



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:29 AM UTC

PDB ID : 4DAS / pdb_00004das
Title : Crystal structure of Bullfrog M ferritin
Authors : Bertini, I.; Lalli, D.; Mangani, S.; Pozzi, C.; Rosa, C.; Turano, P.
Deposited on : 2012-01-13
Resolution : 2.56 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

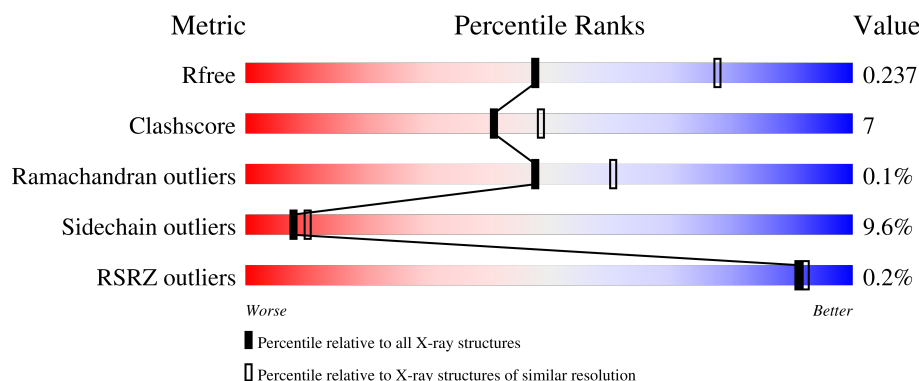
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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.



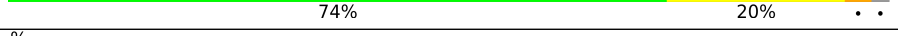
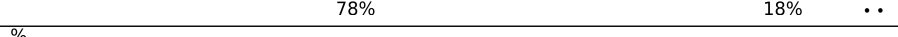
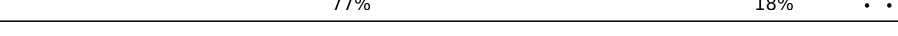
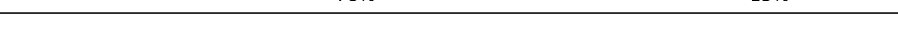
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	176	 78% 18% ..
1	B	176	 77% 19% ..
1	C	176	 80% 17% ..
1	D	176	 80% 16% ..
1	E	176	 80% 16% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	176	
1	G	176	
1	H	176	
1	I	176	
1	J	176	
1	K	176	
1	L	176	
1	M	176	
1	N	176	
1	O	176	
1	P	176	
1	Q	176	
1	R	176	
1	S	176	
1	T	176	
1	U	176	
1	V	176	
1	W	176	
1	X	176	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	R	202	-	-	X	-
3	EDO	U	203	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35835 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 Ferritin, middle subunit.

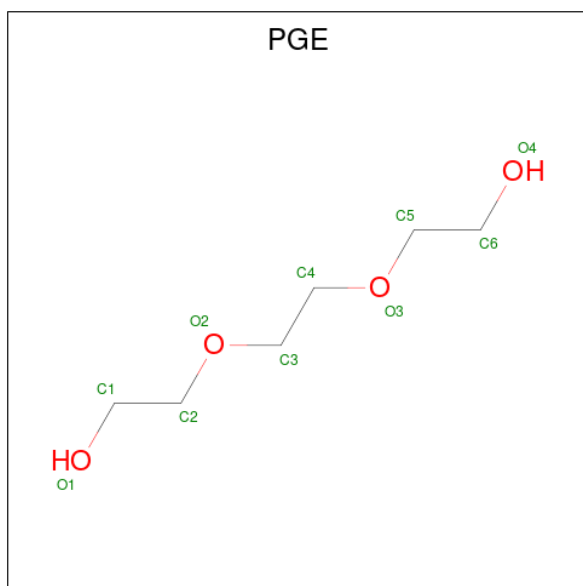
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	B	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	C	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	D	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	E	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	F	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	G	172	Total	C	N	O	S	0	0	0
			1415	891	246	271	7			
1	H	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	I	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	J	172	Total	C	N	O	S	0	0	0
			1415	890	246	272	7			
1	K	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	L	172	Total	C	N	O	S	0	0	0
			1415	891	247	270	7			
1	M	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	N	172	Total	C	N	O	S	0	0	0
			1415	891	247	270	7			
1	O	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	P	172	Total	C	N	O	S	0	0	0
			1414	890	246	271	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	R	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	S	172	Total	C	N	O	S	0	0	0
			1414	890	247	270	7			
1	T	173	Total	C	N	O	S	0	0	0
			1426	897	248	273	8			
1	U	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	V	172	Total	C	N	O	S	0	0	0
			1418	892	247	272	7			
1	X	172	Total	C	N	O	S	0	0	0
			1415	891	247	270	7			
1	W	173	Total	C	N	O	S	0	0	0
			1423	896	247	272	8			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



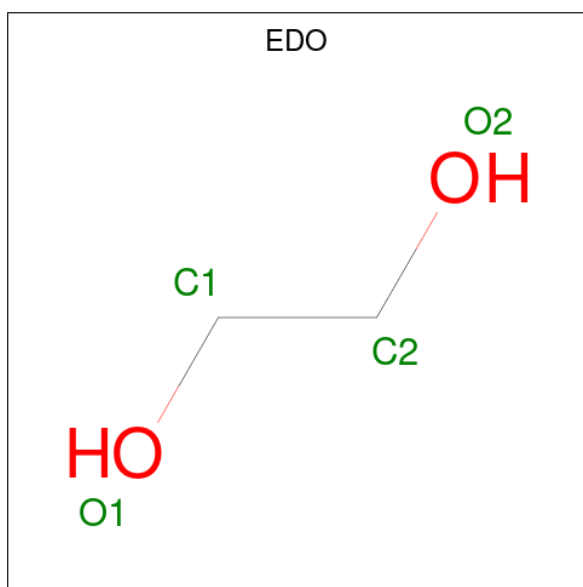
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	G	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		
2	H	1	Total	C	O	0	0
			10	6	4		
2	I	1	Total	C	O	0	0
			10	6	4		
2	P	1	Total	C	O	0	0
			10	6	4		
2	Q	1	Total	C	O	0	0
			10	6	4		
2	Q	1	Total	C	O	0	0
			10	6	4		
2	R	1	Total	C	O	0	0
			10	6	4		
2	R	1	Total	C	O	0	0
			10	6	4		
2	R	1	Total	C	O	0	0
			10	6	4		
2	S	1	Total	C	O	0	0
			10	6	4		
2	U	1	Total	C	O	0	0
			10	6	4		
2	X	1	Total	C	O	0	0
			10	6	4		
2	W	1	Total	C	O	0	0
			10	6	4		
2	W	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	M	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		
3	N	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		
3	P	1	Total	C	O	0	0
			4	2	2		
3	T	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	46	Total O 46 46	0	0
4	C	68	Total O 68 68	0	0
4	D	68	Total O 68 68	0	0
4	E	49	Total O 49 49	0	0
4	F	52	Total O 52 52	0	0
4	G	69	Total O 69 69	0	0
4	H	70	Total O 70 70	0	0
4	I	51	Total O 51 51	0	0
4	J	78	Total O 78 78	0	0
4	K	85	Total O 85 85	0	0
4	L	48	Total O 48 48	0	0
4	M	52	Total O 52 52	0	0
4	N	72	Total O 72 72	0	0
4	O	82	Total O 82 82	0	0
4	P	62	Total O 62 62	0	0
4	Q	71	Total O 71 71	0	0
4	R	73	Total O 73 73	0	0
4	S	60	Total O 60 60	0	0
4	T	36	Total O 36 36	0	0
4	U	63	Total O 63 63	0	0
4	V	38	Total O 38 38	0	0

Continued on next page...

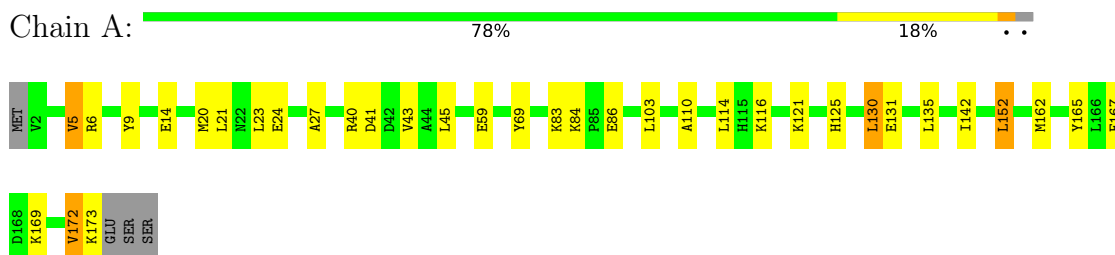
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	87	Total	O	0	0
			87	87		
4	W	71	Total	O	0	0
			71	71		

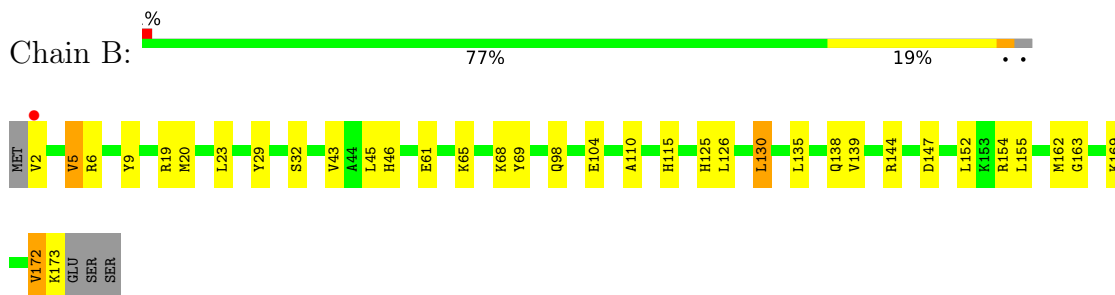
3 Residue-property plots [i](#)

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.

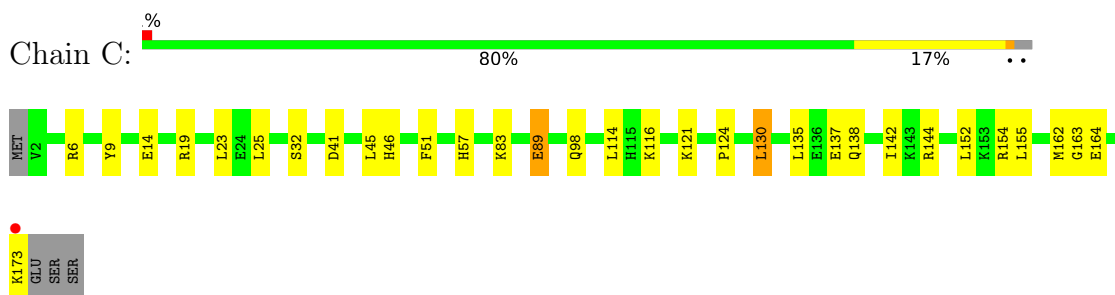
- Molecule 1: Ferritin, middle subunit



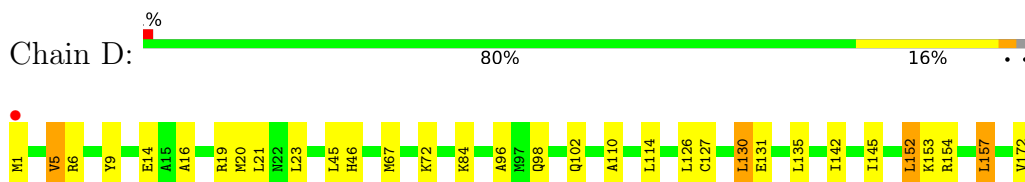
- Molecule 1: Ferritin, middle subunit



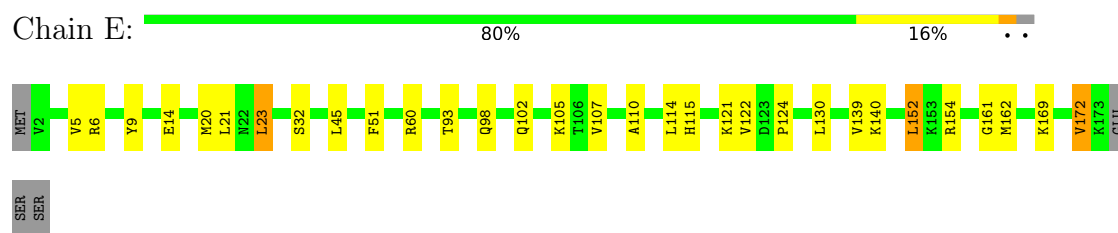
- Molecule 1: Ferritin, middle subunit



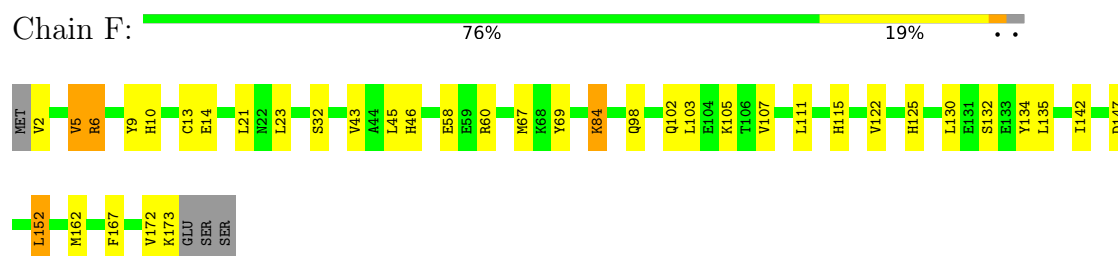
- Molecule 1: Ferritin, middle subunit



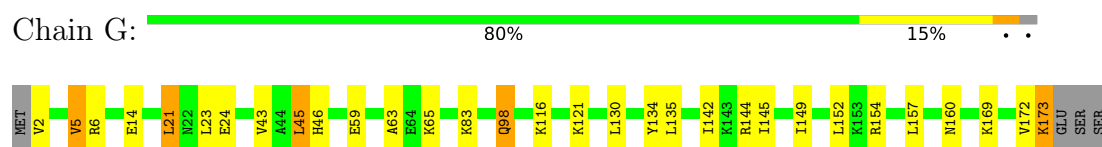
- Molecule 1: Ferritin, middle subunit



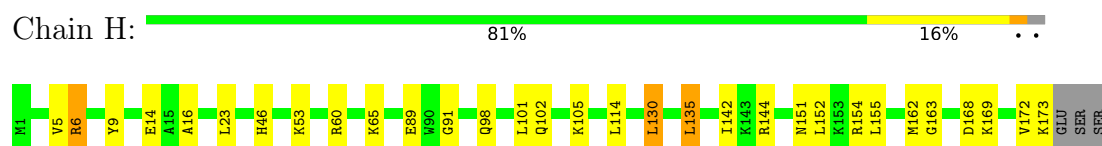
- Molecule 1: Ferritin, middle subunit



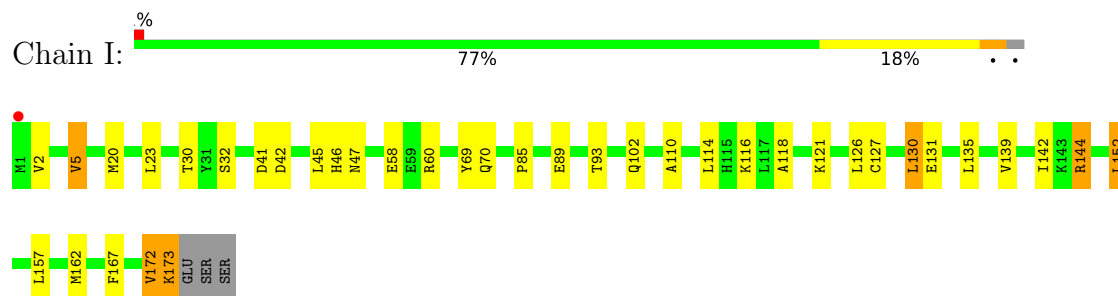
- Molecule 1: Ferritin, middle subunit



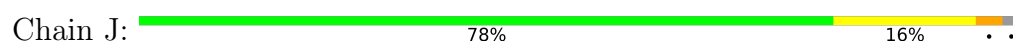
- Molecule 1: Ferritin, middle subunit

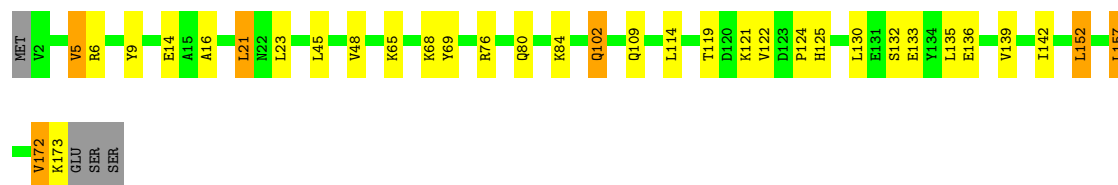


- Molecule 1: Ferritin, middle subunit



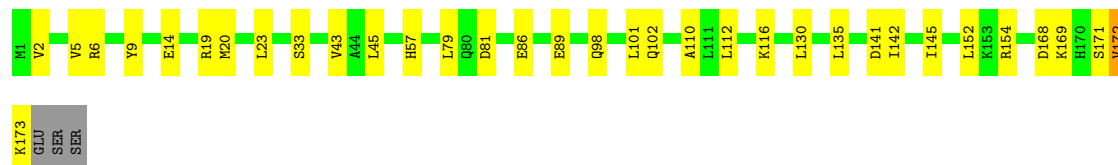
- Molecule 1: Ferritin, middle subunit





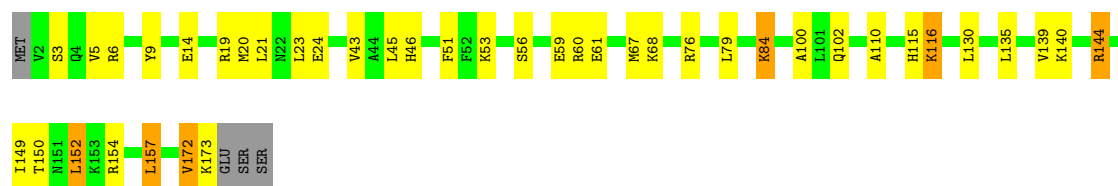
- Molecule 1: Ferritin, middle subunit

Chain K: 79% 19% ..



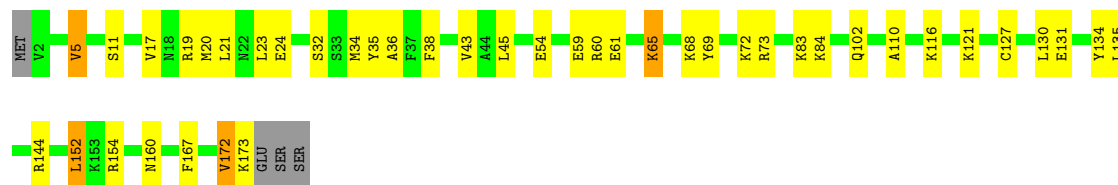
- Molecule 1: Ferritin, middle subunit

Chain L: 74% 20% ..



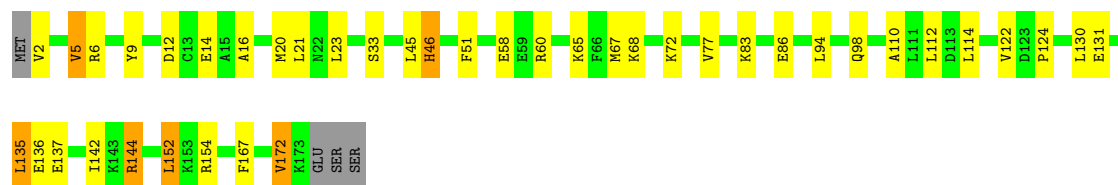
- Molecule 1: Ferritin, middle subunit

Chain M: 74% 22% ..



- Molecule 1: Ferritin, middle subunit

Chain N: 74% 20% ..



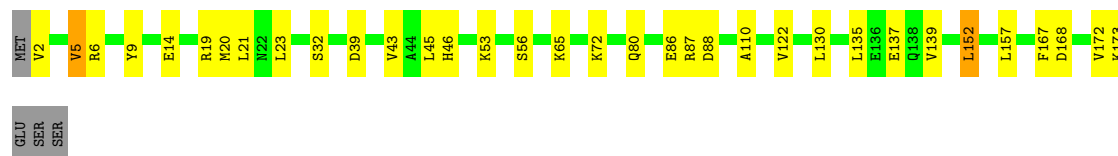
- Molecule 1: Ferritin, middle subunit

Chain O: % 78% 15% ..



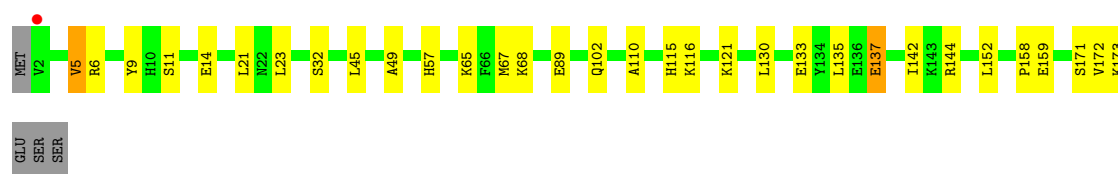
- Molecule 1: Ferritin, middle subunit

Chain P: 78% 18% ..



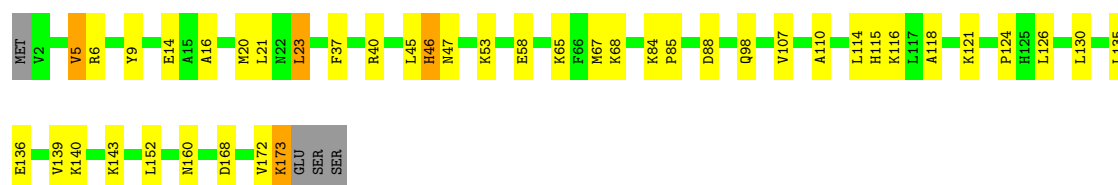
- Molecule 1: Ferritin, middle subunit

Chain Q: 80% 17% ..



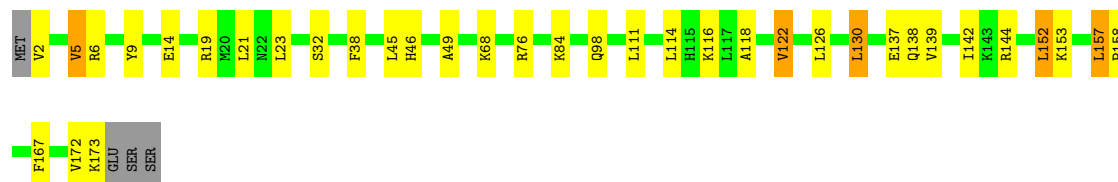
- Molecule 1: Ferritin, middle subunit

Chain R: 74% 22% ..



- Molecule 1: Ferritin, middle subunit

Chain S: 77% 18% ..



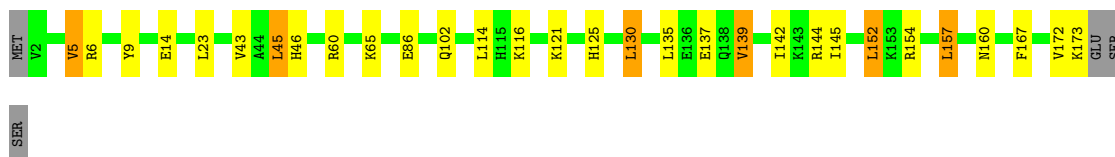
- Molecule 1: Ferritin, middle subunit

Chain T: 84% 12% ..



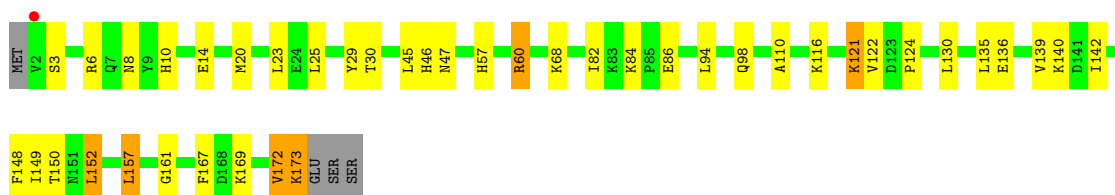
- Molecule 1: Ferritin, middle subunit

Chain U: 81% 14% . .



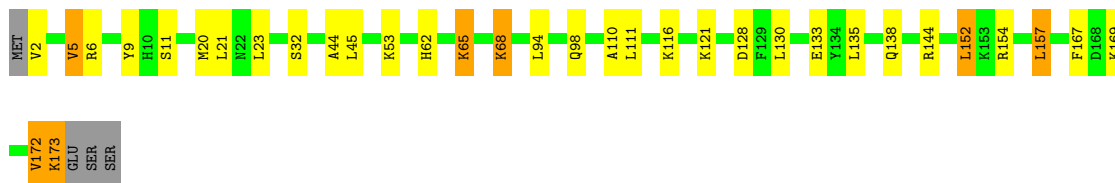
- Molecule 1: Ferritin, middle subunit

Chain V: % 74% 20% . .



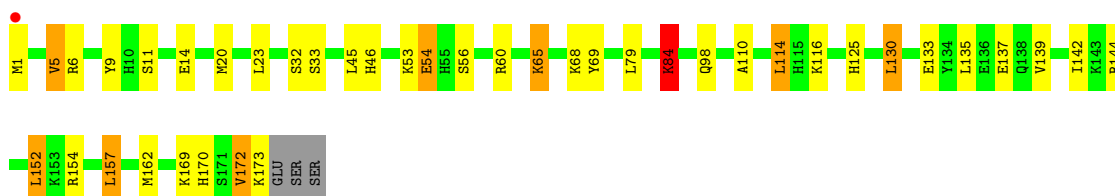
- Molecule 1: Ferritin, middle subunit

Chain X: 78% 15% . .



- Molecule 1: Ferritin, middle subunit

Chain W: % 75% 18% 5% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.95Å 210.95Å 323.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.51 – 2.56 79.51 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.5 (79.51-2.56) 97.5 (79.51-2.56)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.239 0.187 , 0.237	Depositor DCC
R_{free} test set	13392 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35835	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: EDO, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	0/1442	1.08	0/1939
1	B	0.95	0/1446	1.07	1/1944 (0.1%)
1	C	0.98	0/1446	1.10	2/1944 (0.1%)
1	D	1.08	0/1454	1.14	2/1954 (0.1%)
1	E	0.93	0/1442	1.09	0/1939
1	F	0.96	1/1442 (0.1%)	1.01	1/1939 (0.1%)
1	G	0.94	0/1443	1.08	1/1940 (0.1%)
1	H	0.93	0/1454	1.08	3/1954 (0.2%)
1	I	0.97	0/1454	1.09	3/1954 (0.2%)
1	J	1.04	0/1443	1.13	3/1941 (0.2%)
1	K	1.01	0/1454	1.05	1/1954 (0.1%)
1	L	0.90	1/1443 (0.1%)	1.07	3/1940 (0.2%)
1	M	0.88	0/1446	1.08	4/1944 (0.2%)
1	N	1.01	0/1443	1.07	2/1940 (0.1%)
1	O	0.97	1/1446 (0.1%)	1.04	2/1944 (0.1%)
1	P	0.93	0/1442	1.04	3/1939 (0.2%)
1	Q	1.00	1/1446 (0.1%)	1.05	0/1944
1	R	1.03	0/1446	1.10	2/1944 (0.1%)
1	S	0.94	0/1442	0.99	0/1939
1	T	0.97	0/1454	1.05	1/1954 (0.1%)
1	U	1.03	2/1446 (0.1%)	1.03	1/1944 (0.1%)
1	V	0.95	0/1446	1.12	3/1944 (0.2%)
1	W	1.02	0/1451	1.10	3/1950 (0.2%)
1	X	1.00	0/1443	1.06	1/1940 (0.1%)
All	All	0.98	6/34714 (0.0%)	1.07	42/46668 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	43	VAL	CA-CB	-6.70	1.48	1.55
1	L	100	ALA	CA-CB	-5.39	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	70	GLN	N-CA	-5.33	1.40	1.46
1	U	145	ILE	CA-CB	-5.26	1.47	1.54
1	U	139	VAL	CA-CB	5.23	1.61	1.54
1	Q	49	ALA	CA-CB	-5.20	1.45	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	42	ASP	CA-C-N	-7.06	115.95	123.08
1	I	42	ASP	C-N-CA	-7.06	115.95	123.08
1	F	132	SER	N-CA-C	6.61	118.57	111.36
1	J	48	VAL	N-CA-C	-6.60	104.33	110.53
1	W	84	LYS	CA-C-N	-6.16	114.30	120.21
1	W	84	LYS	C-N-CA	-6.16	114.30	120.21
1	D	145	ILE	N-CA-C	6.12	116.79	110.36
1	V	84	LYS	CA-C-N	-6.09	114.36	120.21
1	V	84	LYS	C-N-CA	-6.09	114.36	120.21
1	C	51	PHE	N-CA-C	-6.07	104.66	111.28
1	W	114	LEU	N-CA-C	-5.99	104.83	111.36
1	N	46	HIS	N-CA-C	5.94	117.83	111.36
1	L	84	LYS	CA-C-N	-5.85	114.59	120.21
1	L	84	LYS	C-N-CA	-5.85	114.59	120.21
1	O	138	GLN	N-CA-C	5.84	117.65	111.28
1	B	46	HIS	N-CA-C	5.81	118.56	111.82
1	T	46	HIS	N-CA-C	5.72	118.29	111.71
1	K	172	VAL	CB-CA-C	5.52	118.85	110.62
1	H	46	HIS	N-CA-C	5.51	118.21	111.82
1	M	160	ASN	N-CA-C	5.50	117.69	108.23
1	R	58	GLU	N-CA-C	5.49	117.70	111.11
1	H	151	ASN	N-CA-C	5.47	117.32	111.36
1	J	132	SER	N-CA-C	5.46	116.91	111.07
1	V	169	LYS	N-CA-C	5.42	118.10	111.82
1	L	46	HIS	N-CA-C	5.40	118.34	111.69
1	U	160	ASN	N-CA-C	5.40	117.49	107.99
1	J	109	GLN	N-CA-C	-5.38	105.50	111.36
1	H	135	LEU	N-CA-C	5.34	117.10	111.28
1	M	5	VAL	N-CA-CB	-5.32	106.36	112.21
1	R	46	HIS	N-CA-C	5.32	117.98	111.82
1	N	33	SER	N-CA-C	-5.28	105.52	111.28
1	O	170	HIS	N-CA-C	5.28	120.37	113.88
1	I	46	HIS	N-CA-C	5.23	117.89	111.82
1	C	164	GLU	N-CA-C	-5.17	105.33	111.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ALA	N-CA-C	5.16	116.59	111.07
1	M	84	LYS	CA-C-N	-5.15	115.26	120.21
1	M	84	LYS	C-N-CA	-5.15	115.26	120.21
1	P	2	VAL	CB-CA-C	-5.15	101.62	111.40
1	P	88	ASP	N-CA-C	-5.15	107.13	113.41
1	P	46	HIS	N-CA-C	5.10	116.92	111.36
1	G	134	TYR	N-CA-C	5.09	119.24	112.72
1	X	44	ALA	N-CA-C	5.00	118.29	111.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1414	0	1366	26	0
1	B	1418	0	1370	22	0
1	C	1418	0	1370	18	0
1	D	1426	0	1382	17	0
1	E	1414	0	1366	20	0
1	F	1414	0	1366	26	0
1	G	1415	0	1366	19	0
1	H	1426	0	1382	16	0
1	I	1426	0	1382	21	0
1	J	1415	0	1361	17	0
1	K	1426	0	1382	17	0
1	L	1415	0	1368	22	0
1	M	1418	0	1370	17	0
1	N	1415	0	1368	25	0
1	O	1418	0	1370	27	0
1	P	1414	0	1364	17	0
1	Q	1418	0	1370	12	0
1	R	1418	0	1370	25	0
1	S	1414	0	1366	19	0
1	T	1426	0	1382	13	0
1	U	1418	0	1370	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V	1418	0	1370	30	0
1	W	1423	0	1378	34	0
1	X	1415	0	1368	21	0
2	B	10	0	14	1	0
2	C	20	0	28	1	0
2	D	10	0	14	1	0
2	E	10	0	14	0	0
2	F	10	0	14	0	0
2	G	20	0	28	1	0
2	H	20	0	28	3	0
2	I	10	0	14	0	0
2	P	10	0	14	1	0
2	Q	20	0	28	1	0
2	R	30	0	42	8	0
2	S	10	0	14	1	0
2	U	10	0	14	0	0
2	W	20	0	28	0	0
2	X	10	0	14	0	0
3	B	4	0	6	0	0
3	D	4	0	6	1	0
3	J	4	0	6	0	0
3	L	4	0	6	1	0
3	M	4	0	6	1	0
3	N	8	0	12	2	0
3	O	4	0	6	1	0
3	P	4	0	6	1	0
3	T	4	0	6	0	0
3	U	8	0	12	9	0
4	A	74	0	0	3	0
4	B	46	0	0	4	0
4	C	68	0	0	6	0
4	D	68	0	0	2	0
4	E	49	0	0	1	0
4	F	52	0	0	2	0
4	G	69	0	0	3	0
4	H	70	0	0	3	0
4	I	51	0	0	6	0
4	J	78	0	0	3	0
4	K	85	0	0	3	0
4	L	48	0	0	2	0
4	M	52	0	0	1	0
4	N	72	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	82	0	0	4	0
4	P	62	0	0	4	0
4	Q	71	0	0	5	0
4	R	73	0	0	6	0
4	S	60	0	0	4	0
4	T	36	0	0	1	0
4	U	63	0	0	1	0
4	V	38	0	0	2	0
4	W	71	0	0	3	0
4	X	87	0	0	5	0
All	All	35835	0	33287	441	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (441) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:LYS:HE3	4:G:361:HOH:O	1.42	1.17
1:I:102:GLN:HG3	4:I:348:HOH:O	1.48	1.11
1:D:20:MET:HE1	1:D:110:ALA:HB1	1.29	1.10
1:C:98:GLN:HG2	4:C:362:HOH:O	1.49	1.09
1:I:144:ARG:HD2	4:I:308:HOH:O	1.55	1.06
1:R:46:HIS:HB3	4:R:310:HOH:O	1.58	1.02
1:O:137:GLU:HG2	4:O:372:HOH:O	1.63	0.98
1:A:172:VAL:O	1:A:173:LYS:HB2	1.66	0.94
1:C:142:ILE:HG22	1:S:5:VAL:HG22	1.50	0.93
4:P:351:HOH:O	1:W:169:LYS:HE3	1.69	0.92
1:A:20:MET:HE1	1:A:110:ALA:HB1	1.50	0.91
1:R:37:PHE:HA	2:R:202:PGE:H2	1.52	0.91
1:W:46:HIS:HB3	4:W:302:HOH:O	1.70	0.91
1:J:142:ILE:HG22	1:N:5:VAL:HG22	1.54	0.88
1:G:172:VAL:HG12	1:G:173:LYS:H	1.40	0.87
1:T:172:VAL:O	1:T:173:LYS:HB2	1.74	0.87
1:Q:137:GLU:HG2	4:Q:315:HOH:O	1.76	0.86
1:B:20:MET:HE1	1:B:110:ALA:C	2.02	0.85
1:O:21:LEU:HD11	1:O:67:MET:HG2	1.60	0.84
1:I:5:VAL:CG2	1:W:142:ILE:HG22	2.08	0.84
1:D:20:MET:HE1	1:D:110:ALA:CB	2.06	0.83
1:V:172:VAL:O	1:V:173:LYS:HB2	1.79	0.83
1:C:83:LYS:HE2	4:C:359:HOH:O	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:137:GLU:HG2	4:N:305:HOH:O	1.79	0.82
1:H:98:GLN:HG2	4:H:305:HOH:O	1.81	0.81
1:W:144:ARG:HD3	4:W:337:HOH:O	1.80	0.81
1:A:162:MET:HE1	1:O:162:MET:HE3	1.62	0.79
4:Q:358:HOH:O	1:X:169:LYS:HE3	1.82	0.78
1:W:20:MET:HE1	1:W:110:ALA:HB1	1.66	0.78
1:Q:57:HIS:HB3	4:Q:362:HOH:O	1.85	0.76
1:N:21:LEU:HD11	1:N:67:MET:HG2	1.68	0.76
1:I:5:VAL:HG22	1:W:142:ILE:HG22	1.68	0.75
1:E:6:ARG:NH1	1:E:9:TYR:O	2.20	0.74
1:G:144:ARG:HD3	4:G:333:HOH:O	1.88	0.73
1:F:142:ILE:HG22	1:O:5:VAL:HG22	1.70	0.73
1:J:6:ARG:NH1	1:J:9:TYR:O	2.22	0.72
1:X:20:MET:HE1	1:X:110:ALA:C	2.14	0.72
4:B:305:HOH:O	1:G:154:ARG:HD3	1.89	0.71
1:M:60:ARG:HD2	4:M:304:HOH:O	1.90	0.71
1:V:136:GLU:OE2	1:V:140:LYS:HE3	1.89	0.71
1:S:137:GLU:HG2	4:S:352:HOH:O	1.90	0.71
1:V:152:LEU:HD12	1:V:157:LEU:HD13	1.71	0.71
1:N:136:GLU:HB3	4:N:324:HOH:O	1.90	0.71
1:C:154:ARG:NH2	1:M:43:VAL:O	2.22	0.71
1:F:172:VAL:O	1:F:173:LYS:HB2	1.90	0.70
1:I:47:ASN:HB3	1:I:172:VAL:HG12	1.73	0.70
1:X:172:VAL:O	1:X:173:LYS:HB2	1.90	0.70
1:G:5:VAL:HG22	1:O:142:ILE:HG22	1.74	0.70
1:E:6:ARG:NH2	1:E:14:GLU:OE1	2.24	0.69
1:M:127:CYS:O	1:M:131:GLU:HG3	1.93	0.69
1:N:46:HIS:HB3	4:N:318:HOH:O	1.92	0.69
1:R:40:ARG:HD2	2:R:202:PGE:O2	1.93	0.69
1:A:20:MET:HE1	1:A:110:ALA:CB	2.22	0.69
1:P:5:VAL:HG22	1:U:142:ILE:HG22	1.72	0.69
1:U:6:ARG:NH2	1:U:14:GLU:OE1	2.20	0.69
1:E:23:LEU:HD13	1:E:107:VAL:HG22	1.74	0.69
1:W:20:MET:HE1	1:W:110:ALA:CB	2.22	0.69
1:C:6:ARG:NH2	1:C:14:GLU:OE1	2.26	0.68
1:S:76:ARG:HA	4:S:354:HOH:O	1.94	0.68
1:M:172:VAL:O	1:M:173:LYS:HB2	1.92	0.68
1:M:20:MET:HE1	1:M:110:ALA:C	2.19	0.68
1:B:5:VAL:HG22	1:V:142:ILE:HG22	1.75	0.67
1:C:19:ARG:HH21	2:C:202:PGE:H62	1.59	0.67
1:A:6:ARG:NH1	1:A:9:TYR:O	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:47:ASN:HB3	1:V:172:VAL:HG12	1.75	0.67
1:D:6:ARG:NH1	1:D:9:TYR:O	2.28	0.67
1:J:172:VAL:O	1:J:173:LYS:HB2	1.93	0.67
2:R:202:PGE:H22	4:R:348:HOH:O	1.94	0.67
1:F:6:ARG:NH2	1:F:14:GLU:OE1	2.27	0.67
1:N:136:GLU:HA	1:N:136:GLU:OE1	1.94	0.67
1:O:21:LEU:HD11	1:O:67:MET:CG	2.24	0.67
1:A:131:GLU:HG2	1:X:128:ASP:HB2	1.75	0.66
1:D:6:ARG:NH2	1:D:14:GLU:OE1	2.29	0.66
1:T:6:ARG:NH2	1:T:14:GLU:OE1	2.21	0.66
1:V:20:MET:HE1	1:V:110:ALA:CB	2.26	0.65
1:N:21:LEU:HD11	1:N:67:MET:CG	2.26	0.65
1:V:20:MET:HE1	1:V:110:ALA:HB1	1.77	0.65
1:X:152:LEU:HD12	1:X:157:LEU:HD13	1.79	0.65
1:I:5:VAL:HG23	1:W:142:ILE:HG22	1.79	0.65
1:L:20:MET:HE1	1:L:110:ALA:C	2.21	0.65
1:R:6:ARG:NH2	1:R:14:GLU:OE1	2.27	0.65
1:V:20:MET:HE1	1:V:110:ALA:C	2.21	0.65
1:A:86:GLU:HG2	4:A:232:HOH:O	1.96	0.65
1:F:6:ARG:NH1	1:F:9:TYR:O	2.28	0.65
1:L:76:ARG:HB3	4:L:345:HOH:O	1.96	0.65
1:A:142:ILE:HG22	1:X:5:VAL:HG22	1.78	0.64
1:L:152:LEU:HD12	1:L:157:LEU:HD13	1.79	0.64
1:C:46:HIS:HB3	4:C:308:HOH:O	1.97	0.64
1:O:136:GLU:OE1	1:O:136:GLU:HA	1.97	0.64
1:A:21:LEU:HD23	1:A:21:LEU:C	2.21	0.64
1:E:20:MET:HE1	1:E:110:ALA:C	2.21	0.64
1:H:144:ARG:HD3	4:H:363:HOH:O	1.97	0.64
1:P:6:ARG:NH1	1:P:9:TYR:O	2.31	0.64
1:W:6:ARG:NH1	1:W:9:TYR:O	2.29	0.64
1:A:172:VAL:O	1:A:173:LYS:CB	2.43	0.64
1:B:154:ARG:HD3	4:I:309:HOH:O	1.97	0.63
1:P:6:ARG:NH2	1:P:14:GLU:OE1	2.28	0.63
1:A:169:LYS:HE2	4:A:219:HOH:O	1.98	0.63
1:H:16:ALA:HB1	2:H:202:PGE:H42	1.79	0.63
1:A:6:ARG:NH2	1:A:14:GLU:OE1	2.32	0.63
1:P:20:MET:HE1	1:P:110:ALA:C	2.24	0.62
1:S:152:LEU:HD12	1:S:157:LEU:HD13	1.80	0.62
1:F:122:VAL:HG11	1:G:116:LYS:HD3	1.82	0.62
1:W:65:LYS:HE2	1:W:133:GLU:OE1	2.01	0.61
1:H:6:ARG:NH1	1:H:9:TYR:O	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:46:HIS:HB3	4:S:348:HOH:O	1.99	0.61
1:R:40:ARG:HD2	2:R:202:PGE:C2	2.31	0.61
1:I:47:ASN:HB3	1:I:172:VAL:CG1	2.31	0.60
1:G:6:ARG:NH2	1:G:14:GLU:OE1	2.27	0.60
1:L:172:VAL:HG12	1:L:173:LYS:H	1.65	0.60
1:X:20:MET:HE1	1:X:110:ALA:CB	2.31	0.60
1:U:125:HIS:HB2	3:U:203:EDO:H11	1.84	0.60
1:J:6:ARG:NH2	1:J:14:GLU:OE1	2.35	0.60
1:L:6:ARG:NH1	1:L:9:TYR:O	2.35	0.60
1:L:116:LYS:HE2	1:L:116:LYS:HA	1.82	0.60
1:W:6:ARG:NH2	1:W:14:GLU:OE1	2.35	0.60
1:B:19:ARG:HH21	2:B:201:PGE:H6	1.67	0.59
1:V:94:LEU:O	1:V:98:GLN:HG2	2.01	0.59
1:F:5:VAL:HG22	1:G:142:ILE:HG22	1.84	0.59
1:N:94:LEU:O	1:N:98:GLN:HG3	2.01	0.59
1:N:152:LEU:HD13	1:N:167:PHE:CD1	2.37	0.59
1:U:45:LEU:HA	3:U:202:EDO:H22	1.84	0.59
1:J:152:LEU:HD12	1:J:157:LEU:HD13	1.84	0.59
1:S:157:LEU:HD23	1:S:158:PRO:HA	1.84	0.59
1:K:98:GLN:HG2	4:K:204:HOH:O	2.02	0.59
1:F:46:HIS:HB3	4:F:306:HOH:O	2.00	0.59
1:K:112:LEU:HD11	3:U:203:EDO:H21	1.85	0.59
1:G:46:HIS:HB3	4:G:339:HOH:O	2.02	0.59
1:B:6:ARG:NH1	1:B:9:TYR:O	2.33	0.59
1:L:6:ARG:NH2	1:L:14:GLU:OE1	2.33	0.58
1:H:172:VAL:O	1:H:173:LYS:HB3	2.02	0.58
1:B:126:LEU:O	1:B:130:LEU:HD22	2.03	0.58
1:H:162:MET:CE	4:I:314:HOH:O	2.51	0.58
1:H:162:MET:HE1	4:I:314:HOH:O	2.02	0.58
1:V:60:ARG:HG3	1:V:60:ARG:HH11	1.68	0.58
1:D:21:LEU:HD11	1:D:67:MET:HG2	1.85	0.58
1:E:154:ARG:NH2	1:L:43:VAL:O	2.37	0.58
1:K:142:ILE:HG22	1:U:5:VAL:HG22	1.84	0.57
1:R:5:VAL:HG22	1:S:142:ILE:HG22	1.86	0.57
1:I:172:VAL:O	1:I:173:LYS:HB2	2.03	0.57
1:N:20:MET:HE1	1:N:110:ALA:C	2.30	0.57
1:N:12:ASP:O	3:N:202:EDO:H22	2.04	0.57
1:X:65:LYS:HE2	1:X:133:GLU:OE1	2.03	0.57
1:R:136:GLU:HA	1:R:136:GLU:OE1	2.04	0.57
1:X:20:MET:HE1	1:X:110:ALA:HB1	1.85	0.57
1:T:6:ARG:NH1	1:T:9:TYR:O	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:HIS:HB2	4:X:387:HOH:O	2.05	0.56
1:O:162:MET:HE2	4:R:306:HOH:O	2.05	0.56
1:P:172:VAL:O	1:P:173:LYS:HG3	2.05	0.56
1:U:46:HIS:H	3:U:202:EDO:H22	1.70	0.56
1:L:154:ARG:NH2	1:P:43:VAL:O	2.27	0.56
1:O:86:GLU:HG3	4:O:317:HOH:O	2.05	0.56
1:Q:172:VAL:O	1:Q:173:LYS:HB2	2.05	0.56
1:P:137:GLU:HG2	4:P:340:HOH:O	2.04	0.56
1:V:152:LEU:HD13	1:V:167:PHE:CD1	2.41	0.56
1:V:60:ARG:HH11	1:V:60:ARG:CG	2.19	0.55
1:D:142:ILE:HG22	1:W:5:VAL:HG22	1.88	0.55
1:B:43:VAL:O	1:G:154:ARG:NH2	2.30	0.55
1:W:20:MET:HE1	1:W:110:ALA:C	2.32	0.55
1:N:154:ARG:NH2	1:U:43:VAL:O	2.34	0.55
1:X:62:HIS:CD2	4:X:374:HOH:O	2.59	0.55
1:F:23:LEU:HD11	1:F:107:VAL:HG22	1.88	0.55
2:H:201:PGE:H1	4:H:307:HOH:O	2.06	0.55
1:R:20:MET:HG2	1:R:114:LEU:HD22	1.89	0.54
1:X:62:HIS:HD2	4:X:374:HOH:O	1.90	0.54
1:P:19:ARG:HB3	2:P:201:PGE:H2	1.89	0.54
1:U:125:HIS:HB2	3:U:203:EDO:C1	2.38	0.54
1:B:144:ARG:HD3	4:B:314:HOH:O	2.07	0.54
1:F:172:VAL:O	1:F:173:LYS:CB	2.56	0.54
1:L:53:LYS:O	1:L:56:SER:HB3	2.07	0.54
4:Q:358:HOH:O	1:X:169:LYS:CE	2.48	0.54
1:D:154:ARG:NH2	1:K:43:VAL:O	2.28	0.54
1:V:47:ASN:HB3	1:V:172:VAL:CG1	2.38	0.54
4:B:301:HOH:O	1:F:84:LYS:HE2	2.06	0.54
1:D:5:VAL:HG22	1:I:142:ILE:HG22	1.89	0.54
1:Q:6:ARG:NH2	1:Q:14:GLU:OE1	2.31	0.54
1:U:46:HIS:H	3:U:202:EDO:C2	2.21	0.54
1:G:24:GLU:OE1	1:G:59:GLU:OE1	2.26	0.53
1:G:43:VAL:O	1:H:154:ARG:NH2	2.35	0.53
1:G:172:VAL:HG12	1:G:173:LYS:N	2.19	0.53
1:A:27:ALA:HA	1:A:103:LEU:HD21	1.90	0.53
1:B:162:MET:HE3	1:I:162:MET:SD	2.48	0.53
1:N:136:GLU:OE1	1:N:136:GLU:CA	2.57	0.53
1:O:172:VAL:O	1:O:173:LYS:HB3	2.08	0.53
1:R:172:VAL:O	1:R:173:LYS:HB2	2.08	0.53
1:N:77:VAL:HB	2:R:202:PGE:H12	1.91	0.53
1:X:152:LEU:HD13	1:X:167:PHE:CD1	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LYS:HD3	1:S:122:VAL:HG11	1.90	0.53
1:O:152:LEU:HD13	1:O:167:PHE:CD1	2.44	0.53
1:K:6:ARG:NH2	1:K:14:GLU:OE1	2.32	0.52
1:N:124:PRO:HD2	4:N:310:HOH:O	2.08	0.52
1:S:172:VAL:O	1:S:173:LYS:HB2	2.09	0.52
1:A:162:MET:CE	1:O:162:MET:HE3	2.35	0.52
1:C:46:HIS:HD2	4:C:363:HOH:O	1.92	0.52
1:J:102:GLN:HG3	4:J:364:HOH:O	2.10	0.52
1:E:115:HIS:CE1	1:V:124:PRO:HB3	2.45	0.52
1:G:45:LEU:HD13	1:H:154:ARG:NH2	2.25	0.52
1:S:6:ARG:NH2	1:S:14:GLU:OE1	2.34	0.51
1:S:19:ARG:HB3	2:S:201:PGE:H22	1.92	0.51
1:A:43:VAL:O	1:O:154:ARG:NH2	2.40	0.51
1:J:68:LYS:HE3	4:J:349:HOH:O	2.11	0.51
1:Q:110:ALA:HB1	2:Q:202:PGE:H1	1.93	0.51
1:N:142:ILE:HG22	1:Q:5:VAL:HG22	1.91	0.51
1:V:6:ARG:NH2	1:V:14:GLU:OE1	2.27	0.51
1:D:16:ALA:HB1	1:D:114:LEU:CD1	2.41	0.51
1:P:39:ASP:HB3	1:T:71:ASN:ND2	2.26	0.50
1:I:152:LEU:HD13	1:I:167:PHE:CD1	2.47	0.50
1:J:136:GLU:HB3	4:J:316:HOH:O	2.11	0.50
1:P:87:ARG:HA	3:P:202:EDO:H11	1.93	0.50
1:L:51:PHE:HB2	1:L:172:VAL:HG11	1.92	0.50
1:O:105:LYS:HE3	4:O:378:HOH:O	2.11	0.50
1:O:144:ARG:HH11	1:O:144:ARG:HG2	1.75	0.50
1:W:53:LYS:O	1:W:56:SER:HB3	2.12	0.50
1:E:51:PHE:HB2	1:E:172:VAL:HG11	1.94	0.50
1:G:160:ASN:C	1:G:160:ASN:OD1	2.53	0.50
1:Q:158:PRO:HD2	1:Q:159:GLU:OE1	2.12	0.50
1:I:20:MET:HE1	1:I:110:ALA:HB3	1.93	0.50
1:S:114:LEU:HG	1:S:130:LEU:HD21	1.93	0.50
1:L:144:ARG:NH1	4:L:326:HOH:O	2.45	0.50
1:B:172:VAL:O	1:B:173:LYS:HB3	2.12	0.49
1:U:46:HIS:HB3	4:U:311:HOH:O	2.11	0.49
1:M:19:ARG:HE	3:M:201:EDO:H11	1.77	0.49
1:D:84:LYS:NZ	4:D:302:HOH:O	2.45	0.49
1:R:88:ASP:O	2:R:202:PGE:C3	2.61	0.49
1:R:21:LEU:HD23	1:R:21:LEU:C	2.38	0.49
1:E:21:LEU:C	1:E:21:LEU:HD23	2.38	0.49
1:V:10:HIS:CG	1:V:121:LYS:HG2	2.48	0.49
1:E:162:MET:HE1	1:W:162:MET:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:79:LEU:HD12	1:W:33:SER:HB2	1.94	0.49
1:L:116:LYS:HE2	1:L:116:LYS:CA	2.43	0.49
1:Q:65:LYS:HE2	1:Q:133:GLU:OE1	2.12	0.49
1:A:152:LEU:HD13	1:A:167:PHE:CD1	2.48	0.49
1:M:69:TYR:CE2	1:M:73:ARG:HG3	2.47	0.49
1:P:53:LYS:O	1:P:56:SER:HB3	2.13	0.49
1:R:23:LEU:HD13	1:R:107:VAL:HG22	1.95	0.49
1:H:168:ASP:OD2	1:H:169:LYS:NZ	2.46	0.48
1:R:160:ASN:HB2	4:R:367:HOH:O	2.13	0.48
1:S:111:LEU:HD12	1:S:138:GLN:HG3	1.95	0.48
1:J:5:VAL:HG22	1:Q:142:ILE:HG22	1.95	0.48
1:V:57:HIS:CD2	1:V:60:ARG:HH22	2.31	0.48
1:V:173:LYS:NZ	4:V:224:HOH:O	2.46	0.48
1:A:5:VAL:HG22	1:H:142:ILE:HG22	1.94	0.48
1:W:54:GLU:HG3	4:W:363:HOH:O	2.13	0.48
4:D:303:HOH:O	1:X:154:ARG:HG3	2.13	0.48
1:F:115:HIS:CE1	1:O:124:PRO:HB3	2.49	0.48
1:J:172:VAL:O	1:J:173:LYS:CB	2.60	0.48
1:O:136:GLU:OE1	1:O:136:GLU:CA	2.62	0.48
1:S:6:ARG:NH1	1:S:9:TYR:O	2.46	0.48
1:U:152:LEU:HD13	1:U:167:PHE:CD1	2.49	0.48
1:F:23:LEU:CD1	1:F:107:VAL:HG22	2.43	0.48
1:B:162:MET:CE	1:I:162:MET:SD	3.02	0.48
4:P:351:HOH:O	1:W:169:LYS:CE	2.43	0.48
1:B:115:HIS:CE1	1:E:124:PRO:HB3	2.49	0.48
1:L:115:HIS:CE1	1:T:124:PRO:HB3	2.49	0.48
4:S:345:HOH:O	1:T:154:ARG:HD3	2.13	0.47
1:A:40:ARG:NH1	4:A:231:HOH:O	2.41	0.47
1:K:154:ARG:HD3	4:Q:342:HOH:O	2.14	0.47
1:T:30:THR:OG1	1:T:85:PRO:HB3	2.15	0.47
1:W:172:VAL:O	1:W:173:LYS:HB2	2.14	0.47
1:L:152:LEU:HD12	1:L:157:LEU:CD1	2.43	0.47
1:A:21:LEU:HD23	1:A:21:LEU:O	2.14	0.47
1:R:88:ASP:O	2:R:202:PGE:H32	2.14	0.47
1:X:6:ARG:NH1	1:X:9:TYR:O	2.42	0.47
1:D:19:ARG:HB3	2:D:201:PGE:H22	1.97	0.47
1:H:6:ARG:NH2	1:H:14:GLU:OE1	2.41	0.47
1:H:101:LEU:O	1:H:105:LYS:HG3	2.14	0.46
1:X:144:ARG:HD3	4:X:338:HOH:O	2.15	0.46
1:C:6:ARG:NH1	1:C:9:TYR:O	2.48	0.46
1:K:20:MET:HE1	1:K:110:ALA:HB1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:110:ALA:HB1	2:R:203:PGE:H3	1.97	0.46
1:W:114:LEU:HG	1:W:130:LEU:HD21	1.97	0.46
1:H:114:LEU:HG	1:H:130:LEU:HD21	1.97	0.46
1:V:8:ASN:O	1:V:8:ASN:CG	2.59	0.46
1:G:145:ILE:O	1:G:149:ILE:HG13	2.14	0.46
2:H:201:PGE:H32	2:H:201:PGE:H12	1.60	0.46
1:K:81:ASP:OD1	1:W:84:LYS:HD2	2.16	0.46
1:R:16:ALA:HB1	1:R:114:LEU:HD13	1.98	0.46
1:T:21:LEU:HD11	1:T:67:MET:HG2	1.97	0.46
1:B:169:LYS:HE2	4:B:306:HOH:O	2.15	0.46
1:S:152:LEU:HD12	1:S:157:LEU:CD1	2.44	0.46
1:B:104:GLU:OE1	1:B:138:GLN:NE2	2.48	0.46
1:L:21:LEU:HD11	1:L:67:MET:HG2	1.96	0.46
1:N:2:VAL:HG13	1:N:2:VAL:O	2.16	0.46
3:O:201:EDO:H11	1:R:143:LYS:HG2	1.97	0.46
1:O:144:ARG:HG2	1:O:144:ARG:NH1	2.31	0.46
1:P:152:LEU:HD13	1:P:167:PHE:CD1	2.51	0.46
1:D:127:CYS:O	1:D:131:GLU:HG3	2.16	0.45
1:I:127:CYS:O	1:I:131:GLU:HG3	2.16	0.45
1:L:79:LEU:HD13	1:V:29:TYR:CE1	2.51	0.45
1:U:6:ARG:NH1	1:U:9:TYR:O	2.44	0.45
1:X:94:LEU:O	1:X:98:GLN:HG3	2.16	0.45
1:H:155:LEU:HD13	1:H:163:GLY:O	2.16	0.45
1:I:30:THR:HA	1:I:85:PRO:HG3	1.96	0.45
1:J:65:LYS:NZ	1:J:133:GLU:OE1	2.37	0.45
1:U:125:HIS:CB	3:U:203:EDO:H12	2.47	0.45
1:M:154:ARG:HG3	1:V:161:GLY:CA	2.46	0.45
1:U:125:HIS:CB	3:U:203:EDO:C1	2.95	0.45
1:H:172:VAL:O	1:H:173:LYS:CB	2.64	0.45
1:J:69:TYR:CE1	1:J:125:HIS:CE1	3.05	0.45
1:E:169:LYS:HE2	1:W:170:HIS:HB3	1.99	0.45
1:N:6:ARG:NH1	1:N:9:TYR:O	2.50	0.45
1:F:21:LEU:HD11	1:F:67:MET:HG2	1.98	0.45
2:G:202:PGE:H32	2:G:202:PGE:H52	1.72	0.45
1:O:23:LEU:HD13	1:O:107:VAL:HG22	1.97	0.45
1:S:152:LEU:HD13	1:S:167:PHE:CD1	2.51	0.45
1:V:46:HIS:CD2	4:V:217:HOH:O	2.70	0.45
4:K:216:HOH:O	1:W:60:ARG:HD2	2.16	0.45
1:U:125:HIS:HB3	3:U:203:EDO:H12	1.99	0.45
1:A:21:LEU:C	1:A:21:LEU:CD2	2.89	0.45
1:D:46:HIS:H	3:D:202:EDO:C1	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:20:MET:HE1	1:M:110:ALA:O	2.16	0.44
1:C:41:ASP:HA	1:F:147:ASP:OD1	2.18	0.44
4:E:312:HOH:O	1:I:60:ARG:HD2	2.16	0.44
1:J:21:LEU:C	1:J:21:LEU:HD23	2.42	0.44
1:M:152:LEU:HD13	1:M:167:PHE:CD1	2.52	0.44
1:Q:21:LEU:HD11	1:Q:67:MET:HG2	1.98	0.44
1:W:152:LEU:HD12	1:W:157:LEU:HD13	1.99	0.44
1:K:33:SER:HB2	1:W:79:LEU:HD12	1.98	0.44
1:S:118:ALA:HB2	1:S:126:LEU:HD23	2.00	0.44
1:A:114:LEU:HG	1:A:130:LEU:HD21	1.98	0.44
1:C:89:GLU:HG3	4:C:353:HOH:O	2.18	0.44
1:K:20:MET:HB2	1:K:20:MET:HE2	1.74	0.44
1:A:69:TYR:HE1	1:A:125:HIS:CE1	2.36	0.44
1:G:21:LEU:C	1:G:21:LEU:CD2	2.91	0.44
1:K:141:ASP:O	1:K:145:ILE:HD12	2.17	0.44
1:R:6:ARG:NH1	1:R:9:TYR:O	2.48	0.44
1:O:114:LEU:HG	1:O:130:LEU:HD21	2.00	0.44
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.71	0.43
1:R:85:PRO:HG2	4:R:301:HOH:O	2.18	0.43
1:T:45:LEU:HD13	1:U:154:ARG:NH2	2.32	0.43
1:U:152:LEU:HD12	1:U:157:LEU:HD13	1.99	0.43
1:I:93:THR:HG22	1:I:152:LEU:HD21	1.99	0.43
1:J:69:TYR:HE1	1:J:125:HIS:CE1	2.36	0.43
1:L:19:ARG:HH21	3:L:201:EDO:H12	1.82	0.43
1:M:65:LYS:HB3	1:M:134:TYR:OH	2.18	0.43
1:N:6:ARG:NH2	1:N:14:GLU:OE1	2.32	0.43
1:N:51:PHE:HB2	1:N:172:VAL:HG11	1.99	0.43
1:U:172:VAL:O	1:U:173:LYS:HB2	2.17	0.43
1:E:20:MET:HE1	1:E:110:ALA:CB	2.48	0.43
1:M:24:GLU:OE1	1:M:59:GLU:OE1	2.36	0.43
1:F:69:TYR:HE1	1:F:125:HIS:CE1	2.37	0.43
1:P:137:GLU:CG	4:P:340:HOH:O	2.65	0.43
1:C:114:LEU:HG	1:C:130:LEU:HD21	2.00	0.43
1:E:162:MET:CE	1:W:162:MET:HE2	2.48	0.43
1:C:57:HIS:HB3	4:C:344:HOH:O	2.19	0.43
1:M:35:TYR:O	1:M:36:ALA:C	2.61	0.43
1:G:98:GLN:HE21	1:G:98:GLN:HB2	1.59	0.43
1:R:47:ASN:HB2	1:R:168:ASP:OD1	2.18	0.43
1:X:68:LYS:HE2	4:X:312:HOH:O	2.19	0.43
1:C:155:LEU:HD13	1:C:163:GLY:O	2.19	0.43
1:E:60:ARG:HD2	4:I:302:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:LEU:O	1:F:107:VAL:HG23	2.19	0.43
1:C:162:MET:SD	1:F:162:MET:HE3	2.58	0.42
1:I:69:TYR:O	1:I:70:GLN:C	2.60	0.42
1:O:38:PHE:HB2	1:O:49:ALA:HB2	2.01	0.42
1:W:69:TYR:HE1	1:W:125:HIS:CE1	2.36	0.42
1:A:69:TYR:CE1	1:A:125:HIS:CE1	3.07	0.42
1:D:152:LEU:HD12	1:D:157:LEU:HD13	2.01	0.42
1:M:172:VAL:O	1:M:173:LYS:CB	2.64	0.42
1:O:152:LEU:O	1:O:157:LEU:HB2	2.19	0.42
1:J:16:ALA:HB1	1:J:114:LEU:HD13	2.00	0.42
1:V:25:LEU:HB3	1:V:82:ILE:HD13	2.01	0.42
1:D:126:LEU:HD12	1:D:130:LEU:HD22	2.02	0.42
1:E:122:VAL:O	1:E:122:VAL:HG12	2.18	0.42
1:F:105:LYS:HB3	1:O:7:GLN:NE2	2.35	0.42
1:W:172:VAL:O	1:W:173:LYS:CB	2.67	0.42
1:J:76:ARG:HA	1:J:76:ARG:HD3	1.77	0.42
1:B:29:TYR:O	1:B:32:SER:HB2	2.19	0.42
1:I:118:ALA:HB2	1:I:126:LEU:HD23	2.00	0.42
1:K:79:LEU:CD1	1:W:33:SER:HB2	2.49	0.42
1:L:149:ILE:O	1:L:150:THR:C	2.62	0.42
1:N:144:ARG:NH1	4:N:349:HOH:O	2.22	0.42
1:R:118:ALA:HB2	1:R:126:LEU:HD23	2.01	0.42
1:V:116:LYS:HD2	1:V:116:LYS:HA	1.81	0.42
1:B:20:MET:HE1	1:B:110:ALA:HB1	2.01	0.42
1:M:21:LEU:HD23	1:M:21:LEU:C	2.45	0.42
1:M:154:ARG:O	1:V:161:GLY:HA3	2.20	0.42
1:S:38:PHE:HB2	1:S:49:ALA:HB2	2.02	0.42
1:E:161:GLY:HA3	1:W:154:ARG:HG3	2.01	0.42
1:P:20:MET:HE2	1:P:20:MET:HB2	1.79	0.42
1:E:162:MET:SD	1:W:162:MET:CE	3.08	0.42
1:K:57:HIS:HB3	4:K:276:HOH:O	2.20	0.41
1:M:34:MET:O	1:M:38:PHE:HD2	2.02	0.41
1:N:131:GLU:HA	1:N:135:LEU:HD22	2.01	0.41
1:T:157:LEU:HD21	1:T:164:GLU:HG3	2.03	0.41
1:F:69:TYR:CE1	1:F:125:HIS:HE1	2.39	0.41
1:L:24:GLU:OE1	1:L:59:GLU:OE1	2.38	0.41
1:E:161:GLY:CA	1:W:154:ARG:HG3	2.50	0.41
1:L:60:ARG:CZ	1:L:60:ARG:HB3	2.48	0.41
1:Q:6:ARG:NH1	1:Q:9:TYR:O	2.48	0.41
1:R:124:PRO:HD2	4:R:319:HOH:O	2.20	0.41
1:T:173:LYS:HA	4:T:311:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:149:ILE:O	1:V:150:THR:C	2.61	0.41
1:G:21:LEU:HD23	1:G:63:ALA:HB1	2.02	0.41
1:L:20:MET:HE2	1:L:20:MET:HB2	1.89	0.41
1:O:46:HIS:HB3	4:O:357:HOH:O	2.20	0.41
1:O:138:GLN:HE21	1:O:138:GLN:HB3	1.64	0.41
1:R:136:GLU:OE2	1:R:140:LYS:HE3	2.21	0.41
1:B:155:LEU:HD22	1:B:163:GLY:HA2	2.01	0.41
1:V:60:ARG:CZ	1:V:60:ARG:HB3	2.50	0.41
1:X:172:VAL:O	1:X:173:LYS:CB	2.66	0.41
1:B:147:ASP:OD1	1:I:41:ASP:HA	2.20	0.41
1:B:169:LYS:HA	1:B:169:LYS:HD3	1.91	0.41
1:E:162:MET:SD	1:W:162:MET:HE2	2.60	0.41
1:F:10:HIS:O	1:F:13:CYS:HB2	2.20	0.41
1:F:60:ARG:HD2	4:F:302:HOH:O	2.20	0.41
1:K:168:ASP:OD2	1:K:169:LYS:NZ	2.52	0.41
1:X:111:LEU:HD12	1:X:138:GLN:HG3	2.02	0.41
1:A:165:TYR:OH	1:O:170:HIS:HB2	2.21	0.41
1:P:39:ASP:HB3	1:T:71:ASN:HD22	1.84	0.41
1:K:6:ARG:NH1	1:K:9:TYR:O	2.52	0.41
1:N:20:MET:HE2	3:N:201:EDO:H21	2.03	0.41
1:O:21:LEU:CD1	1:O:67:MET:HG2	2.41	0.41
1:V:148:PHE:O	1:V:152:LEU:HD22	2.19	0.41
1:W:69:TYR:CE1	1:W:125:HIS:CE1	3.09	0.41
1:B:20:MET:HE1	1:B:110:ALA:CB	2.51	0.41
1:F:69:TYR:HE1	1:F:125:HIS:HE1	1.69	0.41
1:F:69:TYR:CE1	1:F:125:HIS:CE1	3.09	0.41
1:F:98:GLN:HE21	1:F:98:GLN:HB2	1.69	0.41
1:I:114:LEU:HG	1:I:130:LEU:HD21	2.01	0.41
1:J:124:PRO:HB3	1:Q:115:HIS:CE1	2.56	0.41
1:P:32:SER:OG	1:T:67:MET:HE1	2.21	0.41
1:S:21:LEU:C	1:S:21:LEU:HD23	2.45	0.41
1:V:60:ARG:NH1	1:V:60:ARG:CB	2.84	0.41
1:A:24:GLU:OE1	1:A:59:GLU:OE1	2.39	0.41
1:D:21:LEU:C	1:D:21:LEU:HD23	2.46	0.41
1:F:111:LEU:HD13	1:F:134:TYR:HB3	2.02	0.41
1:B:69:TYR:HE1	1:B:125:HIS:CE1	2.39	0.40
1:B:155:LEU:HD13	1:B:163:GLY:O	2.21	0.40
1:F:152:LEU:HD13	1:F:167:PHE:CD1	2.56	0.40
1:P:21:LEU:HD23	1:P:21:LEU:C	2.45	0.40
1:R:21:LEU:HD11	1:R:67:MET:HG2	2.03	0.40
1:U:114:LEU:HG	1:U:130:LEU:HD21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:THR:HG22	1:E:152:LEU:HD21	2.04	0.40
1:K:101:LEU:HD12	1:K:101:LEU:HA	1.91	0.40
1:N:112:LEU:HD23	1:N:112:LEU:HA	1.94	0.40
1:A:69:TYR:CE1	1:A:125:HIS:HE1	2.39	0.40
1:V:10:HIS:CD2	1:V:121:LYS:HG2	2.57	0.40
1:X:65:LYS:HE2	1:X:133:GLU:CD	2.46	0.40
1:N:16:ALA:HB1	1:N:114:LEU:HD13	2.02	0.40
1:C:124:PRO:HB3	1:R:115:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	B	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	C	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
1	D	171/176 (97%)	166 (97%)	4 (2%)	1 (1%)	21	28
1	E	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	F	170/176 (97%)	167 (98%)	3 (2%)	0	100	100
1	G	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	H	171/176 (97%)	169 (99%)	1 (1%)	1 (1%)	21	28
1	I	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
1	J	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	K	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
1	L	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	M	170/176 (97%)	166 (98%)	3 (2%)	1 (1%)	21	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	O	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	P	170/176 (97%)	168 (99%)	2 (1%)	0	100	100
1	Q	170/176 (97%)	163 (96%)	7 (4%)	0	100	100
1	R	170/176 (97%)	164 (96%)	6 (4%)	0	100	100
1	S	170/176 (97%)	165 (97%)	5 (3%)	0	100	100
1	T	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
1	U	170/176 (97%)	167 (98%)	3 (2%)	0	100	100
1	V	170/176 (97%)	164 (96%)	5 (3%)	1 (1%)	21	28
1	W	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
1	X	170/176 (97%)	166 (98%)	4 (2%)	0	100	100
All	All	4086/4224 (97%)	3974 (97%)	108 (3%)	4 (0%)	48	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	11	SER
1	V	3	SER
1	D	172	VAL
1	H	91	GLY

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	152/157 (97%)	140 (92%)	12 (8%)	11	16
1	B	153/157 (98%)	140 (92%)	13 (8%)	10	14
1	C	153/157 (98%)	141 (92%)	12 (8%)	11	17
1	D	154/157 (98%)	142 (92%)	12 (8%)	11	17
1	E	152/157 (97%)	138 (91%)	14 (9%)	8	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	152/157 (97%)	141 (93%)	11 (7%)	13	18
1	G	152/157 (97%)	138 (91%)	14 (9%)	8	11
1	H	154/157 (98%)	143 (93%)	11 (7%)	13	19
1	I	154/157 (98%)	137 (89%)	17 (11%)	6	7
1	J	152/157 (97%)	136 (90%)	16 (10%)	6	8
1	K	154/157 (98%)	139 (90%)	15 (10%)	8	10
1	L	152/157 (97%)	135 (89%)	17 (11%)	6	6
1	M	153/157 (98%)	134 (88%)	19 (12%)	4	4
1	N	152/157 (97%)	136 (90%)	16 (10%)	6	8
1	O	153/157 (98%)	142 (93%)	11 (7%)	13	18
1	P	152/157 (97%)	138 (91%)	14 (9%)	8	11
1	Q	153/157 (98%)	137 (90%)	16 (10%)	6	8
1	R	153/157 (98%)	138 (90%)	15 (10%)	7	10
1	S	152/157 (97%)	136 (90%)	16 (10%)	6	8
1	T	154/157 (98%)	141 (92%)	13 (8%)	10	14
1	U	153/157 (98%)	137 (90%)	16 (10%)	6	8
1	V	153/157 (98%)	138 (90%)	15 (10%)	7	10
1	W	153/157 (98%)	134 (88%)	19 (12%)	4	4
1	X	152/157 (97%)	134 (88%)	18 (12%)	5	5
All	All	3667/3768 (97%)	3315 (90%)	352 (10%)	8	10

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	23	LEU
1	A	41	ASP
1	A	45	LEU
1	A	83	LYS
1	A	84	LYS
1	A	116	LYS
1	A	121	LYS
1	A	130	LEU
1	A	135	LEU
1	A	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	VAL
1	B	2	VAL
1	B	5	VAL
1	B	23	LEU
1	B	45	LEU
1	B	61	GLU
1	B	65	LYS
1	B	68	LYS
1	B	98	GLN
1	B	130	LEU
1	B	135	LEU
1	B	139	VAL
1	B	152	LEU
1	B	172	VAL
1	C	23	LEU
1	C	32	SER
1	C	45	LEU
1	C	89	GLU
1	C	121	LYS
1	C	130	LEU
1	C	135	LEU
1	C	137	GLU
1	C	138	GLN
1	C	144	ARG
1	C	152	LEU
1	C	173	LYS
1	D	1	MET
1	D	5	VAL
1	D	23	LEU
1	D	45	LEU
1	D	72	LYS
1	D	98	GLN
1	D	102	GLN
1	D	130	LEU
1	D	135	LEU
1	D	152	LEU
1	D	153	LYS
1	D	157	LEU
1	E	5	VAL
1	E	23	LEU
1	E	32	SER
1	E	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	98	GLN
1	E	102	GLN
1	E	105	LYS
1	E	114	LEU
1	E	121	LYS
1	E	130	LEU
1	E	139	VAL
1	E	140	LYS
1	E	152	LEU
1	E	172	VAL
1	F	2	VAL
1	F	5	VAL
1	F	6	ARG
1	F	32	SER
1	F	45	LEU
1	F	58	GLU
1	F	84	LYS
1	F	102	GLN
1	F	130	LEU
1	F	135	LEU
1	F	152	LEU
1	G	2	VAL
1	G	5	VAL
1	G	21	LEU
1	G	23	LEU
1	G	45	LEU
1	G	65	LYS
1	G	83	LYS
1	G	98	GLN
1	G	121	LYS
1	G	130	LEU
1	G	135	LEU
1	G	152	LEU
1	G	157	LEU
1	G	173	LYS
1	H	5	VAL
1	H	6	ARG
1	H	23	LEU
1	H	53	LYS
1	H	60	ARG
1	H	65	LYS
1	H	89	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	102	GLN
1	H	130	LEU
1	H	135	LEU
1	H	152	LEU
1	I	2	VAL
1	I	5	VAL
1	I	23	LEU
1	I	32	SER
1	I	45	LEU
1	I	58	GLU
1	I	89	GLU
1	I	116	LYS
1	I	121	LYS
1	I	130	LEU
1	I	135	LEU
1	I	139	VAL
1	I	144	ARG
1	I	152	LEU
1	I	157	LEU
1	I	172	VAL
1	I	173	LYS
1	J	5	VAL
1	J	21	LEU
1	J	23	LEU
1	J	45	LEU
1	J	80	GLN
1	J	84	LYS
1	J	102	GLN
1	J	119	THR
1	J	121	LYS
1	J	122	VAL
1	J	130	LEU
1	J	135	LEU
1	J	139	VAL
1	J	152	LEU
1	J	157	LEU
1	J	172	VAL
1	K	2	VAL
1	K	5	VAL
1	K	19	ARG
1	K	23	LEU
1	K	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	86	GLU
1	K	89	GLU
1	K	102	GLN
1	K	116	LYS
1	K	130	LEU
1	K	135	LEU
1	K	152	LEU
1	K	171	SER
1	K	172	VAL
1	K	173	LYS
1	L	3	SER
1	L	5	VAL
1	L	23	LEU
1	L	45	LEU
1	L	61	GLU
1	L	68	LYS
1	L	84	LYS
1	L	102	GLN
1	L	116	LYS
1	L	130	LEU
1	L	135	LEU
1	L	139	VAL
1	L	140	LYS
1	L	144	ARG
1	L	152	LEU
1	L	157	LEU
1	L	172	VAL
1	M	5	VAL
1	M	17	VAL
1	M	23	LEU
1	M	32	SER
1	M	45	LEU
1	M	54	GLU
1	M	61	GLU
1	M	65	LYS
1	M	68	LYS
1	M	72	LYS
1	M	83	LYS
1	M	102	GLN
1	M	116	LYS
1	M	121	LYS
1	M	130	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	135	LEU
1	M	144	ARG
1	M	152	LEU
1	M	172	VAL
1	N	5	VAL
1	N	23	LEU
1	N	45	LEU
1	N	58	GLU
1	N	60	ARG
1	N	65	LYS
1	N	68	LYS
1	N	72	LYS
1	N	83	LYS
1	N	86	GLU
1	N	122	VAL
1	N	130	LEU
1	N	135	LEU
1	N	144	ARG
1	N	152	LEU
1	N	172	VAL
1	O	5	VAL
1	O	23	LEU
1	O	41	ASP
1	O	45	LEU
1	O	68	LYS
1	O	122	VAL
1	O	130	LEU
1	O	135	LEU
1	O	139	VAL
1	O	152	LEU
1	O	157	LEU
1	P	5	VAL
1	P	23	LEU
1	P	45	LEU
1	P	65	LYS
1	P	72	LYS
1	P	80	GLN
1	P	86	GLU
1	P	122	VAL
1	P	130	LEU
1	P	135	LEU
1	P	139	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	152	LEU
1	P	157	LEU
1	P	168	ASP
1	Q	5	VAL
1	Q	11	SER
1	Q	23	LEU
1	Q	32	SER
1	Q	45	LEU
1	Q	68	LYS
1	Q	89	GLU
1	Q	102	GLN
1	Q	116	LYS
1	Q	121	LYS
1	Q	130	LEU
1	Q	135	LEU
1	Q	137	GLU
1	Q	144	ARG
1	Q	152	LEU
1	Q	171	SER
1	R	5	VAL
1	R	23	LEU
1	R	45	LEU
1	R	53	LYS
1	R	65	LYS
1	R	68	LYS
1	R	84	LYS
1	R	98	GLN
1	R	116	LYS
1	R	121	LYS
1	R	130	LEU
1	R	135	LEU
1	R	139	VAL
1	R	152	LEU
1	R	173	LYS
1	S	2	VAL
1	S	5	VAL
1	S	23	LEU
1	S	32	SER
1	S	45	LEU
1	S	68	LYS
1	S	84	LYS
1	S	98	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	116	LYS
1	S	122	VAL
1	S	130	LEU
1	S	139	VAL
1	S	144	ARG
1	S	152	LEU
1	S	153	LYS
1	S	157	LEU
1	T	1	MET
1	T	2	VAL
1	T	5	VAL
1	T	23	LEU
1	T	45	LEU
1	T	84	LYS
1	T	121	LYS
1	T	130	LEU
1	T	135	LEU
1	T	152	LEU
1	T	157	LEU
1	T	172	VAL
1	T	173	LYS
1	U	5	VAL
1	U	23	LEU
1	U	45	LEU
1	U	60	ARG
1	U	65	LYS
1	U	86	GLU
1	U	102	GLN
1	U	116	LYS
1	U	121	LYS
1	U	130	LEU
1	U	135	LEU
1	U	137	GLU
1	U	139	VAL
1	U	144	ARG
1	U	152	LEU
1	U	157	LEU
1	V	23	LEU
1	V	30	THR
1	V	45	LEU
1	V	60	ARG
1	V	68	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	86	GLU
1	V	121	LYS
1	V	122	VAL
1	V	130	LEU
1	V	135	LEU
1	V	139	VAL
1	V	152	LEU
1	V	157	LEU
1	V	172	VAL
1	V	173	LYS
1	X	2	VAL
1	X	5	VAL
1	X	11	SER
1	X	21	LEU
1	X	23	LEU
1	X	32	SER
1	X	45	LEU
1	X	53	LYS
1	X	65	LYS
1	X	68	LYS
1	X	116	LYS
1	X	121	LYS
1	X	130	LEU
1	X	135	LEU
1	X	152	LEU
1	X	157	LEU
1	X	172	VAL
1	X	173	LYS
1	W	1	MET
1	W	5	VAL
1	W	11	SER
1	W	23	LEU
1	W	32	SER
1	W	45	LEU
1	W	54	GLU
1	W	65	LYS
1	W	68	LYS
1	W	84	LYS
1	W	98	GLN
1	W	116	LYS
1	W	130	LEU
1	W	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	137	GLU
1	W	139	VAL
1	W	152	LEU
1	W	157	LEU
1	W	172	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	98	GLN
1	A	138	GLN
1	B	4	GLN
1	B	7	GLN
1	B	98	GLN
1	B	102	GLN
1	B	138	GLN
1	C	46	HIS
1	C	108	ASN
1	C	138	GLN
1	C	151	ASN
1	D	98	GLN
1	D	109	GLN
1	D	138	GLN
1	E	4	GLN
1	E	8	ASN
1	E	115	HIS
1	F	22	ASN
1	F	98	GLN
1	F	108	ASN
1	F	115	HIS
1	G	98	GLN
1	G	115	HIS
1	G	138	GLN
1	G	151	ASN
1	H	55	HIS
1	H	80	GLN
1	H	98	GLN
1	H	108	ASN
1	H	151	ASN
1	I	98	GLN
1	I	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	115	HIS
1	J	7	GLN
1	J	98	GLN
1	J	170	HIS
1	K	55	HIS
1	K	80	GLN
1	L	4	GLN
1	L	70	GLN
1	L	98	GLN
1	L	115	HIS
1	L	151	ASN
1	M	98	GLN
1	M	108	ASN
1	M	115	HIS
1	N	108	ASN
1	O	57	HIS
1	O	102	GLN
1	O	108	ASN
1	O	109	GLN
1	O	138	GLN
1	P	55	HIS
1	P	115	HIS
1	P	138	GLN
1	Q	108	ASN
1	Q	115	HIS
1	R	57	HIS
1	R	98	GLN
1	S	55	HIS
1	S	62	HIS
1	S	98	GLN
1	S	115	HIS
1	S	138	GLN
1	T	115	HIS
1	U	62	HIS
1	U	98	GLN
1	U	138	GLN
1	U	170	HIS
1	V	57	HIS
1	V	80	GLN
1	V	108	ASN
1	V	160	ASN
1	X	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	80	GLN
1	X	115	HIS
1	X	138	GLN
1	W	98	GLN

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](#)

34 ligands are 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	$\# Z > 2$
2	PGE	I	201	-	9,9,9	0.65	0	8,8,8	0.47	0
2	PGE	G	202	-	9,9,9	0.63	0	8,8,8	0.35	0
2	PGE	X	201	-	9,9,9	0.55	0	8,8,8	0.70	0
2	PGE	E	201	-	9,9,9	0.85	0	8,8,8	0.88	0
2	PGE	G	201	-	9,9,9	0.81	0	8,8,8	0.85	0
3	EDO	B	202	-	3,3,3	0.78	0	2,2,2	0.32	0
2	PGE	U	201	-	9,9,9	0.56	0	8,8,8	0.71	0
2	PGE	B	201	-	9,9,9	0.52	0	8,8,8	0.53	0
2	PGE	R	203	-	9,9,9	0.48	0	8,8,8	0.46	0
3	EDO	O	201	-	3,3,3	0.80	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	202	-	3,3,3	0.83	0	2,2,2	0.37	0
2	PGE	H	202	-	9,9,9	0.60	0	8,8,8	0.44	0
3	EDO	N	202	-	3,3,3	0.92	0	2,2,2	0.55	0
3	EDO	U	202	-	3,3,3	0.83	0	2,2,2	0.41	0
2	PGE	H	201	-	9,9,9	0.71	0	8,8,8	0.79	0
3	EDO	N	201	-	3,3,3	0.64	0	2,2,2	0.33	0
3	EDO	U	203	-	3,3,3	1.28	0	2,2,2	0.93	0
2	PGE	C	202	-	9,9,9	0.49	0	8,8,8	0.53	0
2	PGE	W	201	-	9,9,9	0.99	0	8,8,8	1.01	0
2	PGE	R	201	-	9,9,9	0.85	0	8,8,8	0.68	0
2	PGE	W	202	-	9,9,9	0.56	0	8,8,8	0.33	0
3	EDO	J	201	-	3,3,3	0.68	0	2,2,2	0.29	0
2	PGE	C	201	-	9,9,9	0.97	0	8,8,8	1.02	0
2	PGE	S	201	-	9,9,9	0.54	0	8,8,8	0.53	0
2	PGE	D	201	-	9,9,9	0.48	0	8,8,8	0.31	0
3	EDO	M	201	-	3,3,3	0.54	0	2,2,2	0.30	0
3	EDO	P	202	-	3,3,3	0.38	0	2,2,2	0.56	0
2	PGE	Q	202	-	9,9,9	0.46	0	8,8,8	0.58	0
2	PGE	P	201	-	9,9,9	0.73	0	8,8,8	0.60	0
2	PGE	Q	201	-	9,9,9	0.92	0	8,8,8	0.96	0
2	PGE	F	201	-	9,9,9	0.53	0	8,8,8	0.24	0
3	EDO	T	201	-	3,3,3	0.70	0	2,2,2	0.22	0
2	PGE	R	202	-	9,9,9	0.98	0	8,8,8	1.36	1 (12%)
3	EDO	L	201	-	3,3,3	0.52	0	2,2,2	0.43	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
2	PGE	I	201	-	-	3/7/7/7	-
2	PGE	G	202	-	-	4/7/7/7	-
2	PGE	X	201	-	-	4/7/7/7	-
2	PGE	E	201	-	-	5/7/7/7	-
2	PGE	G	201	-	-	3/7/7/7	-
3	EDO	B	202	-	-	1/1/1/1	-
2	PGE	U	201	-	-	3/7/7/7	-
2	PGE	B	201	-	-	5/7/7/7	-
2	PGE	R	203	-	-	3/7/7/7	-
3	EDO	O	201	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	202	-	-	1/1/1/1	-
2	PGE	H	202	-	-	4/7/7/7	-
3	EDO	N	202	-	-	1/1/1/1	-
3	EDO	U	202	-	-	0/1/1/1	-
2	PGE	H	201	-	-	5/7/7/7	-
3	EDO	N	201	-	-	1/1/1/1	-
3	EDO	U	203	-	-	1/1/1/1	-
2	PGE	C	202	-	-	6/7/7/7	-
2	PGE	W	201	-	-	6/7/7/7	-
2	PGE	R	201	-	-	7/7/7/7	-
2	PGE	W	202	-	-	3/7/7/7	-
3	EDO	J	201	-	-	1/1/1/1	-
2	PGE	C	201	-	-	5/7/7/7	-
2	PGE	S	201	-	-	3/7/7/7	-
2	PGE	D	201	-	-	3/7/7/7	-
3	EDO	M	201	-	-	1/1/1/1	-
3	EDO	P	202	-	-	0/1/1/1	-
2	PGE	Q	202	-	-	3/7/7/7	-
2	PGE	P	201	-	-	3/7/7/7	-
2	PGE	Q	201	-	-	4/7/7/7	-
2	PGE	F	201	-	-	2/7/7/7	-
3	EDO	T	201	-	-	1/1/1/1	-
2	PGE	R	202	-	-	4/7/7/7	-
3	EDO	L	201	-	-	1/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	202	PGE	O2-C2-C1	2.42	120.77	110.11

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	201	PGE	C1-C2-O2-C3
2	E	201	PGE	C6-C5-O3-C4
2	C	201	PGE	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	P	201	PGE	O2-C3-C4-O3
2	X	201	PGE	O2-C3-C4-O3
2	G	202	PGE	O2-C3-C4-O3
2	D	201	PGE	O2-C3-C4-O3
2	W	202	PGE	O2-C3-C4-O3
2	U	201	PGE	O2-C3-C4-O3
2	Q	202	PGE	O2-C3-C4-O3
2	R	201	PGE	C1-C2-O2-C3
2	C	202	PGE	O3-C5-C6-O4
2	G	201	PGE	O1-C1-C2-O2
2	G	202	PGE	O1-C1-C2-O2
2	P	201	PGE	O3-C5-C6-O4
2	R	202	PGE	O3-C5-C6-O4
2	G	202	PGE	C3-C4-O3-C5
2	D	201	PGE	O1-C1-C2-O2
2	F	201	PGE	O3-C5-C6-O4
2	I	201	PGE	O3-C5-C6-O4
2	Q	202	PGE	O1-C1-C2-O2
2	W	202	PGE	O1-C1-C2-O2
2	H	202	PGE	O1-C1-C2-O2
2	B	201	PGE	O2-C3-C4-O3
2	Q	201	PGE	O2-C3-C4-O3
2	I	201	PGE	O2-C3-C4-O3
2	G	201	PGE	O3-C5-C6-O4
2	H	201	PGE	O3-C5-C6-O4
2	Q	201	PGE	O3-C5-C6-O4
2	U	201	PGE	O3-C5-C6-O4
2	W	201	PGE	O3-C5-C6-O4
3	D	202	EDO	O1-C1-C2-O2
2	H	201	PGE	O2-C3-C4-O3
2	X	201	PGE	O3-C5-C6-O4
2	B	201	PGE	O1-C1-C2-O2
2	C	202	PGE	O1-C1-C2-O2
2	E	201	PGE	O3-C5-C6-O4
2	H	201	PGE	O1-C1-C2-O2
2	R	201	PGE	O1-C1-C2-O2
2	R	201	PGE	O3-C5-C6-O4
3	B	202	EDO	O1-C1-C2-O2
3	L	201	EDO	O1-C1-C2-O2
2	W	201	PGE	O2-C3-C4-O3
2	C	202	PGE	O2-C3-C4-O3
2	R	203	PGE	O3-C5-C6-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	201	EDO	O1-C1-C2-O2
3	M	201	EDO	O1-C1-C2-O2
2	S	201	PGE	O2-C3-C4-O3
2	E	201	PGE	O1-C1-C2-O2
2	G	202	PGE	C4-C3-O2-C2
2	W	201	PGE	O1-C1-C2-O2
2	B	201	PGE	C3-C4-O3-C5
2	H	202	PGE	C4-C3-O2-C2
2	W	201	PGE	C1-C2-O2-C3
2	S	201	PGE	C6-C5-O3-C4
2	W	201	PGE	C6-C5-O3-C4
2	D	201	PGE	C1-C2-O2-C3
2	C	202	PGE	C3-C4-O3-C5
2	R	201	PGE	C3-C4-O3-C5
2	H	202	PGE	C3-C4-O3-C5
2	C	202	PGE	C1-C2-O2-C3
2	R	202	PGE	C3-C4-O3-C5
2	I	201	PGE	C3-C4-O3-C5
2	Q	202	PGE	C4-C3-O2-C2
2	S	201	PGE	C4-C3-O2-C2
2	R	203	PGE	C4-C3-O2-C2
2	Q	201	PGE	C1-C2-O2-C3
2	Q	201	PGE	C3-C4-O3-C5
2	F	201	PGE	O2-C3-C4-O3
2	R	203	PGE	C6-C5-O3-C4
2	W	201	PGE	C3-C4-O3-C5
2	R	201	PGE	C4-C3-O2-C2
2	U	201	PGE	C3-C4-O3-C5
2	C	201	PGE	C1-C2-O2-C3
2	C	201	PGE	C6-C5-O3-C4
2	X	201	PGE	C6-C5-O3-C4
3	N	201	EDO	O1-C1-C2-O2
2	E	201	PGE	C4-C3-O2-C2
2	R	202	PGE	C6-C5-O3-C4
2	H	202	PGE	C1-C2-O2-C3
2	H	201	PGE	C3-C4-O3-C5
2	B	201	PGE	C6-C5-O3-C4
2	R	201	PGE	C6-C5-O3-C4
3	U	203	EDO	O1-C1-C2-O2
2	B	201	PGE	C1-C2-O2-C3
2	W	202	PGE	C4-C3-O2-C2
2	C	201	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	201	PGE	O2-C3-C4-O3
3	N	202	EDO	O1-C1-C2-O2
3	T	201	EDO	O1-C1-C2-O2
2	C	201	PGE	O3-C5-C6-O4
2	R	202	PGE	O2-C3-C4-O3
2	C	202	PGE	C6-C5-O3-C4
2	X	201	PGE	C4-C3-O2-C2
2	P	201	PGE	C4-C3-O2-C2
2	R	201	PGE	O2-C3-C4-O3
2	G	201	PGE	C1-C2-O2-C3

There are no ring outliers.

20 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	202	PGE	1	0
2	B	201	PGE	1	0
2	R	203	PGE	1	0
3	O	201	EDO	1	0
3	D	202	EDO	1	0
2	H	202	PGE	1	0
3	N	202	EDO	1	0
3	U	202	EDO	3	0
2	H	201	PGE	2	0
3	N	201	EDO	1	0
3	U	203	EDO	6	0
2	C	202	PGE	1	0
2	S	201	PGE	1	0
2	D	201	PGE	1	0
3	M	201	EDO	1	0
3	P	202	EDO	1	0
2	Q	202	PGE	1	0
2	P	201	PGE	1	0
2	R	202	PGE	7	0
3	L	201	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	172/176 (97%)	-0.61	0 100 100	18, 27, 37, 45	0
1	B	172/176 (97%)	-0.34	1 (0%) 85 88	26, 34, 44, 51	0
1	C	172/176 (97%)	-0.58	1 (0%) 85 88	21, 29, 40, 52	0
1	D	173/176 (98%)	-0.54	1 (0%) 85 88	17, 27, 38, 59	0
1	E	172/176 (97%)	-0.28	0 100 100	26, 35, 44, 50	0
1	F	172/176 (97%)	-0.42	0 100 100	22, 32, 42, 55	0
1	G	172/176 (97%)	-0.58	0 100 100	21, 29, 40, 55	0
1	H	173/176 (98%)	-0.59	0 100 100	19, 29, 39, 50	0
1	I	173/176 (98%)	-0.42	1 (0%) 85 88	24, 32, 42, 59	0
1	J	172/176 (97%)	-0.66	0 100 100	19, 25, 36, 48	0
1	K	173/176 (98%)	-0.64	0 100 100	19, 26, 37, 49	0
1	L	172/176 (97%)	-0.23	0 100 100	27, 36, 44, 52	0
1	M	172/176 (97%)	-0.28	0 100 100	27, 36, 45, 52	0
1	N	172/176 (97%)	-0.62	0 100 100	17, 27, 39, 50	0
1	O	172/176 (97%)	-0.63	1 (0%) 85 88	20, 27, 37, 50	0
1	P	172/176 (97%)	-0.46	0 100 100	22, 30, 40, 47	0
1	Q	172/176 (97%)	-0.64	1 (0%) 85 88	17, 27, 37, 43	0
1	R	172/176 (97%)	-0.64	0 100 100	18, 27, 38, 48	0
1	S	172/176 (97%)	-0.43	0 100 100	24, 33, 41, 51	0
1	T	173/176 (98%)	-0.37	0 100 100	22, 34, 45, 62	0
1	U	172/176 (97%)	-0.61	0 100 100	19, 28, 38, 51	0
1	V	172/176 (97%)	-0.26	1 (0%) 85 88	26, 36, 45, 52	0
1	W	173/176 (98%)	-0.59	1 (0%) 85 88	20, 28, 39, 56	0
1	X	172/176 (97%)	-0.69	0 100 100	18, 26, 36, 47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4134/4224 (97%)	-0.50	8 (0%) 91 92	17, 30, 42, 62	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	4.8
1	V	2	VAL	3.4
1	I	1	MET	3.1
1	B	2	VAL	3.0
1	W	1	MET	2.9
1	Q	2	VAL	2.5
1	O	2	VAL	2.4
1	C	173	LYS	2.3

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	EDO	M	201	4/4	0.84	0.28	50,51,52,53	0
3	EDO	N	201	4/4	0.84	0.20	50,51,52,53	0
3	EDO	U	203	4/4	0.85	0.20	28,33,34,34	0
3	EDO	O	201	4/4	0.86	0.23	50,52,53,54	0
2	PGE	R	202	10/10	0.87	0.25	38,46,47,48	0
3	EDO	D	202	4/4	0.87	0.22	42,47,49,50	0
3	EDO	U	202	4/4	0.88	0.18	42,43,43,46	0
3	EDO	N	202	4/4	0.88	0.19	48,48,50,50	0
2	PGE	G	201	10/10	0.89	0.13	39,40,46,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PGE	Q	201	10/10	0.89	0.13	41,44,46,48	0
3	EDO	B	202	4/4	0.90	0.17	45,45,46,47	0
2	PGE	G	202	10/10	0.90	0.17	52,55,59,59	0
2	PGE	E	201	10/10	0.90	0.16	51,53,57,58	0
2	PGE	C	201	10/10	0.90	0.14	37,46,49,50	0
2	PGE	I	201	10/10	0.91	0.15	48,51,56,58	0
2	PGE	W	201	10/10	0.91	0.13	40,43,44,44	0
2	PGE	P	201	10/10	0.91	0.16	53,55,63,64	0
3	EDO	T	201	4/4	0.91	0.18	38,40,40,41	0
2	PGE	D	201	10/10	0.91	0.14	56,58,59,60	0
2	PGE	R	201	10/10	0.91	0.14	41,42,44,44	0
2	PGE	U	201	10/10	0.92	0.13	40,44,52,53	0
2	PGE	X	201	10/10	0.92	0.12	42,47,51,53	0
2	PGE	H	202	10/10	0.93	0.11	40,47,53,55	0
2	PGE	Q	202	10/10	0.93	0.13	54,56,62,64	0
3	EDO	J	201	4/4	0.94	0.15	30,33,35,36	0
2	PGE	R	203	10/10	0.94	0.12	55,57,62,63	0
2	PGE	C	202	10/10	0.94	0.13	56,59,60,60	0
2	PGE	B	201	10/10	0.94	0.13	54,56,59,59	0
3	EDO	L	201	4/4	0.95	0.14	33,34,36,37	0
2	PGE	S	201	10/10	0.95	0.11	42,47,55,56	0
2	PGE	H	201	10/10	0.95	0.10	35,39,42,45	0
2	PGE	W	202	10/10	0.95	0.10	43,45,48,50	0
2	PGE	F	201	10/10	0.96	0.11	45,56,66,67	0
3	EDO	P	202	4/4	0.97	0.09	48,48,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.