



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 AM UTC

PDB ID : 7INS / pdb_00007ins
Title : STRUCTURE OF PORCINE INSULIN COCRYSTALLIZED WITH CLUPEINE Z
Authors : Balschmidt, P.; Hansen, F.B.; Dodson, E.; Dodson, G.; Korber, F.
Deposited on : 1991-09-03
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

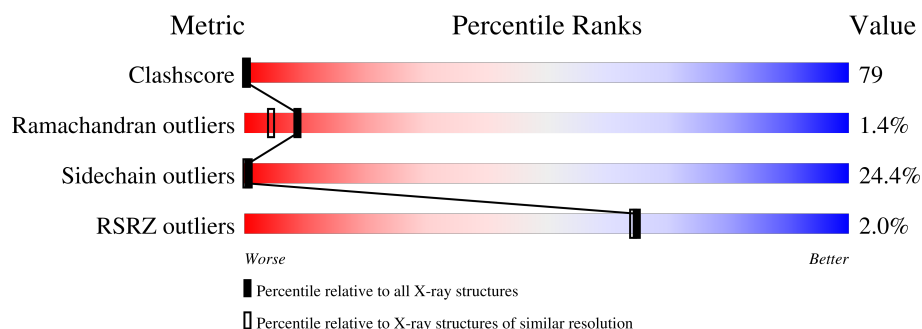
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	21	
1	C	21	
1	E	21	
2	B	30	
2	D	30	
2	F	30	
3	G	16	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 1492 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 (CHAIN A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	3	1	0
			167	101	25	37	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

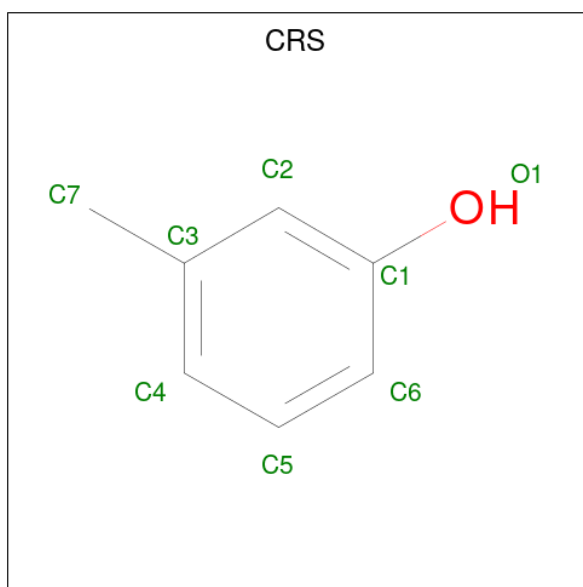
- Molecule 2 is a protein called INSULIN (CHAIN B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	S	0	1	0
			246	163	40	41	2			
2	D	30	Total	C	N	O	S	4	0	0
			240	157	40	41	2			
2	F	30	Total	C	N	O	S	0	0	0
			240	157	40	41	2			

- Molecule 3 is a protein called GENERAL PROTAMINE CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	16	Total	C	N	O	15	0	0
			124	69	39	16			

- Molecule 4 is M-CRESOL (CCD ID: CRS) (formula: C₇H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			15	13	2		
4	C	1	Total	C	O	0	0
			7	6	1		
4	E	1	Total	C	O	0	0
			7	6	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Zn	0	0
			1	1		

- Molecule 6 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	2	Total	C	N	0	0
			10	4	6		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	B	19	Total	O	0	0
			19	19		

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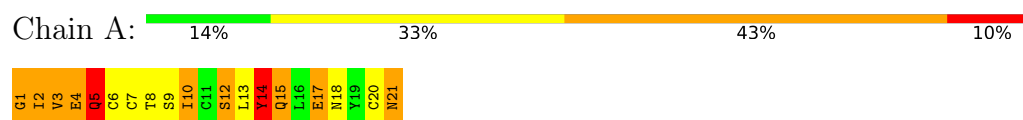
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	5	Total 5	O 5	0	0
7	D	31	Total 31	O 31	0	0
7	E	15	Total 15	O 15	0	0
7	F	13	Total 13	O 13	0	0
7	G	9	Total 9	O 9	0	0

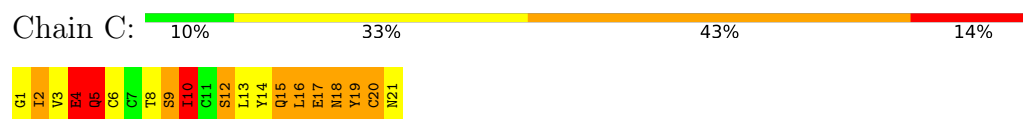
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

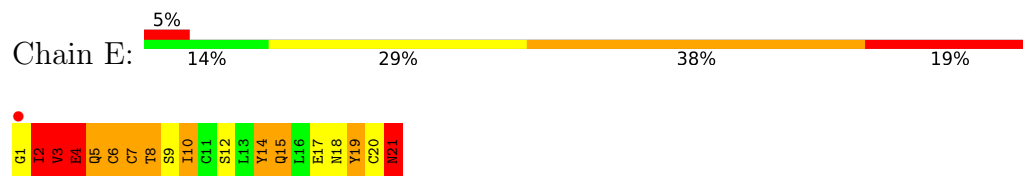
- Molecule 1: INSULIN (CHAIN A)



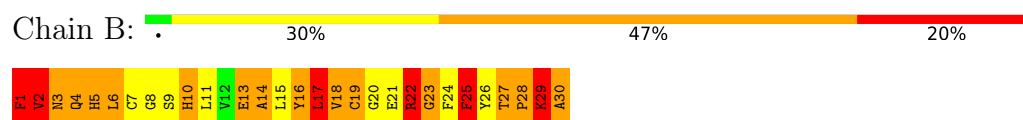
- Molecule 1: INSULIN (CHAIN A)



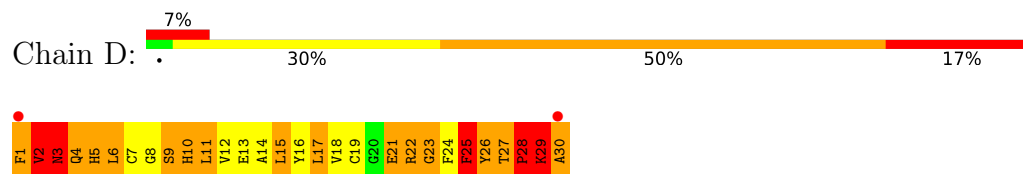
- Molecule 1: INSULIN (CHAIN A)



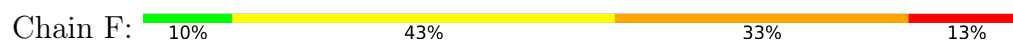
- Molecule 2: INSULIN (CHAIN B)

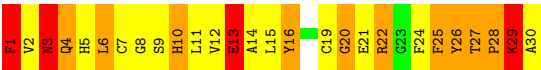


- Molecule 2: INSULIN (CHAIN B)

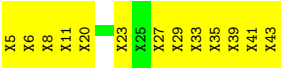


- Molecule 2: INSULIN (CHAIN B)





● Molecule 3: GENERAL PROTAMINE CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.90Å 62.90Å 85.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 50.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 82.0 (50.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 1.99Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available) 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 243.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1492	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, UNL, CRS

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	1.90	3/173 (1.7%)	4.19	47/232 (20.3%)
1	C	1.67	2/164 (1.2%)	4.09	41/220 (18.6%)
1	E	1.65	0/164	3.90	34/220 (15.5%)
2	B	1.73	1/259 (0.4%)	4.06	62/348 (17.8%)
2	D	1.92	3/247 (1.2%)	5.09	74/332 (22.3%)
2	F	1.73	4/247 (1.6%)	4.84	77/332 (23.2%)
All	All	1.78	13/1254 (1.0%)	4.44	335/1684 (19.9%)

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
2	B	0	2
3	G	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	29	LYS	CB-CG	-10.23	1.21	1.52
1	A	10	ILE	CB-CG1	-7.51	1.38	1.53
1	A	8	THR	N-CA	6.67	1.54	1.46
2	F	10	HIS	ND1-CE1	6.57	1.39	1.32
1	A	2	ILE	N-CA	6.18	1.53	1.46
2	F	7	CYS	C-N	-6.14	1.25	1.33
2	F	8	GLY	N-CA	5.72	1.53	1.45
2	D	24	PHE	C-O	5.45	1.29	1.24
2	D	9	SER	N-CA	5.39	1.52	1.46
1	C	4	GLU	N-CA	5.39	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	GLU	C-O	-5.36	1.17	1.24
2	B	14	ALA	N-CA	5.15	1.52	1.46
2	F	4	GLN	C-N	-5.12	1.27	1.33

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	PHE	CA-CB-CG	38.92	152.72	113.80
2	D	29	LYS	CA-CB-CG	24.53	163.17	114.10
2	D	28	PRO	CA-C-N	24.40	168.14	121.54
2	D	28	PRO	C-N-CA	24.40	168.14	121.54
1	C	21	ASN	CA-CB-CG	18.50	131.09	112.60
2	D	3	ASN	OD1-CG-ND2	-17.70	104.90	122.60
2	B	21	GLU	CB-CG-CD	16.32	140.34	112.60
2	D	3	ASN	CA-CB-CG	16.18	128.78	112.60
2	D	29	LYS	N-CA-CB	16.09	137.68	110.49
2	B	27	THR	CB-CA-C	15.97	128.32	109.47
2	F	10	HIS	CA-CB-CG	-15.24	98.56	113.80
1	E	17	GLU	CA-CB-CG	15.18	144.45	114.10
1	A	21	ASN	OD1-CG-ND2	14.90	137.50	122.60
2	D	3	ASN	CB-CG-ND2	14.81	138.62	116.40
2	D	1	PHE	CA-C-O	14.27	145.05	120.80
2	B	24	PHE	O-C-N	14.09	137.41	123.46
2	D	12	VAL	O-C-N	13.85	135.30	121.87
1	A	5	GLN	CA-CB-CG	13.83	141.76	114.10
2	F	7	CYS	CA-C-O	-13.81	106.47	120.70
1	A	2	ILE	CA-C-O	13.60	135.27	120.85
2	D	24	PHE	CA-C-O	13.21	135.65	121.25
2	F	28	PRO	CA-C-O	13.03	130.95	121.31
2	D	29	LYS	CB-CG-CD	-12.63	82.25	111.30
1	E	21	ASN	CA-CB-CG	-12.56	100.04	112.60
1	C	10	ILE	CB-CA-C	12.32	126.19	110.91
1	C	5	GLN	OE1-CD-NE2	-12.30	110.30	122.60
1	C	12	SER	CA-C-O	12.29	136.31	121.81
2	F	24	PHE	CA-C-O	12.28	134.59	121.45
2	F	3	ASN	CA-C-O	-12.05	104.36	119.31
2	D	1	PHE	CA-CB-CG	-11.97	101.83	113.80
1	A	14	TYR	CA-C-O	-11.84	108.51	120.70
1	C	15	GLN	CG-CD-OE1	11.70	144.21	120.80
2	D	13	GLU	CA-C-N	11.63	135.86	120.28
2	D	13	GLU	C-N-CA	11.63	135.86	120.28
2	B	1	PHE	O-C-N	11.49	141.38	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	ALA	CB-CA-C	11.38	127.56	110.50
1	E	21	ASN	OD1-CG-ND2	11.37	133.97	122.60
2	B	8	GLY	CA-C-O	-11.36	107.80	120.30
2	B	5	HIS	CA-CB-CG	-11.03	102.77	113.80
2	F	11	LEU	CA-C-O	-10.93	109.44	120.70
2	F	16	TYR	CA-C-N	10.89	134.60	120.44
2	F	16	TYR	C-N-CA	10.89	134.60	120.44
2	F	25	PHE	N-CA-CB	10.84	129.69	110.83
1	A	8	THR	O-C-N	10.76	136.91	122.49
2	B	23	GLY	O-C-N	10.69	133.54	122.86
1	C	9	SER	CA-C-O	-10.52	108.80	121.11
1	E	3	VAL	N-CA-CB	-10.34	98.96	110.65
2	F	13	GLU	CB-CG-CD	10.20	129.94	112.60
2	D	3	ASN	CA-C-O	-10.18	109.52	120.92
2	D	10	HIS	CE1-NE2-CD2	-10.18	98.82	109.00
1	C	15	GLN	CG-CD-NE2	-10.07	101.29	116.40
2	F	21	GLU	N-CA-CB	10.04	126.00	110.14
1	E	18	ASN	CA-C-O	-9.94	108.86	120.10
2	B	4	GLN	N-CA-CB	-9.83	95.61	110.16
1	E	6	CYS	N-CA-C	9.82	125.55	113.17
2	F	10	HIS	CB-CG-ND1	-9.78	108.03	122.70
2	D	5	HIS	CA-C-N	9.77	133.73	120.44
2	D	5	HIS	C-N-CA	9.77	133.73	120.44
1	A	10	ILE	CB-CG1-CD1	-9.75	93.33	113.80
1	A	5	GLN	CA-C-O	-9.69	110.72	120.70
2	F	21	GLU	CB-CG-CD	-9.69	96.13	112.60
2	F	14	ALA	CA-C-N	9.68	133.02	120.44
2	F	14	ALA	C-N-CA	9.68	133.02	120.44
1	A	5	GLN	OE1-CD-NE2	9.65	132.25	122.60
2	D	10	HIS	ND1-CE1-NE2	9.57	117.97	108.40
2	D	3	ASN	O-C-N	9.56	133.11	122.11
2	D	22	ARG	O-C-N	9.51	132.20	122.12
2	F	25	PHE	CA-CB-CG	-9.45	104.35	113.80
2	D	4	GLN	OE1-CD-NE2	9.43	132.03	122.60
2	D	3	ASN	N-CA-CB	9.41	125.12	109.78
2	F	12	VAL	CA-C-O	-9.35	110.37	120.47
2	B	1	PHE	N-CA-CB	9.33	126.36	110.50
2	B	17	LEU	CA-C-O	-9.33	110.53	120.42
2	D	2	VAL	CA-C-O	-9.32	111.25	120.95
1	A	13	LEU	O-C-N	9.17	131.84	122.12
2	B	3	ASN	OD1-CG-ND2	-9.16	113.44	122.60
2	B	25[A]	PHE	N-CA-C	-9.14	95.09	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25[B]	PHE	N-CA-C	-9.14	95.09	109.72
1	E	3	VAL	CB-CA-C	9.11	123.62	111.87
2	B	22	ARG	CD-NE-CZ	-9.05	111.73	124.40
1	E	10	ILE	CA-C-O	8.87	131.21	120.74
2	D	5	HIS	O-C-N	-8.86	112.73	122.12
1	A	14	TYR	CA-CB-CG	-8.85	97.96	113.90
1	A	13	LEU	CB-CA-C	8.84	125.46	110.79
1	A	4[A]	GLU	CB-CA-C	8.83	125.86	110.85
1	A	4[B]	GLU	CB-CA-C	8.83	125.86	110.85
1	E	4	GLU	CB-CG-CD	8.81	127.58	112.60
2	D	17	LEU	N-CA-CB	-8.75	97.19	110.13
2	B	5	HIS	CA-C-N	8.69	132.28	120.38
2	B	5	HIS	C-N-CA	8.69	132.28	120.38
2	F	4	GLN	CG-CD-OE1	8.60	138.00	120.80
1	E	6	CYS	CA-C-O	-8.58	109.31	119.35
2	D	5	HIS	CE1-NE2-CD2	-8.57	100.43	109.00
2	B	1	PHE	CA-CB-CG	-8.57	105.23	113.80
1	C	19	TYR	N-CA-C	8.55	123.71	113.28
1	C	5	GLN	CB-CG-CD	8.53	127.10	112.60
1	E	14	TYR	CA-CB-CG	8.52	129.23	113.90
2	D	25	PHE	CB-CA-C	8.45	126.53	109.38
1	C	21	ASN	CB-CG-ND2	8.44	129.06	116.40
2	D	26	TYR	CA-C-O	8.38	129.27	120.30
2	D	13	GLU	O-C-N	-8.38	113.23	122.12
1	C	15	GLN	OE1-CD-NE2	-8.34	114.26	122.60
1	C	16	LEU	O-C-N	-8.30	113.32	122.12
2	B	6	LEU	CA-C-O	8.26	129.55	120.63
1	E	6	CYS	O-C-N	8.26	132.66	122.34
1	E	7	CYS	CB-CA-C	8.20	123.78	110.09
2	F	13	GLU	CA-C-N	8.20	131.10	120.44
2	F	13	GLU	C-N-CA	8.20	131.10	120.44
2	F	7	CYS	CA-CB-SG	8.16	133.17	114.40
2	F	7	CYS	CB-CA-C	-8.13	98.05	110.90
2	B	24	PHE	CA-CB-CG	8.13	121.93	113.80
1	C	18	ASN	CA-CB-CG	-8.10	104.50	112.60
2	D	29	LYS	N-CA-C	-8.08	93.59	110.80
2	D	23	GLY	N-CA-C	-8.06	97.54	112.37
2	F	26	TYR	O-C-N	8.04	133.73	123.12
2	D	5	HIS	ND1-CE1-NE2	8.03	116.43	108.40
2	B	21	GLU	CA-C-O	-7.98	109.83	119.49
1	A	1	GLY	CA-C-N	-7.97	109.10	120.42
1	A	1	GLY	C-N-CA	-7.97	109.10	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	SER	CA-C-N	7.92	132.88	121.80
1	E	9	SER	C-N-CA	7.92	132.88	121.80
2	F	21	GLU	OE1-CD-OE2	7.87	141.79	122.90
2	F	4	GLN	CG-CD-NE2	-7.84	104.63	116.40
2	D	22	ARG	CA-CB-CG	-7.83	98.44	114.10
2	F	7	CYS	N-CA-CB	7.82	121.42	110.07
1	A	6	CYS	CA-C-O	-7.80	110.23	119.35
2	F	29	LYS	O-C-N	7.76	132.91	122.59
2	D	1	PHE	CA-C-N	7.74	131.07	120.46
2	D	1	PHE	C-N-CA	7.74	131.07	120.46
1	C	19	TYR	N-CA-CB	7.74	122.61	110.46
2	B	22	ARG	CA-CB-CG	-7.72	98.66	114.10
2	F	5	HIS	CA-CB-CG	-7.71	106.08	113.80
2	B	24	PHE	CA-C-O	-7.70	112.64	121.10
2	F	26	TYR	CB-CA-C	-7.67	98.39	110.74
2	B	13	GLU	CG-CD-OE2	-7.67	100.77	118.40
1	E	17	GLU	CG-CD-OE1	7.65	135.99	118.40
1	E	3	VAL	CA-C-O	-7.63	112.33	121.18
2	D	9	SER	CA-C-O	7.60	128.80	120.82
2	B	29	LYS	CA-CB-CG	7.60	129.30	114.10
2	F	27	THR	CA-C-O	-7.58	111.69	119.49
2	B	5	HIS	O-C-N	-7.52	114.03	122.08
1	E	15	GLN	N-CA-C	-7.51	103.57	112.89
1	A	15	GLN	CG-CD-NE2	-7.47	105.20	116.40
2	B	9	SER	N-CA-CB	7.45	121.04	109.94
2	D	2	VAL	CB-CA-C	7.45	122.19	112.14
1	A	8	THR	CA-C-O	-7.42	110.98	119.14
2	D	17	LEU	O-C-N	7.41	131.13	122.17
2	D	2	VAL	N-CA-CB	-7.41	100.47	110.54
1	A	5	GLN	O-C-N	7.37	130.05	122.09
1	E	19	TYR	O-C-N	-7.29	112.31	122.37
2	B	27	THR	CA-C-N	7.27	128.24	120.83
2	B	27	THR	C-N-CA	7.27	128.24	120.83
2	F	25	PHE	N-CA-C	-7.25	97.59	109.40
2	F	4	GLN	CA-C-N	7.23	130.28	120.44
2	F	4	GLN	C-N-CA	7.23	130.28	120.44
2	D	21	GLU	N-CA-C	7.23	121.36	112.54
2	B	13	GLU	CB-CG-CD	7.20	124.85	112.60
1	E	20	CYS	CA-C-O	-7.20	113.95	121.87
2	D	4	GLN	O-C-N	7.17	131.09	122.27
2	F	21	GLU	CG-CD-OE2	-7.16	101.93	118.40
2	B	4	GLN	OE1-CD-NE2	7.13	129.73	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	SER	O-C-N	-7.07	114.79	122.07
2	D	12	VAL	N-CA-CB	7.06	120.14	110.54
2	F	7	CYS	O-C-N	7.06	129.71	122.09
2	B	28	PRO	CA-C-O	7.00	126.90	118.92
2	B	2	VAL	N-CA-C	-6.94	102.42	111.09
2	F	9	SER	N-CA-CB	-6.92	99.98	110.01
2	F	10	HIS	CB-CG-CD2	6.90	140.17	131.20
1	E	2	ILE	N-CA-CB	-6.88	100.26	110.58
2	D	13	GLU	CB-CA-C	6.79	122.07	110.79
2	B	3	ASN	CB-CG-OD1	6.76	134.33	120.80
2	F	7	CYS	CA-C-N	-6.76	111.69	120.14
2	F	7	CYS	C-N-CA	-6.76	111.69	120.14
2	B	19	CYS	N-CA-C	6.75	121.11	113.01
2	D	15	LEU	CA-C-O	6.72	127.54	120.42
2	F	4	GLN	CB-CA-C	6.72	124.03	109.99
2	F	12	VAL	N-CA-C	-6.72	102.69	111.09
2	B	14	ALA	CA-C-O	6.69	127.51	120.42
2	D	22	ARG	CB-CA-C	-6.66	99.35	110.68
2	B	24	PHE	N-CA-C	-6.66	98.17	108.42
2	D	24	PHE	CA-C-N	-6.65	110.93	122.37
2	D	24	PHE	C-N-CA	-6.65	110.93	122.37
1	A	7	CYS	N-CA-C	-6.64	105.08	113.72
2	F	13	GLU	CG-CD-OE2	6.63	133.66	118.40
1	C	10	ILE	CA-C-O	6.62	128.19	120.71
2	D	12	VAL	CA-CB-CG2	6.60	121.63	110.40
1	C	8	THR	CA-C-O	6.56	128.00	120.00
2	D	25	PHE	CA-C-O	6.53	128.44	120.60
1	E	4	GLU	CG-CD-OE2	6.53	133.41	118.40
1	C	5	GLN	CG-CD-OE1	6.52	133.84	120.80
2	D	10	HIS	CA-C-O	-6.50	112.50	119.97
2	F	1	PHE	N-CA-CB	6.50	121.55	110.50
2	F	28	PRO	O-C-N	-6.48	114.15	122.44
1	A	9	SER	CA-C-O	-6.46	114.35	121.33
2	B	13	GLU	CG-CD-OE1	6.44	133.22	118.40
2	F	24	PHE	CA-CB-CG	-6.44	107.36	113.80
2	F	26	TYR	N-CA-CB	6.43	120.81	110.65
1	E	10	ILE	CB-CA-C	-6.42	103.57	111.08
1	E	17	GLU	N-CA-CB	6.39	120.06	110.22
1	A	15	GLN	CG-CD-OE1	6.38	133.56	120.80
2	F	6	LEU	CA-C-O	6.36	127.29	120.55
2	F	27	THR	O-C-N	6.36	130.31	121.47
2	B	30	ALA	N-CA-C	-6.33	93.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	14	TYR	N-CA-C	6.33	120.74	112.89
1	E	17	GLU	O-C-N	6.33	129.62	122.22
2	D	16	TYR	O-C-N	-6.31	115.43	122.12
1	E	17	GLU	CG-CD-OE2	-6.30	103.91	118.40
1	A	10	ILE	N-CA-C	6.29	117.70	109.58
1	C	19	TYR	CA-C-O	-6.29	111.70	119.18
1	C	2	ILE	CA-C-O	-6.25	113.72	120.47
2	D	22	ARG	NE-CZ-NH2	-6.25	113.58	119.20
2	F	5	HIS	O-C-N	-6.24	115.35	122.09
2	B	17	LEU	N-CA-CB	-6.24	100.92	110.16
1	C	19	TYR	O-C-N	6.20	131.21	122.41
1	E	9	SER	CA-C-O	-6.17	113.95	120.80
2	D	22	ARG	NH1-CZ-NH2	6.17	127.32	119.30
2	F	22	ARG	CG-CD-NE	6.16	125.56	112.00
2	F	22	ARG	N-CA-C	6.16	120.53	112.89
2	D	6	LEU	N-CA-C	-6.14	104.50	111.14
2	D	25	PHE	CA-CB-CG	-6.14	107.66	113.80
1	C	14	TYR	O-C-N	6.12	129.13	122.15
1	A	21	ASN	CB-CA-C	-6.11	98.49	110.10
2	F	22	ARG	NE-CZ-NH1	-6.10	115.40	121.50
2	B	5	HIS	ND1-CE1-NE2	6.10	114.50	108.40
2	F	14	ALA	CA-C-O	-6.10	114.42	120.82
1	E	21	ASN	CB-CG-ND2	-6.09	107.26	116.40
1	A	13	LEU	N-CA-C	-6.09	104.64	111.28
2	F	26	TYR	CA-C-N	-6.09	115.03	122.64
2	F	26	TYR	C-N-CA	-6.09	115.03	122.64
1	A	12	SER	O-C-N	6.09	129.76	122.94
1	C	18	ASN	CA-C-O	6.07	126.99	120.20
1	A	14	TYR	N-CA-CB	6.06	118.86	110.07
1	A	7	CYS	CA-C-N	-6.03	111.49	121.92
1	A	7	CYS	C-N-CA	-6.03	111.49	121.92
1	C	21	ASN	OD1-CG-ND2	-6.02	116.58	122.60
2	D	18	VAL	CG1-CB-CG2	-6.02	97.55	110.80
1	C	16	LEU	CA-C-N	6.02	128.95	120.28
1	C	16	LEU	C-N-CA	6.02	128.95	120.28
2	B	4	GLN	O-C-N	6.01	129.00	122.15
2	F	15	LEU	N-CA-CB	5.99	118.69	110.01
2	B	5	HIS	N-CA-C	-5.98	103.72	111.02
1	E	4	GLU	CA-C-N	-5.98	112.31	120.44
1	E	4	GLU	C-N-CA	-5.98	112.31	120.44
2	F	26	TYR	CA-C-O	-5.97	114.14	120.40
1	C	10	ILE	CA-CB-CG1	5.94	120.50	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	HIS	CB-CG-CD2	5.92	138.90	131.20
1	A	20	CYS	N-CA-C	-5.90	101.80	110.52
2	F	11	LEU	N-CA-CB	5.89	118.61	110.07
1	C	16	LEU	CA-C-O	5.87	126.78	120.55
1	A	10	ILE	CA-CB-CG2	-5.87	100.52	110.50
2	D	14	ALA	N-CA-C	-5.86	104.89	111.28
2	F	5	HIS	CA-C-N	5.83	128.09	120.28
2	F	5	HIS	C-N-CA	5.83	128.09	120.28
1	A	17	GLU	CG-CD-OE1	-5.82	105.02	118.40
1	C	9	SER	CA-C-N	-5.80	114.88	122.37
1	C	9	SER	C-N-CA	-5.80	114.88	122.37
1	A	3	VAL	N-CA-CB	-5.79	103.77	110.55
1	C	14	TYR	CB-CG-CD2	5.79	129.49	120.80
2	F	3	ASN	CA-CB-CG	5.79	118.39	112.60
2	F	13	GLU	O-C-N	-5.78	115.57	122.15
1	E	5	GLN	OE1-CD-NE2	5.75	128.35	122.60
2	F	20	GLY	CA-C-N	5.75	128.77	120.38
2	F	20	GLY	C-N-CA	5.75	128.77	120.38
1	A	12	SER	CA-CB-OG	-5.73	99.64	111.10
2	D	5	HIS	CB-CA-C	5.70	120.25	110.79
2	F	4	GLN	CB-CG-CD	-5.70	102.91	112.60
1	A	5	GLN	CG-CD-NE2	-5.69	107.87	116.40
2	B	21	GLU	CA-C-N	5.67	130.31	120.68
2	B	21	GLU	C-N-CA	5.67	130.31	120.68
2	B	16	TYR	O-C-N	-5.66	116.21	122.09
2	F	29	LYS	CA-C-O	-5.66	112.42	120.51
2	B	18	VAL	CB-CA-C	5.65	119.43	112.02
2	B	15	LEU	N-CA-CB	5.65	118.26	110.07
2	B	2	VAL	O-C-N	-5.65	115.42	121.80
2	D	5	HIS	CG-CD2-NE2	5.62	112.82	107.20
2	F	10	HIS	ND1-CG-CD2	5.62	111.72	106.10
1	C	14	TYR	CB-CG-CD1	-5.60	112.40	120.80
2	B	7	CYS	CA-C-O	-5.59	114.94	120.70
2	D	30	ALA	N-CA-C	5.57	126.61	111.00
1	A	2	ILE	N-CA-CB	5.57	118.93	110.58
1	C	10	ILE	N-CA-CB	5.57	116.79	110.72
1	A	15	GLN	O-C-N	5.53	128.69	122.22
2	B	26	TYR	CA-C-O	5.50	126.18	120.40
1	C	6	CYS	CA-CB-SG	-5.40	101.98	114.40
1	C	19	TYR	CB-CG-CD1	-5.40	112.70	120.80
2	B	8	GLY	N-CA-C	-5.38	106.16	113.37
1	A	4[A]	GLU	CA-C-O	5.37	126.11	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4[B]	GLU	CA-C-O	5.37	126.11	120.42
2	F	10	HIS	CG-CD2-NE2	-5.37	101.83	107.20
2	D	11	LEU	CA-C-O	-5.36	114.29	120.24
2	B	28	PRO	N-CA-CB	5.33	108.84	102.60
2	D	7	CYS	CA-C-N	5.32	126.83	120.13
2	D	7	CYS	C-N-CA	5.32	126.83	120.13
2	F	4	GLN	N-CA-C	-5.32	106.30	112.89
2	F	4	GLN	OE1-CD-NE2	-5.31	117.29	122.60
2	F	13	GLU	CA-CB-CG	5.31	124.72	114.10
1	E	5	GLN	CB-CA-C	5.31	119.28	110.90
1	A	17	GLU	N-CA-C	5.30	119.23	112.87
2	D	12	VAL	CA-C-N	-5.28	113.21	120.28
2	D	12	VAL	C-N-CA	-5.28	113.21	120.28
2	B	29	LYS	O-C-N	5.27	129.59	122.59
2	D	13	GLU	CA-CB-CG	-5.27	103.56	114.10
2	B	15	LEU	CA-C-O	-5.25	115.29	120.70
2	B	27	THR	N-CA-C	-5.25	101.44	109.64
1	A	3	VAL	CA-C-N	-5.25	112.83	120.29
1	A	3	VAL	C-N-CA	-5.25	112.83	120.29
1	E	20	CYS	N-CA-CB	-5.22	102.79	110.26
2	D	29	LYS	CA-C-O	-5.19	113.08	120.51
1	A	18	ASN	CB-CA-C	5.18	120.26	109.95
1	A	17	GLU	CA-CB-CG	-5.18	103.74	114.10
2	B	19	CYS	CA-CB-SG	-5.17	102.50	114.40
2	F	6	LEU	CD1-CG-CD2	-5.17	99.42	110.80
1	A	13	LEU	N-CA-CB	-5.17	102.52	110.12
1	C	2	ILE	N-CA-C	-5.15	104.65	111.09
2	B	9	SER	CA-C-O	-5.14	115.41	120.90
2	D	21	GLU	CA-C-N	5.11	127.39	120.38
2	D	21	GLU	C-N-CA	5.11	127.39	120.38
1	C	20	CYS	CA-C-N	5.11	130.90	121.70
1	C	20	CYS	C-N-CA	5.11	130.90	121.70
1	A	6	CYS	CA-CB-SG	-5.11	102.66	114.40
2	F	22	ARG	O-C-N	-5.11	115.41	122.46
2	B	22	ARG	N-CA-C	5.10	118.66	112.23
2	D	7	CYS	CA-C-O	-5.10	115.44	120.90
2	D	12	VAL	CA-CB-CG1	-5.10	101.73	110.40
1	C	17	GLU	CA-C-N	5.08	127.80	120.38
1	C	17	GLU	C-N-CA	5.08	127.80	120.38
2	F	10	HIS	CE1-NE2-CD2	5.07	114.07	109.00
1	A	3	VAL	CG1-CB-CG2	5.07	121.95	110.80
1	C	9	SER	CB-CA-C	5.06	119.96	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	SER	O-C-N	5.05	129.46	123.24
2	F	28	PRO	N-CA-C	-5.05	104.82	113.70
2	D	25	PHE	O-C-N	5.02	129.40	123.33
2	B	29	LYS	CG-CD-CE	5.01	122.82	111.30
2	D	13	GLU	CG-CD-OE1	-5.01	106.88	118.40
2	B	5	HIS	CE1-NE2-CD2	-5.00	104.00	109.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	25[A]	PHE	Sidechain
2	B	25[B]	PHE	Sidechain
3	G	20	UNK	Mainchain

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5.2 Torsion angles ⓘ

5.2.1 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	20/21 (95%)	20 (100%)	0	0	100	100
1	C	19/21 (90%)	19 (100%)	0	0	100	100
1	E	19/21 (90%)	19 (100%)	0	0	100	100
2	B	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
2	D	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2	1
2	F	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2	1
All	All	143/153 (94%)	138 (96%)	3 (2%)	2 (1%)	9	4

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	28	PRO
2	F	29	LYS

5.2.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	21/20 (105%)	18 (86%)	3 (14%)	3	2
1	C	20/20 (100%)	15 (75%)	5 (25%)	0	0
1	E	20/20 (100%)	13 (65%)	7 (35%)	0	0
2	B	26/25 (104%)	19 (73%)	7 (27%)	0	0
2	D	25/25 (100%)	18 (72%)	7 (28%)	0	0
2	F	25/25 (100%)	20 (80%)	5 (20%)	1	0
All	All	137/135 (102%)	103 (75%)	34 (25%)	1	0

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	10	ILE
1	A	14	TYR
2	B	1	PHE
2	B	2	VAL
2	B	17	LEU
2	B	22	ARG
2	B	25[A]	PHE
2	B	25[B]	PHE
2	B	29	LYS
1	C	4	GLU
1	C	5	GLN
1	C	9	SER
1	C	10	ILE
1	C	13	LEU
2	D	2	VAL
2	D	3	ASN

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Mol	Chain	Res	Type
2	D	17	LEU
2	D	21	GLU
2	D	25	PHE
2	D	27	THR
2	D	29	LYS
1	E	2	ILE
1	E	3	VAL
1	E	4	GLU
1	E	8	THR
1	E	14	TYR
1	E	15	GLN
1	E	21	ASN
2	F	1	PHE
2	F	3	ASN
2	F	4	GLN
2	F	13	GLU
2	F	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
2	B	3	ASN
1	C	21	ASN
2	D	3	ASN
1	E	5	GLN
1	E	21	ASN

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.5 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic and 2 are unknown - leaving 4 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
4	CRS	A	22[B]	-	8,8,8	11.87	1 (12%)	10,10,10	13.32	5 (50%)
4	CRS	E	22	-	7,7,8	0.48	0	8,8,10	1.59	1 (12%)
4	CRS	C	22	-	7,7,8	0.94	0	8,8,10	1.55	2 (25%)
4	CRS	A	22[A]	-	8,8,8	2.48	2 (25%)	10,10,10	1.50	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
4	CRS	A	22[B]	-	-	-	0/1/1/1
4	CRS	E	22	-	-	-	0/1/1/1
4	CRS	C	22	-	-	-	0/1/1/1
4	CRS	A	22[A]	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	22[B]	CRS	C7-C3	33.52	2.51	1.51
4	A	22[A]	CRS	O1-C1	6.58	1.51	1.37
4	A	22[A]	CRS	C2-C3	2.11	1.42	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	22[B]	CRS	C7-C3-C4	-35.60	30.76	120.96
4	A	22[B]	CRS	C7-C3-C2	21.83	150.48	120.92
4	A	22[B]	CRS	C6-C5-C4	3.68	124.97	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	22[A]	CRS	C6-C5-C4	-3.53	115.70	120.24
4	E	22	CRS	C4-C5-C6	-2.96	116.58	120.24
4	A	22[B]	CRS	C5-C6-C1	-2.65	115.70	119.29
4	C	22	CRS	O1-C1-C2	2.57	127.15	120.00
4	A	22[A]	CRS	C5-C6-C1	2.38	122.50	119.29
4	C	22	CRS	O1-C1-C6	-2.16	113.98	120.00
4	A	22[B]	CRS	C6-C1-C2	2.11	122.50	120.19

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
4	C	22	CRS	3	0

5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	27:UNK	C	29:UNK	N	36.83
1	G	25:UNK	C	27:UNK	N	35.11
1	G	29:UNK	C	33:UNK	N	25.47
1	G	23:UNK	C	25:UNK	N	21.39
1	G	39:UNK	C	41:UNK	N	17.94
1	G	11:UNK	C	20:UNK	N	16.02
1	G	8:UNK	C	11:UNK	N	15.90
1	G	6:UNK	C	8:UNK	N	15.81
1	G	35:UNK	C	39:UNK	N	10.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	41:UNK	C	43:UNK	N	3.88
1	G	33:UNK	C	35:UNK	N	2.27
1	G	21:UNK	C	22:UNK	N	1.86
1	G	20:UNK	C	21:UNK	N	0.89
1	G	22:UNK	C	23:UNK	N	0.75

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	21/21 (100%)	0.02	0 100 100	14, 28, 45, 47	3 (14%)
1	C	21/21 (100%)	-0.42	0 100 100	17, 25, 36, 41	1 (4%)
1	E	21/21 (100%)	-0.12	1 (4%) 35 34	20, 32, 40, 54	1 (4%)
2	B	30/30 (100%)	-0.18	0 100 100	9, 22, 53, 63	1 (3%)
2	D	30/30 (100%)	-0.04	2 (6%) 24 22	10, 24, 50, 66	2 (6%)
2	F	30/30 (100%)	-0.29	0 100 100	11, 25, 60, 61	2 (6%)
3	G	0/16	-	-	-	-
All	All	153/169 (90%)	-0.17	3 (1%) 65 64	9, 26, 54, 66	10 (6%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	PHE	2.9
1	E	1	GLY	2.1
2	D	30	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	UNL	D	45	4/-	0.79	0.17	21,23,39,41	4
4	CRS	A	22[B]	8/8	0.83	0.10	12,21,24,32	7
4	CRS	A	22[A]	8/8	0.83	0.10	12,21,25,32	7
6	UNL	D	47	6/-	0.87	0.15	27,46,49,50	6
4	CRS	C	22	7/8	0.96	0.07	20,28,39,64	0
4	CRS	E	22	7/8	0.96	0.07	17,17,25,30	0
5	ZN	D	31	1/1	0.99	0.01	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.