



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 AM UTC

PDB ID : 8BZM / pdb_00008bzm
Title : FOXK1-ELF1-heterodimer bound to DNA
Authors : Morgunova, E.; Popov, A.; Yin, Y.; Taipale, J.
Deposited on : 2022-12-15
Resolution : 2.69 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

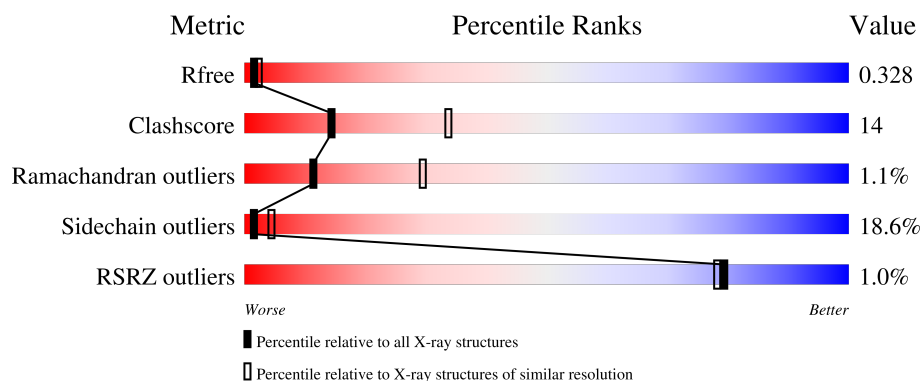
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	D	17	35% 41% 24%
1	G	17	47% 35% 18%
2	A	95	% 57% 36% 6% .
2	E	95	% 66% 29% .
2	I	95	60% 29% 8% .

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Mol	Chain	Length	Quality of chain
2	J	95	2% 63% 27% 8%
3	C	18	61% 22% 17%
3	F	18	50% 22% 22% 6%
4	B	89	% 48% 45% 6%
4	H	89	% 51% 42% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6097 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 DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	17	Total	C	N	O	P	0	0	0
			339	166	50	107	16			
1	D	17	Total	C	N	O	P	0	0	0
			342	166	50	109	17			

- Molecule 2 is a protein called Forkhead box protein K1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	94	Total	C	N	O	0	0	0
			776	496	143	137			
2	E	95	Total	C	N	O	0	1	0
			798	508	151	139			
2	I	93	Total	C	N	O	0	1	0
			784	501	146	137			
2	J	94	Total	C	N	O	0	1	0
			787	502	147	138			

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			355	168	75	95	17			
3	C	18	Total	C	N	O	P	0	0	0
			372	178	80	97	17			

- Molecule 4 is a protein called ETS-related transcription factor Elf-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	88	Total	C	N	O	S	0	0	0
			748	489	130	125	4			
4	H	88	Total	C	N	O	S	0	1	0
			756	494	133	125	4			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		

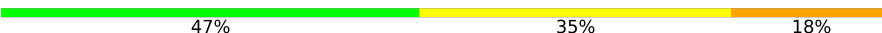
- Molecule 6 is water.

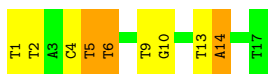
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	E	4	Total	O	0	0
			4	4		
6	F	7	Total	O	0	0
			7	7		
6	C	3	Total	O	0	0
			3	3		
6	D	5	Total	O	0	0
			5	5		
6	I	4	Total	O	0	0
			4	4		
6	J	4	Total	O	0	0
			4	4		
6	H	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

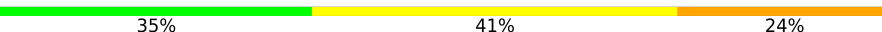
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA

Chain G: 



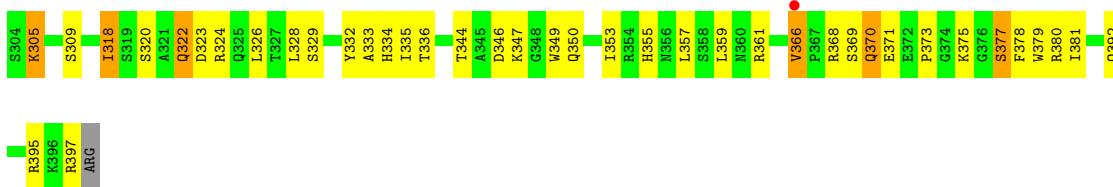
- Molecule 1: DNA

Chain D: 



- Molecule 2: Forkhead box protein K1

Chain A: 



- Molecule 2: Forkhead box protein K1

Chain E: 



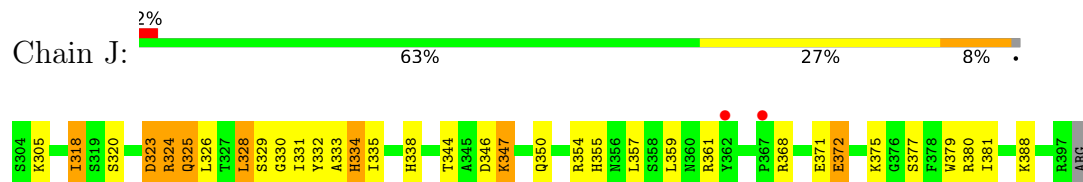
- Molecule 2: Forkhead box protein K1

Chain I: 



ARG
ARG

• Molecule 2: Forkhead box protein K1



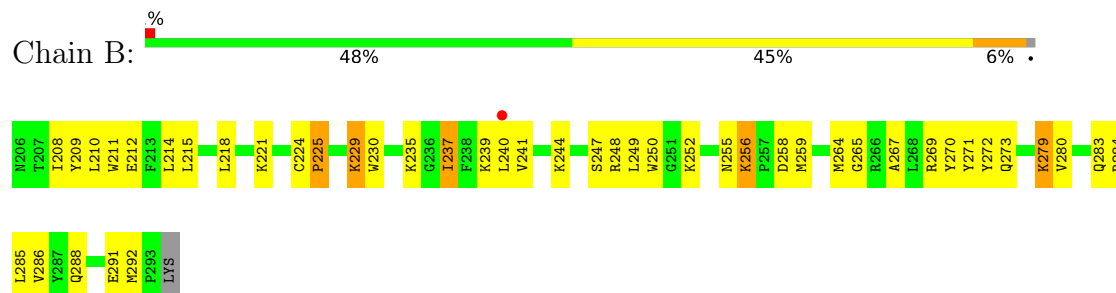
• Molecule 3: DNA



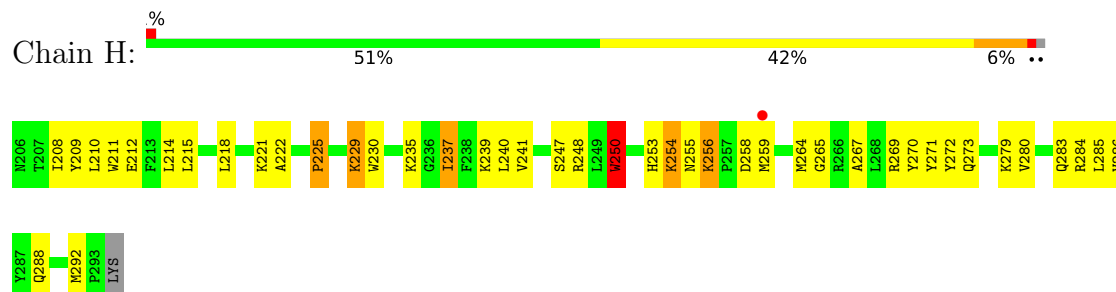
• Molecule 3: DNA



• Molecule 4: ETS-related transcription factor Elf-1



• Molecule 4: ETS-related transcription factor Elf-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.18Å 105.87Å 68.19Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	40.00 – 2.69 40.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-2.69) 96.4 (40.00-2.69)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.271 , 0.324 0.283 , 0.328	Depositor DCC
R_{free} test set	1255 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.256 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6097	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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: GOL

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	D	0.81	0/379	1.55	7/582 (1.2%)
1	G	0.84	0/376	1.48	7/578 (1.2%)
2	A	0.99	0/798	1.45	2/1078 (0.2%)
2	E	0.99	0/820	1.46	2/1106 (0.2%)
2	I	0.98	0/809	1.46	3/1092 (0.3%)
2	J	1.00	0/809	1.44	3/1092 (0.3%)
3	C	0.73	0/421	1.26	5/649 (0.8%)
3	F	0.77	0/401	1.38	7/617 (1.1%)
4	B	0.97	0/767	1.39	0/1030
4	H	0.97	0/778	1.41	2/1044 (0.2%)
All	All	0.94	0/6358	1.43	38/8868 (0.4%)

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	E	0	1
4	H	0	1
All	All	0	2

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	DT	C4'-C3'-O3'	11.00	126.50	110.00
1	G	9	DT	P-O3'-C3'	-7.88	108.39	120.20
1	D	9	DT	P-O3'-C3'	-7.76	108.55	120.20
3	F	14	DA	C8-N9-C1'	-7.12	116.37	127.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	DA	P-O3'-C3'	7.08	130.81	120.20
1	G	5	DT	C2'-C3'-O3'	6.91	121.87	111.50
3	F	14	DA	C4-N9-C1'	6.89	137.39	127.05
3	C	3	DC	P-O3'-C3'	-6.69	110.16	120.20
3	F	3	DC	P-O3'-C3'	-6.67	110.20	120.20
3	C	12	DG	P-O3'-C3'	-6.56	110.36	120.20
4	H	250	TRP	CA-C-O	-6.54	113.95	120.82
3	F	12	DG	P-O3'-C3'	-6.29	110.76	120.20
1	D	1	DT	P-O3'-C3'	-6.07	111.09	120.20
1	G	1	DT	P-O3'-C3'	-6.05	111.12	120.20
1	D	3	DA	P-O3'-C3'	-6.01	111.18	120.20
1	D	16	DG	P-O3'-C3'	-5.85	111.42	120.20
1	G	5	DT	C4'-C3'-O3'	-5.84	101.23	110.00
1	D	15	DC	C4'-C3'-O3'	-5.71	101.43	110.00
2	I	333	ALA	O-C-N	5.52	127.75	122.07
1	D	6	DT	P-O3'-C3'	-5.49	111.97	120.20
1	G	2	DT	P-O3'-C3'	-5.39	112.12	120.20
2	J	333	ALA	O-C-N	5.37	127.60	122.07
3	F	7	DA	P-O3'-C3'	-5.34	112.19	120.20
3	C	7	DA	P-O3'-C3'	-5.33	112.21	120.20
2	I	334	HIS	O-C-N	5.30	127.53	122.07
2	E	333	ALA	O-C-N	5.30	127.53	122.07
2	A	333	ALA	O-C-N	5.27	127.50	122.07
3	C	8	DA	P-O3'-C3'	-5.27	112.30	120.20
2	E	334	HIS	O-C-N	5.26	127.49	122.07
1	G	6	DT	P-O3'-C3'	-5.26	112.31	120.20
1	G	14	DA	O3'-P-O5'	-5.24	96.14	104.00
2	J	334	HIS	O-C-N	5.18	127.40	122.07
4	H	250	TRP	O-C-N	5.12	127.34	122.07
2	A	334	HIS	O-C-N	5.11	127.33	122.07
2	J	331	ILE	O-C-N	5.08	126.89	121.91
3	C	10	DA	P-O3'-C3'	-5.05	112.62	120.20
3	F	8	DA	P-O3'-C3'	-5.05	112.63	120.20
2	I	331	ILE	O-C-N	5.03	126.84	121.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	397	ARG	Sidechain
4	H	250	TRP	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	D	342	0	197	9	1
1	G	339	0	198	10	0
2	A	776	0	770	29	0
2	E	798	0	795	19	0
2	I	784	0	780	20	0
2	J	787	0	782	20	0
3	C	372	0	199	6	0
3	F	355	0	190	15	0
4	B	748	0	768	23	0
4	H	756	0	781	22	0
5	F	6	0	8	1	0
6	A	5	0	0	0	0
6	C	3	0	0	1	0
6	D	5	0	0	2	0
6	E	4	0	0	3	0
6	F	7	0	0	8	0
6	H	2	0	0	0	0
6	I	4	0	0	3	0
6	J	4	0	0	5	1
All	All	6097	0	5468	163	1

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 (163) 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)
3:F:14:DA:N7	6:F:201:HOH:O	1.60	1.24
2:I:312:GLN:HG3	6:I:403:HOH:O	1.59	1.03
1:D:4:DC:H2''	1:D:5:DT:H5'	1.41	1.01
1:G:4:DC:H2''	1:G:5:DT:H5'	1.50	0.94
1:D:15:DC:OP2	6:D:101:HOH:O	1.85	0.94
3:F:4:DG:N7	6:F:202:HOH:O	2.01	0.94
2:J:354[A]:ARG:NE	6:J:402:HOH:O	2.03	0.92
3:F:8:DA:H8	6:F:203:HOH:O	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:LYS:HE2	6:E:401:HOH:O	1.79	0.82
3:C:3:DC:H3'	6:C:103:HOH:O	1.81	0.81
2:I:353:ILE:C	2:I:354[B]:ARG:CA	2.54	0.80
2:J:323:ASP:O	6:J:401:HOH:O	1.98	0.79
3:F:3:DC:H3'	6:F:206:HOH:O	1.82	0.77
2:J:325:GLN:OE1	6:J:401:HOH:O	2.03	0.76
1:G:4:DC:H2''	1:G:5:DT:H71	1.68	0.75
1:D:4:DC:H2''	1:D:5:DT:C5'	2.16	0.75
2:I:354[B]:ARG:NH2	6:I:401:HOH:O	2.20	0.74
2:A:377:SER:OG	1:D:10:DG:OP1	2.04	0.74
1:G:4:DC:H2''	1:G:5:DT:C5'	2.18	0.73
1:D:4:DC:H2'	1:D:5:DT:H71	1.69	0.72
4:H:280:VAL:HG21	4:H:286:VAL:HG12	1.72	0.72
2:A:349:TRP:O	2:A:353:ILE:HD12	1.90	0.72
2:E:349:TRP:O	2:E:353:ILE:HD12	1.89	0.72
2:I:354[B]:ARG:CA	2:I:355:HIS:N	2.54	0.71
4:B:280:VAL:HG21	4:B:286:VAL:HG12	1.72	0.70
2:A:366:VAL:HG13	2:A:378:PHE:O	1.91	0.69
4:H:240:LEU:O	4:H:285:LEU:HD23	1.93	0.68
1:D:16:DG:H5''	6:D:102:HOH:O	1.93	0.68
2:E:347:LYS:HG2	6:E:401:HOH:O	1.93	0.68
4:B:240:LEU:O	4:B:285:LEU:HD23	1.93	0.67
2:A:366:VAL:HG13	2:A:378:PHE:C	2.20	0.67
2:E:349:TRP:O	2:E:353:ILE:CD1	2.44	0.66
2:A:349:TRP:O	2:A:353:ILE:CD1	2.44	0.65
3:F:8:DA:C8	6:F:203:HOH:O	2.38	0.65
2:I:323:ASP:OD1	2:I:323:ASP:N	2.30	0.65
3:F:8:DA:O5'	6:F:203:HOH:O	2.15	0.64
2:J:323:ASP:N	2:J:323:ASP:OD1	2.30	0.64
4:H:210:LEU:HD13	4:H:250:TRP:CE2	2.34	0.63
1:G:10:DG:OP1	2:E:377:SER:OG	2.16	0.62
4:B:210:LEU:HD13	4:B:250:TRP:CE2	2.34	0.61
2:J:368:ARG:NH2	2:J:372:GLU:OE2	2.35	0.60
2:I:368:ARG:NH2	2:I:372:GLU:OE2	2.32	0.60
3:F:7:DA:H2''	6:F:203:HOH:O	2.00	0.60
4:B:210:LEU:HB3	4:B:271:TYR:OH	2.02	0.59
4:H:210:LEU:HB3	4:H:271:TYR:OH	2.02	0.59
4:B:247:SER:HA	4:B:264:MET:SD	2.43	0.58
2:I:354[B]:ARG:CZ	6:I:401:HOH:O	2.52	0.57
2:E:349:TRP:N	6:E:402:HOH:O	2.33	0.57
4:H:247:SER:HA	4:H:264:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:DT:C2'	1:G:6:DT:H71	2.36	0.56
3:F:8:DA:P	6:F:203:HOH:O	2.62	0.56
4:H:253:HIS:CE1	4:H:254:LYS:HG2	2.40	0.56
1:G:5:DT:H2'	1:G:6:DT:H71	1.87	0.56
2:A:355:HIS:CE1	3:C:5:DT:O4	2.59	0.55
1:D:5:DT:H2'	1:D:6:DT:H72	1.88	0.55
2:J:326:LEU:HD11	2:J:330:GLY:HA3	1.87	0.55
2:J:347:LYS:HA	2:J:350:GLN:HG3	1.89	0.55
2:A:309:SER:HA	3:C:4:DG:OP1	2.07	0.55
2:E:309:SER:HA	3:F:4:DG:OP1	2.06	0.55
2:J:332:TYR:HB3	6:J:403:HOH:O	2.06	0.55
4:B:218:LEU:HD13	4:B:230:TRP:CZ2	2.42	0.55
4:B:225:PRO:HA	4:B:229:LYS:HG2	1.89	0.54
4:H:218:LEU:HD13	4:H:230:TRP:CZ2	2.42	0.54
2:A:366:VAL:HG22	2:A:378:PHE:HB2	1.90	0.54
2:A:370:GLN:HA	2:A:373:PRO:HG3	1.89	0.54
2:I:395:ARG:O	2:I:396:LYS:C	2.51	0.54
4:B:211:TRP:NE1	4:B:212:GLU:HG3	2.24	0.53
2:I:312:GLN:HE22	2:I:392:GLN:HG3	1.74	0.53
2:I:347:LYS:HA	2:I:350:GLN:HG3	1.89	0.53
4:H:211:TRP:NE1	4:H:212:GLU:HG3	2.24	0.53
2:J:328:LEU:HD22	2:J:332:TYR:CZ	2.44	0.53
2:A:318:ILE:HG21	2:A:381:ILE:HG13	1.91	0.52
2:J:344:THR:HG23	2:J:350:GLN:HE22	1.74	0.52
2:J:354[A]:ARG:CZ	6:J:402:HOH:O	2.50	0.52
2:E:394:PHE:O	2:E:396:LYS:HD3	2.10	0.52
2:J:318:ILE:HG21	2:J:381:ILE:HG13	1.91	0.51
2:I:328:LEU:HD22	2:I:332:TYR:CZ	2.45	0.51
2:J:354[B]:ARG:O	2:J:354[B]:ARG:NE	2.44	0.51
4:H:267:ALA:O	4:H:270:TYR:HB3	2.11	0.51
2:E:328:LEU:HG	2:E:332:TYR:CE2	2.46	0.50
2:A:328:LEU:HG	2:A:332:TYR:CE2	2.46	0.50
4:B:267:ALA:O	4:B:270:TYR:HB3	2.12	0.50
2:I:318:ILE:HG21	2:I:381:ILE:HG13	1.94	0.50
2:I:357:LEU:HD22	2:I:379:TRP:CD2	2.47	0.49
2:J:326:LEU:CD1	2:J:330:GLY:HA3	2.42	0.49
1:G:5:DT:H3	3:F:14:DA:H62	1.60	0.49
2:A:357:LEU:HD22	2:A:379:TRP:CD2	2.48	0.49
2:E:357:LEU:HD22	2:E:379:TRP:CD2	2.48	0.49
2:E:318:ILE:HG21	2:E:381:ILE:HG13	1.94	0.49
4:H:239:LYS:HA	4:H:285:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:269:ARG:HA	4:H:272:TYR:CE2	2.47	0.48
2:A:328:LEU:HD11	2:A:332:TYR:CZ	2.48	0.48
2:J:357:LEU:HD22	2:J:379:TRP:CD2	2.48	0.48
4:B:269:ARG:HA	4:B:272:TYR:CE2	2.47	0.48
2:E:355:HIS:CE1	3:F:5:DT:O4	2.66	0.48
2:A:322:GLN:H	2:A:322:GLN:CD	2.22	0.48
3:F:3:DC:H2''	3:F:4:DG:OP2	2.14	0.47
2:A:369:SER:HB3	2:A:371:GLU:HG3	1.95	0.47
2:A:305:LYS:O	2:A:305:LYS:HG2	2.13	0.47
2:A:322:GLN:H	2:A:322:GLN:NE2	2.12	0.47
2:A:366:VAL:HG13	2:A:378:PHE:CB	2.45	0.47
2:E:328:LEU:HD11	2:E:332:TYR:CZ	2.49	0.47
3:C:3:DC:H2''	3:C:4:DG:OP2	2.15	0.47
4:B:239:LYS:HA	4:B:285:LEU:O	2.14	0.47
1:G:10:DG:H8	2:E:354[B]:ARG:HD3	1.80	0.47
2:A:392:GLN:HA	2:A:395:ARG:HG3	1.98	0.46
1:D:5:DT:C6	1:D:6:DT:H72	2.50	0.46
2:I:334:HIS:O	2:I:337:LYS:HG2	2.15	0.46
4:B:283:GLN:N	4:B:283:GLN:OE1	2.48	0.46
2:A:368:ARG:HG3	2:A:377:SER:HA	1.96	0.46
4:B:208:ILE:HG22	4:B:209:TYR:O	2.16	0.46
1:G:14:DA:H5''	4:H:284[B]:ARG:NH2	2.31	0.46
2:A:347:LYS:HA	2:A:350:GLN:OE1	2.16	0.46
4:H:208:ILE:HG22	4:H:209:TYR:O	2.16	0.46
4:H:283:GLN:N	4:H:283:GLN:OE1	2.49	0.46
2:I:312:GLN:HA	2:I:312:GLN:OE1	2.15	0.46
4:B:211:TRP:CD1	4:B:212:GLU:N	2.84	0.46
2:J:324:ARG:NH1	4:H:222:ALA:HB2	2.31	0.45
2:J:354[B]:ARG:NH2	2:J:357:LEU:HB3	2.32	0.45
4:H:211:TRP:CD1	4:H:212:GLU:N	2.85	0.45
4:H:225:PRO:HA	4:H:229:LYS:HG2	1.99	0.45
3:F:3:DC:C4	5:F:100:GOL:H11	2.52	0.44
1:G:13:DT:H1'	1:G:14:DA:H5'	1.99	0.44
4:B:291:GLU:O	4:B:292:MET:HG2	2.18	0.44
2:A:336:THR:HG21	2:A:344:THR:HG23	1.98	0.44
1:D:13:DT:H1'	1:D:14:DA:H5'	1.98	0.44
4:B:211:TRP:CD1	4:B:212:GLU:H	2.36	0.44
2:E:349:TRP:HE3	2:E:353:ILE:HD13	1.83	0.43
3:F:4:DG:H1'	3:F:5:DT:H5'	2.00	0.43
4:B:265:GLY:O	4:B:269:ARG:HG3	2.19	0.43
2:E:347:LYS:HA	2:E:350:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:211:TRP:CD1	4:H:212:GLU:H	2.37	0.43
2:A:349:TRP:HE3	2:A:353:ILE:HD13	1.84	0.42
4:H:265:GLY:O	4:H:269:ARG:HG3	2.19	0.42
2:A:349:TRP:HE3	2:A:353:ILE:CD1	2.32	0.42
2:E:349:TRP:HE3	2:E:353:ILE:CD1	2.33	0.42
3:C:4:DG:H1'	3:C:5:DT:H5'	2.00	0.42
2:J:334:HIS:CE1	2:J:338:HIS:CE1	3.08	0.42
2:E:355:HIS:NE2	2:E:359:LEU:HD11	2.35	0.42
4:B:255:ASN:O	4:B:256:LYS:C	2.63	0.42
2:A:326:LEU:HD23	2:A:326:LEU:HA	1.89	0.42
3:F:7:DA:C2	3:F:8:DA:C5	3.08	0.42
4:H:255:ASN:O	4:H:256:LYS:C	2.62	0.42
4:H:210:LEU:HD13	4:H:250:TRP:CD2	2.55	0.42
4:B:237:ILE:HD13	4:B:288:GLN:HB2	2.02	0.42
2:A:332:TYR:CE1	2:A:350:GLN:CG	3.03	0.42
2:A:355:HIS:NE2	2:A:359:LEU:HD11	2.34	0.42
2:E:332:TYR:CE1	2:E:350:GLN:CG	3.03	0.41
2:J:355:HIS:NE2	2:J:359:LEU:HD11	2.35	0.41
3:C:7:DA:C2	3:C:8:DA:C5	3.08	0.41
4:B:210:LEU:HD13	4:B:250:TRP:CD2	2.56	0.41
2:I:324:ARG:NH2	2:I:386:GLU:OE1	2.53	0.41
2:I:332:TYR:CE1	2:I:350:GLN:HB3	2.56	0.41
4:B:224:CYS:HB3	4:B:225:PRO:HD3	2.03	0.41
2:I:355:HIS:NE2	2:I:359:LEU:HD11	2.35	0.41
2:J:332:TYR:CE1	2:J:350:GLN:HB3	2.56	0.41
4:B:249:LEU:O	4:B:252:LYS:HB2	2.20	0.41
4:H:237:ILE:HD13	4:H:288:GLN:HB2	2.02	0.41
2:A:349:TRP:O	2:A:353:ILE:HD13	2.19	0.41
2:I:326:LEU:HD23	2:I:326:LEU:HA	1.89	0.41
2:A:322:GLN:HG2	2:A:323:ASP:OD1	2.21	0.40
4:B:279:LYS:H	4:B:279:LYS:HG3	1.74	0.40
2:I:336:THR:HG21	2:I:344:THR:HG23	2.04	0.40

All (1) 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:16:DG:O6	6:J:402:HOH:O[2_555]	2.17	0.03

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	
2	A	92/95 (97%)	87 (95%)	5 (5%)	0	100	100
2	E	94/95 (99%)	89 (95%)	5 (5%)	0	100	100
2	I	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
2	J	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
4	B	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	3	6
4	H	87/89 (98%)	77 (88%)	7 (8%)	3 (3%)	3	7
All	All	545/558 (98%)	507 (93%)	32 (6%)	6 (1%)	11	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	225	PRO
4	H	225	PRO
4	B	241	VAL
4	B	256	LYS
4	H	256	LYS
4	H	241	VAL

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	
2	A	82/83 (99%)	67 (82%)	15 (18%)	2	5
2	E	84/83 (101%)	68 (81%)	16 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	83/83 (100%)	68 (82%)	15 (18%)	2	5
2	J	83/83 (100%)	65 (78%)	18 (22%)	1	3
4	B	78/79 (99%)	65 (83%)	13 (17%)	2	6
4	H	79/79 (100%)	66 (84%)	13 (16%)	2	6
All	All	489/490 (100%)	399 (82%)	90 (18%)	1	4

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	305	LYS
2	A	318	ILE
2	A	320	SER
2	A	322	GLN
2	A	324	ARG
2	A	329	SER
2	A	335	ILE
2	A	346	ASP
2	A	361	ARG
2	A	366	VAL
2	A	370	GLN
2	A	375	LYS
2	A	377	SER
2	A	380	ARG
2	A	397	ARG
2	E	305	LYS
2	E	318	ILE
2	E	320	SER
2	E	324	ARG
2	E	325	GLN
2	E	329	SER
2	E	335	ILE
2	E	346	ASP
2	E	361	ARG
2	E	375	LYS
2	E	377	SER
2	E	380	ARG
2	E	388	LYS
2	E	396	LYS
2	E	397	ARG
2	E	398	ARG
2	I	318	ILE

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Mol	Chain	Res	Type
2	I	320	SER
2	I	323	ASP
2	I	324	ARG
2	I	328	LEU
2	I	329	SER
2	I	335	ILE
2	I	337	LYS
2	I	347	LYS
2	I	361	ARG
2	I	375	LYS
2	I	377	SER
2	I	380	ARG
2	I	381	ILE
2	I	388	LYS
2	J	305	LYS
2	J	318	ILE
2	J	320	SER
2	J	323	ASP
2	J	324	ARG
2	J	325	GLN
2	J	328	LEU
2	J	329	SER
2	J	335	ILE
2	J	346	ASP
2	J	347	LYS
2	J	361	ARG
2	J	371	GLU
2	J	372	GLU
2	J	375	LYS
2	J	377	SER
2	J	380	ARG
2	J	388	LYS
4	B	214	LEU
4	B	215	LEU
4	B	221	LYS
4	B	229	LYS
4	B	235	LYS
4	B	237	ILE
4	B	244	LYS
4	B	248	ARG
4	B	258	ASP
4	B	259	MET

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Mol	Chain	Res	Type
4	B	273	GLN
4	B	279	LYS
4	B	284	ARG
4	H	214	LEU
4	H	215	LEU
4	H	221	LYS
4	H	229	LYS
4	H	235	LYS
4	H	237	ILE
4	H	248	ARG
4	H	254	LYS
4	H	258	ASP
4	H	259	MET
4	H	273	GLN
4	H	279	LYS
4	H	292	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	338	HIS
2	A	351	ASN
2	A	370	GLN
2	E	338	HIS
2	E	351	ASN
2	I	334	HIS
2	I	351	ASN
2	J	325	GLN
2	J	334	HIS
2	J	338	HIS
2	J	350	GLN
2	J	351	ASN
4	B	255	ASN
4	B	273	GLN
4	H	255	ASN
4	H	273	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	F	100	-	5,5,5	0.09	0	5,5,5	0.49	0

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
5	GOL	F	100	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	100	GOL	O1-C1-C2-C3
5	F	100	GOL	O1-C1-C2-O2
5	F	100	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	100	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	D	17/17 (100%)	-0.71	0 100 100	74, 85, 99, 102	0
1	G	17/17 (100%)	-0.83	0 100 100	70, 85, 97, 98	0
2	A	94/95 (98%)	-0.03	1 (1%) 78 76	87, 130, 199, 264	0
2	E	95/95 (100%)	0.09	1 (1%) 78 76	44, 128, 217, 247	1 (1%)
2	I	93/95 (97%)	0.06	0 100 100	30, 123, 177, 217	1 (1%)
2	J	94/95 (98%)	0.15	2 (2%) 63 61	40, 134, 194, 243	1 (1%)
3	C	18/18 (100%)	-0.87	0 100 100	76, 87, 96, 117	0
3	F	17/18 (94%)	-0.92	0 100 100	80, 91, 97, 115	0
4	B	88/89 (98%)	-0.07	1 (1%) 78 76	70, 110, 148, 170	0
4	H	88/89 (98%)	-0.04	1 (1%) 78 76	58, 112, 150, 168	1 (1%)
All	All	621/628 (98%)	-0.07	6 (0%) 79 78	30, 118, 182, 264	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	362	TYR	3.4
2	J	367	PRO	2.3
2	E	379	TRP	2.2
4	H	259	MET	2.2
2	A	366	VAL	2.1
4	B	240	LEU	2.0

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($\text{\AA}^2$)	Q<0.9
5	GOL	F	100	6/6	0.77	0.09	51,54,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.