



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:23 PM UTC

PDB ID : 8PP2 / pdb_00008pp2
Title : Binary crystal structure of positively supercharged ferritin variant Ftn(pos) and native(K86Q) human heavy chain ferritin (Mg formate condition)
Authors : Lang, L.; Beck, T.
Deposited on : 2023-07-06
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

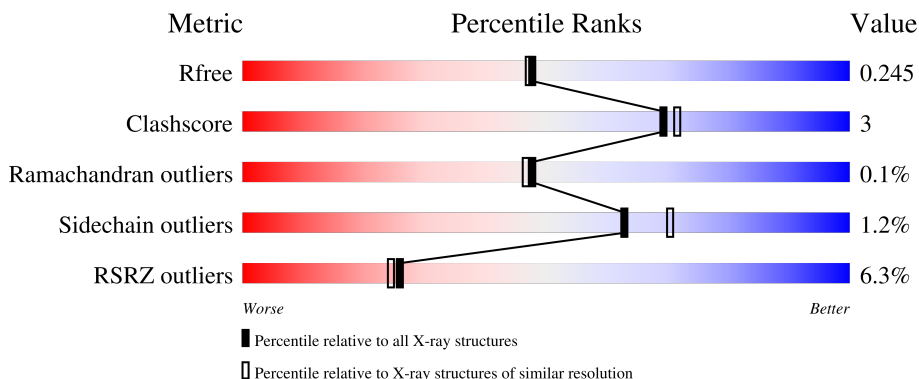
1 Overall quality at a glance

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.



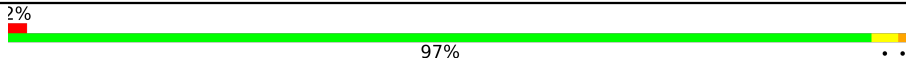
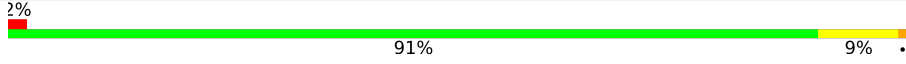
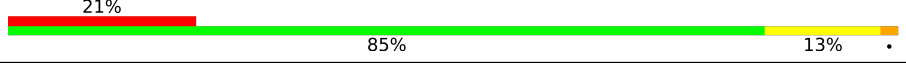
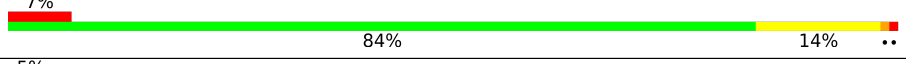

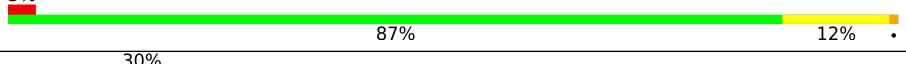
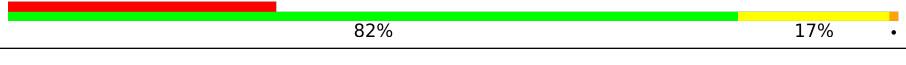
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	172	 93% 6%
1	B	172	 95% 5%
1	C	172	 97%
1	D	172	 94% 6%
1	E	172	 94% 6%

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Mol	Chain	Length	Quality of chain
1	F	172	 <p>2% 97%</p>
2	G	172	 <p>2% 91% 9%</p>
2	H	172	 <p>21% 85% 13%</p>
2	I	172	 <p>7% 84% 14%</p>
2	J	172	 <p>5% 88% 11%</p>
2	K	172	 <p>3% 87% 12%</p>
2	L	172	 <p>30% 82% 17%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34658 atoms, of which 16829 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 Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	172	2863	903	1431	258	266	5	42	0	0
1	B	172	2863	903	1431	258	266	5	42	0	0
1	C	172	2887	909	1444	262	267	5	42	1	0
1	D	172	2863	903	1431	258	266	5	42	0	0
1	E	172	2863	903	1431	258	266	5	42	0	0
1	F	172	2863	903	1431	258	266	5	42	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	LYS	ALA	engineered mutation	UNP P02794
A	26	ARG	ASN	engineered mutation	UNP P02794
A	87	GLN	LYS	engineered mutation	UNP P02794
A	91	LYS	CYS	engineered mutation	UNP P02794
A	99	ARG	ASN	engineered mutation	UNP P02794
A	103	LYS	CYS	engineered mutation	UNP P02794
A	106	LYS	HIS	engineered mutation	UNP P02794
A	110	LYS	ASN	engineered mutation	UNP P02794
A	124	LYS	ASP	engineered mutation	UNP P02794
A	163	ARG	GLU	engineered mutation	UNP P02794
B	19	LYS	ALA	engineered mutation	UNP P02794
B	26	ARG	ASN	engineered mutation	UNP P02794
B	87	GLN	LYS	engineered mutation	UNP P02794
B	91	LYS	CYS	engineered mutation	UNP P02794
B	99	ARG	ASN	engineered mutation	UNP P02794
B	103	LYS	CYS	engineered mutation	UNP P02794
B	106	LYS	HIS	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	110	LYS	ASN	engineered mutation	UNP P02794
B	124	LYS	ASP	engineered mutation	UNP P02794
B	163	ARG	GLU	engineered mutation	UNP P02794
C	19	LYS	ALA	engineered mutation	UNP P02794
C	26	ARG	ASN	engineered mutation	UNP P02794
C	87	GLN	LYS	engineered mutation	UNP P02794
C	91	LYS	CYS	engineered mutation	UNP P02794
C	99	ARG	ASN	engineered mutation	UNP P02794
C	103	LYS	CYS	engineered mutation	UNP P02794
C	106	LYS	HIS	engineered mutation	UNP P02794
C	110	LYS	ASN	engineered mutation	UNP P02794
C	124	LYS	ASP	engineered mutation	UNP P02794
C	163	ARG	GLU	engineered mutation	UNP P02794
D	19	LYS	ALA	engineered mutation	UNP P02794
D	26	ARG	ASN	engineered mutation	UNP P02794
D	87	GLN	LYS	engineered mutation	UNP P02794
D	91	LYS	CYS	engineered mutation	UNP P02794
D	99	ARG	ASN	engineered mutation	UNP P02794
D	103	LYS	CYS	engineered mutation	UNP P02794
D	106	LYS	HIS	engineered mutation	UNP P02794
D	110	LYS	ASN	engineered mutation	UNP P02794
D	124	LYS	ASP	engineered mutation	UNP P02794
D	163	ARG	GLU	engineered mutation	UNP P02794
E	19	LYS	ALA	engineered mutation	UNP P02794
E	26	ARG	ASN	engineered mutation	UNP P02794
E	87	GLN	LYS	engineered mutation	UNP P02794
E	91	LYS	CYS	engineered mutation	UNP P02794
E	99	ARG	ASN	engineered mutation	UNP P02794
E	103	LYS	CYS	engineered mutation	UNP P02794
E	106	LYS	HIS	engineered mutation	UNP P02794
E	110	LYS	ASN	engineered mutation	UNP P02794
E	124	LYS	ASP	engineered mutation	UNP P02794
E	163	ARG	GLU	engineered mutation	UNP P02794
F	19	LYS	ALA	engineered mutation	UNP P02794
F	26	ARG	ASN	engineered mutation	UNP P02794
F	87	GLN	LYS	engineered mutation	UNP P02794
F	91	LYS	CYS	engineered mutation	UNP P02794
F	99	ARG	ASN	engineered mutation	UNP P02794
F	103	LYS	CYS	engineered mutation	UNP P02794
F	106	LYS	HIS	engineered mutation	UNP P02794
F	110	LYS	ASN	engineered mutation	UNP P02794
F	124	LYS	ASP	engineered mutation	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	163	ARG	GLU	engineered mutation	UNP P02794

- Molecule 2 is a protein called Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	G	172	Total	C	H	N	O	S	46	0	0
			2778	885	1365	248	273	7			
2	H	172	Total	C	H	N	O	S	46	0	0
			2778	885	1365	248	273	7			
2	I	172	Total	C	H	N	O	S	46	0	0
			2778	885	1365	248	273	7			
2	J	172	Total	C	H	N	O	S	46	0	0
			2778	885	1365	248	273	7			
2	K	172	Total	C	H	N	O	S	46	0	0
			2778	885	1365	248	273	7			
2	L	172	Total	C	H	N	O	S	46	0	0
			2778	885	1365	248	273	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	87	GLN	LYS	engineered mutation	UNP P02794
H	87	GLN	LYS	engineered mutation	UNP P02794
I	87	GLN	LYS	engineered mutation	UNP P02794
J	87	GLN	LYS	engineered mutation	UNP P02794
K	87	GLN	LYS	engineered mutation	UNP P02794
L	87	GLN	LYS	engineered mutation	UNP P02794

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	A	1	Total	C	H	O	2	0
			14	3	8	3		
3	B	1	Total	C	H	O	2	0
			14	3	8	3		
3	C	1	Total	C	H	O	2	0
			14	3	8	3		
3	E	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		
4	B	1	Total	Fe	0	0
			1	1		
4	C	1	Total	Fe	0	0
			1	1		
4	D	1	Total	Fe	0	0
			1	1		
4	E	1	Total	Fe	0	0
			1	1		
4	F	1	Total	Fe	0	0
			1	1		
4	G	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Fe 1 1	0	0
4	I	1	Total Fe 1 1	0	0
4	J	1	Total Fe 1 1	0	0
4	K	1	Total Fe 1 1	0	0
4	L	1	Total Fe 1 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	84	Total O 84 84	0	0
6	B	71	Total O 71 71	0	0
6	C	97	Total O 97 97	0	0
6	D	106	Total O 106 106	0	0
6	E	105	Total O 105 105	0	0
6	F	102	Total O 102 102	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	29	Total 29	O 29	0	0
6	H	9	Total 9	O 9	0	0
6	I	30	Total 30	O 30	0	0
6	J	29	Total 29	O 29	0	0
6	K	27	Total 27	O 27	0	0
6	L	11	Total 11	O 11	0	0

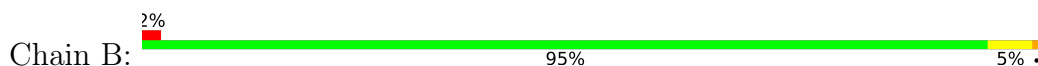
3 Residue-property plots [i](#)

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.

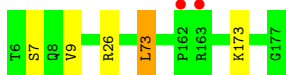
- Molecule 1: Ferritin heavy chain, N-terminally processed



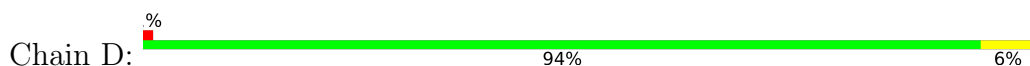
- Molecule 1: Ferritin heavy chain, N-terminally processed



- Molecule 1: Ferritin heavy chain, N-terminally processed



- Molecule 1: Ferritin heavy chain, N-terminally processed



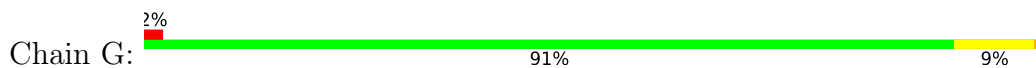
- Molecule 1: Ferritin heavy chain, N-terminally processed



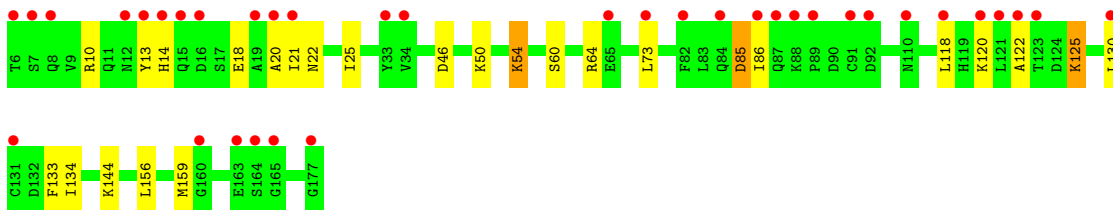
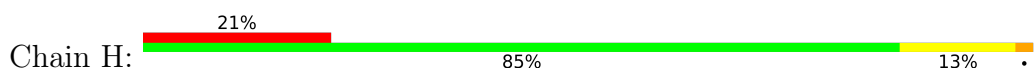
- Molecule 1: Ferritin heavy chain, N-terminally processed



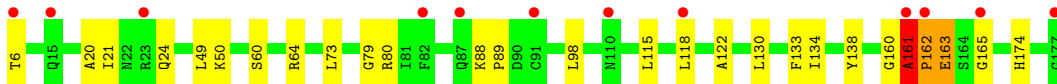
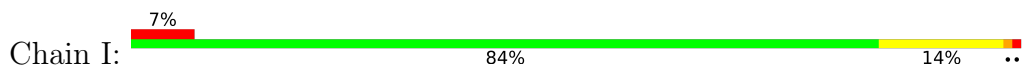
- Molecule 2: Ferritin heavy chain, N-terminally processed



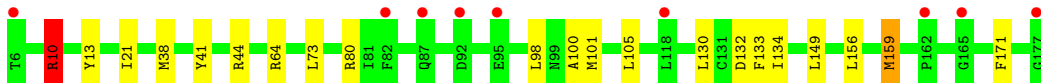
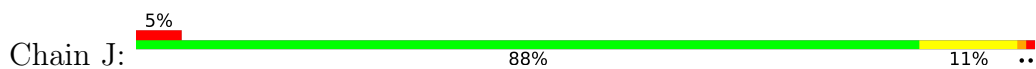
- Molecule 2: Ferritin heavy chain, N-terminally processed



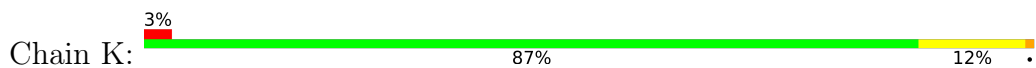
- Molecule 2: Ferritin heavy chain, N-terminally processed



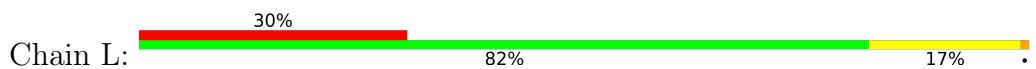
- Molecule 2: Ferritin heavy chain, N-terminally processed

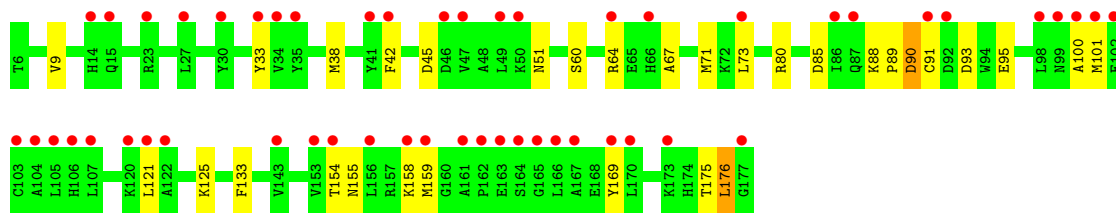


- Molecule 2: Ferritin heavy chain, N-terminally processed



- Molecule 2: Ferritin heavy chain, N-terminally processed





4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	126.80Å 126.80Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.00 49.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.06-2.00) 99.9 (49.06-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.247 0.202 , 0.245	Depositor DCC
R_{free} test set	9313 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtrriage
Anisotropy	0.369	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34658	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FE

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	1.03	0/1460	1.40	4/1957 (0.2%)
1	B	1.06	1/1460 (0.1%)	1.36	0/1957
1	C	1.10	0/1471	1.34	0/1971
1	D	1.06	1/1460 (0.1%)	1.39	0/1957
1	E	1.09	1/1460 (0.1%)	1.37	1/1957 (0.1%)
1	F	1.09	0/1460	1.38	1/1957 (0.1%)
2	G	1.10	1/1442 (0.1%)	1.45	0/1943
2	H	1.02	0/1442	1.56	2/1943 (0.1%)
2	I	1.08	0/1442	1.49	3/1943 (0.2%)
2	J	1.07	0/1442	1.45	1/1943 (0.1%)
2	K	1.09	0/1442	1.48	2/1943 (0.1%)
2	L	1.02	0/1442	1.50	1/1943 (0.1%)
All	All	1.07	4/17423 (0.0%)	1.43	15/23414 (0.1%)

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	I	0	1
2	L	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	165	GLY	C-O	5.81	1.31	1.23
1	B	71	MET	C-O	5.38	1.30	1.24
2	G	66	HIS	C-O	5.04	1.29	1.24
1	E	165	GLY	C-O	5.01	1.29	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	177	GLY	CA-C-O	-7.30	105.47	120.80
2	J	10	ARG	CG-CD-NE	6.29	125.85	112.00
2	K	171	PHE	CA-C-N	6.05	128.38	120.28
2	K	171	PHE	C-N-CA	6.05	128.38	120.28
1	A	177	GLY	CA-C-O	-5.75	108.71	120.80
2	I	50	LYS	N-CA-CB	-5.53	101.99	110.12
1	F	64	ARG	CG-CD-NE	-5.46	99.98	112.00
2	I	49	LEU	CA-C-N	5.32	127.40	120.28
2	I	49	LEU	C-N-CA	5.32	127.40	120.28
1	A	89	PRO	CA-C-N	5.27	128.07	120.38
1	A	89	PRO	C-N-CA	5.27	128.07	120.38
2	L	85	ASP	CA-CB-CG	5.19	117.79	112.60
2	H	85	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	87	GLN	CB-CA-C	5.07	118.31	109.65
2	H	144	LYS	CB-CA-C	5.03	120.33	110.67

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	161	ALA	Peptide
2	L	90	ASP	Peptide

5.2 Too-close contacts [i](#)

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	1432	1431	1419	7	0
1	B	1432	1431	1419	8	0
1	C	1443	1444	1431	4	0
1	D	1432	1431	1419	5	0
1	E	1432	1431	1419	6	0
1	F	1432	1431	1419	5	0
2	G	1413	1365	1352	9	0
2	H	1413	1365	1352	19	0
2	I	1413	1365	1352	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1413	1365	1352	17	0
2	K	1413	1365	1352	16	0
2	L	1413	1365	1352	17	2
3	A	12	16	16	0	0
3	B	6	8	8	0	0
3	C	6	8	8	0	0
3	E	6	8	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	A	84	0	0	2	0
6	B	71	0	0	1	0
6	C	97	0	0	2	0
6	D	106	0	0	1	0
6	E	105	0	0	0	0
6	F	102	0	0	0	0
6	G	29	0	0	1	1
6	H	9	0	0	0	0
6	I	30	0	0	0	1
6	J	29	0	0	4	0
6	K	27	0	0	0	0
6	L	11	0	0	0	0
All	All	17829	16829	16678	117	3

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 3.

All (117) 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)
2:J:101:MET:O	6:J:301:HOH:O	1.80	0.97
2:I:160:GLY:O	2:I:161:ALA:O	1.96	0.83
2:H:10:ARG:NH2	2:H:18:GLU:OE1	2.17	0.77
2:J:41:TYR:O	2:J:44:ARG:HG2	1.91	0.71
1:D:173:LYS:HE2	6:D:302:HOH:O	1.91	0.70
2:G:158:LYS:HG3	2:I:165:GLY:HA3	1.74	0.69
2:H:60:SER:OG	2:L:64:ARG:NH2	2.28	0.67
2:I:73:LEU:HD22	2:I:133:PHE:CE1	2.30	0.66
1:B:15:GLN:HG3	1:B:19:LYS:HE2	1.77	0.66
2:I:98:LEU:HD23	2:I:162:PRO:HD3	1.79	0.65
2:H:10:ARG:NH1	2:H:13:TYR:O	2.31	0.64
2:I:98:LEU:CD2	2:I:162:PRO:HD3	2.28	0.64
2:G:160:GLY:O	2:G:163:GLU:HG2	1.98	0.64
2:J:132:ASP:OD1	6:J:302:HOH:O	2.15	0.63
2:K:130:LEU:O	2:K:134:ILE:HG12	1.98	0.63
2:I:21:ILE:HD13	2:I:118:LEU:HD21	1.81	0.62
2:I:73:LEU:HD22	2:I:133:PHE:CD1	2.35	0.61
2:H:21:ILE:HD13	2:H:118:LEU:HD21	1.83	0.61
2:I:161:ALA:O	2:I:163:GLU:N	2.34	0.60
2:G:73:LEU:HG	2:G:73:LEU:O	2.00	0.59
1:F:73:LEU:HD22	1:F:133:PHE:CE2	2.38	0.59
2:G:20:ALA:HB1	2:G:118:LEU:CD1	2.33	0.58
1:A:163:ARG:HG2	6:A:341:HOH:O	2.03	0.58
2:J:149:LEU:HB3	6:J:301:HOH:O	2.04	0.57
2:H:50:LYS:HE2	2:H:54:LYS:HE3	1.87	0.57
2:H:156:LEU:O	2:H:159:MET:O	2.23	0.56
2:H:122:ALA:HB2	2:H:130:LEU:CD2	2.35	0.56
1:C:26:ARG:HD2	6:C:378:HOH:O	2.03	0.56
1:B:73:LEU:HD22	1:B:133:PHE:CE2	2.40	0.56
1:A:60:SER:OG	1:B:64:ARG:NH2	2.35	0.55
2:J:38:MET:HE3	2:J:100:ALA:HB1	1.86	0.55
1:D:132:ASP:O	1:D:136:THR:HG23	2.06	0.54
2:H:64:ARG:NH2	2:L:60:SER:OG	2.35	0.54
1:E:154:THR:O	1:E:158:LYS:HG2	2.06	0.54
2:H:130:LEU:O	2:H:134:ILE:HG12	2.08	0.54
2:G:98:LEU:O	2:G:102:GLU:HG3	2.08	0.53
1:B:152:HIS:HD2	6:B:363:HOH:O	1.90	0.53
2:K:146:ILE:HG22	2:L:9:VAL:HB	1.90	0.53
1:B:73:LEU:HD22	1:B:133:PHE:CD2	2.44	0.53
2:J:105:LEU:N	6:J:301:HOH:O	2.43	0.52
1:E:64:ARG:NH1	1:F:64:ARG:HG2	2.25	0.51
2:J:73:LEU:HD22	2:J:133:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:60:SER:OG	2:J:64:ARG:NH2	2.36	0.51
1:F:95:GLU:OE1	1:F:99:ARG:NH1	2.43	0.51
2:H:73:LEU:HD22	2:H:133:PHE:CD1	2.46	0.51
2:H:86:ILE:HG13	2:L:33:TYR:CE2	2.45	0.50
1:F:73:LEU:HD22	1:F:133:PHE:CD2	2.46	0.50
2:H:50:LYS:CE	2:H:54:LYS:HE3	2.41	0.50
2:H:14:HIS:CE1	2:H:125:LYS:HE3	2.46	0.50
2:J:130:LEU:O	2:J:134:ILE:HG12	2.12	0.50
2:K:14:HIS:CG	2:K:125:LYS:HD3	2.47	0.50
2:K:121:LEU:O	2:K:125:LYS:HG3	2.12	0.50
2:I:79:GLY:O	2:I:80:ARG:NH1	2.45	0.49
2:I:130:LEU:O	2:I:134:ILE:HG12	2.11	0.49
2:I:20:ALA:HB1	2:I:118:LEU:HD13	1.94	0.49
2:L:73:LEU:HD22	2:L:133:PHE:CD1	2.47	0.49
2:L:121:LEU:O	2:L:125:LYS:HG2	2.12	0.49
1:C:26:ARG:CD	6:C:378:HOH:O	2.60	0.48
2:J:73:LEU:HD22	2:J:133:PHE:CD1	2.47	0.48
2:L:73:LEU:HD22	2:L:133:PHE:CE1	2.48	0.48
1:D:73:LEU:C	1:D:73:LEU:HD13	2.38	0.48
1:E:142:GLN:O	1:E:146:ILE:HG12	2.14	0.48
1:A:20:ALA:HB1	1:A:118:LEU:HD13	1.95	0.48
2:I:64:ARG:NH1	2:J:64:ARG:HG2	2.30	0.47
1:B:19:LYS:HE3	2:L:90:ASP:OD1	2.15	0.47
2:L:51:ASN:HB3	2:L:176:LEU:HB3	1.96	0.47
2:H:20:ALA:HB1	2:H:118:LEU:HD13	1.96	0.47
2:H:73:LEU:HD22	2:H:133:PHE:CE1	2.50	0.47
2:I:122:ALA:HB2	2:I:130:LEU:HD23	1.97	0.47
1:E:130:LEU:O	1:E:134:ILE:HG12	2.16	0.46
1:A:73:LEU:O	1:A:73:LEU:HG	2.15	0.45
1:C:73:LEU:O	1:C:73:LEU:HG	2.11	0.45
2:H:14:HIS:CE1	2:H:125:LYS:CE	3.00	0.45
2:J:80:ARG:HD3	2:J:80:ARG:HA	1.77	0.45
2:J:159:MET:HE1	2:J:171:PHE:HD1	1.82	0.45
2:I:115:LEU:HD13	2:I:138:TYR:HB3	1.99	0.45
2:K:102:GLU:OE2	2:K:157:ARG:NH2	2.45	0.45
2:L:80:ARG:HD3	2:L:80:ARG:HA	1.79	0.45
1:D:26:ARG:HD2	1:D:87:GLN:HE22	1.80	0.45
1:A:36:LEU:HG	1:B:71:MET:HE1	1.99	0.44
1:B:155:ASN:O	1:B:159:MET:HG3	2.18	0.44
2:H:122:ALA:HB2	2:H:130:LEU:HD22	1.99	0.44
2:K:73:LEU:HD13	2:K:133:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:LYS:NZ	2:J:10:ARG:O	2.42	0.44
2:K:35:TYR:OH	2:K:108:GLU:OE2	2.25	0.44
2:L:93:ASP:OD1	2:L:93:ASP:C	2.60	0.44
2:H:46:ASP:C	2:K:154:THR:HG21	2.43	0.43
2:L:38:MET:CE	2:L:100:ALA:HB1	2.49	0.43
2:L:88:LYS:HG2	2:L:89:PRO:O	2.19	0.43
2:L:67:ALA:O	2:L:71:MET:HG3	2.18	0.43
2:K:69:LYS:HE2	2:K:137:HIS:CG	2.54	0.42
2:K:155:ASN:O	2:K:159:MET:HG3	2.19	0.42
1:E:73:LEU:C	1:E:73:LEU:HD13	2.44	0.42
2:K:14:HIS:CB	2:K:125:LYS:HD3	2.49	0.42
2:G:173:LYS:HE2	6:G:307:HOH:O	2.18	0.42
2:J:13:TYR:OH	2:J:21:ILE:HD12	2.20	0.42
1:A:45:ASP:HA	1:F:151:ASP:OD1	2.19	0.42
1:D:26:ARG:HD3	1:D:84:GLN:HB2	2.01	0.42
2:I:98:LEU:HD22	2:I:162:PRO:HD3	2.01	0.42
2:L:91:CYS:HB3	2:L:93:ASP:O	2.19	0.42
2:L:155:ASN:O	2:L:159:MET:HG3	2.20	0.42
1:A:90:ASP:HB2	6:A:328:HOH:O	2.19	0.41
2:J:98:LEU:HA	2:J:156:LEU:HD13	2.02	0.41
2:K:73:LEU:HD22	2:K:133:PHE:CD1	2.55	0.41
2:H:22:ASN:HA	2:H:25:ILE:HD12	2.02	0.41
2:I:88:LYS:HG2	2:I:89:PRO:O	2.21	0.41
2:K:42:PHE:CZ	2:K:97:GLY:HA2	2.56	0.41
1:E:108:GLU:C	1:E:146:ILE:HD11	2.45	0.41
2:I:80:ARG:HD3	2:I:80:ARG:HA	1.89	0.41
2:L:38:MET:O	2:L:42:PHE:CD2	2.74	0.41
2:G:149:LEU:O	2:G:153:VAL:HG23	2.21	0.41
2:G:73:LEU:HD13	2:G:133:PHE:CD1	2.56	0.41
2:I:174:HIS:HB3	2:K:173:LYS:HG3	2.02	0.40
2:J:159:MET:HB2	2:J:159:MET:HE3	1.89	0.40
2:K:14:HIS:CD2	2:K:125:LYS:HD3	2.56	0.40
2:K:69:LYS:HE2	2:K:137:HIS:ND1	2.36	0.40
1:C:7:SER:OG	1:C:9:VAL:HG22	2.21	0.40

All (3) 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)
2:L:45:ASP:O	2:L:154:THR:HG1[3_655]	1.42	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:169:TYR:HH	2:L:175:THR:OG1[3_655]	1.42	0.18
6:G:312:HOH:O	6:I:319:HOH:O[3_655]	2.11	0.09

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	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
1	B	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
1	C	171/172 (99%)	167 (98%)	4 (2%)	0	100	100
1	D	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
1	E	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
1	F	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	G	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	H	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	21	17
2	I	170/172 (99%)	164 (96%)	4 (2%)	2 (1%)	10	6
2	J	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	K	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
2	L	170/172 (99%)	154 (91%)	16 (9%)	0	100	100
All	All	2041/2064 (99%)	1978 (97%)	60 (3%)	3 (0%)	48	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	161	ALA
2	H	85	ASP
2	I	162	PRO

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	154/154 (100%)	152 (99%)	2 (1%)	61	68
1	B	154/154 (100%)	154 (100%)	0	100	100
1	C	155/154 (101%)	153 (99%)	2 (1%)	61	68
1	D	154/154 (100%)	152 (99%)	2 (1%)	61	68
1	E	154/154 (100%)	154 (100%)	0	100	100
1	F	154/154 (100%)	154 (100%)	0	100	100
2	G	153/153 (100%)	150 (98%)	3 (2%)	48	54
2	H	153/153 (100%)	150 (98%)	3 (2%)	48	54
2	I	153/153 (100%)	150 (98%)	3 (2%)	48	54
2	J	153/153 (100%)	151 (99%)	2 (1%)	61	68
2	K	153/153 (100%)	151 (99%)	2 (1%)	61	68
2	L	153/153 (100%)	149 (97%)	4 (3%)	40	44
All	All	1843/1842 (100%)	1820 (99%)	23 (1%)	63	70

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	73	LEU
1	C	73	LEU
1	C	173	LYS
1	D	118	LEU
1	D	163	ARG
2	G	15	GLN
2	G	73	LEU
2	G	113	GLN
2	H	54	LYS
2	H	120	LYS
2	H	125	LYS
2	I	6	THR
2	I	24	GLN

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Mol	Chain	Res	Type
2	I	163	GLU
2	J	10	ARG
2	J	159	MET
2	K	80	ARG
2	K	173	LYS
2	L	95	GLU
2	L	101	MET
2	L	158	LYS
2	L	176	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	155	ASN
1	B	152	HIS
1	C	51	ASN
1	D	112	ASN
1	E	87	GLN
1	E	126	ASN
1	F	58	HIS
2	G	51	ASN
2	G	112	ASN
2	G	174	HIS
2	H	51	ASN
2	I	174	HIS
2	J	58	HIS
2	J	84	GLN
2	J	99	ASN
2	L	15	GLN
2	L	26	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 23 ligands modelled in this entry, 18 are monoatomic - leaving 5 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
3	GOL	A	202	-	5,5,5	0.12	0	5,5,5	0.33	0
3	GOL	A	201	-	5,5,5	0.14	0	5,5,5	0.27	0
3	GOL	C	201	-	5,5,5	0.16	0	5,5,5	0.28	0
3	GOL	B	201	-	5,5,5	0.17	0	5,5,5	0.45	0
3	GOL	E	201	-	5,5,5	0.16	0	5,5,5	0.76	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
3	GOL	A	202	-	-	1/4/4/4	-
3	GOL	A	201	-	-	2/4/4/4	-
3	GOL	C	201	-	-	0/4/4/4	-
3	GOL	B	201	-	-	1/4/4/4	-
3	GOL	E	201	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	E	201	GOL	C1-C2-C3-O3
3	A	201	GOL	O1-C1-C2-O2
3	B	201	GOL	O2-C2-C3-O3
3	A	202	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	A	172/172 (100%)	-0.49	1 (0%) 85 85	19, 24, 40, 67	0
1	B	172/172 (100%)	-0.48	3 (1%) 69 68	19, 24, 41, 72	0
1	C	172/172 (100%)	-0.60	2 (1%) 76 76	10, 22, 39, 69	1 (0%)
1	D	172/172 (100%)	-0.57	2 (1%) 76 76	18, 22, 39, 69	0
1	E	172/172 (100%)	-0.54	4 (2%) 61 60	18, 22, 38, 78	0
1	F	172/172 (100%)	-0.57	3 (1%) 69 68	17, 22, 38, 72	0
2	G	172/172 (100%)	0.36	3 (1%) 69 68	25, 33, 48, 62	0
2	H	172/172 (100%)	1.24	36 (20%) 2 2	28, 43, 62, 75	0
2	I	172/172 (100%)	0.51	12 (6%) 22 21	24, 35, 51, 65	0
2	J	172/172 (100%)	0.62	9 (5%) 33 31	27, 37, 55, 70	0
2	K	172/172 (100%)	0.51	5 (2%) 53 52	24, 36, 48, 57	0
2	L	172/172 (100%)	1.62	51 (29%) 1 1	34, 48, 71, 95	0
All	All	2064/2064 (100%)	0.13	131 (6%) 26 24	10, 31, 55, 95	1 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	161	ALA	6.2
2	L	162	PRO	4.9
2	L	164	SER	4.7
1	E	162	PRO	4.6
2	H	87	GLN	4.6
2	L	177	GLY	4.5
2	L	158	LYS	4.4
2	L	91	CYS	4.2
2	H	82	PHE	4.2
2	L	153	VAL	4.1
2	H	177	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	L	86	ILE	3.8
1	F	162	PRO	3.7
2	H	121	LEU	3.6
2	H	160	GLY	3.6
2	L	92	ASP	3.6
2	I	162	PRO	3.5
2	H	92	ASP	3.4
2	L	120	LYS	3.4
2	I	87	GLN	3.4
2	H	86	ILE	3.3
2	J	177	GLY	3.3
2	L	104	ALA	3.3
2	G	177	GLY	3.3
2	L	15	GLN	3.3
2	L	103	CYS	3.2
2	H	89	PRO	3.2
2	L	161	ALA	3.2
2	I	177	GLY	3.2
2	K	6	THR	3.1
1	E	165	GLY	3.0
1	D	87	GLN	3.0
2	H	84	GLN	3.0
2	I	6	THR	2.9
2	L	73	LEU	2.9
2	L	166	LEU	2.9
2	H	21	ILE	2.9
2	J	95	GLU	2.9
2	L	106	HIS	2.8
2	H	14	HIS	2.8
2	J	82	PHE	2.8
2	K	177	GLY	2.8
2	L	33	TYR	2.8
2	H	19	ALA	2.8
2	L	154	THR	2.8
2	H	34	VAL	2.8
2	K	91	CYS	2.8
1	B	163	ARG	2.8
2	L	165	GLY	2.8
2	L	156	LEU	2.7
2	L	41	TYR	2.7
1	E	163	ARG	2.7
2	L	121	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	163	GLU	2.7
2	L	47	VAL	2.7
2	H	15	GLN	2.6
2	H	6	THR	2.6
2	L	100	ALA	2.6
2	I	118	LEU	2.6
2	H	33	TYR	2.6
2	L	167	ALA	2.6
2	L	35	TYR	2.6
2	J	165	GLY	2.6
2	H	122	ALA	2.6
2	H	164	SER	2.6
2	L	101	MET	2.5
2	H	118	LEU	2.5
2	L	98	LEU	2.5
1	B	165	GLY	2.5
2	L	143	VAL	2.5
2	H	13	TYR	2.5
2	H	16	ASP	2.5
2	L	122	ALA	2.5
2	L	105	LEU	2.5
2	J	87	GLN	2.5
2	L	87	GLN	2.5
2	L	107	LEU	2.5
2	L	169	TYR	2.4
2	L	102	GLU	2.4
2	H	91	CYS	2.4
1	F	165	GLY	2.4
2	I	15	GLN	2.4
1	E	164	SER	2.4
2	L	14	HIS	2.4
2	L	30	TYR	2.3
2	L	49	LEU	2.3
2	H	110	ASN	2.3
2	I	110	ASN	2.3
2	H	165	GLY	2.3
2	L	34	VAL	2.3
2	H	12	ASN	2.3
2	L	27	LEU	2.3
2	L	159	MET	2.3
2	L	42	PHE	2.2
2	L	170	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	113	GLN	2.2
1	F	164	SER	2.2
2	H	7	SER	2.2
2	I	23	ARG	2.2
2	L	64	ARG	2.2
2	H	65	GLU	2.2
2	I	91	CYS	2.2
2	J	118	LEU	2.2
2	L	66	HIS	2.2
1	D	165	GLY	2.2
2	H	120	LYS	2.2
2	L	99	ASN	2.2
1	C	163	ARG	2.1
2	J	92	ASP	2.1
2	L	46	ASP	2.1
2	J	6	THR	2.1
2	I	82	PHE	2.1
2	L	50	LYS	2.1
2	G	164	SER	2.1
1	C	162	PRO	2.1
2	H	8	GLN	2.1
2	I	165	GLY	2.1
2	H	88	LYS	2.1
2	L	173	LYS	2.1
1	A	164	SER	2.1
1	B	164	SER	2.1
2	H	20	ALA	2.1
2	K	122	ALA	2.1
2	H	130	LEU	2.0
2	K	73	LEU	2.0
2	H	131	CYS	2.0
2	L	23	ARG	2.0
2	J	162	PRO	2.0
2	H	163	GLU	2.0
2	H	73	LEU	2.0
2	H	123	THR	2.0

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

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
3	GOL	E	201	6/6	0.87	0.15	34,40,42,42	2
5	MG	F	202	1/1	0.89	0.20	51,51,51,51	0
4	FE	L	201	1/1	0.91	0.11	73,73,73,73	0
3	GOL	A	202	6/6	0.91	0.11	35,37,40,42	2
3	GOL	A	201	6/6	0.92	0.10	32,40,46,46	2
3	GOL	C	201	6/6	0.93	0.09	26,32,35,36	2
3	GOL	B	201	6/6	0.93	0.10	31,36,36,37	2
4	FE	H	201	1/1	0.94	0.08	63,63,63,63	0
5	MG	J	202	1/1	0.94	0.08	62,62,62,62	0
5	MG	G	202	1/1	0.96	0.04	33,33,33,33	0
5	MG	K	202	1/1	0.97	0.08	42,42,42,42	0
4	FE	K	201	1/1	0.98	0.05	53,53,53,53	0
4	FE	G	201	1/1	0.98	0.06	48,48,48,48	0
4	FE	I	201	1/1	0.99	0.06	48,48,48,48	0
4	FE	J	201	1/1	0.99	0.05	52,52,52,52	0
4	FE	C	202	1/1	0.99	0.05	35,35,35,35	0
4	FE	D	201	1/1	0.99	0.05	35,35,35,35	0
5	MG	B	203	1/1	0.99	0.03	21,21,21,21	0
5	MG	C	203	1/1	0.99	0.03	26,26,26,26	0
4	FE	E	202	1/1	0.99	0.06	34,34,34,34	0
4	FE	F	201	1/1	0.99	0.06	35,35,35,35	0
4	FE	A	203	1/1	0.99	0.07	37,37,37,37	0
4	FE	B	202	1/1	0.99	0.06	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.