



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:30 PM UTC

PDB ID : 1ZEI / pdb_00001zei
Title : CROSS-LINKED B28 ASP INSULIN
Authors : Whittingham, J.L.; Edwards, E.J.; Antson, A.A.; Clarkson, J.M.; Dodson, G.G.
Deposited on : 1998-07-14
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

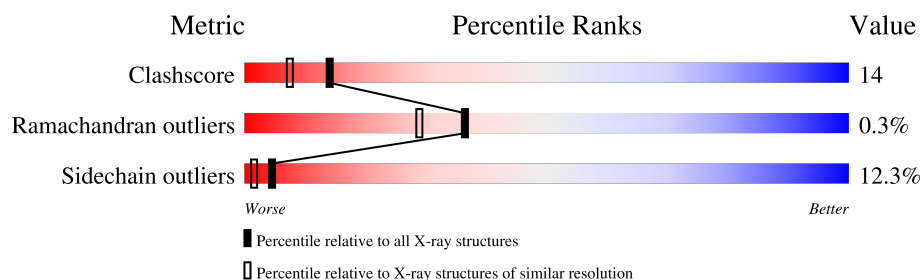
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	53	
1	B	53	
1	C	53	
1	D	53	
1	E	53	
1	F	53	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CRS	B	56	-	X	-	-
2	CRS	D	54	-	X	-	-
2	CRS	E	55	-	X	-	-
2	CRS	F	55	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2806 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 INSULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	41	0	0
			417	264	68	79	6			
1	B	53	Total	C	N	O	S	8	1	0
			420	265	69	80	6			
1	C	53	Total	C	N	O	S	16	1	0
			421	266	68	81	6			
1	D	53	Total	C	N	O	S	16	0	0
			417	264	68	79	6			
1	E	53	Total	C	N	O	S	6	0	0
			417	264	68	79	6			
1	F	53	Total	C	N	O	S	7	1	0
			418	264	68	80	6			

There are 18 discrepancies between the modelled and reference sequences:

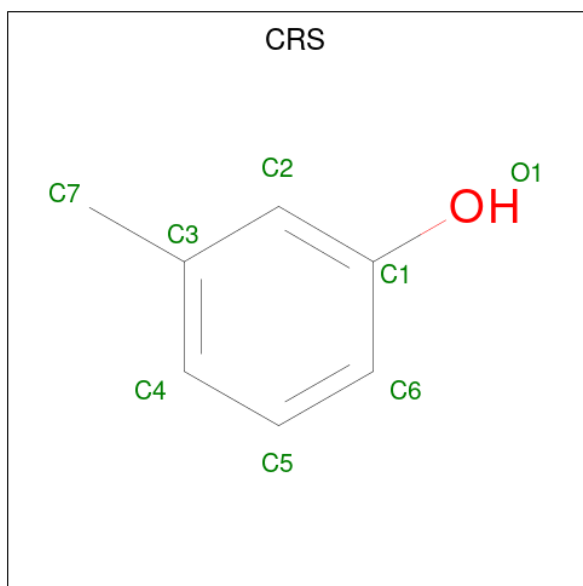
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	PRO	engineered mutation	UNP P01315
A	31	ALA	-	insertion	UNP P01315
A	32	LYS	-	insertion	UNP P01315
B	28	ASP	PRO	engineered mutation	UNP P01315
B	31	ALA	-	insertion	UNP P01315
B	32	LYS	-	insertion	UNP P01315
C	28	ASP	PRO	engineered mutation	UNP P01315
C	31	ALA	-	insertion	UNP P01315
C	32	LYS	-	insertion	UNP P01315
D	28	ASP	PRO	engineered mutation	UNP P01315
D	31	ALA	-	insertion	UNP P01315
D	32	LYS	-	insertion	UNP P01315
E	28	ASP	PRO	engineered mutation	UNP P01315
E	31	ALA	-	insertion	UNP P01315
E	32	LYS	-	insertion	UNP P01315
F	28	ASP	PRO	engineered mutation	UNP P01315
F	31	ALA	-	insertion	UNP P01315

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Chain	Residue	Modelled	Actual	Comment	Reference
F	32	LYS	-	insertion	UNP P01315

- Molecule 2 is M-CRESOL (CCD ID: CRS) (formula: C_7H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	7	1		
2	B	1	Total	C	O	0	0
			8	7	1		
2	C	1	Total	C	O	0	0
			8	7	1		
2	D	1	Total	C	O	0	0
			8	7	1		
2	E	1	Total	C	O	0	0
			8	7	1		
2	E	1	Total	C	O	0	0
			8	7	1		
2	F	1	Total	C	O	0	0
			8	7	1		
2	F	1	Total	C	O	0	0
			8	7	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Zn 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

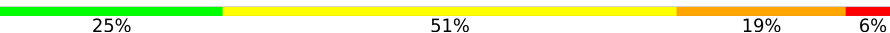
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	B	34	Total 34	O 34	0	0
5	C	40	Total 40	O 40	0	0
5	D	36	Total 36	O 36	0	0
5	E	49	Total 49	O 49	0	0
5	F	44	Total 44	O 44	0	0

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. 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.

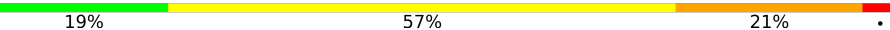
Note EDS was not executed.

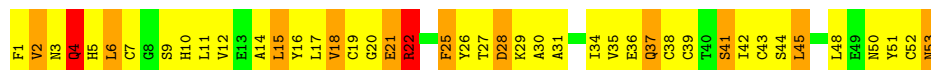
• Molecule 1: INSULIN

Chain A: 

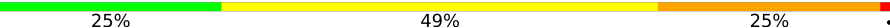


• Molecule 1: INSULIN

Chain B: 

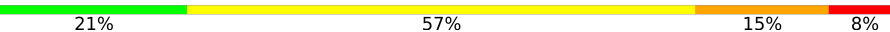


• Molecule 1: INSULIN

Chain C: 

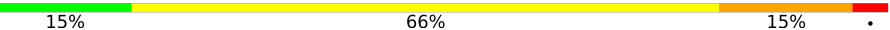


• Molecule 1: INSULIN

Chain D: 



• Molecule 1: INSULIN

Chain E: 



• Molecule 1: INSULIN

Chain F: 

F1	V2	N3	Q4	H5	L6	C7	G8	S9	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	F25	Y26	T27		K32	G33	I34	V35	E36	Q37	C38	C39	T40	S41	I42	C43	S44	L45	Y46	Q47	L48	E49	N50	Y51	G52	N53
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.95Å 64.77Å 48.91Å 90.00° 109.81° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	87.8 (20.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2806	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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: CL, CRS, ZN

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	1.86	12/425 (2.8%)	2.82	48/572 (8.4%)
1	B	2.23	21/434 (4.8%)	3.11	66/584 (11.3%)
1	C	2.27	19/434 (4.4%)	2.97	60/584 (10.3%)
1	D	2.47	25/425 (5.9%)	3.18	67/572 (11.7%)
1	E	2.70	35/425 (8.2%)	3.33	81/572 (14.2%)
1	F	2.23	21/431 (4.9%)	3.01	56/580 (9.7%)
All	All	2.31	133/2574 (5.2%)	3.07	378/3464 (10.9%)

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	2
1	B	0	6
1	C	0	3
1	D	0	2
1	E	0	5
1	F	0	2
All	All	0	20

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	HIS	CE1-NE2	12.83	1.45	1.32
1	A	27	THR	C-N	-11.54	1.18	1.34
1	D	10	HIS	ND1-CE1	10.31	1.42	1.32
1	E	23	GLY	CA-C	10.12	1.67	1.52
1	F	10	HIS	CE1-NE2	10.01	1.42	1.32
1	E	6	LEU	C-O	9.78	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	5	HIS	N-CA	9.24	1.57	1.46
1	C	10	HIS	CG-CD2	9.23	1.46	1.35
1	C	8	GLY	CA-C	8.94	1.62	1.52
1	C	36	GLU	CA-CB	8.70	1.66	1.53
1	C	7	CYS	CA-CB	8.44	1.66	1.53
1	C	7	CYS	C-O	8.32	1.33	1.24
1	D	11	LEU	CA-C	8.28	1.63	1.52
1	C	10	HIS	N-CA	-8.25	1.35	1.46
1	C	10	HIS	CB-CG	7.62	1.60	1.50
1	E	30	ALA	CA-C	7.58	1.62	1.52
1	B	2	VAL	CA-CB	7.56	1.64	1.54
1	E	24	PHE	N-CA	7.53	1.55	1.45
1	E	31	ALA	N-CA	7.39	1.55	1.46
1	F	7	CYS	C-O	7.36	1.32	1.24
1	D	38	CYS	CA-CB	7.24	1.65	1.53
1	F	12	VAL	CA-CB	7.20	1.63	1.54
1	F	10	HIS	N-CA	-7.13	1.37	1.46
1	F	8	GLY	N-CA	7.11	1.55	1.45
1	A	39	CYS	N-CA	7.10	1.55	1.46
1	E	16	TYR	CA-C	-7.08	1.43	1.52
1	E	40	THR	CA-CB	7.07	1.65	1.53
1	A	11	LEU	CA-C	7.03	1.62	1.52
1	A	7	CYS	C-O	6.98	1.32	1.24
1	D	46	TYR	N-CA	6.97	1.54	1.46
1	E	53	ASN	C-OXT	6.97	1.37	1.23
1	C	10	HIS	C-N	6.92	1.43	1.34
1	D	18	VAL	N-CA	6.91	1.54	1.46
1	D	11	LEU	C-N	-6.90	1.25	1.33
1	B	10	HIS	ND1-CE1	6.82	1.39	1.32
1	A	12	VAL	C-O	6.80	1.32	1.24
1	E	16	TYR	C-O	6.79	1.31	1.24
1	D	2	VAL	CA-C	-6.75	1.43	1.52
1	A	17	LEU	CA-CB	-6.70	1.42	1.53
1	E	2	VAL	N-CA	6.67	1.54	1.46
1	E	18	VAL	C-O	6.65	1.31	1.24
1	A	12	VAL	N-CA	6.64	1.54	1.46
1	E	24	PHE	CA-C	-6.56	1.44	1.52
1	E	29	LYS	CA-C	-6.54	1.44	1.52
1	D	33	GLY	C-O	-6.47	1.15	1.23
1	C	11	LEU	C-N	-6.44	1.25	1.33
1	D	42	ILE	CA-CB	-6.44	1.47	1.54
1	A	41	SER	C-N	-6.43	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	10	HIS	ND1-CE1	6.38	1.39	1.32
1	E	34	ILE	N-CA	6.32	1.54	1.46
1	E	18	VAL	C-N	-6.31	1.24	1.33
1	B	36	GLU	N-CA	6.27	1.53	1.46
1	D	33	GLY	N-CA	6.27	1.54	1.45
1	F	36	GLU	C-O	6.25	1.31	1.24
1	C	16	TYR	N-CA	6.22	1.53	1.46
1	B	48	LEU	C-N	6.19	1.42	1.33
1	F	11	LEU	CA-C	6.19	1.60	1.52
1	B	44	SER	C-O	6.18	1.32	1.23
1	D	5	HIS	C-O	6.17	1.31	1.24
1	C	32	LYS	CA-CB	-6.13	1.43	1.53
1	E	4	GLN	CA-C	6.12	1.61	1.52
1	E	39	CYS	N-CA	6.11	1.53	1.46
1	D	10	HIS	CD2-NE2	-6.10	1.31	1.37
1	B	4[A]	GLN	C-O	6.09	1.31	1.24
1	B	4[B]	GLN	C-O	6.09	1.31	1.24
1	B	44	SER	C-N	6.04	1.42	1.34
1	F	1	PHE	N-CA	6.04	1.57	1.46
1	D	10	HIS	C-O	6.02	1.31	1.24
1	F	32	LYS	C-O	6.02	1.31	1.24
1	E	28	ASP	N-CA	6.01	1.53	1.46
1	F	12	VAL	C-N	5.99	1.41	1.33
1	E	15	LEU	C-O	-5.94	1.16	1.24
1	F	16	TYR	C-O	5.92	1.31	1.24
1	D	40	THR	N-CA	5.88	1.53	1.46
1	C	43	CYS	C-O	5.87	1.30	1.23
1	B	15	LEU	CA-C	5.86	1.60	1.52
1	E	3	ASN	C-O	5.85	1.30	1.24
1	B	37	GLN	C-N	5.80	1.42	1.33
1	B	7	CYS	N-CA	5.79	1.53	1.46
1	D	23	GLY	C-N	5.79	1.40	1.33
1	B	4[A]	GLN	CA-C	5.75	1.60	1.52
1	B	4[B]	GLN	CA-C	5.75	1.60	1.52
1	D	39	CYS	N-CA	5.74	1.53	1.46
1	F	10	HIS	ND1-CE1	5.71	1.38	1.32
1	E	25	PHE	CA-CB	5.70	1.63	1.53
1	F	22	ARG	CA-C	5.70	1.60	1.52
1	E	16	TYR	N-CA	5.69	1.53	1.46
1	F	32	LYS	C-N	-5.68	1.26	1.33
1	C	50	ASN	C-N	5.63	1.41	1.33
1	F	46	TYR	CB-CG	5.62	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	30	ALA	C-N	-5.62	1.26	1.33
1	B	15	LEU	CB-CG	5.61	1.64	1.53
1	D	2	VAL	CA-CB	5.56	1.62	1.54
1	C	33	GLY	CA-C	5.56	1.58	1.52
1	D	9	SER	CA-CB	5.55	1.62	1.53
1	D	4	GLN	C-N	-5.54	1.26	1.33
1	E	10	HIS	C-N	5.52	1.41	1.33
1	E	17	LEU	CA-CB	5.47	1.61	1.53
1	B	3	ASN	C-N	-5.45	1.26	1.33
1	F	24	PHE	CA-C	5.42	1.59	1.52
1	D	43	CYS	CA-CB	-5.38	1.41	1.53
1	E	38	CYS	N-CA	5.37	1.53	1.46
1	C	4	GLN	C-N	-5.36	1.27	1.33
1	E	8	GLY	C-N	5.36	1.41	1.34
1	A	10	HIS	N-CA	5.32	1.52	1.46
1	E	38	CYS	C-O	5.32	1.31	1.24
1	E	11	LEU	N-CA	5.32	1.52	1.46
1	B	3	ASN	CA-CB	5.27	1.61	1.53
1	F	27	THR	N-CA	5.25	1.52	1.46
1	E	10	HIS	ND1-CE1	5.24	1.37	1.32
1	C	9	SER	N-CA	5.20	1.52	1.46
1	E	17	LEU	N-CA	-5.20	1.40	1.46
1	F	27	THR	C-O	5.19	1.29	1.23
1	A	8	GLY	C-O	5.18	1.30	1.23
1	E	47	GLN	C-N	5.18	1.41	1.34
1	C	4	GLN	CA-C	5.17	1.59	1.52
1	F	51	TYR	C-N	-5.15	1.26	1.33
1	F	6	LEU	CA-CB	5.14	1.61	1.53
1	A	16	TYR	C-O	5.14	1.30	1.24
1	D	38	CYS	CA-C	5.12	1.59	1.52
1	A	4	GLN	N-CA	-5.11	1.40	1.46
1	E	9	SER	CB-OG	-5.10	1.31	1.42
1	F	38	CYS	C-N	-5.10	1.26	1.33
1	C	15	LEU	C-N	-5.07	1.27	1.33
1	E	8	GLY	N-CA	5.07	1.52	1.45
1	B	18	VAL	C-N	-5.05	1.26	1.33
1	B	10	HIS	CD2-NE2	5.04	1.43	1.37
1	D	13	GLU	CA-CB	5.03	1.61	1.53
1	E	22	ARG	N-CA	5.03	1.52	1.46
1	B	11	LEU	CA-CB	5.02	1.61	1.53
1	B	9	SER	N-CA	-5.01	1.40	1.46
1	D	8	GLY	C-N	5.01	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	5	HIS	CB-CG	5.00	1.57	1.50

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ARG	NE-CZ-NH2	17.24	134.72	119.20
1	A	25	PHE	CA-CB-CG	15.92	129.72	113.80
1	E	30	ALA	O-C-N	15.20	140.96	122.27
1	B	10	HIS	CE1-NE2-CD2	-12.81	96.19	109.00
1	B	34	ILE	O-C-N	-12.74	107.40	121.80
1	D	47	GLN	OE1-CD-NE2	12.45	135.05	122.60
1	D	50	ASN	OD1-CG-ND2	-12.42	110.18	122.60
1	D	38	CYS	O-C-N	12.11	136.90	122.24
1	F	25	PHE	CA-CB-CG	-11.55	102.25	113.80
1	F	16	TYR	CA-C-N	11.40	135.26	120.44
1	F	16	TYR	C-N-CA	11.40	135.26	120.44
1	D	10	HIS	CE1-NE2-CD2	11.03	120.03	109.00
1	D	38	CYS	CA-C-N	-11.01	103.21	122.26
1	D	38	CYS	C-N-CA	-11.01	103.21	122.26
1	B	10	HIS	CG-CD2-NE2	10.97	118.17	107.20
1	E	17	LEU	CA-C-O	10.79	131.82	120.70
1	D	10	HIS	ND1-CE1-NE2	-10.36	98.04	108.40
1	E	30	ALA	CA-C-O	-10.36	108.06	119.97
1	C	3	ASN	O-C-N	-10.20	111.31	122.12
1	B	3	ASN	CA-C-O	-10.07	110.32	120.70
1	C	8	GLY	O-C-N	9.82	131.62	122.19
1	F	21	GLU	CB-CG-CD	9.77	129.21	112.60
1	A	7	CYS	CA-C-O	-9.64	110.70	120.82
1	B	41	SER	CA-C-O	-9.31	110.32	120.75
1	E	40	THR	CA-C-O	9.21	130.26	119.67
1	E	23	GLY	O-C-N	9.20	131.51	122.77
1	F	16	TYR	O-C-N	-9.14	112.43	122.12
1	B	37	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	E	10	HIS	ND1-CE1-NE2	-9.02	99.38	108.40
1	C	12	VAL	N-CA-CB	9.01	122.80	110.54
1	E	24	PHE	O-C-N	-9.01	111.44	123.15
1	D	11	LEU	CA-C-O	-9.00	111.37	120.82
1	B	22	ARG	NE-CZ-NH1	-8.97	112.53	121.50
1	D	38	CYS	CA-C-O	-8.97	108.64	119.32
1	D	24	PHE	CA-C-O	-8.96	111.24	121.10
1	C	36	GLU	O-C-N	-8.96	112.63	122.12
1	F	32	LYS	CA-C-N	8.89	129.84	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	32	LYS	C-N-CA	8.89	129.84	119.98
1	B	22	ARG	CD-NE-CZ	8.73	136.62	124.40
1	A	18	VAL	CA-C-N	8.69	131.93	120.28
1	A	18	VAL	C-N-CA	8.69	131.93	120.28
1	E	21	GLU	CA-CB-CG	-8.68	96.74	114.10
1	A	22	ARG	NE-CZ-NH2	-8.66	111.41	119.20
1	E	33	GLY	N-CA-C	8.47	122.90	112.73
1	E	10	HIS	CE1-NE2-CD2	8.45	117.45	109.00
1	D	11	LEU	O-C-N	8.43	130.76	122.07
1	C	32	LYS	CA-C-N	8.39	129.25	119.94
1	C	32	LYS	C-N-CA	8.39	129.25	119.94
1	A	53	ASN	CA-CB-CG	-8.33	104.27	112.60
1	C	26	TYR	CA-C-O	8.31	131.09	121.78
1	D	12	VAL	N-CA-CB	8.28	119.70	110.51
1	C	6	LEU	O-C-N	-8.27	113.49	122.09
1	C	51	TYR	O-C-N	-8.26	111.80	122.37
1	F	4	GLN	CA-CB-CG	-8.26	97.59	114.10
1	D	18	VAL	CA-C-O	-8.25	112.42	121.17
1	E	16	TYR	O-C-N	-8.25	113.51	122.09
1	C	34	ILE	CB-CA-C	-8.24	101.42	111.97
1	A	31	ALA	O-C-N	-8.24	110.66	122.36
1	D	53	ASN	OD1-CG-ND2	8.17	130.77	122.60
1	E	13	GLU	O-C-N	-8.11	113.71	122.07
1	E	29	LYS	O-C-N	-8.09	113.35	122.09
1	F	12	VAL	CA-CB-CG2	-8.03	96.75	110.40
1	C	3	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	E	17	LEU	O-C-N	-7.93	113.53	122.09
1	C	31	ALA	O-C-N	7.91	134.91	122.81
1	B	3	ASN	CA-CB-CG	-7.88	104.72	112.60
1	E	40	THR	O-C-N	-7.87	110.33	122.13
1	D	44	SER	N-CA-C	-7.83	99.23	110.59
1	F	50	ASN	CA-CB-CG	-7.82	104.78	112.60
1	D	44	SER	O-C-N	-7.80	113.55	122.68
1	E	34	ILE	CA-C-O	-7.79	112.06	120.47
1	D	46	TYR	N-CA-CB	-7.76	98.71	110.12
1	E	11	LEU	N-CA-CB	-7.76	98.67	110.16
1	E	48	LEU	N-CA-CB	-7.74	98.28	110.28
1	A	15	LEU	O-C-N	7.73	131.78	122.27
1	C	30	ALA	O-C-N	7.72	130.96	122.15
1	E	8	GLY	O-C-N	-7.66	114.12	122.24
1	C	6	LEU	CA-C-O	7.59	129.03	120.90
1	D	4	GLN	O-C-N	7.56	132.06	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LEU	CA-C-O	-7.51	111.33	119.97
1	D	25	PHE	CA-CB-CG	7.50	121.30	113.80
1	F	22	ARG	CD-NE-CZ	7.50	134.90	124.40
1	E	28	ASP	O-C-N	-7.46	114.21	122.12
1	B	10	HIS	CA-CB-CG	-7.45	106.35	113.80
1	C	50	ASN	CA-CB-CG	-7.45	105.15	112.60
1	E	38	CYS	CA-C-O	-7.45	110.31	119.18
1	F	38	CYS	O-C-N	-7.44	113.04	122.34
1	E	25	PHE	CA-CB-CG	-7.42	106.38	113.80
1	D	32	LYS	CA-C-O	-7.38	112.02	120.58
1	A	52	CYS	N-CA-CB	7.36	120.46	110.38
1	A	11	LEU	CB-CA-C	-7.32	96.61	110.67
1	D	46	TYR	CA-C-O	7.32	128.31	120.55
1	F	39	CYS	N-CA-CB	7.31	121.31	110.49
1	A	18	VAL	CA-CB-CG2	-7.30	98.00	110.40
1	B	4[A]	GLN	OE1-CD-NE2	7.29	129.90	122.60
1	B	4[B]	GLN	OE1-CD-NE2	7.29	129.90	122.60
1	A	38	CYS	CA-C-N	-7.29	109.65	122.26
1	A	38	CYS	C-N-CA	-7.29	109.65	122.26
1	A	4	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	E	7	CYS	CA-C-N	7.25	129.21	120.14
1	E	7	CYS	C-N-CA	7.25	129.21	120.14
1	A	27	THR	O-C-N	-7.24	114.85	123.03
1	E	8	GLY	N-CA-C	-7.24	103.76	113.24
1	A	14	ALA	CA-C-O	-7.22	112.76	120.42
1	A	12	VAL	CA-C-O	-7.22	113.20	120.85
1	D	3	ASN	N-CA-C	-7.21	103.46	111.82
1	E	2	VAL	N-CA-C	-7.13	106.05	112.90
1	C	43	CYS	N-CA-CB	-7.11	98.78	110.52
1	D	40	THR	OG1-CB-CG2	-7.10	95.09	109.30
1	E	32	LYS	CA-C-O	-7.10	113.36	120.82
1	F	8	GLY	CA-C-N	-7.08	110.79	120.28
1	F	8	GLY	C-N-CA	-7.08	110.79	120.28
1	B	5	HIS	CA-C-O	-7.07	112.93	120.42
1	E	51	TYR	N-CA-C	7.06	121.92	113.16
1	A	10	HIS	CB-CG-CD2	7.05	140.36	131.20
1	C	48	LEU	O-C-N	-7.03	113.99	122.22
1	B	14	ALA	N-CA-C	-6.99	103.74	111.36
1	E	17	LEU	N-CA-C	6.99	118.69	111.14
1	B	1	PHE	CE1-CZ-CE2	6.95	132.50	120.00
1	E	38	CYS	CA-C-N	-6.93	111.56	122.65
1	E	38	CYS	C-N-CA	-6.93	111.56	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	LEU	O-C-N	-6.93	114.25	122.15
1	D	17	LEU	O-C-N	6.92	129.50	122.03
1	C	16	TYR	CA-C-O	-6.91	113.57	120.82
1	C	36	GLU	CA-C-O	6.90	127.86	120.55
1	F	32	LYS	N-CA-C	-6.86	103.89	111.36
1	B	3	ASN	CB-CA-C	-6.85	100.08	110.90
1	E	30	ALA	CA-C-N	-6.84	110.57	120.29
1	E	30	ALA	C-N-CA	-6.84	110.57	120.29
1	A	41	SER	CA-C-O	-6.84	113.33	120.99
1	C	34	ILE	N-CA-CB	6.84	118.55	110.55
1	B	37	GLN	CB-CG-CD	6.81	124.18	112.60
1	F	22	ARG	NH1-CZ-NH2	-6.79	110.48	119.30
1	D	32	LYS	CA-C-N	-6.78	108.13	121.41
1	D	32	LYS	C-N-CA	-6.78	108.13	121.41
1	C	11	LEU	CA-C-O	-6.77	112.45	120.10
1	A	48	LEU	O-C-N	-6.75	114.97	122.12
1	F	21	GLU	CA-C-O	-6.74	110.48	119.11
1	E	24	PHE	CB-CG-CD2	-6.72	109.27	120.70
1	E	2	VAL	CA-C-N	6.71	129.57	120.38
1	E	2	VAL	C-N-CA	6.71	129.57	120.38
1	B	5	HIS	O-C-N	6.71	129.79	122.15
1	F	10	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
1	B	53	ASN	CA-CB-CG	-6.69	105.91	112.60
1	F	9	SER	CA-C-N	6.67	129.22	120.28
1	F	9	SER	C-N-CA	6.67	129.22	120.28
1	C	34	ILE	O-C-N	-6.67	115.37	121.91
1	C	4	GLN	N-CA-C	-6.65	104.10	111.82
1	B	21	GLU	O-C-N	-6.65	114.09	122.27
1	B	37	GLN	CG-CD-OE1	6.65	134.10	120.80
1	E	10	HIS	CA-C-O	6.64	127.62	119.79
1	C	28	ASP	N-CA-CB	6.63	120.55	110.28
1	E	1	PHE	CA-C-N	-6.62	112.83	122.69
1	E	1	PHE	C-N-CA	-6.62	112.83	122.69
1	E	28	ASP	CA-C-O	6.58	127.53	120.55
1	E	14	ALA	CA-C-O	-6.55	111.56	119.49
1	E	17	LEU	CD1-CG-CD2	-6.55	96.39	110.80
1	E	5	HIS	CA-CB-CG	-6.53	107.27	113.80
1	E	50	ASN	CB-CA-C	-6.53	98.55	110.63
1	B	6	LEU	CA-C-N	-6.53	110.39	120.31
1	B	6	LEU	C-N-CA	-6.53	110.39	120.31
1	D	32	LYS	N-CA-C	-6.52	100.00	109.59
1	D	37	GLN	N-CA-C	6.51	118.46	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	SER	CA-C-N	-6.51	110.42	120.31
1	B	44	SER	C-N-CA	-6.51	110.42	120.31
1	D	33	GLY	N-CA-C	-6.50	97.78	113.18
1	A	25	PHE	CA-C-O	-6.49	113.18	120.32
1	F	10	HIS	CG-CD2-NE2	6.49	113.69	107.20
1	E	5	HIS	N-CA-C	-6.49	104.29	111.36
1	E	22	ARG	CA-CB-CG	6.46	127.01	114.10
1	E	26	TYR	O-C-N	6.44	130.97	123.30
1	A	19	CYS	N-CA-CB	6.43	119.57	110.12
1	C	12	VAL	CA-C-N	-6.42	111.18	120.29
1	C	12	VAL	C-N-CA	-6.42	111.18	120.29
1	F	14	ALA	CA-C-N	-6.41	110.56	120.31
1	F	14	ALA	C-N-CA	-6.41	110.56	120.31
1	F	16	TYR	CA-C-O	6.39	127.33	120.55
1	B	3	ASN	O-C-N	6.39	128.99	122.09
1	C	5	HIS	N-CA-C	-6.38	104.24	111.07
1	B	39	CYS	O-C-N	6.37	130.31	122.34
1	A	10	HIS	CA-C-O	-6.29	113.75	120.42
1	C	12	VAL	O-C-N	6.27	127.95	121.87
1	A	6	LEU	O-C-N	6.27	129.30	122.15
1	E	22	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	A	18	VAL	O-C-N	-6.24	115.41	121.90
1	B	14	ALA	O-C-N	-6.24	115.04	122.15
1	E	22	ARG	N-CA-C	-6.22	104.39	112.23
1	F	12	VAL	CB-CA-C	-6.20	103.77	112.14
1	D	37	GLN	CB-CG-CD	6.17	123.09	112.60
1	B	36	GLU	CA-CB-CG	-6.17	101.77	114.10
1	D	10	HIS	CA-C-N	6.15	128.43	120.44
1	D	10	HIS	C-N-CA	6.15	128.43	120.44
1	E	50	ASN	OD1-CG-ND2	6.14	128.74	122.60
1	C	13	GLU	O-C-N	-6.12	115.18	122.15
1	C	4	GLN	CA-C-O	-6.08	112.97	119.97
1	A	14	ALA	O-C-N	6.08	129.08	122.15
1	F	5	HIS	CA-C-O	-6.08	112.98	119.97
1	E	33	GLY	O-C-N	-6.07	116.36	122.19
1	B	12	VAL	N-CA-C	-6.07	104.59	110.72
1	B	22	ARG	CA-C-O	-6.07	113.24	120.10
1	C	31	ALA	CB-CA-C	-6.06	103.43	112.09
1	E	3	ASN	N-CA-CB	6.05	119.14	110.06
1	B	25	PHE	N-CA-CB	-6.05	100.52	110.68
1	B	52	CYS	CA-C-O	-6.04	114.59	121.72
1	D	12	VAL	O-C-N	-6.03	115.91	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	12	VAL	CG1-CB-CG2	-6.03	97.54	110.80
1	F	13	GLU	OE1-CD-OE2	-6.02	108.44	122.90
1	B	42	ILE	O-C-N	-6.01	116.12	122.68
1	E	18	VAL	N-CA-C	-6.01	104.88	110.53
1	F	21	GLU	CB-CA-C	6.00	121.89	109.95
1	C	35	VAL	CA-C-N	-5.99	112.25	120.28
1	C	35	VAL	C-N-CA	-5.99	112.25	120.28
1	E	21	GLU	CB-CG-CD	-5.99	102.42	112.60
1	B	38	CYS	N-CA-CB	-5.98	101.29	110.44
1	A	6	LEU	N-CA-CB	5.97	119.00	110.16
1	D	25	PHE	N-CA-C	-5.97	100.88	110.14
1	F	42	ILE	CA-C-N	-5.97	113.26	122.09
1	F	42	ILE	C-N-CA	-5.97	113.26	122.09
1	A	21	GLU	CB-CG-CD	-5.95	102.49	112.60
1	C	33	GLY	N-CA-C	-5.93	105.62	112.50
1	B	10	HIS	CA-C-O	5.89	126.67	120.42
1	A	12	VAL	CG1-CB-CG2	-5.89	97.84	110.80
1	A	47	GLN	CG-CD-NE2	-5.88	107.57	116.40
1	F	13	GLU	CG-CD-OE1	5.88	131.93	118.40
1	B	25	PHE	O-C-N	-5.88	116.30	123.30
1	D	24	PHE	CA-C-N	-5.88	112.58	122.92
1	D	24	PHE	C-N-CA	-5.88	112.58	122.92
1	C	48	LEU	CA-C-O	5.86	126.72	120.10
1	A	22	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	B	51	TYR	O-C-N	-5.83	115.31	122.25
1	B	52	CYS	N-CA-CB	5.83	119.78	110.46
1	C	12	VAL	CA-CB-CG2	5.82	120.30	110.40
1	A	50	ASN	CA-CB-CG	-5.82	106.78	112.60
1	C	10	HIS	O-C-N	-5.80	114.69	122.23
1	F	10	HIS	CA-CB-CG	-5.79	108.00	113.80
1	B	18	VAL	N-CA-C	-5.79	104.69	111.00
1	F	17	LEU	O-C-N	5.78	128.02	122.07
1	E	14	ALA	N-CA-C	5.78	119.43	112.38
1	C	7	CYS	CA-C-N	5.77	126.38	119.98
1	C	7	CYS	C-N-CA	5.77	126.38	119.98
1	D	11	LEU	N-CA-CB	5.77	118.37	110.01
1	C	3	ASN	N-CA-C	5.75	117.55	111.28
1	E	4	GLN	CB-CG-CD	5.75	122.38	112.60
1	A	5	HIS	N-CA-C	-5.72	105.18	111.82
1	E	6	LEU	CA-C-O	-5.72	114.80	120.70
1	D	44	SER	CA-C-N	5.72	128.52	120.28
1	D	44	SER	C-N-CA	5.72	128.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLN	N-CA-C	-5.71	105.13	111.36
1	B	42	ILE	CA-C-N	5.70	128.93	120.95
1	B	42	ILE	C-N-CA	5.70	128.93	120.95
1	C	51	TYR	CA-C-N	5.70	131.82	122.07
1	C	51	TYR	C-N-CA	5.70	131.82	122.07
1	D	41	SER	CA-CB-OG	-5.70	99.70	111.10
1	A	41	SER	CB-CA-C	-5.70	97.81	109.94
1	F	22	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	C	38	CYS	O-C-N	-5.69	115.23	122.34
1	F	11	LEU	N-CA-CB	-5.68	101.75	110.16
1	D	13	GLU	N-CA-C	5.67	117.46	111.28
1	E	35	VAL	O-C-N	-5.67	114.05	121.82
1	B	50	ASN	CA-CB-CG	-5.67	106.93	112.60
1	E	10	HIS	CG-CD2-NE2	-5.67	101.53	107.20
1	A	25	PHE	CB-CA-C	-5.66	100.91	110.19
1	B	50	ASN	CA-C-O	5.66	126.23	119.10
1	D	3	ASN	CA-C-O	-5.65	113.47	119.97
1	F	15	LEU	CA-C-O	-5.64	113.48	119.97
1	F	40	THR	O-C-N	-5.64	114.54	122.10
1	D	22	ARG	CD-NE-CZ	-5.63	116.52	124.40
1	E	26	TYR	N-CA-CB	-5.62	101.23	110.68
1	B	1	PHE	CA-CB-CG	-5.62	108.18	113.80
1	D	9	SER	N-CA-C	-5.61	105.24	111.36
1	E	10	HIS	CA-C-N	-5.61	112.32	120.29
1	E	10	HIS	C-N-CA	-5.61	112.32	120.29
1	C	43	CYS	O-C-N	-5.59	116.65	123.19
1	D	37	GLN	CG-CD-NE2	-5.59	108.02	116.40
1	E	11	LEU	O-C-N	5.58	128.52	122.15
1	A	35	VAL	O-C-N	-5.58	116.10	121.90
1	B	35	VAL	CA-C-N	-5.57	112.81	120.28
1	B	35	VAL	C-N-CA	-5.57	112.81	120.28
1	F	22	ARG	CA-CB-CG	-5.57	102.96	114.10
1	E	22	ARG	CD-NE-CZ	-5.57	116.61	124.40
1	C	38	CYS	N-CA-CB	-5.56	102.26	110.49
1	E	15	LEU	O-C-N	5.56	129.46	122.23
1	F	21	GLU	CA-CB-CG	-5.55	103.00	114.10
1	F	11	LEU	CD1-CG-CD2	-5.54	98.60	110.80
1	F	41	SER	CA-C-N	-5.53	113.45	120.98
1	F	41	SER	C-N-CA	-5.53	113.45	120.98
1	E	34	ILE	O-C-N	5.53	128.05	121.80
1	C	36	GLU	CB-CA-C	-5.52	101.62	110.79
1	D	20	GLY	CA-C-O	5.52	130.18	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	8	GLY	CA-C-O	-5.52	115.39	120.80
1	E	51	TYR	O-C-N	5.51	129.98	122.37
1	C	8	GLY	CA-C-N	-5.51	112.47	120.29
1	C	8	GLY	C-N-CA	-5.51	112.47	120.29
1	B	4[A]	GLN	CG-CD-NE2	-5.50	108.15	116.40
1	B	4[B]	GLN	CG-CD-NE2	-5.50	108.15	116.40
1	D	24	PHE	O-C-N	5.50	128.90	123.46
1	D	18	VAL	N-CA-CB	-5.50	104.12	110.55
1	D	1	PHE	CB-CA-C	5.49	120.53	110.10
1	E	50	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	27	THR	CA-C-N	5.48	128.38	120.38
1	A	27	THR	C-N-CA	5.48	128.38	120.38
1	D	2	VAL	O-C-N	-5.47	116.34	121.87
1	B	2	VAL	CA-CB-CG1	-5.47	101.10	110.40
1	D	53	ASN	N-CA-CB	-5.47	101.20	110.50
1	D	47	GLN	CA-C-O	5.46	126.34	120.55
1	F	49	GLU	CA-CB-CG	-5.44	103.22	114.10
1	B	16	TYR	CG-CD1-CE1	-5.43	113.05	121.20
1	E	11	LEU	CA-C-O	-5.43	114.66	120.42
1	C	25	PHE	CA-C-O	-5.43	114.84	121.36
1	A	53	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	B	9	SER	N-CA-CB	5.41	118.17	110.16
1	C	6	LEU	CB-CG-CD1	5.41	126.93	110.70
1	D	1	PHE	CA-C-O	-5.40	111.61	120.80
1	D	17	LEU	CA-C-O	-5.40	115.34	120.90
1	E	24	PHE	CA-C-O	5.39	127.75	121.44
1	B	16	TYR	CA-C-N	-5.38	112.65	120.29
1	B	16	TYR	C-N-CA	-5.38	112.65	120.29
1	D	48	LEU	N-CA-CB	-5.38	101.94	110.28
1	E	53	ASN	CA-CB-CG	5.36	117.95	112.60
1	D	33	GLY	O-C-N	5.34	129.65	122.70
1	D	1	PHE	N-CA-CB	-5.34	101.42	110.50
1	F	27	THR	CA-CB-CG2	5.34	119.57	110.50
1	E	15	LEU	CA-C-O	-5.33	114.32	120.24
1	F	10	HIS	CB-CG-CD2	5.30	138.09	131.20
1	E	32	LYS	O-C-N	5.30	127.53	122.07
1	A	11	LEU	CA-C-N	-5.30	112.90	120.42
1	A	11	LEU	C-N-CA	-5.30	112.90	120.42
1	C	47	GLN	N-CA-C	-5.30	105.42	111.14
1	B	43	CYS	O-C-N	5.29	129.44	122.93
1	D	10	HIS	CG-CD2-NE2	-5.28	101.92	107.20
1	B	39	CYS	CA-C-N	-5.27	114.25	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	CYS	C-N-CA	-5.27	114.25	122.37
1	C	20	GLY	CA-C-N	-5.27	111.31	121.58
1	C	20	GLY	C-N-CA	-5.27	111.31	121.58
1	E	42	ILE	CB-CG1-CD1	-5.26	102.74	113.80
1	E	44	SER	CA-C-O	-5.25	116.01	121.99
1	B	18	VAL	O-C-N	-5.25	114.92	121.84
1	D	39	CYS	CA-C-N	-5.24	111.63	120.58
1	D	39	CYS	C-N-CA	-5.24	111.63	120.58
1	E	22	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	B	35	VAL	N-CA-CB	-5.21	102.77	110.58
1	C	16	TYR	N-CA-C	-5.19	105.52	111.07
1	F	13	GLU	O-C-N	-5.17	116.74	122.07
1	B	22	ARG	CA-CB-CG	5.16	124.42	114.10
1	E	7	CYS	O-C-N	-5.16	116.72	122.09
1	A	40	THR	CA-C-N	5.16	130.98	121.85
1	A	40	THR	C-N-CA	5.16	130.98	121.85
1	D	34	ILE	CA-C-O	-5.16	114.68	120.25
1	C	44	SER	O-C-N	-5.14	115.47	122.36
1	D	52	CYS	CB-CA-C	-5.14	99.76	110.40
1	F	2	VAL	O-C-N	-5.14	117.49	122.99
1	D	44	SER	CA-CB-OG	-5.14	100.83	111.10
1	B	36	GLU	N-CA-CB	-5.13	102.58	110.12
1	F	9	SER	CA-C-O	-5.12	115.12	120.55
1	F	5	HIS	CB-CG-CD2	5.11	137.85	131.20
1	D	7	CYS	N-CA-C	-5.11	105.79	111.36
1	A	9	SER	CA-CB-OG	-5.11	100.88	111.10
1	E	23	GLY	CA-C-N	-5.11	114.57	122.59
1	E	23	GLY	C-N-CA	-5.11	114.57	122.59
1	F	19	CYS	CA-C-N	5.11	131.42	121.41
1	F	19	CYS	C-N-CA	5.11	131.42	121.41
1	D	45	LEU	CA-C-N	-5.11	113.44	120.28
1	D	45	LEU	C-N-CA	-5.11	113.44	120.28
1	F	49	GLU	O-C-N	-5.10	115.76	122.39
1	C	18	VAL	N-CA-CB	-5.09	101.56	110.77
1	C	10	HIS	N-CA-C	-5.09	105.43	111.69
1	E	16	TYR	CB-CA-C	-5.08	102.68	110.81
1	C	42	ILE	CA-C-N	-5.08	115.08	122.65
1	C	42	ILE	C-N-CA	-5.08	115.08	122.65
1	D	47	GLN	CG-CD-OE1	-5.07	110.65	120.80
1	F	42	ILE	N-CA-CB	-5.06	104.08	110.31
1	E	4	GLN	CG-CD-NE2	5.04	123.97	116.40
1	B	22	ARG	NH1-CZ-NH2	-5.04	112.75	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PHE	CZ-CE2-CD2	-5.04	110.93	120.00
1	B	15	LEU	CB-CA-C	-5.04	102.29	110.85
1	C	1	PHE	CA-C-O	-5.03	112.25	120.80
1	A	40	THR	CB-CA-C	-5.03	101.50	110.70
1	A	1	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	LEU	Mainchain
1	A	18	VAL	Mainchain
1	B	2	VAL	Mainchain
1	B	26	TYR	Mainchain
1	B	37	GLN	Mainchain
1	B	4[A]	GLN	Mainchain
1	B	4[B]	GLN	Mainchain
1	B	41	SER	Mainchain
1	C	16	TYR	Sidechain
1	C	44	SER	Mainchain
1	C	51	TYR	Mainchain
1	D	18	VAL	Mainchain
1	D	22	ARG	Mainchain
1	E	14	ALA	Mainchain
1	E	29	LYS	Mainchain
1	E	31	ALA	Mainchain
1	E	44	SER	Mainchain
1	E	46	TYR	Mainchain
1	F	23	GLY	Mainchain
1	F	35	VAL	Mainchain

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	417	0	392	21	0
1	B	420	0	392	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	421	0	394	13	0
1	D	417	0	392	20	2
1	E	417	0	392	8	0
1	F	418	0	393	5	2
2	A	8	0	8	3	0
2	B	8	0	8	0	0
2	C	8	0	8	0	0
2	D	8	0	8	0	0
2	E	16	0	16	0	0
2	F	16	0	16	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	25	0	0	2	0
5	B	34	0	0	2	0
5	C	40	0	0	2	0
5	D	36	0	0	4	0
5	E	49	0	0	3	0
5	F	44	0	0	0	0
All	All	2806	0	2419	69	2

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 14.

All (69) 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:D:22:ARG:HD2	5:D:77:HOH:O	1.48	1.14
1:A:45:LEU:HD21	1:D:17:LEU:CD1	1.90	1.02
1:A:45:LEU:HD21	1:D:17:LEU:HD11	1.51	0.92
1:A:2:VAL:CG1	1:A:2:VAL:O	2.25	0.84
1:D:44:SER:H	1:D:47:GLN:HE21	1.30	0.80
1:B:22:ARG:HH11	1:B:22:ARG:HG2	1.47	0.79
1:C:13:GLU:HG2	1:D:13:GLU:OE2	1.87	0.74
1:B:22:ARG:NH1	1:B:53:ASN:O	2.24	0.70
1:B:27:THR:O	1:B:31:ALA:N	2.24	0.69
1:A:2:VAL:O	1:A:2:VAL:HG12	1.91	0.68
1:B:21:GLU:OE1	5:B:77:HOH:O	2.12	0.65
1:D:17:LEU:HD13	1:D:17:LEU:O	1.97	0.65
1:A:2:VAL:O	1:A:2:VAL:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:HG2	5:D:89:HOH:O	1.98	0.63
1:A:45:LEU:HD21	1:D:17:LEU:HD12	1.80	0.62
1:C:1:PHE:N	5:C:96:HOH:O	2.32	0.62
1:A:2:VAL:HG22	1:E:42:ILE:CD1	2.31	0.61
1:F:44[B]:SER:OG	1:F:45:LEU:N	2.32	0.61
2:A:54:CRS:C7	1:D:17:LEU:HD21	2.33	0.59
1:A:35:VAL:O	1:A:36:GLU:C	2.41	0.59
1:E:5:HIS:CE1	5:E:103:HOH:O	2.56	0.59
1:C:21:GLU:O	1:D:28:ASP:HB2	2.03	0.58
1:C:9:SER:O	1:C:13:GLU:HG3	2.02	0.58
1:B:22:ARG:HH11	1:B:22:ARG:CG	2.17	0.55
1:B:18:VAL:HG21	1:B:45:LEU:HD12	1.89	0.55
1:E:12:VAL:CG1	1:F:12:VAL:HG12	2.37	0.55
1:B:27:THR:O	1:B:30:ALA:N	2.38	0.54
1:C:13:GLU:CG	1:D:13:GLU:OE2	2.55	0.54
1:B:15:LEU:HD12	5:B:81:HOH:O	2.09	0.53
1:A:11:LEU:HD13	1:A:34:ILE:HG12	1.91	0.53
1:A:22:ARG:NH2	1:A:49:GLU:OE2	2.42	0.53
1:C:18:VAL:HG13	1:C:49[B]:GLU:OE1	2.09	0.52
1:C:19:CYS:O	1:C:22:ARG:HB2	2.10	0.52
2:A:54:CRS:H71	1:D:17:LEU:HD21	1.91	0.52
1:A:2:VAL:HG22	1:E:42:ILE:HD13	1.91	0.51
1:D:17:LEU:HD13	1:D:17:LEU:C	2.36	0.50
1:A:45:LEU:CD2	1:D:17:LEU:HD11	2.33	0.50
1:D:6:LEU:HD23	5:D:90:HOH:O	2.12	0.49
1:A:21:GLU:HA	1:B:28:ASP:CG	2.37	0.49
1:E:32:LYS:O	1:E:36:GLU:HG3	2.12	0.49
1:C:3:ASN:ND2	5:C:63:HOH:O	2.33	0.48
1:A:41:SER:HA	1:C:1:PHE:CE2	2.48	0.48
1:D:32:LYS:HD2	1:D:32:LYS:HA	1.59	0.48
1:A:25:PHE:HE1	1:A:53:ASN:HD21	1.62	0.47
1:D:22:ARG:NH1	5:D:77:HOH:O	2.47	0.47
1:B:19:CYS:O	1:B:20:GLY:C	2.57	0.46
1:B:18:VAL:CG2	1:B:45:LEU:HD12	2.44	0.46
2:A:54:CRS:H73	5:A:72:HOH:O	2.14	0.46
1:A:21:GLU:O	1:B:28:ASP:HB2	2.17	0.45
1:A:41:SER:CB	1:C:1:PHE:HE2	2.30	0.44
1:B:45:LEU:HD13	1:B:45:LEU:HA	1.79	0.44
1:A:34:ILE:HD12	1:A:51:TYR:CD2	2.52	0.44
1:D:17:LEU:CD1	1:D:17:LEU:C	2.90	0.43
1:E:37:GLN:HG3	5:E:96:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:HA	1:B:28:ASP:OD1	2.19	0.43
1:A:2:VAL:HG22	1:E:42:ILE:HD11	2.01	0.43
1:B:27:THR:C	1:B:29:LYS:N	2.77	0.43
1:C:46:TYR:N	1:C:46:TYR:CD1	2.87	0.43
1:E:29:LYS:HD2	5:E:80:HOH:O	2.19	0.43
1:C:42:ILE:O	1:C:42:ILE:CG2	2.67	0.43
1:A:46:TYR:HE1	5:A:76:HOH:O	2.02	0.42
1:B:25:PHE:HD1	1:B:53:ASN:OD1	2.03	0.41
1:D:53:ASN:HD22	1:D:53:ASN:C	2.29	0.41
1:F:34:ILE:HD12	1:F:51:TYR:CD1	2.56	0.41
1:D:27:THR:C	1:D:29:LYS:H	2.30	0.40
1:C:26:TYR:CE1	1:C:31:ALA:HB1	2.57	0.40

All (2) 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)
1:D:29:LYS:NZ	1:F:53:ASN:O[2_455]	1.63	0.57
1:D:29:LYS:NZ	1:F:22:ARG:NH2[2_455]	1.87	0.33

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
1	B	52/53 (98%)	49 (94%)	3 (6%)	0	100	100
1	C	52/53 (98%)	50 (96%)	1 (2%)	1 (2%)	6	1
1	D	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
1	E	51/53 (96%)	51 (100%)	0	0	100	100
1	F	52/53 (98%)	52 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	309/318 (97%)	298 (96%)	10 (3%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	32	LYS

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	46/46 (100%)	37 (80%)	9 (20%)	1	0
1	B	47/46 (102%)	41 (87%)	6 (13%)	4	1
1	C	47/46 (102%)	43 (92%)	4 (8%)	10	4
1	D	46/46 (100%)	38 (83%)	8 (17%)	2	0
1	E	46/46 (100%)	41 (89%)	5 (11%)	6	2
1	F	47/46 (102%)	44 (94%)	3 (6%)	16	8
All	All	279/276 (101%)	244 (88%)	35 (12%)	4	1

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	17	LEU
1	A	25	PHE
1	A	27	THR
1	A	29	LYS
1	A	36	GLU
1	A	37	GLN
1	A	48	LEU
1	A	53	ASN
1	B	4[A]	GLN
1	B	4[B]	GLN

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	22	ARG
1	B	28	ASP
1	B	45	LEU
1	C	1	PHE
1	C	2	VAL
1	C	6	LEU
1	C	46	TYR
1	D	9	SER
1	D	17	LEU
1	D	21	GLU
1	D	25	PHE
1	D	32	LYS
1	D	41	SER
1	D	42	ILE
1	D	53	ASN
1	E	3	ASN
1	E	6	LEU
1	E	29	LYS
1	E	32	LYS
1	E	48	LEU
1	F	17	LEU
1	F	32	LYS
1	F	46	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	53	ASN
1	B	53	ASN
1	C	3	ASN
1	C	4	GLN
1	D	37	GLN
1	D	47	GLN
1	D	53	ASN
1	E	53	ASN
1	F	5	HIS
1	F	47	GLN
1	F	50	ASN
1	F	53	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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
2	CRS	E	54	-	8,8,8	1.53	1 (12%)	10,10,10	6.61	6 (60%)
2	CRS	A	54	-	8,8,8	1.13	1 (12%)	10,10,10	2.81	6 (60%)
2	CRS	B	56	-	8,8,8	2.10	3 (37%)	10,10,10	3.71	5 (50%)
2	CRS	F	54	-	8,8,8	2.25	3 (37%)	10,10,10	2.32	3 (30%)
2	CRS	E	55	-	8,8,8	2.05	3 (37%)	10,10,10	4.06	8 (80%)
2	CRS	D	54	-	8,8,8	3.65	5 (62%)	10,10,10	8.05	5 (50%)
2	CRS	F	55	-	8,8,8	2.21	3 (37%)	10,10,10	8.28	9 (90%)
2	CRS	C	56	-	8,8,8	1.88	2 (25%)	10,10,10	1.79	2 (20%)

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
2	CRS	E	54	-	-	-	0/1/1/1
2	CRS	A	54	-	-	-	0/1/1/1
2	CRS	B	56	-	-	-	0/1/1/1
2	CRS	F	54	-	-	-	0/1/1/1
2	CRS	E	55	-	-	-	0/1/1/1
2	CRS	D	54	-	-	-	0/1/1/1
2	CRS	F	55	-	-	-	0/1/1/1
2	CRS	C	56	-	-	-	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	54	CRS	C5-C6	7.58	1.51	1.38
2	B	56	CRS	C5-C6	4.51	1.46	1.38
2	D	54	CRS	O1-C1	4.39	1.46	1.37
2	F	54	CRS	C5-C4	-4.09	1.31	1.38
2	F	55	CRS	C2-C1	3.91	1.45	1.39
2	E	55	CRS	O1-C1	3.73	1.45	1.37
2	C	56	CRS	C5-C6	3.66	1.45	1.38
2	E	54	CRS	C2-C3	3.62	1.44	1.39
2	D	54	CRS	C2-C1	3.44	1.44	1.39
2	F	54	CRS	C2-C1	-3.38	1.34	1.39
2	F	55	CRS	C5-C4	3.22	1.44	1.38
2	D	54	CRS	C5-C4	-3.02	1.33	1.38
2	C	56	CRS	C2-C1	-2.98	1.34	1.39
2	D	54	CRS	C6-C1	-2.94	1.33	1.39
2	E	55	CRS	C5-C4	-2.69	1.34	1.38
2	E	55	CRS	C5-C6	2.63	1.43	1.38
2	F	55	CRS	C6-C1	-2.21	1.34	1.39
2	F	54	CRS	C5-C6	2.19	1.42	1.38
2	B	56	CRS	C2-C3	2.14	1.42	1.39
2	A	54	CRS	C5-C6	2.06	1.42	1.38
2	B	56	CRS	C2-C1	2.01	1.42	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	54	CRS	C1-C2-C3	-20.01	107.75	120.10
2	F	55	CRS	C1-C2-C3	-19.32	108.17	120.10
2	E	54	CRS	C1-C2-C3	-17.74	109.14	120.10
2	F	55	CRS	C6-C5-C4	-11.16	105.90	120.24
2	E	55	CRS	C7-C3-C2	9.52	133.81	120.92
2	D	54	CRS	C6-C5-C4	-9.51	108.02	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	54	CRS	C4-C3-C2	9.22	131.56	117.96
2	B	56	CRS	C1-C2-C3	-8.81	114.66	120.10
2	F	55	CRS	C7-C3-C2	-7.26	111.09	120.92
2	D	54	CRS	C5-C6-C1	6.71	128.35	119.29
2	E	54	CRS	C4-C3-C2	6.43	127.44	117.96
2	F	55	CRS	O1-C1-C2	-5.73	104.87	119.85
2	F	55	CRS	C5-C6-C1	5.66	126.94	119.29
2	F	55	CRS	C4-C3-C2	5.48	126.05	117.96
2	E	54	CRS	C6-C5-C4	-5.00	113.82	120.24
2	D	54	CRS	C7-C3-C4	-4.87	108.62	120.96
2	E	54	CRS	C7-C3-C2	-4.80	114.42	120.92
2	F	55	CRS	C6-C1-C2	4.74	125.39	120.19
2	F	54	CRS	C5-C6-C1	-4.60	113.08	119.29
2	A	54	CRS	C5-C6-C1	4.57	125.46	119.29
2	B	56	CRS	C6-C1-C2	4.42	125.04	120.19
2	E	54	CRS	C5-C6-C1	4.37	125.20	119.29
2	A	54	CRS	C4-C3-C2	4.23	124.20	117.96
2	B	56	CRS	C7-C3-C2	-4.22	115.21	120.92
2	E	55	CRS	O1-C1-C6	-4.11	108.54	120.00
2	C	56	CRS	C7-C3-C2	-3.99	115.51	120.92
2	F	54	CRS	C6-C1-C2	3.99	124.56	120.19
2	E	55	CRS	C7-C3-C4	-3.62	111.78	120.96
2	F	54	CRS	C6-C5-C4	3.51	124.75	120.24
2	F	55	CRS	O1-C1-C6	3.50	129.74	120.00
2	A	54	CRS	C6-C5-C4	-3.37	115.92	120.24
2	E	54	CRS	C6-C1-C2	3.30	123.81	120.19
2	E	55	CRS	C6-C1-C2	3.24	123.74	120.19
2	B	56	CRS	C6-C5-C4	-3.11	116.24	120.24
2	A	54	CRS	C7-C3-C2	-3.02	116.83	120.92
2	E	55	CRS	O1-C1-C2	2.98	127.65	119.85
2	A	54	CRS	C1-C2-C3	-2.71	118.43	120.10
2	E	55	CRS	C5-C6-C1	-2.66	115.69	119.29
2	B	56	CRS	C4-C3-C2	2.59	121.78	117.96
2	A	54	CRS	C6-C1-C2	-2.48	117.47	120.19
2	E	55	CRS	C4-C3-C2	-2.43	114.38	117.96
2	E	55	CRS	C1-C2-C3	2.27	121.50	120.10
2	C	56	CRS	C4-C3-C2	2.14	121.12	117.96
2	F	55	CRS	C5-C4-C3	2.09	127.48	120.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	54	CRS	3	0

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	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	27:THR	C	28:ASP	N	1.18

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.