



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:49 AM UTC

PDB ID : 3QGA / pdb_00003qga
Title : 3.0 A Model of Iron Containing Urease UreA2B2 from Helicobacter mustelae
Authors : Tronrud, D.E.; Robbins, A.; Karplus, P.A.
Deposited on : 2011-01-24
Resolution : 3.00 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

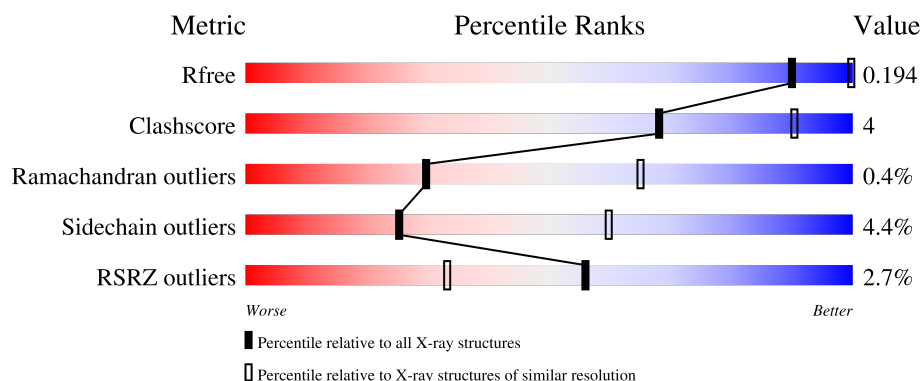
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	225	
1	D	225	
1	G	225	
1	J	225	
1	M	225	

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Mol	Chain	Length	Quality of chain
1	P	225	88%11%
2	C	568	4% 85%13%..
2	F	568	3% 84%14%..
2	I	568	3% 83%14%..
2	L	568	3% 84%14%..
2	O	568	4% 85%12%..
2	R	568	4% 85%13%..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37026 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 Fusion of urease beta and gamma subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1767	1124	310	326	7			
1	D	225	Total	C	N	O	S	0	0	0
			1767	1124	310	326	7			
1	G	225	Total	C	N	O	S	0	0	0
			1767	1124	310	326	7			
1	J	225	Total	C	N	O	S	0	0	0
			1767	1124	310	326	7			
1	M	225	Total	C	N	O	S	0	0	0
			1767	1124	310	326	7			
1	P	225	Total	C	N	O	S	0	0	0
			1767	1124	310	326	7			

- Molecule 2 is a protein called Urease subunit beta 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	564	Total	C	N	O	S	0	0	0
			4301	2701	740	836	24			
2	F	564	Total	C	N	O	S	0	0	0
			4301	2701	740	836	24			
2	I	564	Total	C	N	O	S	0	0	0
			4301	2701	740	836	24			
2	L	564	Total	C	N	O	S	0	0	0
			4301	2701	740	836	24			
2	O	564	Total	C	N	O	S	0	0	0
			4301	2701	740	836	24			
2	R	564	Total	C	N	O	S	0	0	0
			4301	2701	740	836	24			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total Fe 2 2	0	0
3	F	2	Total Fe 2 2	0	0
3	I	2	Total Fe 2 2	0	0
3	L	2	Total Fe 2 2	0	0
3	O	2	Total Fe 2 2	0	0
3	R	2	Total Fe 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	C	92	Total O 92 92	0	0
4	D	9	Total O 9 9	0	0
4	F	90	Total O 90 90	0	0
4	G	10	Total O 10 10	0	0
4	I	92	Total O 92 92	0	0
4	J	10	Total O 10 10	0	0
4	L	92	Total O 92 92	0	0
4	M	10	Total O 10 10	0	0
4	O	92	Total O 92 92	0	0
4	P	9	Total O 9 9	0	0
4	R	91	Total O 91 91	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: Fusion of urease beta and gamma subunits

Chain A:  91% 9%



- Molecule 1: Fusion of urease beta and gamma subunits

Chain D:  88% 12%



- Molecule 1: Fusion of urease beta and gamma subunits

Chain G:  89% 10%



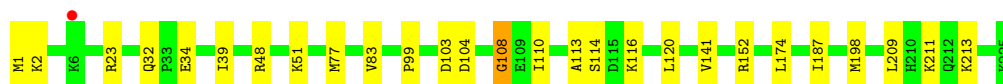
- Molecule 1: Fusion of urease beta and gamma subunits

Chain J:  89% 11%



- Molecule 1: Fusion of urease beta and gamma subunits

Chain M:  88% 12%



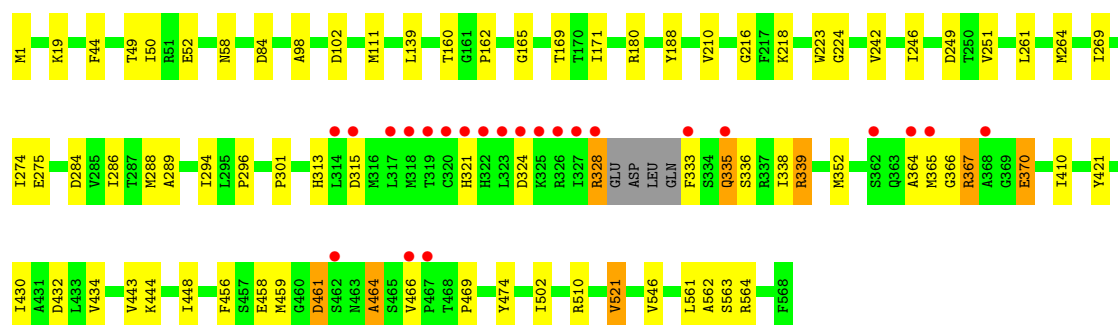
- Molecule 1: Fusion of urease beta and gamma subunits

Chain P:  88% 11%



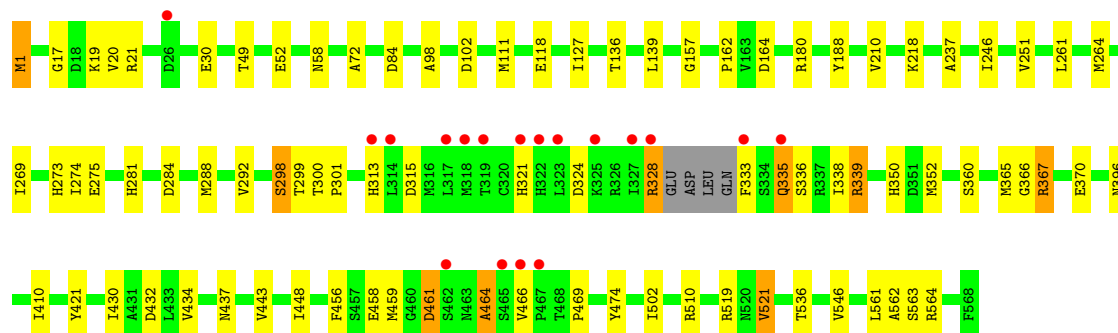
• Molecule 2: Urease subunit beta 2

Chain C:  85% 13% 2%



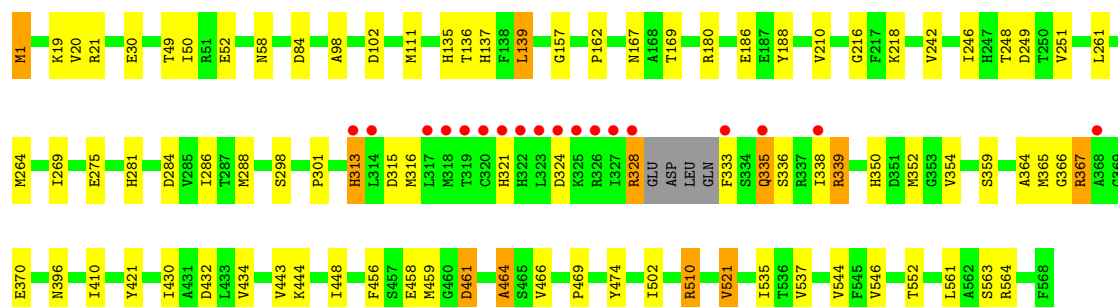
• Molecule 2: Urease subunit beta 2

Chain F:  84% 14% 2%



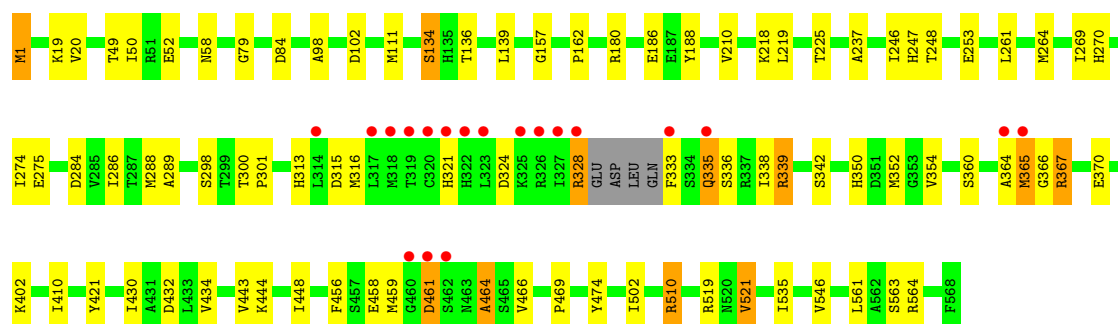
• Molecule 2: Urease subunit beta 2

Chain I:  83% 14% 3%

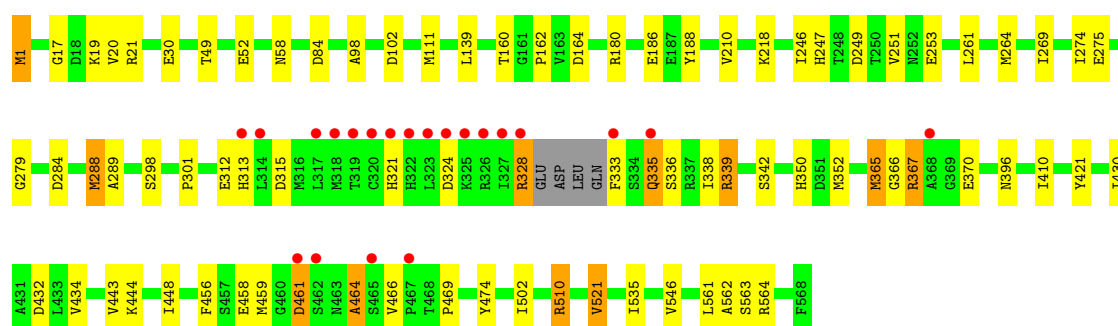
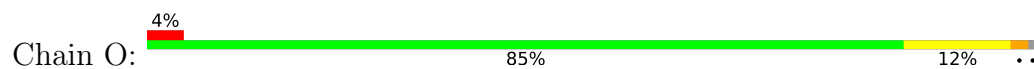


• Molecule 2: Urease subunit beta 2

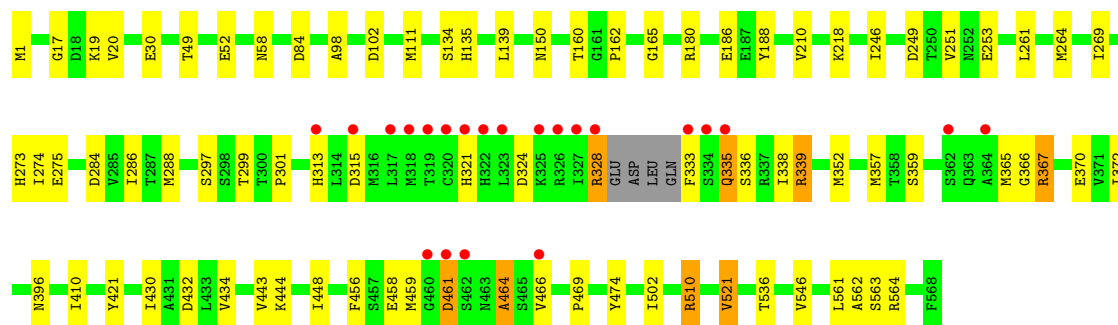
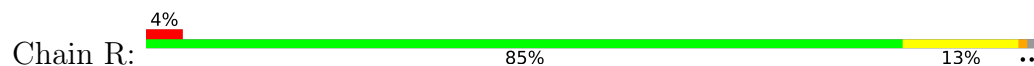
Chain L:  84% 14% 2%



• Molecule 2: Urease subunit beta 2



• Molecule 2: Urease subunit beta 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.98Å 223.94Å 395.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.29 – 3.00 67.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (67.29-3.00) 98.4 (67.29-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.170 , 0.189 0.177 , 0.194	Depositor DCC
R_{free} test set	7283 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	37026	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: FME, FE, KCX

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	0.77	0/1791	1.28	1/2401 (0.0%)
1	D	0.78	0/1791	1.30	6/2401 (0.2%)
1	G	0.77	1/1791 (0.1%)	1.29	4/2401 (0.2%)
1	J	0.74	0/1791	1.29	6/2401 (0.2%)
1	M	0.75	0/1791	1.29	4/2401 (0.2%)
1	P	0.75	0/1791	1.29	2/2401 (0.1%)
2	C	0.82	1/4376 (0.0%)	1.36	21/5925 (0.4%)
2	F	0.82	1/4376 (0.0%)	1.36	21/5925 (0.4%)
2	I	0.81	2/4376 (0.0%)	1.34	17/5925 (0.3%)
2	L	0.81	1/4376 (0.0%)	1.36	19/5925 (0.3%)
2	O	0.81	2/4376 (0.0%)	1.35	17/5925 (0.3%)
2	R	0.80	1/4376 (0.0%)	1.36	19/5925 (0.3%)
All	All	0.80	9/37002 (0.0%)	1.34	137/49956 (0.3%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	321	HIS	ND1-CE1	6.21	1.38	1.32
2	F	321	HIS	ND1-CE1	5.87	1.38	1.32
2	L	321	HIS	ND1-CE1	5.75	1.38	1.32
2	C	321	HIS	ND1-CE1	5.62	1.38	1.32
2	R	321	HIS	ND1-CE1	5.58	1.38	1.32
2	O	321	HIS	ND1-CE1	5.55	1.38	1.32
2	O	288	MET	SD-CE	-5.42	1.66	1.79
2	I	316	MET	SD-CE	-5.19	1.66	1.79
1	G	77	MET	SD-CE	-5.04	1.67	1.79

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	284	ASP	N-CA-C	8.10	121.96	112.72
2	I	410	ILE	N-CA-C	7.77	117.83	110.53
2	F	410	ILE	N-CA-C	7.72	117.79	110.53
2	R	410	ILE	N-CA-C	7.72	117.78	110.53
2	O	249	ASP	CA-CB-CG	7.67	120.27	112.60
2	O	410	ILE	N-CA-C	7.63	117.71	110.53
2	C	410	ILE	N-CA-C	7.60	117.67	110.53
2	L	321	HIS	CB-CG-CD2	-7.47	121.48	131.20
2	O	321	HIS	CB-CG-CD2	-7.44	121.53	131.20
2	C	321	HIS	CB-CG-CD2	-7.43	121.54	131.20
2	R	321	HIS	CB-CG-CD2	-7.38	121.60	131.20
2	F	321	HIS	CB-CG-CD2	-7.38	121.60	131.20
2	I	321	HIS	CB-CG-CD2	-7.36	121.63	131.20
2	L	410	ILE	N-CA-C	7.36	117.45	110.53
2	F	284	ASP	N-CA-C	7.29	121.03	112.72
2	O	246	ILE	N-CA-C	7.08	118.51	108.17
2	C	246	ILE	N-CA-C	6.91	118.25	108.17
2	C	284	ASP	N-CA-C	6.70	120.76	112.59
2	I	188	TYR	N-CA-C	6.58	120.14	110.59
2	R	284	ASP	N-CA-C	6.58	120.62	112.59
2	L	284	ASP	N-CA-C	6.53	120.56	112.59
2	R	249	ASP	CA-CB-CG	6.49	119.09	112.60
2	O	284	ASP	N-CA-C	6.47	120.49	112.59
2	R	521	VAL	N-CA-CB	6.46	118.77	111.21
2	R	246	ILE	N-CA-C	6.45	117.40	108.12
2	O	188	TYR	N-CA-C	6.44	119.93	110.59
2	I	246	ILE	N-CA-C	6.38	117.97	108.46
2	C	102	ASP	CA-CB-CG	6.37	118.97	112.60
2	L	188	TYR	N-CA-C	6.28	119.69	110.59
2	F	188	TYR	N-CA-C	6.27	119.68	110.59
2	I	102	ASP	CA-CB-CG	6.26	118.86	112.60
2	C	188	TYR	N-CA-C	6.24	119.64	110.59
2	L	432	ASP	CA-CB-CG	6.20	118.80	112.60
2	C	160	THR	N-CA-C	-6.19	106.36	114.04
2	F	521	VAL	N-CA-CB	6.15	118.41	111.21
2	I	249	ASP	CA-CB-CG	6.14	118.74	112.60
2	O	432	ASP	CA-CB-CG	6.13	118.73	112.60
2	R	367	ARG	N-CA-C	6.13	118.72	108.73
2	L	521	VAL	N-CA-CB	6.13	118.38	111.21
2	I	432	ASP	CA-CB-CG	6.08	118.69	112.60
2	L	102	ASP	CA-CB-CG	6.06	118.66	112.60
2	R	188	TYR	N-CA-C	6.06	119.38	110.59
2	F	432	ASP	CA-CB-CG	6.06	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	360	SER	N-CA-C	6.05	121.18	113.55
2	O	521	VAL	N-CA-CB	6.02	118.25	111.21
2	C	432	ASP	CA-CB-CG	5.98	118.58	112.60
2	I	521	VAL	N-CA-CB	5.98	118.20	111.21
2	I	367	ARG	CA-C-N	5.97	128.60	120.54
2	I	367	ARG	C-N-CA	5.97	128.60	120.54
2	R	432	ASP	CA-CB-CG	5.96	118.56	112.60
2	I	284	ASP	CA-CB-CG	5.95	118.55	112.60
2	O	102	ASP	CA-CB-CG	5.95	118.55	112.60
2	F	461	ASP	CA-CB-CG	5.93	118.53	112.60
2	I	248	THR	N-CA-C	5.93	117.98	110.33
2	F	102	ASP	CA-CB-CG	5.92	118.52	112.60
2	R	461	ASP	CA-CB-CG	5.92	118.52	112.60
2	O	461	ASP	CA-CB-CG	5.91	118.51	112.60
2	F	367	ARG	N-CA-C	5.88	118.32	108.73
1	P	211	LYS	N-CA-C	5.87	118.16	111.11
2	I	461	ASP	CA-CB-CG	5.85	118.45	112.60
2	R	102	ASP	CA-CB-CG	5.82	118.42	112.60
2	R	562	ALA	CA-C-N	5.82	128.35	120.38
2	R	562	ALA	C-N-CA	5.82	128.35	120.38
2	F	246	ILE	N-CA-C	5.78	116.60	108.17
2	L	246	ILE	N-CA-C	5.75	116.56	108.17
2	C	461	ASP	CA-CB-CG	5.74	118.34	112.60
2	C	521	VAL	N-CA-CB	5.72	117.90	111.21
1	M	103	ASP	CA-CB-CG	5.70	118.30	112.60
2	C	562	ALA	CA-C-N	5.69	128.18	120.38
2	C	562	ALA	C-N-CA	5.69	128.18	120.38
2	R	165	GLY	CA-C-N	5.69	128.37	120.29
2	R	165	GLY	C-N-CA	5.69	128.37	120.29
1	D	76	ASN	CA-C-N	5.69	128.96	120.31
1	D	76	ASN	C-N-CA	5.69	128.96	120.31
2	L	367	ARG	N-CA-C	5.68	117.99	108.73
1	G	211	LYS	N-CA-C	5.68	117.92	111.11
2	O	84	ASP	CA-CB-CG	5.67	118.27	112.60
2	C	367	ARG	N-CA-C	5.62	117.89	108.73
2	L	461	ASP	CA-CB-CG	5.61	118.21	112.60
1	J	211	LYS	N-CA-C	5.59	117.82	111.11
2	C	367	ARG	CA-C-N	5.56	128.04	120.54
2	C	367	ARG	C-N-CA	5.56	128.04	120.54
2	L	367	ARG	CA-C-N	5.55	128.04	120.54
2	L	367	ARG	C-N-CA	5.55	128.04	120.54
1	M	211	LYS	N-CA-C	5.55	117.77	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	367	ARG	CA-C-N	5.55	128.03	120.54
2	O	367	ARG	C-N-CA	5.55	128.03	120.54
2	F	84	ASP	CA-CB-CG	5.54	118.14	112.60
1	D	211	LYS	N-CA-C	5.54	117.75	111.11
2	L	364	ALA	CA-C-N	5.50	132.04	121.54
2	L	364	ALA	C-N-CA	5.50	132.04	121.54
2	L	284	ASP	CA-CB-CG	5.49	118.09	112.60
2	O	562	ALA	CA-C-N	5.48	128.38	120.38
2	O	562	ALA	C-N-CA	5.48	128.38	120.38
2	I	367	ARG	N-CA-C	5.47	117.65	108.73
2	I	84	ASP	CA-CB-CG	5.46	118.06	112.60
2	F	284	ASP	CA-CB-CG	5.46	118.06	112.60
2	L	300	THR	N-CA-C	5.44	121.01	113.45
1	J	76	ASN	CA-C-N	5.44	128.11	120.28
1	J	76	ASN	C-N-CA	5.44	128.11	120.28
2	F	437	ASN	N-CA-C	-5.42	102.95	109.72
2	C	364	ALA	CA-C-N	5.37	131.80	121.54
2	C	364	ALA	C-N-CA	5.37	131.80	121.54
1	G	62	VAL	N-CA-CB	5.34	116.88	110.31
2	O	164	ASP	N-CA-C	5.34	117.79	111.33
2	F	367	ARG	CA-C-N	5.33	127.73	120.54
2	F	367	ARG	C-N-CA	5.33	127.73	120.54
2	L	84	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	211	LYS	N-CA-C	5.27	117.44	111.11
2	C	284	ASP	CA-CB-CG	5.26	117.86	112.60
2	F	360	SER	N-CA-C	5.25	119.36	111.96
2	R	84	ASP	CA-CB-CG	5.24	117.84	112.60
1	J	108	GLY	CA-C-N	5.24	128.28	120.95
1	J	108	GLY	C-N-CA	5.24	128.28	120.95
2	F	562	ALA	CA-C-N	5.22	128.01	120.38
2	F	562	ALA	C-N-CA	5.22	128.01	120.38
2	O	367	ARG	N-CA-C	5.20	117.21	108.73
2	F	300	THR	N-CA-C	5.19	121.28	109.81
1	D	212	GLN	CA-C-N	5.16	127.15	120.44
1	D	212	GLN	C-N-CA	5.16	127.15	120.44
2	R	367	ARG	CA-C-N	5.11	127.44	120.54
2	R	367	ARG	C-N-CA	5.11	127.44	120.54
1	M	108	GLY	CA-C-N	5.09	127.99	120.82
1	M	108	GLY	C-N-CA	5.09	127.99	120.82
1	D	62	VAL	N-CA-CB	5.08	116.46	110.82
1	G	76	ASN	CA-C-N	5.08	128.03	120.31
1	G	76	ASN	C-N-CA	5.08	128.03	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	62	VAL	N-CA-CB	5.07	116.55	110.31
2	C	84	ASP	CA-CB-CG	5.07	117.67	112.60
2	C	249	ASP	CA-CB-CG	5.07	117.67	112.60
2	C	370	GLU	CB-CG-CD	5.06	121.20	112.60
2	L	248	THR	N-CA-C	5.05	116.84	110.33
1	P	62	VAL	N-CA-CB	5.05	116.52	110.31
2	I	313	HIS	N-CA-C	5.02	116.83	111.36
2	R	299	THR	CB-CA-C	5.02	117.99	109.50
2	F	299	THR	CB-CA-C	5.02	117.91	109.48
2	F	164	ASP	N-CA-C	5.01	118.16	111.75

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	1767	0	1802	8	0
1	D	1767	0	1802	13	0
1	G	1767	0	1802	9	0
1	J	1767	0	1802	12	0
1	M	1767	0	1802	13	0
1	P	1767	0	1802	14	0
2	C	4301	0	4216	38	0
2	F	4301	0	4216	41	0
2	I	4301	0	4216	42	0
2	L	4301	0	4216	42	0
2	O	4301	0	4216	41	0
2	R	4301	0	4216	40	0
3	C	2	0	0	0	0
3	F	2	0	0	0	0
3	I	2	0	0	0	0
3	L	2	0	0	0	0
3	O	2	0	0	0	0
3	R	2	0	0	0	0
4	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	92	0	0	0	0
4	D	9	0	0	0	0
4	F	90	0	0	1	0
4	G	10	0	0	0	0
4	I	92	0	0	0	0
4	J	10	0	0	0	0
4	L	92	0	0	0	0
4	M	10	0	0	0	0
4	O	92	0	0	0	0
4	P	9	0	0	0	0
4	R	91	0	0	1	0
All	All	37026	0	36108	258	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 4.

All (258) 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:C:335:GLN:HG3	2:C:339:ARG:HD2	1.56	0.88
2:R:335:GLN:HG3	2:R:339:ARG:HD2	1.56	0.87
2:L:335:GLN:HG3	2:L:339:ARG:HD2	1.57	0.86
2:O:335:GLN:HG3	2:O:339:ARG:HD2	1.58	0.86
2:I:335:GLN:HG3	2:I:339:ARG:HD2	1.58	0.85
2:F:335:GLN:HG3	2:F:339:ARG:HD2	1.58	0.85
1:G:77:MET:HE1	2:I:564:ARG:HD2	1.69	0.75
2:F:328:ARG:HE	2:F:333:PHE:HD1	1.38	0.70
2:R:328:ARG:HE	2:R:333:PHE:HD1	1.39	0.70
2:I:328:ARG:HE	2:I:333:PHE:HD1	1.38	0.70
2:L:328:ARG:HE	2:L:333:PHE:HD1	1.39	0.69
2:C:328:ARG:HE	2:C:333:PHE:HD1	1.39	0.69
2:O:328:ARG:HE	2:O:333:PHE:HD1	1.39	0.69
1:A:77:MET:HE1	2:C:564:ARG:HD2	1.74	0.69
2:I:367:ARG:CB	2:I:370:GLU:HG3	2.24	0.67
2:F:367:ARG:CB	2:F:370:GLU:HG3	2.25	0.67
2:O:367:ARG:CB	2:O:370:GLU:HG3	2.25	0.67
2:L:367:ARG:CB	2:L:370:GLU:HG3	2.25	0.66
1:P:77:MET:HE1	2:R:564:ARG:HD2	1.76	0.66
2:R:367:ARG:CB	2:R:370:GLU:HG3	2.25	0.66
1:D:77:MET:HE1	2:F:564:ARG:HD2	1.78	0.66
2:C:367:ARG:CB	2:C:370:GLU:HG3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:MET:HE1	2:L:564:ARG:HD2	1.78	0.65
2:R:367:ARG:HB3	2:R:370:GLU:HG3	1.79	0.65
1:M:77:MET:HE1	2:O:564:ARG:HD2	1.81	0.63
2:L:367:ARG:HB3	2:L:370:GLU:HG3	1.79	0.63
2:I:367:ARG:HB3	2:I:370:GLU:HG3	1.81	0.62
2:O:352:MET:HE1	2:O:546:VAL:HG11	1.81	0.62
2:L:335:GLN:O	2:L:339:ARG:HB2	1.99	0.61
2:C:367:ARG:HB3	2:C:370:GLU:HG3	1.82	0.61
2:F:352:MET:HE1	2:F:546:VAL:HG11	1.81	0.61
2:R:335:GLN:O	2:R:339:ARG:HB2	2.01	0.61
2:F:335:GLN:O	2:F:339:ARG:HB2	2.00	0.61
2:F:367:ARG:HB3	2:F:370:GLU:HG3	1.81	0.61
2:C:335:GLN:O	2:C:339:ARG:HB2	2.00	0.60
2:O:335:GLN:O	2:O:339:ARG:HB2	2.01	0.60
2:I:335:GLN:O	2:I:339:ARG:HB2	2.01	0.59
2:I:443:VAL:HB	2:I:561:LEU:HB3	1.84	0.59
2:O:367:ARG:HB3	2:O:370:GLU:HG3	1.83	0.59
2:R:30:GLU:HB2	2:R:396:ASN:HB3	1.85	0.58
2:F:443:VAL:HB	2:F:561:LEU:HB3	1.84	0.58
2:I:352:MET:HE1	2:I:546:VAL:HG11	1.86	0.57
1:D:1:FME:HCN	1:D:2:LYS:HZ2	1.68	0.57
2:R:443:VAL:HB	2:R:561:LEU:HB3	1.87	0.57
2:L:352:MET:HE1	2:L:546:VAL:HG11	1.87	0.56
2:O:443:VAL:HB	2:O:561:LEU:HB3	1.86	0.56
2:F:461:ASP:HB3	2:F:464:ALA:HB2	1.88	0.56
2:O:466:VAL:HG23	2:O:469:PRO:HD3	1.88	0.56
2:C:443:VAL:HB	2:C:561:LEU:HB3	1.86	0.56
2:L:443:VAL:HB	2:L:561:LEU:HB3	1.86	0.56
2:L:464:ALA:HB1	2:L:469:PRO:HG2	1.88	0.56
2:R:461:ASP:HB3	2:R:464:ALA:HB2	1.88	0.56
2:R:466:VAL:HG23	2:R:469:PRO:HD3	1.88	0.56
1:M:120:LEU:HD12	2:O:1:MET:HE2	1.87	0.56
1:G:110:ILE:HG12	2:I:20:VAL:HG22	1.88	0.55
2:F:162:PRO:HB3	2:I:459:MET:HE1	1.87	0.55
1:A:140:HIS:HB2	2:I:251:VAL:HB	1.89	0.55
2:C:352:MET:HE1	2:C:546:VAL:HG11	1.88	0.55
2:C:461:ASP:HB3	2:C:464:ALA:HB2	1.88	0.55
2:F:464:ALA:HB1	2:F:469:PRO:HG2	1.89	0.55
2:O:275:GLU:HG2	2:O:342:SER:HB2	1.87	0.55
2:I:466:VAL:HG23	2:I:469:PRO:HD3	1.89	0.54
1:J:140:HIS:HB2	2:R:251:VAL:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:459:MET:HE1	2:I:162:PRO:HB3	1.90	0.54
2:I:537:VAL:HG22	2:I:544:VAL:HG22	1.88	0.54
2:L:466:VAL:HG23	2:L:469:PRO:HD3	1.89	0.54
2:I:461:ASP:HB3	2:I:464:ALA:HB2	1.90	0.54
2:L:461:ASP:HB3	2:L:464:ALA:HB2	1.90	0.54
2:C:464:ALA:HB1	2:C:469:PRO:HG2	1.90	0.54
2:C:466:VAL:HG23	2:C:469:PRO:HD3	1.89	0.54
2:O:461:ASP:HB3	2:O:464:ALA:HB2	1.90	0.53
2:C:162:PRO:HB3	2:F:459:MET:HE1	1.89	0.53
1:J:1:FME:HCN	1:J:2:LYS:HZ3	1.73	0.53
2:R:464:ALA:HB1	2:R:469:PRO:HG2	1.91	0.53
2:R:328:ARG:HH11	2:R:333:PHE:HE1	1.57	0.53
2:O:444:LYS:HD3	1:P:2:LYS:HB2	1.91	0.53
1:P:1:FME:HCN	1:P:2:LYS:HZ2	1.74	0.53
2:F:466:VAL:HG23	2:F:469:PRO:HD3	1.90	0.53
1:P:113:ALA:HB2	2:R:17:GLY:C	2.34	0.53
2:O:367:ARG:HB2	2:O:370:GLU:HG3	1.92	0.52
2:O:464:ALA:HB1	2:O:469:PRO:HG2	1.90	0.52
2:R:274:ILE:HD11	2:R:288:MET:HB2	1.90	0.52
2:C:328:ARG:HH11	2:C:333:PHE:HE1	1.58	0.51
2:I:367:ARG:HB2	2:I:370:GLU:HG3	1.92	0.51
2:L:162:PRO:HB3	2:O:459:MET:HE1	1.93	0.51
2:F:367:ARG:HB2	2:F:370:GLU:HG3	1.93	0.51
2:I:135:HIS:HB3	2:I:359:SER:HB2	1.91	0.51
2:O:328:ARG:HH11	2:O:333:PHE:HE1	1.58	0.51
1:G:120:LEU:HD12	2:I:1:MET:HE2	1.93	0.51
2:F:328:ARG:HH11	2:F:333:PHE:HE1	1.59	0.50
2:O:162:PRO:HB3	2:R:459:MET:HE1	1.93	0.50
2:R:297:SER:HB3	2:R:357:MET:HB2	1.94	0.50
1:G:106:LYS:HB3	1:G:109:GLU:HB2	1.93	0.50
2:L:328:ARG:HH11	2:L:333:PHE:HE1	1.58	0.50
2:O:251:VAL:HB	1:P:140:HIS:HB2	1.94	0.50
2:C:367:ARG:HB2	2:C:370:GLU:HG3	1.94	0.50
2:I:464:ALA:HB1	2:I:469:PRO:HG2	1.93	0.50
2:F:52:GLU:HG2	2:F:58:ASN:HD21	1.76	0.50
1:D:106:LYS:HB3	1:D:109:GLU:HB2	1.93	0.49
1:D:110:ILE:HG12	2:F:20:VAL:HG22	1.94	0.49
2:I:328:ARG:HH11	2:I:333:PHE:HE1	1.59	0.49
2:L:275:GLU:OE2	2:L:339:ARG:NH2	2.46	0.49
1:J:110:ILE:HG12	2:L:20:VAL:HG22	1.95	0.49
2:F:274:ILE:HD11	2:F:288:MET:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:VAL:HA	2:R:253:GLU:HG3	1.95	0.48
2:O:421:TYR:HB3	2:O:430:ILE:HD12	1.95	0.48
2:I:421:TYR:HB3	2:I:430:ILE:HD12	1.96	0.48
1:J:48:ARG:HG3	1:P:23:ARG:CZ	2.43	0.48
2:L:421:TYR:HB3	2:L:430:ILE:HD12	1.96	0.48
2:R:367:ARG:HB2	2:R:370:GLU:HG3	1.96	0.48
2:I:30:GLU:HB2	2:I:396:ASN:HB3	1.96	0.48
2:R:135:HIS:HB3	2:R:359:SER:HB2	1.96	0.48
2:C:421:TYR:HB3	2:C:430:ILE:HD12	1.96	0.48
2:L:459:MET:HE1	2:R:162:PRO:HB3	1.96	0.48
2:R:52:GLU:HG2	2:R:58:ASN:HD21	1.78	0.48
2:C:275:GLU:HA	2:C:286:ILE:HD12	1.94	0.48
2:L:367:ARG:HB2	2:L:370:GLU:HG3	1.96	0.48
2:C:301:PRO:HD3	2:C:366:GLY:HA2	1.97	0.47
2:F:421:TYR:HB3	2:F:430:ILE:HD12	1.96	0.47
2:R:275:GLU:HA	2:R:286:ILE:HD12	1.97	0.47
2:C:98:ALA:HB2	2:C:111:MET:HE2	1.97	0.47
2:L:298:SER:CB	2:L:350:HIS:HE2	2.27	0.47
2:F:301:PRO:HD3	2:F:366:GLY:HA2	1.97	0.47
2:F:251:VAL:HB	1:G:140:HIS:HB2	1.97	0.47
2:O:30:GLU:HB2	2:O:396:ASN:HB3	1.96	0.46
2:L:301:PRO:HD3	2:L:366:GLY:HA2	1.97	0.46
2:R:301:PRO:HD3	2:R:366:GLY:HA2	1.98	0.46
2:I:137:HIS:CD2	2:I:364:ALA:HB3	2.50	0.46
1:J:34:GLU:OE1	1:M:48:ARG:NH2	2.48	0.46
2:O:247:HIS:CE1	2:O:279:GLY:HA3	2.51	0.46
2:F:30:GLU:HB2	2:F:396:ASN:HB3	1.97	0.46
1:G:108:GLY:HA2	2:I:21:ARG:O	2.15	0.46
2:F:273:HIS:CD2	4:F:780:HOH:O	2.68	0.46
2:O:301:PRO:HD3	2:O:366:GLY:HA2	1.98	0.45
2:R:421:TYR:HB3	2:R:430:ILE:HD12	1.98	0.45
2:F:98:ALA:HB2	2:F:111:MET:HE2	1.98	0.45
2:F:261:LEU:HD21	2:F:288:MET:HG2	1.98	0.45
2:I:275:GLU:HA	2:I:286:ILE:HD12	1.99	0.45
2:I:301:PRO:HD3	2:I:366:GLY:HA2	1.97	0.45
2:L:136:THR:O	2:L:157:GLY:HA3	2.17	0.45
2:L:316:MET:HE3	2:L:365:MET:HG2	1.99	0.45
2:C:456:PHE:CE2	2:C:474:TYR:HB3	2.51	0.45
2:C:275:GLU:OE2	2:C:339:ARG:NH2	2.50	0.45
1:D:113:ALA:HB2	2:F:17:GLY:C	2.42	0.45
1:D:120:LEU:HD12	2:F:1:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:264:MET:HE2	2:F:269:ILE:HD13	1.99	0.45
1:J:2:LYS:HB2	2:R:444:LYS:HD3	1.98	0.45
2:L:275:GLU:HA	2:L:286:ILE:HD12	1.97	0.45
1:A:72:PRO:HG2	2:C:564:ARG:HH12	1.82	0.45
2:I:52:GLU:HG2	2:I:58:ASN:HD21	1.81	0.44
1:A:48:ARG:HG3	1:G:23:ARG:CZ	2.47	0.44
2:O:434:VAL:HG13	2:O:448:ILE:HD13	1.98	0.44
2:I:216:GLY:HA2	2:I:242:VAL:HB	1.99	0.44
2:L:456:PHE:CE2	2:L:474:TYR:HB3	2.53	0.44
2:R:456:PHE:CE2	2:R:474:TYR:HB3	2.53	0.44
1:A:2:LYS:HB2	2:I:444:LYS:HD3	2.00	0.44
2:L:275:GLU:HG2	2:L:342:SER:HB2	1.98	0.44
2:R:98:ALA:HB2	2:R:111:MET:HE2	2.00	0.44
2:L:219:LEU:HB3	2:L:225:THR:HG23	2.00	0.44
2:C:216:GLY:HA2	2:C:242:VAL:HB	2.00	0.44
2:C:444:LYS:HD3	1:D:2:LYS:HB2	2.00	0.44
2:I:354:VAL:HG11	2:I:535:ILE:HD11	1.99	0.44
2:L:52:GLU:HG2	2:L:58:ASN:HD21	1.82	0.44
2:L:98:ALA:HB2	2:L:111:MET:HE2	1.99	0.44
2:R:434:VAL:HG13	2:R:448:ILE:HD13	2.00	0.44
2:I:98:ALA:HB2	2:I:111:MET:HE2	2.00	0.44
1:J:23:ARG:CZ	1:M:48:ARG:HG3	2.48	0.44
2:L:134:SER:HB2	2:L:270:HIS:HE1	1.83	0.44
2:R:264:MET:HE2	2:R:269:ILE:HD13	1.99	0.43
2:F:298:SER:CB	2:F:350:HIS:HE2	2.30	0.43
2:R:352:MET:HE1	2:R:546:VAL:HG11	2.00	0.43
2:C:52:GLU:HG2	2:C:58:ASN:HD21	1.81	0.43
2:C:169:THR:HB	2:C:171:ILE:HD12	2.00	0.43
2:F:237:ALA:O	2:F:519:ARG:HD3	2.18	0.43
2:C:165:GLY:HA3	2:F:118:GLU:OE2	2.18	0.43
2:O:98:ALA:HB2	2:O:111:MET:HE2	1.99	0.43
2:C:264:MET:HE2	2:C:269:ILE:HD13	2.01	0.43
2:C:251:VAL:HB	1:D:140:HIS:HB2	2.00	0.43
2:I:275:GLU:OE2	2:I:339:ARG:NH2	2.51	0.43
2:I:313:HIS:C	2:I:315:ASP:H	2.27	0.43
1:P:72:PRO:HG2	2:R:564:ARG:HH12	1.83	0.43
1:D:28:LEU:HD13	1:G:48:ARG:HD2	2.01	0.43
2:I:456:PHE:CE2	2:I:474:TYR:HB3	2.54	0.43
1:J:48:ARG:HH22	1:P:71:MET:HE3	1.84	0.43
2:O:52:GLU:HG2	2:O:58:ASN:HD21	1.83	0.43
2:O:264:MET:HE2	2:O:269:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:SER:OG	1:G:116:LYS:HB2	2.19	0.43
2:I:139:LEU:HD11	2:I:167:ASN:HA	2.00	0.43
2:I:298:SER:CB	2:I:350:HIS:HE2	2.32	0.43
1:M:23:ARG:CZ	1:P:48:ARG:HG3	2.48	0.43
2:O:456:PHE:CE2	2:O:474:TYR:HB3	2.54	0.43
2:C:274:ILE:HG12	2:C:289:ALA:HB2	2.01	0.43
2:F:313:HIS:C	2:F:315:ASP:H	2.27	0.43
2:I:261:LEU:HD21	2:I:288:MET:HG2	2.01	0.43
1:M:108:GLY:HA2	2:O:21:ARG:O	2.18	0.43
2:F:292:VAL:CG1	1:J:205:ILE:HG21	2.49	0.43
2:L:237:ALA:O	2:L:519:ARG:HD3	2.19	0.43
2:L:274:ILE:HG12	2:L:289:ALA:HB2	2.01	0.43
1:D:108:GLY:HA2	2:F:21:ARG:O	2.19	0.42
2:L:434:VAL:HG13	2:L:448:ILE:HD13	2.00	0.42
2:F:298:SER:HB2	2:F:350:HIS:HE2	1.84	0.42
2:F:456:PHE:CE2	2:F:474:TYR:HB3	2.54	0.42
2:I:264:MET:HE2	2:I:269:ILE:HD13	2.00	0.42
2:O:313:HIS:C	2:O:315:ASP:H	2.27	0.42
2:C:169:THR:HG21	2:C:223:TRP:NE1	2.33	0.42
2:L:338:ILE:HG22	2:L:339:ARG:NH1	2.34	0.42
1:M:34:GLU:OE1	1:P:48:ARG:NH2	2.51	0.42
2:L:261:LEU:HD21	2:L:288:MET:HG2	2.01	0.42
2:L:264:MET:HE2	2:L:269:ILE:HD13	2.01	0.42
1:A:39:ILE:HD13	1:A:99:PRO:HB2	2.01	0.42
2:C:338:ILE:HG22	2:C:339:ARG:NH1	2.34	0.42
1:M:39:ILE:HD13	1:M:99:PRO:HB2	2.01	0.42
1:D:39:ILE:HD13	1:D:99:PRO:HB2	2.02	0.42
2:F:434:VAL:HG13	2:F:448:ILE:HD13	2.02	0.42
2:C:261:LEU:HD21	2:C:288:MET:HG2	2.02	0.42
2:R:338:ILE:HG22	2:R:339:ARG:NH1	2.35	0.42
1:A:23:ARG:CZ	1:D:48:ARG:HG3	2.50	0.42
2:O:535:ILE:HG12	2:O:546:VAL:HG22	2.01	0.42
2:F:72:ALA:HB1	2:F:127:ILE:HD13	2.02	0.41
2:I:338:ILE:HG22	2:I:339:ARG:NH1	2.35	0.41
2:O:186:GLU:HA	2:O:510:ARG:HD2	2.01	0.41
2:F:338:ILE:HG22	2:F:339:ARG:NH1	2.34	0.41
2:R:273:HIS:CD2	4:R:780:HOH:O	2.72	0.41
2:R:275:GLU:OE2	2:R:339:ARG:NH2	2.53	0.41
2:R:313:HIS:C	2:R:315:ASP:H	2.27	0.41
2:O:301:PRO:HG3	2:O:365:MET:O	2.20	0.41
2:C:44:PHE:HB2	2:C:50:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:OE1	1:D:48:ARG:NH2	2.49	0.41
2:I:434:VAL:HG13	2:I:448:ILE:HD13	2.02	0.41
2:L:253:GLU:HG3	1:M:141:VAL:HA	2.02	0.41
2:F:136:THR:O	2:F:157:GLY:HA3	2.21	0.41
1:J:120:LEU:HD12	2:L:1:MET:HE2	2.03	0.41
1:P:110:ILE:HG12	2:R:20:VAL:HG22	2.02	0.41
2:L:313:HIS:C	2:L:315:ASP:H	2.28	0.41
2:L:444:LYS:HD3	1:M:2:LYS:HB2	2.02	0.41
2:O:274:ILE:HG12	2:O:289:ALA:HB2	2.03	0.41
2:O:298:SER:CB	2:O:350:HIS:HE2	2.34	0.41
2:O:338:ILE:HG22	2:O:339:ARG:NH1	2.35	0.41
2:R:150:ASN:O	2:R:372:ILE:HD12	2.21	0.41
2:C:169:THR:HG21	2:C:223:TRP:HE1	1.86	0.41
2:I:136:THR:O	2:I:157:GLY:HA3	2.21	0.41
2:C:294:ILE:O	2:C:296:PRO:HD3	2.21	0.40
2:R:186:GLU:HA	2:R:510:ARG:HD2	2.03	0.40
2:F:275:GLU:OE2	2:F:339:ARG:NH2	2.54	0.40
2:I:186:GLU:HA	2:I:510:ARG:HD2	2.03	0.40
2:L:354:VAL:HG11	2:L:535:ILE:HD11	2.03	0.40
1:P:39:ILE:HD13	1:P:99:PRO:HB2	2.03	0.40
1:M:32:GLN:HE22	1:P:1:FME:HCN	1.86	0.40
1:M:113:ALA:HB2	2:O:17:GLY:C	2.46	0.40
2:C:313:HIS:C	2:C:315:ASP:H	2.29	0.40
2:C:434:VAL:HG13	2:C:448:ILE:HD13	2.03	0.40
2:O:253:GLU:HG3	1:P:141:VAL:HA	2.03	0.40
2:L:79:GLY:HA2	2:L:402:LYS:HE2	2.04	0.40
2:L:186:GLU:HA	2:L:510:ARG:HD2	2.03	0.40
1:M:110:ILE:HG12	2:O:20:VAL:HG22	2.04	0.40
2:O:261:LEU:HD21	2:O:288:MET:HG2	2.03	0.40
2:O:312:GLU:OE2	2:O:367:ARG:NH2	2.55	0.40
2:R:261:LEU:HD21	2:R:288:MET:HG2	2.04	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	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
1	D	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
1	G	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
1	J	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
1	M	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
1	P	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
2	C	559/568 (98%)	525 (94%)	31 (6%)	3 (0%)	24	60
2	F	559/568 (98%)	523 (94%)	33 (6%)	3 (0%)	24	60
2	I	559/568 (98%)	526 (94%)	29 (5%)	4 (1%)	18	53
2	L	559/568 (98%)	520 (93%)	36 (6%)	3 (0%)	24	60
2	O	559/568 (98%)	525 (94%)	32 (6%)	2 (0%)	30	65
2	R	559/568 (98%)	527 (94%)	30 (5%)	2 (0%)	30	65
All	All	4692/4758 (99%)	4456 (95%)	219 (5%)	17 (0%)	30	65

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	464	ALA
2	O	464	ALA
2	C	365	MET
2	C	464	ALA
2	F	365	MET
2	I	464	ALA
2	L	365	MET
2	L	464	ALA
2	R	365	MET
2	R	464	ALA
2	F	281	HIS
2	I	365	MET
2	I	281	HIS
2	O	365	MET
2	C	224	GLY
2	I	50	ILE
2	L	50	ILE

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	185/185 (100%)	176 (95%)	9 (5%)	22	56
1	D	185/185 (100%)	175 (95%)	10 (5%)	20	53
1	G	185/185 (100%)	173 (94%)	12 (6%)	15	47
1	J	185/185 (100%)	175 (95%)	10 (5%)	20	53
1	M	185/185 (100%)	174 (94%)	11 (6%)	18	50
1	P	185/185 (100%)	174 (94%)	11 (6%)	18	50
2	C	459/466 (98%)	443 (96%)	16 (4%)	32	65
2	F	459/466 (98%)	441 (96%)	18 (4%)	28	62
2	I	459/466 (98%)	441 (96%)	18 (4%)	28	62
2	L	459/466 (98%)	441 (96%)	18 (4%)	28	62
2	O	459/466 (98%)	442 (96%)	17 (4%)	30	64
2	R	459/466 (98%)	440 (96%)	19 (4%)	27	61
All	All	3864/3906 (99%)	3695 (96%)	169 (4%)	25	60

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	83	VAL
1	A	104	ASP
1	A	116	LYS
1	A	174	LEU
1	A	187	ILE
1	A	198	MET
1	A	209	LEU
1	A	213	LYS
2	C	1	MET
2	C	19	LYS
2	C	49	THR
2	C	139	LEU
2	C	180	ARG

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Mol	Chain	Res	Type
2	C	210	VAL
2	C	324	ASP
2	C	328	ARG
2	C	335	GLN
2	C	336	SER
2	C	339	ARG
2	C	458	GLU
2	C	502	ILE
2	C	510	ARG
2	C	521	VAL
2	C	563	SER
1	D	51	LYS
1	D	83	VAL
1	D	104	ASP
1	D	116	LYS
1	D	152	ARG
1	D	174	LEU
1	D	187	ILE
1	D	198	MET
1	D	209	LEU
1	D	213	LYS
2	F	1	MET
2	F	19	LYS
2	F	49	THR
2	F	139	LEU
2	F	180	ARG
2	F	210	VAL
2	F	298	SER
2	F	324	ASP
2	F	328	ARG
2	F	335	GLN
2	F	336	SER
2	F	339	ARG
2	F	458	GLU
2	F	502	ILE
2	F	510	ARG
2	F	521	VAL
2	F	536	THR
2	F	563	SER
1	G	51	LYS
1	G	83	VAL
1	G	104	ASP

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Mol	Chain	Res	Type
1	G	114	SER
1	G	116	LYS
1	G	119	GLU
1	G	152	ARG
1	G	174	LEU
1	G	187	ILE
1	G	198	MET
1	G	209	LEU
1	G	213	LYS
2	I	1	MET
2	I	19	LYS
2	I	49	THR
2	I	139	LEU
2	I	169	THR
2	I	180	ARG
2	I	210	VAL
2	I	324	ASP
2	I	328	ARG
2	I	335	GLN
2	I	336	SER
2	I	339	ARG
2	I	458	GLU
2	I	502	ILE
2	I	510	ARG
2	I	521	VAL
2	I	552	THR
2	I	563	SER
1	J	51	LYS
1	J	83	VAL
1	J	104	ASP
1	J	116	LYS
1	J	152	ARG
1	J	174	LEU
1	J	187	ILE
1	J	198	MET
1	J	209	LEU
1	J	213	LYS
2	L	1	MET
2	L	19	LYS
2	L	49	THR
2	L	134	SER
2	L	139	LEU

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Mol	Chain	Res	Type
2	L	180	ARG
2	L	210	VAL
2	L	247	HIS
2	L	324	ASP
2	L	328	ARG
2	L	335	GLN
2	L	336	SER
2	L	339	ARG
2	L	458	GLU
2	L	502	ILE
2	L	510	ARG
2	L	521	VAL
2	L	563	SER
1	M	51	LYS
1	M	83	VAL
1	M	104	ASP
1	M	114	SER
1	M	116	LYS
1	M	152	ARG
1	M	174	LEU
1	M	187	ILE
1	M	198	MET
1	M	209	LEU
1	M	213	LYS
2	O	1	MET
2	O	19	LYS
2	O	49	THR
2	O	139	LEU
2	O	160	THR
2	O	180	ARG
2	O	210	VAL
2	O	324	ASP
2	O	328	ARG
2	O	335	GLN
2	O	336	SER
2	O	339	ARG
2	O	458	GLU
2	O	502	ILE
2	O	510	ARG
2	O	521	VAL
2	O	563	SER
1	P	51	LYS

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Mol	Chain	Res	Type
1	P	83	VAL
1	P	104	ASP
1	P	116	LYS
1	P	119	GLU
1	P	152	ARG
1	P	174	LEU
1	P	187	ILE
1	P	198	MET
1	P	209	LEU
1	P	213	LYS
2	R	1	MET
2	R	19	LYS
2	R	49	THR
2	R	134	SER
2	R	139	LEU
2	R	160	THR
2	R	180	ARG
2	R	210	VAL
2	R	324	ASP
2	R	328	ARG
2	R	335	GLN
2	R	336	SER
2	R	339	ARG
2	R	458	GLU
2	R	502	ILE
2	R	510	ARG
2	R	521	VAL
2	R	536	THR
2	R	563	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	56	GLN
1	A	86	ASN
1	A	97	ASN
2	C	100	ASN
2	C	143	GLN
2	C	377	GLN
1	D	8	GLN
1	D	56	GLN

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Mol	Chain	Res	Type
1	D	97	ASN
2	F	100	ASN
2	F	143	GLN
2	F	167	ASN
2	F	463	ASN
1	G	8	GLN
1	G	56	GLN
1	G	97	ASN
2	I	100	ASN
2	I	143	GLN
2	I	377	GLN
1	J	8	GLN
1	J	56	GLN
1	J	86	ASN
1	J	97	ASN
2	L	143	GLN
2	L	265	ASN
1	M	8	GLN
1	M	56	GLN
1	M	86	ASN
1	M	97	ASN
2	O	6	GLN
2	O	143	GLN
2	O	377	GLN
2	O	463	ASN
1	P	8	GLN
1	P	56	GLN
1	P	97	ASN
2	R	6	GLN
2	R	100	ASN
2	R	143	GLN
2	R	167	ASN
2	R	377	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	KCX	L	218	2,3	10,11,12	1.10	1 (10%)	6,12,14	1.65	1 (16%)
1	FME	M	1	1	8,9,10	0.54	0	8,9,11	1.05	1 (12%)
2	KCX	C	218	2,3	10,11,12	1.02	1 (10%)	6,12,14	1.68	1 (16%)
2	KCX	R	218	2,3	10,11,12	1.16	1 (10%)	6,12,14	1.56	1 (16%)
1	FME	G	1	1	8,9,10	0.50	0	8,9,11	1.05	1 (12%)
2	KCX	F	218	2,3	10,11,12	1.04	1 (10%)	6,12,14	1.65	1 (16%)
2	KCX	O	218	2,3	10,11,12	1.06	1 (10%)	6,12,14	1.77	1 (16%)
1	FME	J	1	1	8,9,10	0.57	0	8,9,11	0.97	0
1	FME	P	1	1	8,9,10	0.57	0	8,9,11	1.00	1 (12%)
1	FME	D	1	1	8,9,10	0.50	0	8,9,11	0.95	0
1	FME	A	1	1	8,9,10	0.54	0	8,9,11	1.00	1 (12%)
2	KCX	I	218	2,3	10,11,12	0.98	1 (10%)	6,12,14	1.66	1 (16%)

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	KCX	L	218	2,3	-	0/9/10/12	-
1	FME	M	1	1	-	2/7/9/11	-
2	KCX	C	218	2,3	-	0/9/10/12	-
2	KCX	R	218	2,3	-	1/9/10/12	-
1	FME	G	1	1	-	2/7/9/11	-
2	KCX	F	218	2,3	-	0/9/10/12	-
2	KCX	O	218	2,3	-	1/9/10/12	-
1	FME	J	1	1	-	2/7/9/11	-
1	FME	P	1	1	-	2/7/9/11	-
1	FME	D	1	1	-	2/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
2	KCX	I	218	2,3	-	1/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	218	KCX	OQ1-CX	2.91	1.27	1.21
2	L	218	KCX	OQ1-CX	2.80	1.26	1.21
2	O	218	KCX	OQ1-CX	2.72	1.26	1.21
2	F	218	KCX	OQ1-CX	2.55	1.26	1.21
2	C	218	KCX	OQ1-CX	2.32	1.26	1.21
2	I	218	KCX	OQ1-CX	2.26	1.25	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	218	KCX	OQ1-CX-NZ	-4.07	118.74	124.92
2	C	218	KCX	OQ1-CX-NZ	-3.87	119.04	124.92
2	I	218	KCX	OQ1-CX-NZ	-3.82	119.12	124.92
2	F	218	KCX	OQ1-CX-NZ	-3.70	119.30	124.92
2	L	218	KCX	OQ1-CX-NZ	-3.66	119.35	124.92
2	R	218	KCX	OQ1-CX-NZ	-3.31	119.89	124.92
1	G	1	FME	O-C-CA	-2.25	118.97	124.77
1	P	1	FME	O-C-CA	-2.20	119.12	124.77
1	M	1	FME	O-C-CA	-2.17	119.20	124.77
1	A	1	FME	O-C-CA	-2.16	119.22	124.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	D	1	FME	O1-CN-N-CA
1	G	1	FME	O1-CN-N-CA
1	J	1	FME	O1-CN-N-CA
1	M	1	FME	O1-CN-N-CA
1	P	1	FME	O1-CN-N-CA
1	J	1	FME	C-CA-CB-CG
2	I	218	KCX	C-CA-CB-CG
2	O	218	KCX	C-CA-CB-CG
2	R	218	KCX	C-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
1	D	1	FME	C-CA-CB-CG
1	G	1	FME	C-CA-CB-CG
1	M	1	FME	C-CA-CB-CG
1	P	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	1	FME	1	0
1	P	1	FME	2	0
1	D	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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	224/225 (99%)	-0.45	0 100 100	20, 30, 51, 65	0
1	D	224/225 (99%)	-0.27	2 (0%) 81 61	22, 31, 52, 69	0
1	G	224/225 (99%)	-0.41	0 100 100	21, 31, 54, 66	0
1	J	224/225 (99%)	-0.33	1 (0%) 88 76	25, 36, 57, 74	0
1	M	224/225 (99%)	-0.38	1 (0%) 88 76	19, 32, 55, 73	0
1	P	224/225 (99%)	-0.35	1 (0%) 88 76	25, 36, 56, 71	0
2	C	563/568 (99%)	-0.44	23 (4%) 41 23	14, 24, 57, 107	0
2	F	563/568 (99%)	-0.44	18 (3%) 50 29	15, 25, 57, 105	0
2	I	563/568 (99%)	-0.44	18 (3%) 50 29	13, 24, 57, 104	0
2	L	563/568 (99%)	-0.41	19 (3%) 48 27	16, 26, 59, 109	0
2	O	563/568 (99%)	-0.42	21 (3%) 45 25	15, 26, 61, 111	0
2	R	563/568 (99%)	-0.39	22 (3%) 43 24	18, 29, 62, 112	0
All	All	4722/4758 (99%)	-0.40	126 (2%) 56 33	13, 28, 57, 112	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	462	SER	5.7
2	C	327	ILE	5.1
2	R	317	LEU	5.0
2	C	319	THR	4.9
2	R	319	THR	4.9
2	C	325	LYS	4.7
2	O	327	ILE	4.5
2	O	328	ARG	4.5
2	C	328	ARG	4.4
2	F	327	ILE	4.4
2	L	327	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
2	R	328	ARG	4.3
2	L	319	THR	4.3
2	R	321	HIS	4.2
2	C	321	HIS	4.1
2	O	325	LYS	4.1
2	R	327	ILE	4.1
2	L	322	HIS	4.1
2	F	328	ARG	4.1
2	L	462	SER	4.0
2	L	328	ARG	3.9
2	I	328	ARG	3.8
2	I	327	ILE	3.8
2	I	321	HIS	3.7
2	O	322	HIS	3.7
2	O	317	LEU	3.6
2	F	325	LYS	3.6
2	I	319	THR	3.6
2	L	325	LYS	3.6
2	I	320	CYS	3.5
1	M	6	LYS	3.5
2	C	317	LEU	3.5
2	L	321	HIS	3.5
2	O	319	THR	3.4
2	C	326	ARG	3.4
2	L	323	LEU	3.4
2	R	318	MET	3.4
2	C	322	HIS	3.3
2	I	322	HIS	3.3
1	J	6	LYS	3.3
2	R	462	SER	3.3
2	F	322	HIS	3.3
2	I	325	LYS	3.2
2	L	318	MET	3.2
2	F	319	THR	3.2
2	R	325	LYS	3.2
2	C	364	ALA	3.1
2	L	317	LEU	3.1
2	C	318	MET	3.1
2	F	462	SER	3.0
2	R	333	PHE	3.0
2	L	320	CYS	3.0
2	F	321	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	318	MET	3.0
2	L	460	GLY	3.0
1	D	104	ASP	2.9
2	C	368	ALA	2.9
2	C	333	PHE	2.9
2	R	323	LEU	2.9
2	F	465	SER	2.9
2	I	313	HIS	2.9
2	I	317	LEU	2.9
2	F	323	LEU	2.8
2	O	318	MET	2.8
2	L	461	ASP	2.8
2	I	314	LEU	2.8
2	C	315	ASP	2.7
2	O	326	ARG	2.7
2	R	313	HIS	2.6
2	I	326	ARG	2.6
2	R	466	VAL	2.6
2	F	313	HIS	2.6
2	O	321	HIS	2.6
2	L	364	ALA	2.6
2	I	318	MET	2.6
2	O	461	ASP	2.6
1	D	6	LYS	2.6
2	O	314	LEU	2.6
2	R	364	ALA	2.6
2	I	338	ILE	2.5
2	R	322	HIS	2.5
2	O	323	LEU	2.5
2	O	333	PHE	2.5
2	L	326	ARG	2.5
2	C	314	LEU	2.5
2	I	323	LEU	2.5
2	R	315	ASP	2.5
2	O	313	HIS	2.5
2	R	320	CYS	2.4
2	F	26	ASP	2.4
2	C	320	CYS	2.4
2	C	323	LEU	2.4
2	L	314	LEU	2.4
2	F	467	PRO	2.4
2	O	320	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	324	ASP	2.4
2	I	368	ALA	2.4
2	O	465	SER	2.3
2	I	333	PHE	2.3
2	C	335	GLN	2.3
2	O	324	ASP	2.3
2	I	335	GLN	2.3
2	C	466	VAL	2.3
2	F	466	VAL	2.3
2	R	362	SER	2.2
2	R	335	GLN	2.2
2	C	467	PRO	2.2
2	L	335	GLN	2.2
2	R	334	SER	2.2
2	F	335	GLN	2.2
2	L	333	PHE	2.2
2	O	335	GLN	2.2
2	C	365	MET	2.2
2	C	362	SER	2.1
2	L	365	MET	2.1
2	R	326	ARG	2.1
1	P	6	LYS	2.1
2	O	368	ALA	2.1
2	O	467	PRO	2.1
2	C	462	SER	2.1
2	F	314	LEU	2.1
2	R	460	GLY	2.1
2	F	333	PHE	2.1
2	F	317	LEU	2.0
2	C	324	ASP	2.0
2	R	461	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	FME	J	1	10/11	0.94	0.12	50,53,57,57	0
1	FME	A	1	10/11	0.95	0.10	42,44,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	FME	M	1	10/11	0.95	0.12	49,51,55,56	0
1	FME	P	1	10/11	0.95	0.12	47,50,54,55	0
1	FME	D	1	10/11	0.96	0.09	45,48,52,52	0
1	FME	G	1	10/11	0.97	0.09	40,42,47,48	0
2	KCX	F	218	12/13	0.97	0.06	19,21,24,26	0
2	KCX	L	218	12/13	0.98	0.05	18,20,22,23	0
2	KCX	I	218	12/13	0.98	0.07	18,19,25,27	0
2	KCX	C	218	12/13	0.98	0.06	19,20,23,24	0
2	KCX	R	218	12/13	0.98	0.06	20,23,28,29	0
2	KCX	O	218	12/13	0.99	0.05	23,27,29,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FE	L	774	1/1	0.98	0.03	24,24,24,24	0
3	FE	F	774	1/1	0.99	0.03	26,26,26,26	0
3	FE	F	775	1/1	0.99	0.01	25,25,25,25	0
3	FE	I	774	1/1	0.99	0.04	25,25,25,25	0
3	FE	I	775	1/1	0.99	0.03	29,29,29,29	0
3	FE	C	774	1/1	0.99	0.03	23,23,23,23	0
3	FE	O	774	1/1	0.99	0.02	31,31,31,31	0
3	FE	R	774	1/1	0.99	0.05	36,36,36,36	0
3	FE	R	775	1/1	0.99	0.02	31,31,31,31	0
3	FE	O	775	1/1	1.00	0.01	28,28,28,28	0
3	FE	L	775	1/1	1.00	0.02	31,31,31,31	0
3	FE	C	775	1/1	1.00	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.