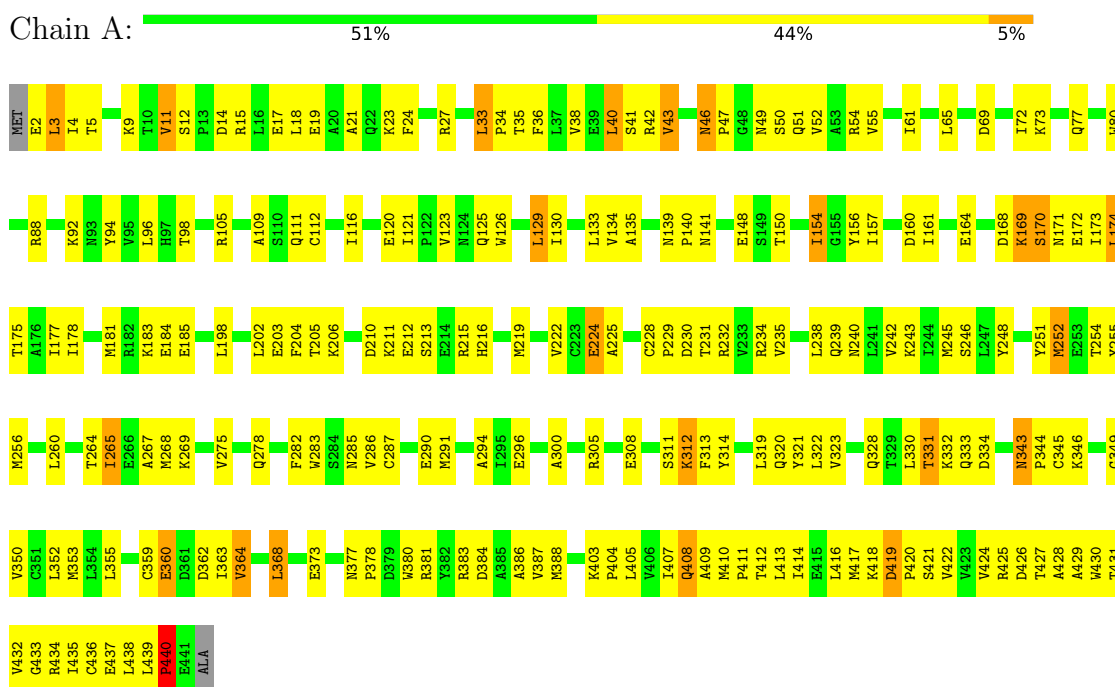
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	2	Total	O	0	0
			2	2		
3	C	5	Total	O	0	0
			5	5		

3 Residue-property plots

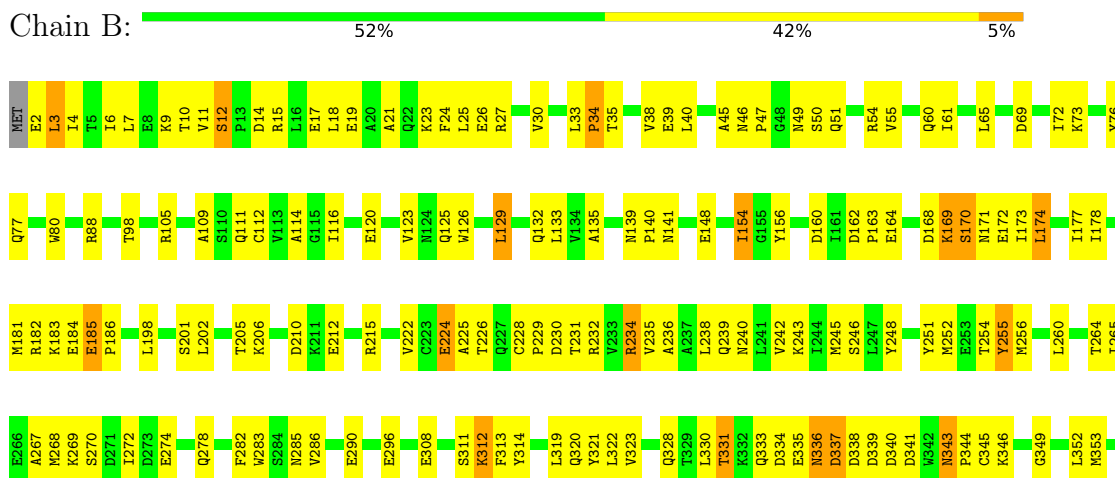
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

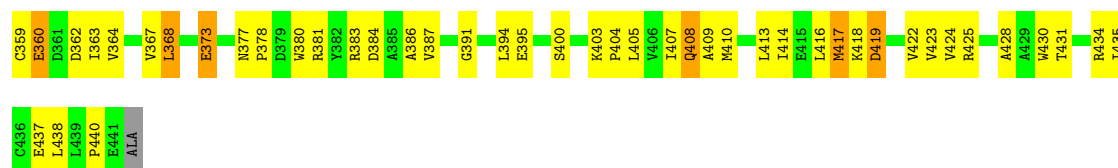
Note EDS was not executed.

• Molecule 1: IMPORTIN BETA-1 SUBUNIT



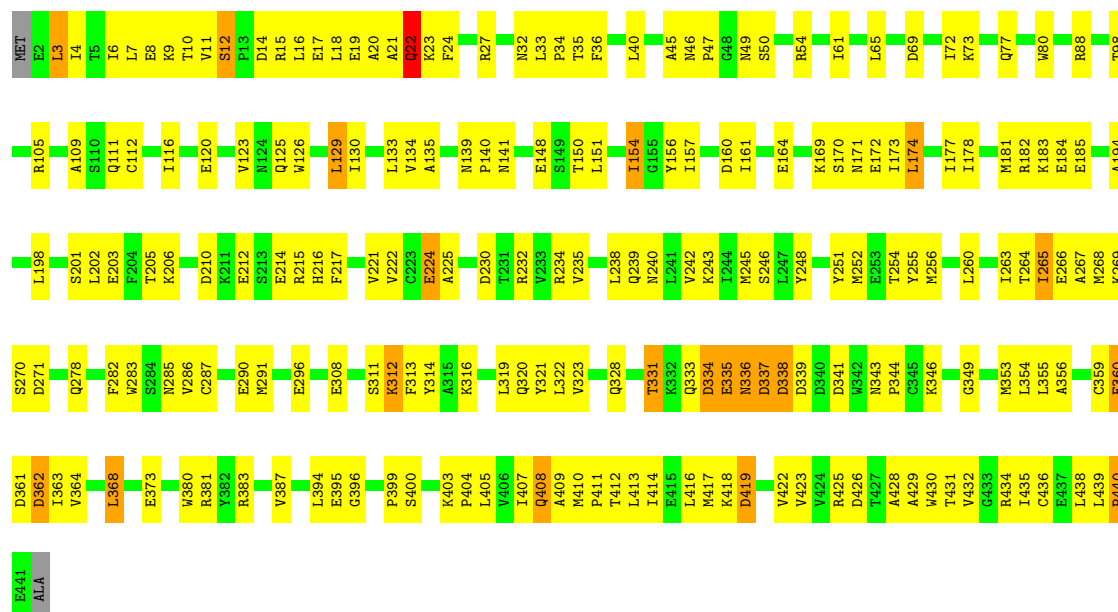
• Molecule 1: IMPORTIN BETA-1 SUBUNIT





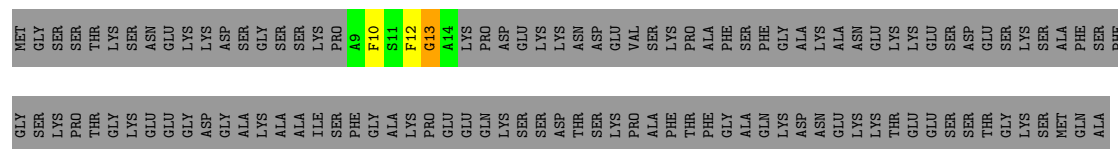
• Molecule 1: IMPORTIN BETA-1 SUBUNIT

Chain C: 52% 43% 5%



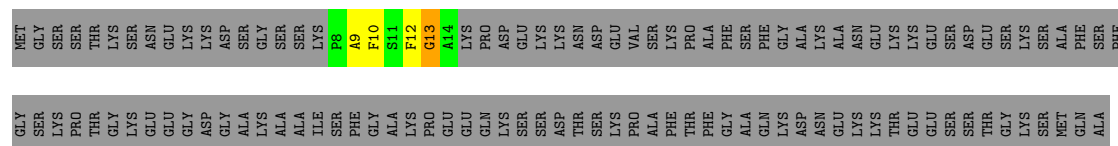
• Molecule 2: NUCLEOPORIN NSP1

Chain D: 95%



• Molecule 2: NUCLEOPORIN NSP1

Chain E: 94%



• Molecule 2: NUCLEOPORIN NSP1

Chain F: 95%

MET	GLY	SER	SER	THR	LYS	LYS	ASN	GLU	GLY	LYS	LYS	ASP	GLY	SER	GLY	SER	ALA	SER	ILE	SER	PHE	GLY	ALA	LYS	PRO	GLU	GLN	LYS	SER	THR	SER	LYS	PRO	ALA	PHE	THR	PHE	GLY	ALA	GLN	LYS	ASP	ASN	LYS	GLU	ALA	LYS	THR	LYS	GLU	SER	THR	GLY	LYS	SER	LYS	GLN	MET	GLN	PHE	ALA	SER	PHE
GLY	SER	LYS	PRO	THR	GLY	LYS	ASN	GLU	GLY	LYS	LYS	ASP	GLY	SER	GLY	SER	ALA	SER	ILE	SER	PHE	GLY	ALA	LYS	PRO	GLU	GLN	LYS	SER	THR	SER	LYS	PRO	ALA	PHE	THR	PHE	GLY	ALA	GLN	LYS	ASP	ASN	LYS	GLU	ALA	LYS	THR	LYS	GLU	SER	THR	GLY	LYS	SER	LYS	GLN	MET	GLN	PHE	ALA	SER	PHE

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	67.11Å 125.35Å 266.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	94.7 (20.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10433	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.60	4/3497 (0.1%)	1.03	17/4761 (0.4%)
1	B	0.56	4/3497 (0.1%)	1.00	12/4761 (0.3%)
1	C	0.54	1/3496 (0.0%)	0.99	12/4758 (0.3%)
2	D	1.06	1/39 (2.6%)	0.57	0/51
2	E	1.39	2/47 (4.3%)	1.39	1/62 (1.6%)
2	F	1.12	1/39 (2.6%)	0.55	0/51
All	All	0.58	13/10615 (0.1%)	1.01	42/14444 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	169	LYS	CA-CB	-7.99	1.41	1.53
1	A	169	LYS	CA-CB	-7.49	1.42	1.53
1	A	168	ASP	C-O	-6.57	1.16	1.24
1	B	168	ASP	C-O	-6.27	1.16	1.24
2	F	13	GLY	C-N	-5.98	1.25	1.33
1	B	170	SER	CA-C	5.70	1.60	1.52
1	C	440	PRO	C-N	-5.70	1.25	1.33
2	D	13	GLY	C-N	-5.68	1.25	1.33
1	A	440	PRO	C-N	-5.58	1.25	1.33
2	E	13	GLY	C-N	-5.54	1.25	1.33
2	E	9	ALA	CA-CB	-5.51	1.45	1.53
1	B	440	PRO	C-N	-5.49	1.25	1.33
1	A	170	SER	CA-C	5.46	1.60	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	SER	N-CA-C	11.77	125.25	111.71
1	B	170	SER	N-CA-C	9.73	123.10	111.33
1	C	336	ASN	N-CA-C	-9.02	103.41	112.97
1	B	252	MET	N-CA-C	8.24	123.11	112.89
1	B	185	GLU	CA-C-N	8.09	127.39	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	GLU	C-N-CA	8.09	127.39	118.97
1	C	252	MET	N-CA-C	7.42	122.08	112.89
1	A	252	MET	N-CA-C	7.37	122.02	112.89
2	E	9	ALA	N-CA-C	7.16	120.60	109.07
1	B	312	LYS	N-CA-C	-7.12	103.62	114.16
1	A	12	SER	CA-C-N	7.12	126.74	119.19
1	A	12	SER	C-N-CA	7.12	126.74	119.19
1	B	336	ASN	N-CA-C	-7.05	103.61	113.20
1	C	335	GLU	N-CA-C	-6.35	104.64	112.38
1	A	312	LYS	N-CA-C	-6.29	104.34	114.09
1	C	160	ASP	N-CA-C	6.14	120.91	113.17
1	C	417	MET	N-CA-C	-6.13	104.66	111.71
1	A	417	MET	N-CA-C	-6.11	104.69	111.71
1	C	185	GLU	CA-C-N	5.97	125.67	119.05
1	C	185	GLU	C-N-CA	5.97	125.67	119.05
1	C	312	LYS	N-CA-C	-5.93	103.82	113.19
1	B	417	MET	N-CA-C	-5.91	104.96	111.82
1	A	169	LYS	CB-CG-CD	5.70	124.42	111.30
1	A	46	ASN	CA-C-N	5.69	126.07	119.47
1	A	46	ASN	C-N-CA	5.69	126.07	119.47
1	A	185	GLU	CA-C-N	5.63	125.30	119.05
1	A	185	GLU	C-N-CA	5.63	125.30	119.05
1	B	160	ASP	N-CA-C	5.63	120.26	113.17
1	B	12	SER	CA-C-N	5.61	125.22	119.56
1	B	12	SER	C-N-CA	5.61	125.22	119.56
1	B	169	LYS	CB-CG-CD	5.58	124.14	111.30
1	C	154	ILE	N-CA-C	-5.51	104.57	110.36
1	A	160	ASP	N-CA-C	5.49	120.09	113.17
1	C	12	SER	CA-C-N	5.30	125.00	119.64
1	C	12	SER	C-N-CA	5.30	125.00	119.64
1	C	364	VAL	CB-CA-C	-5.25	108.71	113.70
1	A	364	VAL	CB-CA-C	-5.23	108.73	113.70
1	A	43	VAL	CB-CA-C	-5.19	105.32	111.81
1	A	40	LEU	N-CA-C	-5.17	105.64	111.28
1	B	154	ILE	N-CA-C	-5.17	104.94	110.36
1	A	33	LEU	N-CA-C	5.16	119.52	112.55
1	A	154	ILE	CB-CA-C	-5.04	105.42	111.88

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	3433	0	3419	177	0
1	B	3433	0	3419	166	0
1	C	3433	0	3418	184	0
2	D	38	0	30	6	0
2	E	45	0	38	7	0
2	F	38	0	30	3	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
3	C	5	0	0	0	0
All	All	10433	0	10354	528	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 25.

All (528) 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:A:343:ASN:HD21	1:A:346:LYS:HD3	1.18	1.04
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.49	0.95
1:C:181:MET:HE1	1:C:198:LEU:HD22	1.49	0.94
1:B:202:LEU:HD12	1:B:243:LYS:HD3	1.49	0.93
1:C:215:ARG:HE	1:C:251:TYR:HD1	1.08	0.91
1:C:202:LEU:HD12	1:C:243:LYS:HD3	1.54	0.87
1:A:343:ASN:ND2	1:A:346:LYS:HD3	1.90	0.87
1:A:202:LEU:HD12	1:A:243:LYS:HD3	1.57	0.86
1:B:410:MET:O	1:B:414:ILE:HG12	1.75	0.85
1:A:219:MET:HE2	1:A:252:MET:HE1	1.59	0.84
1:C:120:GLU:HB3	1:C:125:GLN:HB3	1.59	0.84
1:A:410:MET:O	1:A:414:ILE:HG12	1.77	0.83
1:C:430:TRP:CZ2	1:C:434:ARG:HD2	2.14	0.82
1:B:215:ARG:CZ	1:B:251:TYR:HD1	1.94	0.80
1:A:120:GLU:HB3	1:A:125:GLN:HB3	1.63	0.80
1:C:215:ARG:NE	1:C:251:TYR:HD1	1.79	0.80
1:A:181:MET:HE1	1:A:198:LEU:HD22	1.64	0.78
1:C:212:GLU:HB3	1:C:215:ARG:HH22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HB3	1:B:34:PRO:HD3	1.69	0.75
1:C:123:VAL:HG12	1:C:123:VAL:O	1.85	0.75
1:A:123:VAL:HG12	1:A:123:VAL:O	1.88	0.74
1:B:120:GLU:HB3	1:B:125:GLN:HB3	1.70	0.73
1:B:256:MET:HG2	1:B:314:TYR:CD1	2.23	0.73
1:C:14:ASP:HB3	1:C:17:GLU:HB2	1.70	0.73
1:C:256:MET:HG2	1:C:314:TYR:CD1	2.24	0.73
1:A:69:ASP:HB3	1:A:72:ILE:HG12	1.71	0.72
1:A:206:LYS:HD2	1:A:248:TYR:HE1	1.54	0.72
1:B:431:THR:O	1:B:435:ILE:HG12	1.90	0.72
1:B:69:ASP:HB3	1:B:72:ILE:HG12	1.72	0.71
1:A:216:HIS:CE1	1:A:254:THR:HG21	2.25	0.71
1:A:216:HIS:HE1	1:A:254:THR:HG21	1.55	0.71
1:C:410:MET:O	1:C:414:ILE:HG12	1.91	0.71
1:B:256:MET:HE3	1:B:260:LEU:HB2	1.73	0.70
1:B:46:ASN:HB3	1:B:49:ASN:HD22	1.57	0.69
1:C:215:ARG:NE	1:C:251:TYR:CD1	2.57	0.69
1:C:368:LEU:HD11	1:C:405:LEU:HD21	1.74	0.69
1:B:14:ASP:HB3	1:B:17:GLU:HB2	1.75	0.68
1:B:123:VAL:HG12	1:B:123:VAL:O	1.92	0.68
1:A:178:ILE:HD13	1:A:181:MET:HE3	1.76	0.68
1:C:69:ASP:HB3	1:C:72:ILE:HG12	1.75	0.68
1:C:268:MET:HE1	1:C:322:LEU:HD22	1.76	0.67
1:A:413:LEU:HG	1:A:432:VAL:HG22	1.77	0.66
1:A:171:ASN:HD22	2:D:12:PHE:C	2.04	0.66
1:C:206:LYS:HD2	1:C:248:TYR:HE1	1.60	0.66
1:B:230:ASP:OD1	1:B:232:ARG:HB2	1.96	0.66
1:B:268:MET:HE1	1:B:322:LEU:HD22	1.76	0.66
1:B:46:ASN:HB3	1:B:49:ASN:ND2	2.11	0.66
1:C:343:ASN:OD1	1:C:346:LYS:HD3	1.95	0.65
1:C:256:MET:HE3	1:C:260:LEU:HB2	1.78	0.65
1:C:256:MET:HG2	1:C:314:TYR:CE1	2.32	0.65
1:B:264:THR:HG21	1:B:282:PHE:CD2	2.31	0.65
1:B:335:GLU:C	1:B:337:ASP:H	2.05	0.65
1:C:216:HIS:HE1	1:C:254:THR:HG21	1.61	0.64
1:A:256:MET:HE3	1:A:260:LEU:HB2	1.79	0.64
1:C:169:LYS:C	1:C:170:SER:N	2.56	0.64
1:B:256:MET:HG2	1:B:314:TYR:CE1	2.33	0.63
1:A:286:VAL:O	1:A:290:GLU:HG3	1.99	0.62
1:C:337:ASP:CG	1:C:338:ASP:H	2.06	0.62
1:A:431:THR:O	1:A:435:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:THR:HG21	1:C:282:PHE:CD2	2.33	0.62
1:A:343:ASN:HB2	1:A:344:PRO:HD2	1.82	0.62
1:C:171:ASN:ND2	2:E:13:GLY:HA3	2.14	0.62
1:B:183:LYS:HD2	1:B:224:GLU:HG2	1.80	0.62
1:C:434:ARG:HG2	1:C:434:ARG:HH11	1.64	0.62
1:A:434:ARG:HG3	1:A:434:ARG:HH11	1.65	0.62
1:C:19:GLU:O	1:C:23:LYS:HG2	1.99	0.61
1:A:19:GLU:O	1:A:23:LYS:HG2	2.00	0.61
1:A:256:MET:HG2	1:A:314:TYR:CD1	2.35	0.61
1:C:105:ARG:NH1	1:C:148:GLU:OE1	2.32	0.61
1:A:387:VAL:HG11	1:A:428:ALA:HA	1.80	0.61
1:C:431:THR:O	1:C:435:ILE:HG12	2.00	0.61
1:B:206:LYS:NZ	1:B:210:ASP:HB2	2.15	0.61
1:C:246:SER:HB2	1:C:285:ASN:ND2	2.16	0.61
1:A:157:ILE:O	1:A:161:ILE:HG22	2.00	0.61
1:C:286:VAL:O	1:C:290:GLU:HG3	2.01	0.61
1:B:133:LEU:HD13	1:B:154:ILE:HD13	1.83	0.60
1:A:18:LEU:O	1:A:19:GLU:C	2.44	0.60
1:A:215:ARG:CZ	1:A:251:TYR:HD1	2.13	0.60
1:B:19:GLU:O	1:B:23:LYS:HG2	2.01	0.60
1:C:238:LEU:O	1:C:242:VAL:HG23	2.01	0.60
1:A:183:LYS:HD2	1:A:224:GLU:HG2	1.84	0.60
1:B:333:GLN:HE22	1:B:384:ASP:HB3	1.66	0.60
1:C:256:MET:HA	1:C:260:LEU:HB2	1.82	0.60
1:C:184:GLU:OE1	1:C:184:GLU:N	2.34	0.60
1:C:268:MET:HE1	1:C:322:LEU:CD2	2.32	0.59
1:B:133:LEU:HB3	1:B:154:ILE:HD11	1.83	0.59
1:C:320:GLN:HG3	1:C:321:TYR:CD1	2.37	0.59
1:B:328:GLN:O	1:B:331:THR:HB	2.01	0.59
1:C:214:GLU:HG2	2:E:12:PHE:CD2	2.38	0.59
1:A:41:SER:OG	1:A:94:TYR:HB2	2.02	0.59
1:A:437:GLU:HB2	1:B:400:SER:HB3	1.84	0.59
1:C:422:VAL:HG12	1:C:426:ASP:OD2	2.02	0.59
1:A:198:LEU:HD23	1:A:240:ASN:ND2	2.18	0.58
1:A:256:MET:HA	1:A:260:LEU:HB2	1.84	0.58
1:C:206:LYS:NZ	1:C:210:ASP:HB2	2.18	0.58
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.84	0.58
1:C:418:LYS:O	1:C:419:ASP:O	2.21	0.58
1:C:212:GLU:HB3	1:C:215:ARG:NH2	2.19	0.58
1:A:264:THR:HG21	1:A:282:PHE:CD2	2.39	0.58
1:A:343:ASN:HD21	1:A:346:LYS:CD	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ASN:HB2	1:C:344:PRO:HD2	1.86	0.58
1:A:170:SER:HB2	1:A:204:PHE:HD1	1.69	0.57
1:B:417:MET:O	1:B:425:ARG:HG2	2.04	0.57
1:C:337:ASP:CG	1:C:338:ASP:N	2.60	0.57
1:A:320:GLN:HG3	1:A:321:TYR:CD1	2.39	0.57
1:A:343:ASN:HB2	1:A:344:PRO:CD	2.33	0.57
1:A:328:GLN:O	1:A:331:THR:HB	2.04	0.57
1:C:133:LEU:HB3	1:C:154:ILE:HD11	1.85	0.57
1:C:426:ASP:O	1:C:429:ALA:HB3	2.05	0.57
1:A:421:SER:HB3	1:A:424:VAL:HG23	1.86	0.57
1:B:235:VAL:O	1:B:239:GLN:HG3	2.05	0.57
1:C:123:VAL:O	1:C:123:VAL:CG1	2.53	0.57
1:A:235:VAL:O	1:A:239:GLN:HG3	2.05	0.57
1:A:202:LEU:HD12	1:A:243:LYS:CD	2.32	0.57
1:A:333:GLN:NE2	1:A:384:ASP:OD2	2.35	0.57
1:B:105:ARG:NH1	1:B:148:GLU:OE1	2.37	0.57
1:A:43:VAL:HG13	1:A:49:ASN:HD22	1.69	0.56
1:A:230:ASP:OD1	1:A:232:ARG:HB2	2.06	0.56
1:A:418:LYS:O	1:A:419:ASP:O	2.24	0.56
1:C:130:ILE:O	1:C:134:VAL:HG23	2.05	0.56
1:C:287:CYS:SG	1:C:355:LEU:HD23	2.46	0.56
1:B:65:LEU:HD13	1:B:116:ILE:HG13	1.87	0.56
1:B:245:MET:HE3	1:B:245:MET:O	2.04	0.56
1:C:181:MET:HE1	1:C:198:LEU:CD2	2.30	0.56
1:B:320:GLN:HG3	1:B:321:TYR:CD1	2.41	0.56
1:B:256:MET:HA	1:B:260:LEU:HB2	1.86	0.56
1:B:422:VAL:HG22	1:B:425:ARG:NH1	2.21	0.56
1:C:395:GLU:HB2	1:C:438:LEU:HD13	1.88	0.56
1:A:105:ARG:NH1	1:A:148:GLU:OE1	2.39	0.55
1:C:169:LYS:O	1:C:170:SER:N	2.39	0.55
1:A:14:ASP:HB3	1:A:17:GLU:HB2	1.88	0.55
1:A:123:VAL:O	1:A:123:VAL:CG1	2.54	0.55
1:C:395:GLU:HB2	1:C:438:LEU:CD1	2.37	0.55
1:A:349:GLY:O	1:A:353:MET:HG3	2.07	0.55
1:B:15:ARG:O	1:B:19:GLU:HG2	2.05	0.55
1:A:210:ASP:HA	1:A:251:TYR:CE1	2.41	0.55
1:C:65:LEU:HD13	1:C:116:ILE:HG13	1.88	0.55
1:C:319:LEU:HD12	1:C:323:VAL:HG23	1.89	0.55
1:C:50:SER:O	1:C:54:ARG:HG3	2.07	0.55
1:C:394:LEU:HD12	1:C:434:ARG:HB2	1.89	0.55
1:C:73:LYS:O	1:C:77:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD22	1:C:150:THR:HG23	1.89	0.54
1:A:265:ILE:HA	1:A:268:MET:HE3	1.89	0.54
1:A:184:GLU:N	1:A:184:GLU:OE1	2.39	0.54
1:B:178:ILE:HD13	1:B:181:MET:HE3	1.89	0.54
1:C:216:HIS:CE1	1:C:254:THR:HG21	2.42	0.54
1:B:238:LEU:O	1:B:242:VAL:HG23	2.07	0.54
1:A:24:PHE:C	1:A:24:PHE:CD1	2.85	0.54
1:C:373:GLU:O	1:C:373:GLU:HG2	2.06	0.54
1:C:428:ALA:O	1:C:432:VAL:HG23	2.06	0.54
1:A:80:TRP:CZ2	1:A:88:ARG:HG2	2.43	0.54
1:C:80:TRP:CZ2	1:C:88:ARG:HG2	2.43	0.54
1:C:230:ASP:OD1	1:C:232:ARG:HB2	2.08	0.54
1:A:5:THR:O	1:A:9:LYS:HD3	2.07	0.54
1:B:338:ASP:O	1:B:341:ASP:N	2.40	0.54
1:A:34:PRO:O	1:A:38:VAL:HG23	2.07	0.53
1:B:418:LYS:O	1:B:419:ASP:O	2.26	0.53
1:C:215:ARG:HB3	1:C:215:ARG:NH1	2.23	0.53
1:A:331:THR:CG2	1:A:331:THR:O	2.56	0.53
1:B:26:GLU:O	1:B:30:VAL:HG23	2.09	0.53
1:B:334:ASP:O	1:B:337:ASP:N	2.42	0.53
1:C:33:LEU:HB3	1:C:34:PRO:HD3	1.90	0.53
1:A:46:ASN:OD1	1:A:46:ASN:C	2.51	0.53
1:A:175:THR:HG23	2:D:10:PHE:O	2.09	0.53
1:A:360:GLU:O	1:A:363:ILE:HG22	2.09	0.53
1:B:171:ASN:HD22	2:F:12:PHE:C	2.17	0.53
1:B:373:GLU:HG2	1:B:373:GLU:O	2.09	0.53
1:C:264:THR:HG21	1:C:282:PHE:CG	2.44	0.53
1:A:206:LYS:NZ	1:A:210:ASP:HB2	2.23	0.53
1:B:268:MET:HE1	1:B:322:LEU:CD2	2.38	0.53
1:C:18:LEU:O	1:C:19:GLU:C	2.51	0.53
1:A:268:MET:HE2	1:A:283:TRP:CD1	2.43	0.52
1:A:50:SER:O	1:A:54:ARG:HG3	2.08	0.52
1:A:319:LEU:HD12	1:A:323:VAL:HG23	1.90	0.52
1:A:343:ASN:C	1:A:343:ASN:HD22	2.15	0.52
1:B:430:TRP:CZ2	1:B:434:ARG:HD2	2.43	0.52
1:C:184:GLU:H	1:C:184:GLU:CD	2.18	0.52
1:C:203:GLU:OE2	1:C:243:LYS:NZ	2.40	0.52
1:A:403:LYS:N	1:A:404:PRO:HD2	2.24	0.52
1:B:319:LEU:HD12	1:B:323:VAL:HG23	1.91	0.52
1:A:405:LEU:HD23	1:A:408:GLN:OE1	2.10	0.52
1:B:184:GLU:N	1:B:184:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:HD3	1:C:251:TYR:HB3	1.90	0.52
1:A:422:VAL:HG22	1:A:425:ARG:NH1	2.25	0.52
1:C:171:ASN:HD22	2:E:13:GLY:HA3	1.75	0.52
1:A:211:LYS:NZ	2:D:13:GLY:HA2	2.24	0.52
1:C:263:ILE:O	1:C:266:GLU:HB3	2.09	0.52
1:A:111:GLN:NE2	1:A:156:TYR:CE1	2.78	0.52
1:B:111:GLN:NE2	1:B:156:TYR:CE1	2.78	0.52
1:C:328:GLN:O	1:C:331:THR:HB	2.09	0.52
1:A:380:TRP:CZ2	1:A:381:ARG:NH1	2.78	0.52
1:A:256:MET:HG2	1:A:314:TYR:CE1	2.46	0.51
1:A:333:GLN:HE22	1:A:384:ASP:HB3	1.73	0.51
1:A:433:GLY:HA2	1:A:436:CYS:SG	2.51	0.51
1:B:333:GLN:NE2	1:B:384:ASP:OD2	2.39	0.51
1:C:111:GLN:NE2	1:C:156:TYR:CE1	2.78	0.51
1:C:164:GLU:HA	1:C:164:GLU:OE1	2.09	0.51
1:C:405:LEU:HD23	1:C:408:GLN:OE1	2.10	0.51
1:C:4:ILE:O	1:C:8:GLU:HG3	2.10	0.51
1:B:18:LEU:O	1:B:19:GLU:C	2.54	0.51
1:A:246:SER:HB2	1:A:285:ASN:ND2	2.26	0.51
1:A:430:TRP:CZ2	1:A:434:ARG:HD2	2.44	0.51
1:C:434:ARG:HG2	1:C:434:ARG:NH1	2.26	0.51
1:A:164:GLU:OE1	1:A:164:GLU:HA	2.10	0.51
1:A:387:VAL:CG2	1:A:416:LEU:HD13	2.41	0.51
1:B:264:THR:HG21	1:B:282:PHE:CG	2.46	0.51
1:C:181:MET:CE	1:C:198:LEU:HB2	2.41	0.51
1:C:380:TRP:HZ3	1:C:423:VAL:HG11	1.75	0.51
1:C:413:LEU:HA	1:C:416:LEU:HD12	1.93	0.51
1:A:219:MET:CE	1:A:252:MET:HE1	2.37	0.50
1:C:245:MET:HE3	1:C:245:MET:O	2.11	0.50
1:C:380:TRP:CZ2	1:C:381:ARG:NH1	2.79	0.50
1:A:65:LEU:HD13	1:A:116:ILE:HG13	1.93	0.50
1:B:123:VAL:O	1:B:123:VAL:CG1	2.59	0.50
1:A:219:MET:HE2	1:A:252:MET:CE	2.37	0.50
1:B:14:ASP:HB3	1:B:17:GLU:CB	2.40	0.50
1:B:177:ILE:HG21	1:B:198:LEU:HB2	1.94	0.50
1:A:169:LYS:O	1:A:173:ILE:HG12	2.12	0.50
1:A:413:LEU:HA	1:A:416:LEU:HD12	1.92	0.50
1:B:226:THR:O	1:B:234:ARG:HG2	2.11	0.50
1:B:268:MET:HE2	1:B:283:TRP:CD1	2.47	0.50
1:B:338:ASP:O	1:B:340:ASP:N	2.45	0.50
1:C:178:ILE:HD13	1:C:181:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:GLU:O	1:B:363:ILE:HG22	2.12	0.50
1:A:98:THR:CG2	1:A:109:ALA:HB2	2.42	0.50
1:A:343:ASN:ND2	1:A:343:ASN:H	2.10	0.50
1:A:384:ASP:OD1	1:A:427:THR:HB	2.11	0.50
1:A:133:LEU:HB3	1:A:154:ILE:HD11	1.94	0.50
1:B:215:ARG:CZ	1:B:251:TYR:CD1	2.86	0.50
1:A:373:GLU:O	1:A:373:GLU:HG2	2.11	0.49
1:B:403:LYS:N	1:B:404:PRO:HD2	2.27	0.49
1:B:413:LEU:HA	1:B:416:LEU:HD12	1.93	0.49
1:C:171:ASN:HD22	2:E:12:PHE:C	2.19	0.49
1:B:333:GLN:NE2	1:B:384:ASP:HB3	2.27	0.49
1:A:296:GLU:OE2	1:A:308:GLU:HB2	2.13	0.49
1:B:343:ASN:ND2	1:B:345:CYS:HB3	2.28	0.49
1:C:69:ASP:CB	1:C:72:ILE:HG12	2.43	0.49
1:C:98:THR:CG2	1:C:109:ALA:HB2	2.43	0.49
1:C:334:ASP:C	1:C:336:ASN:N	2.70	0.49
1:A:428:ALA:O	1:A:432:VAL:HG23	2.13	0.49
1:C:296:GLU:OE2	1:C:308:GLU:HB2	2.13	0.49
1:C:313:PHE:N	1:C:313:PHE:CD1	2.80	0.49
1:B:335:GLU:C	1:B:337:ASP:N	2.70	0.49
1:B:343:ASN:HD21	1:B:345:CYS:HB3	1.78	0.49
1:B:24:PHE:CD1	1:B:24:PHE:C	2.91	0.49
1:B:126:TRP:CE3	1:B:129:LEU:HD22	2.48	0.49
1:B:359:CYS:O	1:B:360:GLU:C	2.56	0.49
1:C:360:GLU:O	1:C:363:ILE:HG22	2.13	0.49
1:B:377:ASN:OD1	1:B:378:PRO:HD2	2.12	0.49
1:B:405:LEU:HD23	1:B:408:GLN:OE1	2.13	0.49
1:C:14:ASP:HB3	1:C:17:GLU:CB	2.42	0.49
1:C:210:ASP:HA	1:C:251:TYR:CE1	2.47	0.49
1:A:268:MET:HE1	1:A:322:LEU:CD2	2.43	0.48
1:B:174:LEU:HG	1:B:205:THR:HG21	1.95	0.48
1:C:36:PHE:CZ	1:C:40:LEU:HD11	2.48	0.48
1:C:403:LYS:N	1:C:404:PRO:HD2	2.28	0.48
1:A:73:LYS:O	1:A:77:GLN:HG3	2.14	0.48
1:B:343:ASN:HB2	1:B:344:PRO:HD2	1.94	0.48
1:C:24:PHE:CD1	1:C:24:PHE:C	2.92	0.48
1:A:211:LYS:HZ2	2:D:13:GLY:HA2	1.78	0.48
1:B:246:SER:HB2	1:B:285:ASN:ND2	2.28	0.48
1:C:246:SER:HB2	1:C:285:ASN:HD22	1.78	0.48
1:A:80:TRP:CE2	1:A:88:ARG:HG2	2.49	0.48
1:A:438:LEU:O	1:A:439:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LEU:HA	1:B:201:SER:OG	2.14	0.48
1:C:338:ASP:HB3	1:C:341:ASP:HB2	1.96	0.48
1:C:387:VAL:HG22	1:C:416:LEU:HD13	1.95	0.48
1:A:426:ASP:O	1:A:429:ALA:HB3	2.14	0.48
1:B:215:ARG:NH2	1:B:251:TYR:HD1	2.11	0.48
1:A:2:GLU:CD	1:A:2:GLU:N	2.72	0.48
1:A:9:LYS:HB3	1:A:21:ALA:HB2	1.95	0.48
1:A:177:ILE:HG22	1:A:181:MET:HE2	1.96	0.48
1:B:177:ILE:CG2	1:B:198:LEU:HB2	2.43	0.48
1:C:380:TRP:CZ3	1:C:423:VAL:HG21	2.49	0.48
1:A:133:LEU:HD22	1:A:150:THR:HG23	1.96	0.48
1:B:383:ARG:HH11	1:B:419:ASP:CG	2.22	0.48
1:C:334:ASP:O	1:C:337:ASP:HB2	2.14	0.48
1:A:222:VAL:O	1:A:225:ALA:HB3	2.14	0.48
1:B:206:LYS:HD2	1:B:248:TYR:HE1	1.79	0.48
1:C:235:VAL:O	1:C:239:GLN:HG3	2.14	0.48
1:A:171:ASN:ND2	2:D:13:GLY:HA3	2.29	0.48
1:B:34:PRO:O	1:B:38:VAL:HG23	2.13	0.48
1:C:130:ILE:HG23	1:C:173:ILE:HD11	1.96	0.48
1:B:50:SER:O	1:B:54:ARG:HG3	2.14	0.47
1:C:183:LYS:HD2	1:C:224:GLU:HG2	1.94	0.47
1:A:42:ARG:HG2	1:A:94:TYR:CE2	2.49	0.47
1:A:174:LEU:HG	1:A:205:THR:HG21	1.95	0.47
1:A:228:CYS:SG	1:A:229:PRO:HD2	2.54	0.47
1:A:405:LEU:HA	1:A:408:GLN:OE1	2.14	0.47
1:B:164:GLU:OE1	1:B:164:GLU:HA	2.13	0.47
1:C:126:TRP:CE3	1:C:129:LEU:HD22	2.49	0.47
1:A:140:PRO:C	1:A:141:ASN:HD22	2.22	0.47
1:A:429:ALA:O	1:A:430:TRP:C	2.57	0.47
1:B:416:LEU:HD22	1:B:424:VAL:HG11	1.96	0.47
1:A:80:TRP:O	1:A:88:ARG:HD2	2.14	0.47
1:C:331:THR:O	1:C:331:THR:CG2	2.62	0.47
1:A:170:SER:HB2	1:A:204:PHE:CD1	2.48	0.47
1:B:7:LEU:O	1:B:10:THR:HG23	2.14	0.47
1:B:430:TRP:CE2	1:B:434:ARG:HD2	2.49	0.47
1:C:181:MET:HE2	1:C:198:LEU:HB2	1.96	0.47
1:A:330:LEU:HD11	1:A:352:LEU:HD12	1.96	0.47
1:B:27:ARG:HH11	1:B:27:ARG:HG3	1.80	0.47
1:C:174:LEU:HG	1:C:205:THR:HG21	1.96	0.47
1:A:3:LEU:O	1:A:4:ILE:C	2.58	0.47
1:C:334:ASP:O	1:C:337:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:CYS:O	1:C:360:GLU:C	2.57	0.47
1:A:36:PHE:CZ	1:A:40:LEU:HD11	2.50	0.47
1:A:69:ASP:CB	1:A:72:ILE:HG12	2.40	0.47
1:A:313:PHE:CD1	1:A:313:PHE:N	2.83	0.47
1:B:171:ASN:ND2	2:F:13:GLY:HA3	2.30	0.47
1:B:331:THR:O	1:B:331:THR:CG2	2.62	0.47
1:C:15:ARG:O	1:C:19:GLU:HG2	2.14	0.47
1:B:51:GLN:O	1:B:55:VAL:HG23	2.16	0.46
1:B:228:CYS:SG	1:B:229:PRO:HD2	2.55	0.46
1:C:387:VAL:CG2	1:C:416:LEU:HD13	2.45	0.46
1:B:286:VAL:O	1:B:290:GLU:HG3	2.15	0.46
1:C:418:LYS:O	1:C:425:ARG:HD2	2.15	0.46
1:A:245:MET:O	1:A:245:MET:HG3	2.15	0.46
1:C:319:LEU:HD11	1:C:363:ILE:CD1	2.45	0.46
1:A:130:ILE:O	1:A:134:VAL:HG23	2.15	0.46
1:B:349:GLY:O	1:B:353:MET:HG3	2.15	0.46
1:B:404:PRO:O	1:B:408:GLN:HG3	2.15	0.46
1:C:133:LEU:HD13	1:C:154:ILE:HD13	1.96	0.46
1:A:11:VAL:HG21	1:A:52:VAL:HG13	1.98	0.46
1:B:45:ALA:HA	1:B:98:THR:OG1	2.15	0.46
1:B:46:ASN:HA	1:B:47:PRO:HD3	1.80	0.46
1:B:343:ASN:ND2	1:B:346:LYS:HD3	2.30	0.46
1:C:157:ILE:O	1:C:161:ILE:HG22	2.16	0.46
1:B:313:PHE:CD1	1:B:313:PHE:N	2.84	0.46
1:B:387:VAL:CG2	1:B:416:LEU:HD13	2.46	0.46
1:C:80:TRP:CE2	1:C:88:ARG:HG2	2.51	0.46
1:A:436:CYS:O	1:A:440:PRO:HD3	2.15	0.46
1:C:419:ASP:O	1:C:425:ARG:CD	2.64	0.46
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.81	0.46
1:A:267:ALA:HB1	1:A:275:VAL:HG12	1.96	0.46
1:A:404:PRO:O	1:A:408:GLN:HG3	2.16	0.46
1:B:69:ASP:CB	1:B:72:ILE:HG12	2.41	0.46
1:C:202:LEU:HD12	1:C:243:LYS:CD	2.37	0.46
1:A:174:LEU:HD13	2:D:12:PHE:CD2	2.50	0.46
1:A:268:MET:HE1	1:A:322:LEU:HD22	1.98	0.46
1:A:434:ARG:HG3	1:A:434:ARG:NH1	2.29	0.46
1:C:22:GLN:O	1:C:23:LYS:C	2.59	0.46
1:C:215:ARG:CD	1:C:251:TYR:HB3	2.46	0.46
1:C:335:GLU:C	1:C:337:ASP:H	2.21	0.46
1:B:140:PRO:C	1:B:141:ASN:HD22	2.23	0.45
1:C:271:ASP:OD1	1:C:271:ASP:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ALA:O	1:C:396:GLY:HA3	2.17	0.45
1:A:126:TRP:CE3	1:A:129:LEU:HD22	2.51	0.45
1:B:98:THR:CG2	1:B:109:ALA:HB2	2.47	0.45
1:B:395:GLU:HB2	1:B:438:LEU:HD13	1.98	0.45
1:C:140:PRO:C	1:C:141:ASN:HD22	2.24	0.45
1:A:387:VAL:HG21	1:A:416:LEU:HD13	1.98	0.45
1:A:384:ASP:OD1	1:A:427:THR:CB	2.65	0.45
1:B:3:LEU:O	1:B:4:ILE:C	2.59	0.45
1:C:27:ARG:HG3	1:C:27:ARG:HH11	1.82	0.45
1:C:383:ARG:HH11	1:C:419:ASP:CG	2.23	0.45
1:A:359:CYS:O	1:A:360:GLU:C	2.59	0.45
1:B:215:ARG:HD2	1:B:255:TYR:OH	2.16	0.45
1:B:387:VAL:HG11	1:B:428:ALA:HA	1.99	0.45
1:C:316:LYS:HE3	1:C:362:ASP:OD2	2.17	0.45
1:A:245:MET:O	1:A:245:MET:HE3	2.17	0.45
1:C:333:GLN:N	1:C:381:ARG:HH21	2.15	0.45
1:B:73:LYS:O	1:B:77:GLN:HG3	2.17	0.45
1:B:181:MET:O	1:B:182:ARG:C	2.60	0.45
1:B:343:ASN:C	1:B:343:ASN:HD22	2.25	0.45
1:B:380:TRP:CZ2	1:B:381:ARG:NH1	2.85	0.45
1:A:43:VAL:HG13	1:A:49:ASN:ND2	2.30	0.44
1:A:238:LEU:O	1:A:242:VAL:HG23	2.17	0.44
1:A:267:ALA:C	1:A:269:LYS:N	2.74	0.44
1:B:15:ARG:HH11	1:B:15:ARG:HG2	1.81	0.44
1:C:265:ILE:HA	1:C:268:MET:HE3	1.98	0.44
1:C:339:ASP:C	1:C:341:ASP:H	2.24	0.44
1:A:51:GLN:O	1:A:55:VAL:HG23	2.18	0.44
1:B:9:LYS:HB3	1:B:21:ALA:HB2	1.98	0.44
1:C:343:ASN:HB2	1:C:344:PRO:CD	2.47	0.44
1:C:404:PRO:O	1:C:408:GLN:HG3	2.17	0.44
1:C:439:LEU:O	1:C:440:PRO:C	2.60	0.44
1:B:181:MET:HE1	1:B:198:LEU:CD2	2.34	0.44
1:B:184:GLU:H	1:B:184:GLU:CD	2.26	0.44
1:C:198:LEU:HA	1:C:201:SER:OG	2.17	0.44
1:C:380:TRP:HZ2	1:C:381:ARG:NH1	2.16	0.44
1:C:419:ASP:O	1:C:425:ARG:HD3	2.17	0.44
1:A:38:VAL:O	1:A:42:ARG:HG3	2.18	0.44
1:B:185:GLU:HA	1:B:186:PRO:HD3	1.81	0.44
1:C:32:ASN:ND2	1:C:35:THR:HB	2.32	0.44
1:A:98:THR:HG21	1:A:109:ALA:HB2	2.00	0.44
1:A:264:THR:HG21	1:A:282:PHE:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ASP:HB3	1:B:72:ILE:CG1	2.45	0.44
1:B:343:ASN:HD21	1:B:346:LYS:HD3	1.82	0.44
1:A:246:SER:HB2	1:A:285:ASN:HD22	1.82	0.44
1:B:363:ILE:HG23	1:B:364:VAL:N	2.33	0.44
2:E:10:PHE:C	2:E:10:PHE:CD2	2.96	0.44
1:A:72:ILE:HD13	1:A:72:ILE:N	2.33	0.44
1:A:343:ASN:HD22	1:A:343:ASN:H	1.64	0.44
1:B:40:LEU:HB2	1:B:61:ILE:HD11	2.00	0.44
1:B:222:VAL:O	1:B:225:ALA:HB3	2.18	0.44
1:B:235:VAL:HG11	1:B:274:GLU:HG3	2.00	0.44
1:A:215:ARG:HD2	1:A:255:TYR:OH	2.17	0.43
1:A:380:TRP:HZ2	1:A:381:ARG:NH1	2.15	0.43
1:C:268:MET:HE2	1:C:283:TRP:CD1	2.54	0.43
1:A:287:CYS:SG	1:A:355:LEU:HD23	2.58	0.43
1:C:405:LEU:HA	1:C:408:GLN:OE1	2.17	0.43
1:B:296:GLU:OE2	1:B:308:GLU:HB2	2.18	0.43
1:B:407:ILE:C	1:B:409:ALA:H	2.26	0.43
1:B:422:VAL:HG13	1:B:425:ARG:NH2	2.33	0.43
1:A:343:ASN:ND2	1:A:343:ASN:C	2.77	0.43
1:C:3:LEU:O	1:C:4:ILE:C	2.62	0.43
1:C:45:ALA:O	1:C:47:PRO:HD3	2.19	0.43
1:C:69:ASP:CG	1:C:72:ILE:HG12	2.44	0.43
1:B:267:ALA:C	1:B:269:LYS:N	2.77	0.43
1:C:181:MET:O	1:C:182:ARG:C	2.62	0.43
1:C:399:PRO:O	1:C:403:LYS:HG3	2.17	0.43
1:C:432:VAL:O	1:C:436:CYS:SG	2.72	0.43
1:A:388:MET:HB2	1:A:427:THR:HG21	2.00	0.43
1:B:114:ALA:HB2	1:B:156:TYR:HB3	2.00	0.43
1:B:80:TRP:CZ2	1:B:88:ARG:HG2	2.54	0.43
1:B:367:VAL:O	1:B:368:LEU:C	2.61	0.43
1:C:267:ALA:C	1:C:269:LYS:N	2.76	0.43
1:C:291:MET:HE1	1:C:354:LEU:HD23	2.01	0.43
1:A:212:GLU:HG3	1:A:213:SER:N	2.34	0.43
1:C:217:PHE:O	1:C:221:VAL:HG23	2.19	0.43
1:C:400:SER:O	1:C:404:PRO:HD3	2.19	0.43
1:A:177:ILE:HG21	1:A:198:LEU:HB2	2.00	0.42
1:B:338:ASP:O	1:B:341:ASP:HB2	2.19	0.42
1:C:171:ASN:ND2	2:E:13:GLY:CA	2.81	0.42
1:A:172:GLU:H	1:A:172:GLU:CD	2.27	0.42
1:B:330:LEU:HD11	1:B:352:LEU:HD12	2.01	0.42
1:C:177:ILE:HG21	1:C:198:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:CG	1:A:72:ILE:HG12	2.44	0.42
1:A:184:GLU:H	1:A:184:GLU:CD	2.25	0.42
1:B:21:ALA:O	1:B:25:LEU:HG	2.19	0.42
1:A:311:SER:O	1:A:312:LYS:HD3	2.19	0.42
1:C:339:ASP:C	1:C:341:ASP:N	2.77	0.42
1:C:349:GLY:O	1:C:353:MET:HG3	2.19	0.42
1:C:383:ARG:NH1	1:C:419:ASP:OD1	2.53	0.42
1:A:96:LEU:HD12	1:A:96:LEU:HA	1.93	0.42
1:A:332:LYS:O	1:A:345:CYS:HB2	2.18	0.42
1:B:254:THR:HB	1:B:255:TYR:CE1	2.55	0.42
1:C:169:LYS:O	1:C:170:SER:CA	2.68	0.42
1:A:46:ASN:HA	1:A:47:PRO:HD3	1.81	0.42
1:B:60:GLN:O	1:B:61:ILE:C	2.62	0.42
1:B:346:LYS:N	1:B:346:LYS:HD2	2.35	0.42
1:B:405:LEU:HA	1:B:408:GLN:OE1	2.18	0.42
1:B:10:THR:O	1:B:18:LEU:HD22	2.20	0.42
1:B:265:ILE:HA	1:B:268:MET:HE3	2.01	0.42
1:C:9:LYS:HB3	1:C:21:ALA:HB2	2.01	0.42
1:C:32:ASN:O	1:C:36:PHE:HB2	2.20	0.42
1:A:121:ILE:C	1:A:123:VAL:H	2.27	0.42
1:A:135:ALA:O	1:A:139:ASN:HB2	2.20	0.42
1:A:368:LEU:HD11	1:A:405:LEU:HD11	2.00	0.42
1:B:61:ILE:HB	1:B:112:CYS:SG	2.60	0.42
2:F:10:PHE:C	2:F:10:PHE:CD2	2.97	0.42
1:A:350:VAL:HA	1:A:353:MET:HE2	2.00	0.42
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.85	0.42
1:B:6:ILE:O	1:B:10:THR:HG23	2.20	0.41
1:C:407:ILE:C	1:C:409:ALA:H	2.28	0.41
1:A:231:THR:O	1:A:235:VAL:HG23	2.20	0.41
1:B:2:GLU:N	1:B:2:GLU:CD	2.78	0.41
1:B:129:LEU:O	1:B:132:GLN:HB3	2.20	0.41
1:B:231:THR:HG21	1:B:272:ILE:HD13	2.02	0.41
1:B:336:ASN:O	1:B:336:ASN:CG	2.62	0.41
1:B:416:LEU:HD22	1:B:424:VAL:CG1	2.50	0.41
1:B:434:ARG:O	1:B:435:ILE:C	2.63	0.41
1:C:206:LYS:HZ2	1:C:210:ASP:HB2	1.84	0.41
1:C:311:SER:O	1:C:312:LYS:HD3	2.19	0.41
1:B:69:ASP:CG	1:B:72:ILE:HG12	2.46	0.41
1:C:7:LEU:O	1:C:10:THR:OG1	2.37	0.41
1:C:20:ALA:O	1:C:21:ALA:C	2.64	0.41
1:C:174:LEU:HD13	2:E:12:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:HD2	1:A:126:TRP:CE2	2.56	0.41
1:A:377:ASN:OD1	1:A:378:PRO:HD2	2.20	0.41
1:B:40:LEU:CB	1:B:61:ILE:HD11	2.50	0.41
1:C:69:ASP:HB3	1:C:72:ILE:CG1	2.47	0.41
1:C:245:MET:O	1:C:245:MET:HG3	2.18	0.41
1:A:331:THR:O	1:A:331:THR:HG22	2.19	0.41
1:C:319:LEU:HD11	1:C:363:ILE:HD12	2.03	0.41
1:C:430:TRP:CE2	1:C:434:ARG:HD2	2.54	0.41
1:A:291:MET:O	1:A:294:ALA:HB3	2.20	0.41
1:B:343:ASN:HB2	1:B:344:PRO:CD	2.51	0.41
1:C:214:GLU:O	1:C:215:ARG:C	2.62	0.41
1:C:418:LYS:O	1:C:419:ASP:C	2.63	0.41
1:A:61:ILE:HB	1:A:112:CYS:SG	2.60	0.41
1:A:202:LEU:HD12	1:A:243:LYS:CG	2.51	0.41
1:B:246:SER:HB2	1:B:285:ASN:HD22	1.85	0.41
1:A:27:ARG:HH11	1:A:27:ARG:HG3	1.85	0.41
1:A:363:ILE:HG23	1:A:364:VAL:N	2.36	0.41
1:A:383:ARG:O	1:A:386:ALA:HB3	2.21	0.41
1:B:46:ASN:OD1	1:B:46:ASN:C	2.64	0.41
1:B:72:ILE:HG22	1:B:76:TYR:CE2	2.56	0.41
1:B:169:LYS:O	1:B:173:ILE:HG12	2.21	0.41
1:B:383:ARG:O	1:B:386:ALA:HB3	2.20	0.41
1:B:387:VAL:HG22	1:B:416:LEU:HD13	2.03	0.41
1:B:408:GLN:HG3	1:B:408:GLN:H	1.74	0.41
1:C:222:VAL:O	1:C:225:ALA:HB3	2.20	0.41
1:A:133:LEU:HD13	1:A:154:ILE:HD13	2.03	0.41
1:A:410:MET:N	1:A:411:PRO:CD	2.84	0.41
1:B:236:ALA:O	1:B:239:GLN:HB2	2.20	0.41
1:B:290:GLU:OE2	1:B:314:TYR:N	2.54	0.41
1:B:311:SER:O	1:B:312:LYS:HD3	2.21	0.41
1:C:6:ILE:HG23	1:C:21:ALA:HA	2.02	0.41
1:C:46:ASN:HB3	1:C:49:ASN:ND2	2.35	0.41
1:C:65:LEU:CD1	1:C:116:ILE:HG13	2.51	0.41
1:B:198:LEU:HD23	1:B:240:ASN:ND2	2.35	0.40
1:B:380:TRP:HZ3	1:B:423:VAL:HG11	1.85	0.40
1:C:198:LEU:HD23	1:C:240:ASN:ND2	2.36	0.40
1:C:343:ASN:O	1:C:344:PRO:C	2.64	0.40
1:A:300:ALA:O	1:A:305:ARG:O	2.39	0.40
1:A:412:THR:O	1:A:416:LEU:HG	2.20	0.40
1:B:80:TRP:O	1:B:88:ARG:HD2	2.21	0.40
1:B:135:ALA:O	1:B:139:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:VAL:HG21	1:C:172:GLU:HB3	2.03	0.40
1:C:361:ASP:O	1:C:363:ILE:N	2.55	0.40
1:B:169:LYS:HA	1:B:172:GLU:OE1	2.20	0.40
1:C:61:ILE:HB	1:C:112:CYS:SG	2.61	0.40
1:C:151:LEU:HD13	1:C:194:ALA:HB2	2.04	0.40
1:C:410:MET:N	1:C:411:PRO:CD	2.85	0.40
1:A:212:GLU:O	1:A:213:SER:C	2.65	0.40
1:A:407:ILE:C	1:A:409:ALA:H	2.30	0.40
1:A:408:GLN:HE21	1:A:408:GLN:HB2	1.59	0.40
1:B:35:THR:O	1:B:39:GLU:HG2	2.22	0.40
1:B:391:GLY:HA2	1:B:394:LEU:CD1	2.52	0.40
1:C:9:LYS:O	1:C:18:LEU:HD23	2.22	0.40
1:C:412:THR:O	1:C:416:LEU:HG	2.22	0.40
1:A:38:VAL:O	1:A:41:SER:HB3	2.21	0.40
1:A:215:ARG:NH2	1:A:251:TYR:HD1	2.20	0.40
1:B:15:ARG:HA	1:B:15:ARG:HD2	1.94	0.40
1:B:162:ASP:O	1:B:163:PRO:C	2.64	0.40
1:C:135:ALA:O	1:C:139:ASN:HB2	2.21	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	438/442 (99%)	379 (86%)	53 (12%)	6 (1%)	9	30
1	B	438/442 (99%)	379 (86%)	49 (11%)	10 (2%)	5	18
1	C	436/442 (99%)	379 (87%)	50 (12%)	7 (2%)	7	27
2	D	4/119 (3%)	3 (75%)	1 (25%)	0	100	100
2	E	5/119 (4%)	4 (80%)	1 (20%)	0	100	100
2	F	4/119 (3%)	3 (75%)	1 (25%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1325/1683 (79%)	1147 (87%)	155 (12%)	23 (2%)	7	25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU
1	A	419	ASP
1	B	339	ASP
1	B	360	GLU
1	B	419	ASP
1	C	337	ASP
1	C	360	GLU
1	C	419	ASP
1	A	129	LEU
1	A	362	ASP
1	B	129	LEU
1	B	212	GLU
1	B	362	ASP
1	C	129	LEU
1	C	362	ASP
1	A	440	PRO
1	B	337	ASP
1	C	22	GLN
1	A	420	PRO
1	B	437	GLU
1	C	12	SER
1	B	373	GLU
1	B	12	SER

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	380/382 (100%)	366 (96%)	14 (4%)	30	65
1	B	380/382 (100%)	366 (96%)	14 (4%)	30	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	380/382 (100%)	364 (96%)	16 (4%)	26	61
2	D	3/95 (3%)	3 (100%)	0	100	100
2	E	4/95 (4%)	4 (100%)	0	100	100
2	F	3/95 (3%)	3 (100%)	0	100	100
All	All	1150/1431 (80%)	1106 (96%)	44 (4%)	29	64

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	11	VAL
1	A	35	THR
1	A	174	LEU
1	A	203	GLU
1	A	224	GLU
1	A	234	ARG
1	A	265	ILE
1	A	278	GLN
1	A	331	THR
1	A	334	ASP
1	A	343	ASN
1	A	368	LEU
1	A	408	GLN
1	B	3	LEU
1	B	11	VAL
1	B	34	PRO
1	B	170	SER
1	B	174	LEU
1	B	224	GLU
1	B	234	ARG
1	B	255	TYR
1	B	270	SER
1	B	278	GLN
1	B	331	THR
1	B	343	ASN
1	B	368	LEU
1	B	408	GLN
1	C	3	LEU
1	C	11	VAL
1	C	16	LEU
1	C	22	GLN

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Mol	Chain	Res	Type
1	C	174	LEU
1	C	224	GLU
1	C	234	ARG
1	C	255	TYR
1	C	265	ILE
1	C	270	SER
1	C	278	GLN
1	C	331	THR
1	C	334	ASP
1	C	338	ASP
1	C	368	LEU
1	C	408	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	32	ASN
1	A	51	GLN
1	A	60	GLN
1	A	77	GLN
1	A	141	ASN
1	A	171	ASN
1	A	179	GLN
1	A	216	HIS
1	A	240	ASN
1	A	285	ASN
1	A	343	ASN
1	B	22	GLN
1	B	32	ASN
1	B	49	ASN
1	B	51	GLN
1	B	60	GLN
1	B	111	GLN
1	B	141	ASN
1	B	171	ASN
1	B	179	GLN
1	B	220	GLN
1	B	240	ASN
1	B	285	ASN
1	B	343	ASN
1	C	22	GLN

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Mol	Chain	Res	Type
1	C	32	ASN
1	C	49	ASN
1	C	51	GLN
1	C	141	ASN
1	C	171	ASN
1	C	179	GLN
1	C	216	HIS
1	C	240	ASN
1	C	285	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	169:LYS	C	170:SER	N	2.56

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.