



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 AM UTC

PDB ID : 3QGK / pdb_00003qgk
Title : 3.0 A Model of Iron Containing Urease UreA2B2 from Helicobacter mustelae
(refined w/ no ordered solvent)
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

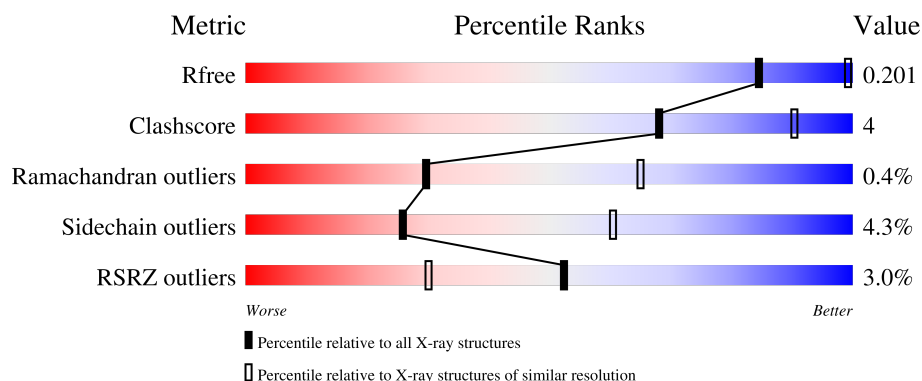
1 Overall quality at a glance

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	 90% 9%
1	D	225	 89% 11%
1	G	225	 88% 11%
1	J	225	 88% 12%
1	M	225	 89% 11%

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Mol	Chain	Length	Quality of chain
1	P	225	90%10%
2	C	568	4% 85%12%..
2	F	568	4% 84%14%..
2	I	568	4% 84%14%..
2	L	568	4% 84%14%..
2	O	568	4% 85%12%..
2	R	568	5% 84%14%..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36420 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).

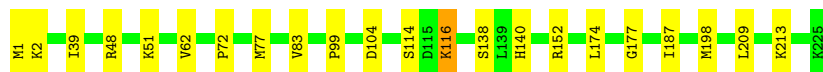
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total 2	Fe 2	0	0
3	F	2	Total 2	Fe 2	0	0
3	I	2	Total 2	Fe 2	0	0
3	L	2	Total 2	Fe 2	0	0
3	O	2	Total 2	Fe 2	0	0
3	R	2	Total 2	Fe 2	0	0

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: 



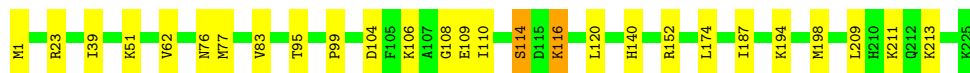
- Molecule 1: Fusion of urease beta and gamma subunits

Chain D: 



- Molecule 1: Fusion of urease beta and gamma subunits

Chain G: 

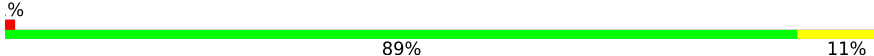


- Molecule 1: Fusion of urease beta and gamma subunits

Chain J: 



- Molecule 1: Fusion of urease beta and gamma subunits

Chain M: 



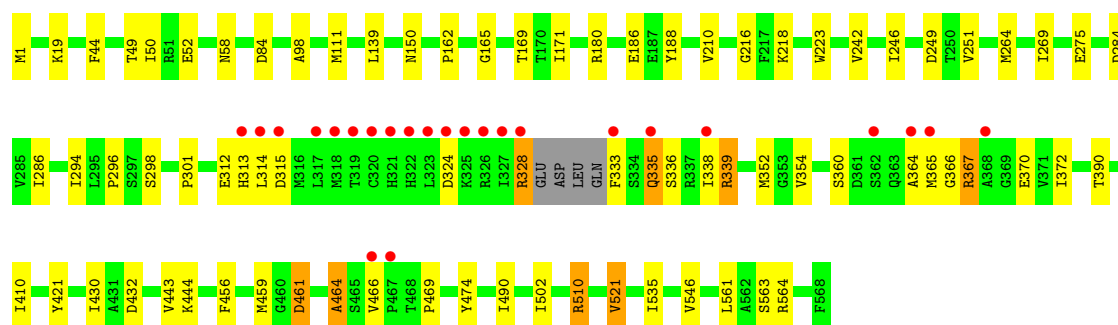
- Molecule 1: Fusion of urease beta and gamma subunits

Chain P:  90% 10%



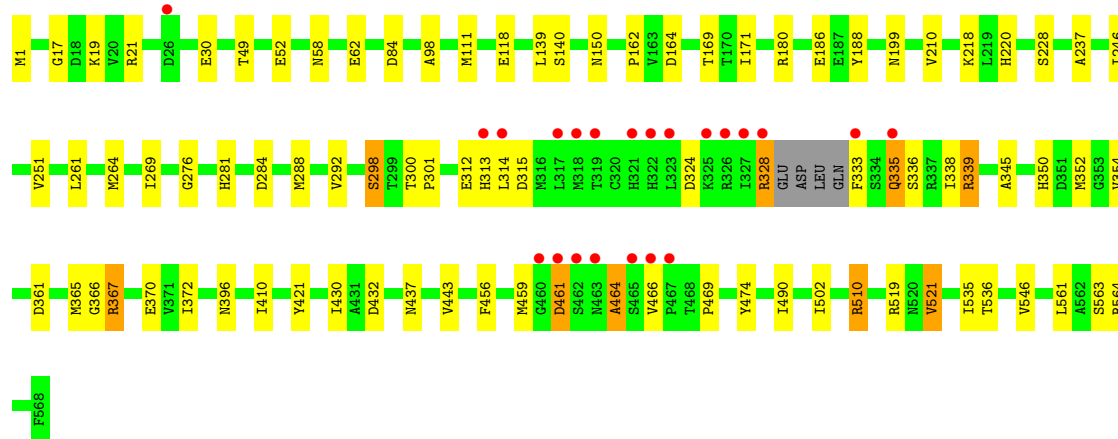
• Molecule 2: Urease subunit beta 2

Chain C:  4% 85% 12% ..



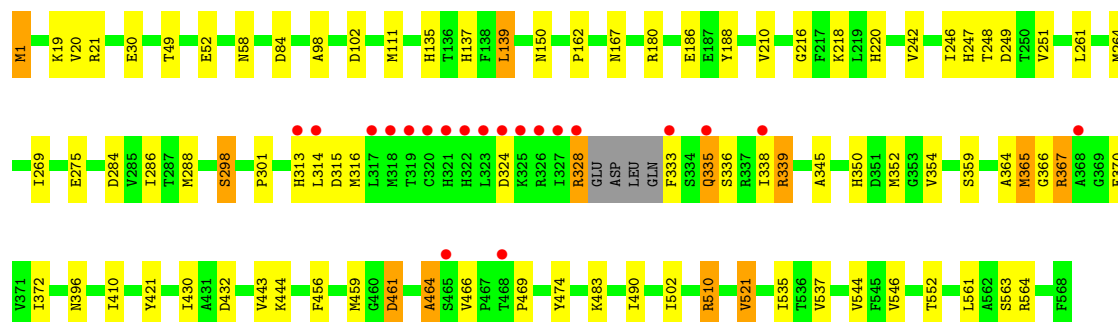
• Molecule 2: Urease subunit beta 2

Chain F:  4% 84% 14% ..

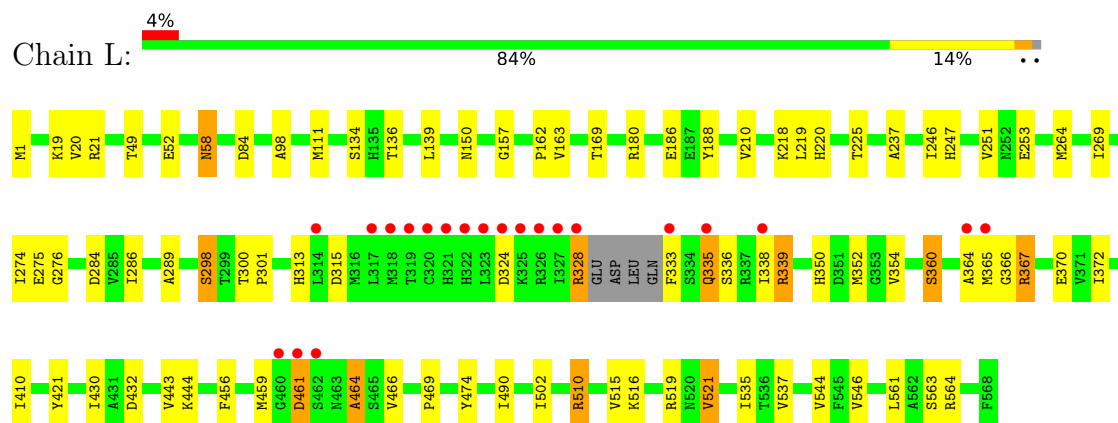


• Molecule 2: Urease subunit beta 2

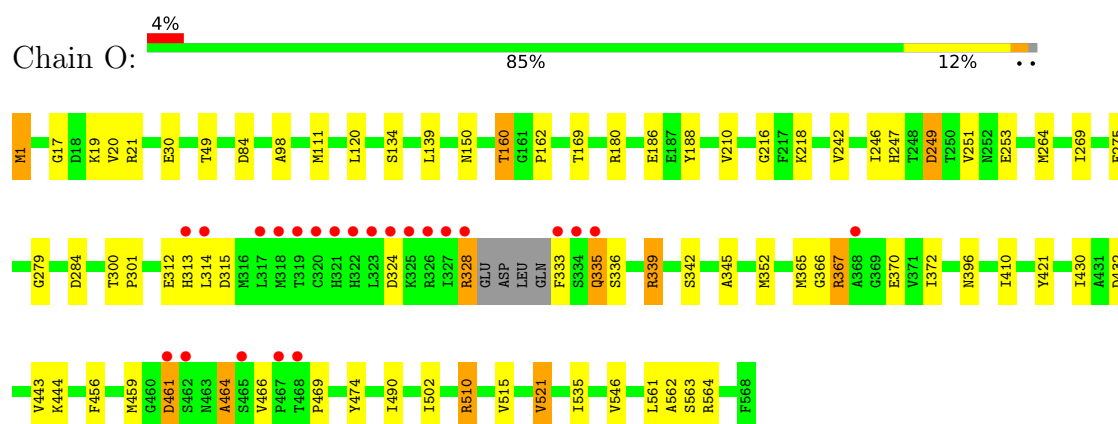
Chain I:  4% 84% 14% ..



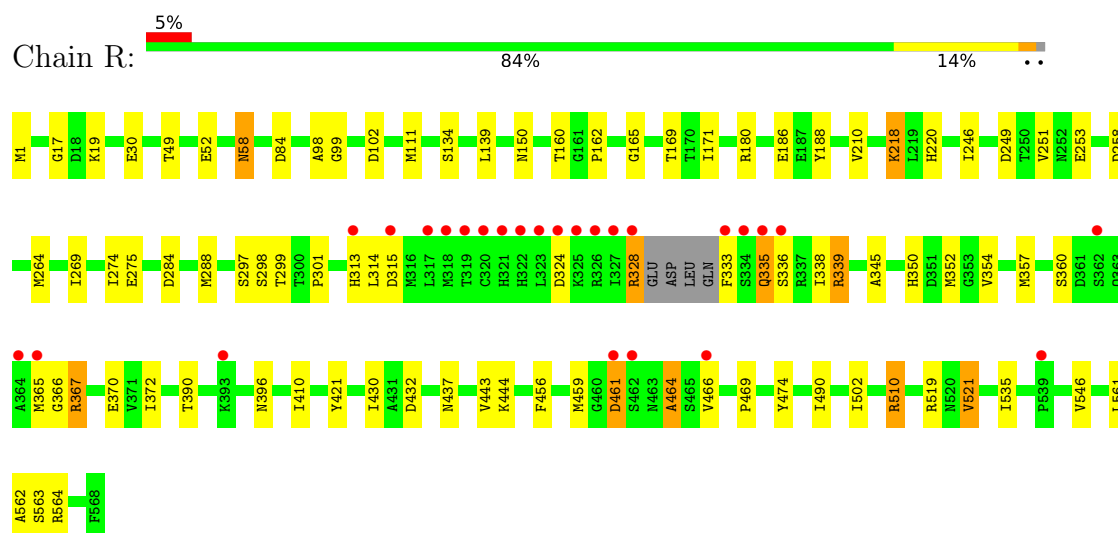
• Molecule 2: Urease subunit beta 2



• 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}	0.177 , 0.197 0.184 , 0.201	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 , 29.3	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	36420	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 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	0.76	0/1791	1.29	1/2401 (0.0%)
1	D	0.77	0/1791	1.31	6/2401 (0.2%)
1	G	0.77	0/1791	1.29	4/2401 (0.2%)
1	J	0.74	0/1791	1.29	4/2401 (0.2%)
1	M	0.74	0/1791	1.30	2/2401 (0.1%)
1	P	0.74	0/1791	1.29	2/2401 (0.1%)
2	C	0.81	0/4376	1.35	17/5925 (0.3%)
2	F	0.81	0/4376	1.36	21/5925 (0.4%)
2	I	0.80	0/4376	1.35	16/5925 (0.3%)
2	L	0.80	0/4376	1.35	19/5925 (0.3%)
2	O	0.80	0/4376	1.35	18/5925 (0.3%)
2	R	0.78	0/4376	1.36	26/5925 (0.4%)
All	All	0.79	0/37002	1.34	136/49956 (0.3%)

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	410	ILE	N-CA-C	8.13	118.17	110.53
2	I	410	ILE	N-CA-C	8.12	118.16	110.53
2	R	410	ILE	N-CA-C	8.02	118.07	110.53
2	O	410	ILE	N-CA-C	7.91	117.97	110.53
2	C	410	ILE	N-CA-C	7.88	117.94	110.53
2	L	410	ILE	N-CA-C	7.71	117.78	110.53
2	I	284	ASP	N-CA-C	7.39	121.60	112.59
2	O	249	ASP	CA-CB-CG	6.92	119.52	112.60
2	F	284	ASP	N-CA-C	6.86	120.96	112.59
2	C	284	ASP	N-CA-C	6.84	120.94	112.59
2	O	284	ASP	N-CA-C	6.83	120.93	112.59
2	O	246	ILE	N-CA-C	6.74	118.42	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	284	ASP	N-CA-C	6.59	120.63	112.59
2	I	188	TYR	N-CA-C	6.43	119.92	110.59
2	R	249	ASP	CA-CB-CG	6.38	118.98	112.60
2	O	188	TYR	N-CA-C	6.37	119.83	110.59
2	C	188	TYR	N-CA-C	6.25	119.65	110.59
2	L	188	TYR	N-CA-C	6.21	119.60	110.59
2	F	432	ASP	CA-CB-CG	6.21	118.81	112.60
2	I	248	THR	N-CA-C	6.18	118.01	110.41
2	F	188	TYR	N-CA-C	6.17	119.53	110.59
2	I	249	ASP	CA-CB-CG	6.12	118.72	112.60
2	L	284	ASP	N-CA-C	6.11	120.05	112.59
2	L	432	ASP	CA-CB-CG	6.07	118.67	112.60
2	O	432	ASP	CA-CB-CG	6.06	118.66	112.60
2	R	188	TYR	N-CA-C	6.05	119.37	110.59
2	I	284	ASP	CA-CB-CG	6.05	118.65	112.60
2	C	432	ASP	CA-CB-CG	6.01	118.61	112.60
2	L	360	SER	N-CA-C	6.00	121.48	114.04
2	I	521	VAL	N-CA-CB	6.00	118.23	111.21
2	R	432	ASP	CA-CB-CG	5.95	118.55	112.60
2	C	246	ILE	N-CA-C	5.92	117.27	108.46
2	I	432	ASP	CA-CB-CG	5.90	118.50	112.60
2	R	367	ARG	N-CA-C	5.80	118.69	109.24
2	O	84	ASP	CA-CB-CG	5.79	118.39	112.60
2	I	367	ARG	CA-C-N	5.78	128.34	120.54
2	I	367	ARG	C-N-CA	5.78	128.34	120.54
2	R	521	VAL	N-CA-CB	5.77	118.72	111.46
2	R	461	ASP	CA-CB-CG	5.72	118.32	112.60
2	R	165	GLY	CA-C-N	5.71	128.39	120.29
2	R	165	GLY	C-N-CA	5.71	128.39	120.29
2	F	461	ASP	CA-CB-CG	5.69	118.29	112.60
2	F	521	VAL	N-CA-CB	5.68	118.62	111.46
2	L	367	ARG	N-CA-C	5.67	117.97	108.73
2	C	461	ASP	CA-CB-CG	5.64	118.24	112.60
2	F	300	THR	N-CA-C	5.63	122.25	109.81
2	L	364	ALA	CA-C-N	5.63	132.29	121.54
2	L	364	ALA	C-N-CA	5.63	132.29	121.54
1	J	76	ASN	CA-C-N	5.62	128.38	120.28
1	J	76	ASN	C-N-CA	5.62	128.38	120.28
2	O	367	ARG	CA-C-N	5.62	127.75	120.44
2	O	367	ARG	C-N-CA	5.62	127.75	120.44
2	F	84	ASP	CA-CB-CG	5.61	118.21	112.60
2	L	284	ASP	CA-CB-CG	5.60	118.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	211	LYS	N-CA-C	5.60	117.83	111.11
1	D	76	ASN	CA-C-N	5.59	128.81	120.31
1	D	76	ASN	C-N-CA	5.59	128.81	120.31
2	O	461	ASP	CA-CB-CG	5.59	118.19	112.60
2	R	246	ILE	N-CA-C	5.58	116.78	108.46
2	I	84	ASP	CA-CB-CG	5.58	118.18	112.60
2	I	246	ILE	N-CA-C	5.57	116.76	108.46
1	M	103	ASP	CA-CB-CG	5.56	118.16	112.60
2	I	461	ASP	CA-CB-CG	5.56	118.16	112.60
2	I	367	ARG	N-CA-C	5.56	117.79	108.73
2	F	164	ASP	N-CA-C	5.55	118.05	111.33
1	G	62	VAL	N-CA-CB	5.55	117.13	110.31
2	F	367	ARG	N-CA-C	5.54	118.27	109.24
2	L	521	VAL	N-CA-CB	5.51	118.40	111.46
2	R	390	THR	CA-C-N	5.50	129.39	120.60
2	R	390	THR	C-N-CA	5.50	129.39	120.60
2	L	367	ARG	CA-C-N	5.49	127.95	120.54
2	L	367	ARG	C-N-CA	5.49	127.95	120.54
2	F	284	ASP	CA-CB-CG	5.48	118.08	112.60
2	L	276	GLY	N-CA-C	5.46	122.29	114.64
2	C	284	ASP	CA-CB-CG	5.46	118.06	112.60
2	L	84	ASP	CA-CB-CG	5.42	118.02	112.60
1	J	62	VAL	N-CA-CB	5.42	116.97	110.31
2	C	367	ARG	CA-C-N	5.42	127.85	120.54
2	C	367	ARG	C-N-CA	5.42	127.85	120.54
2	R	84	ASP	CA-CB-CG	5.41	118.01	112.60
2	O	521	VAL	N-CA-CB	5.41	118.28	111.46
2	F	437	ASN	N-CA-C	-5.39	102.98	109.72
2	C	367	ARG	N-CA-C	5.39	118.02	109.24
2	L	461	ASP	CA-CB-CG	5.39	117.99	112.60
2	O	515	VAL	N-CA-CB	5.37	116.38	110.53
1	J	211	LYS	N-CA-C	5.36	117.55	111.11
1	M	211	LYS	N-CA-C	5.36	117.54	111.11
2	I	345	ALA	CA-C-N	5.34	127.70	120.38
2	I	345	ALA	C-N-CA	5.34	127.70	120.38
2	R	299	THR	CB-CA-C	5.34	118.45	109.48
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
1	G	211	LYS	N-CA-C	5.29	117.47	111.11
2	F	276	GLY	N-CA-C	5.28	121.98	114.85
2	R	367	ARG	CA-C-N	5.28	127.30	120.44
2	R	367	ARG	C-N-CA	5.28	127.30	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	562	ALA	CA-C-N	5.26	128.06	120.38
2	O	562	ALA	C-N-CA	5.26	128.06	120.38
1	P	62	VAL	N-CA-CB	5.25	116.77	110.31
2	C	84	ASP	CA-CB-CG	5.25	117.85	112.60
1	D	62	VAL	N-CA-CB	5.25	116.77	110.31
2	R	437	ASN	N-CA-C	-5.24	103.17	109.72
1	D	211	LYS	N-CA-C	5.23	117.39	111.11
2	L	246	ILE	N-CA-C	5.20	115.61	108.12
2	O	300	THR	N-CA-C	5.20	121.30	109.81
2	R	284	ASP	CA-CB-CG	5.18	117.78	112.60
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
1	G	76	ASN	CA-C-N	5.16	128.15	120.31
1	G	76	ASN	C-N-CA	5.16	128.15	120.31
2	R	519	ARG	N-CA-C	5.12	117.76	111.82
2	L	300	THR	N-CA-C	5.10	121.08	109.81
2	F	345	ALA	CA-C-N	5.10	127.42	120.54
2	F	345	ALA	C-N-CA	5.10	127.42	120.54
2	O	345	ALA	CA-C-N	5.09	127.36	120.38
2	O	345	ALA	C-N-CA	5.09	127.36	120.38
2	F	246	ILE	N-CA-C	5.09	115.45	108.12
2	O	160	THR	CB-CA-C	5.09	116.98	109.29
2	C	521	VAL	N-CA-CB	5.09	117.87	111.46
2	L	58	ASN	N-CA-C	-5.09	107.11	113.72
2	C	364	ALA	CA-C-N	5.08	131.24	121.54
2	C	364	ALA	C-N-CA	5.08	131.24	121.54
2	C	249	ASP	CA-CB-CG	5.07	117.67	112.60
2	R	562	ALA	CA-C-N	5.07	127.78	120.38
2	R	562	ALA	C-N-CA	5.07	127.78	120.38
2	R	345	ALA	CA-C-N	5.05	127.30	120.38
2	R	345	ALA	C-N-CA	5.05	127.30	120.38
2	L	515	VAL	N-CA-CB	5.04	116.03	110.53
2	R	99	GLY	N-CA-C	5.03	116.73	110.29
2	C	390	THR	CA-C-N	5.03	128.65	120.60
2	C	390	THR	C-N-CA	5.03	128.65	120.60
2	F	228	SER	CA-C-N	5.03	127.02	120.28
2	F	228	SER	C-N-CA	5.03	127.02	120.28
2	R	58	ASN	N-CA-C	-5.02	107.20	113.72
2	F	361	ASP	N-CA-C	-5.02	106.46	112.58
1	A	62	VAL	N-CA-CB	5.00	116.47	110.31

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	8	0
1	G	1767	0	1802	10	0
1	J	1767	0	1802	11	0
1	M	1767	0	1802	10	0
1	P	1767	0	1802	11	0
2	C	4301	0	4216	41	0
2	F	4301	0	4216	43	0
2	I	4301	0	4216	48	0
2	L	4301	0	4216	45	0
2	O	4301	0	4216	38	0
2	R	4301	0	4216	41	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
All	All	36420	0	36108	263	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 (263) 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	1.60	0.84
2:L:335:GLN:HG3	2:L:339:ARG:HD2	1.60	0.83
2:R:335:GLN:HG3	2:R:339:ARG:HD2	1.60	0.83
2:O:335:GLN:HG3	2:O:339:ARG:HD2	1.61	0.82
2:I:335:GLN:HG3	2:I:339:ARG:HD2	1.61	0.82
2:F:335:GLN:HG3	2:F:339:ARG:HD2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:MET:HE1	2:I:564:ARG:HD2	1.70	0.74
2:R:328:ARG:HE	2:R:333:PHE:HD1	1.38	0.71
2:F:328:ARG:HE	2:F:333:PHE:HD1	1.38	0.70
2:I:328:ARG:HE	2:I:333:PHE:HD1	1.38	0.70
2:O:328:ARG:HE	2:O:333:PHE:HD1	1.39	0.69
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
1:A:77:MET:HE1	2:C:564:ARG:HD2	1.77	0.67
1:P:77:MET:HE1	2:R:564:ARG:HD2	1.77	0.66
1:D:77:MET:HE1	2:F:564:ARG:HD2	1.79	0.65
1:J:77:MET:HE1	2:L:564:ARG:HD2	1.79	0.65
2:I:367:ARG:CB	2:I:370:GLU:HG3	2.27	0.65
2:R:367:ARG:HB3	2:R:370:GLU:HG3	1.80	0.64
2:L:367:ARG:CB	2:L:370:GLU:HG3	2.28	0.63
1:M:77:MET:HE1	2:O:564:ARG:HD2	1.81	0.63
2:R:367:ARG:CB	2:R:370:GLU:HG3	2.28	0.63
2:C:367:ARG:CB	2:C:370:GLU:HG3	2.29	0.63
2:F:367:ARG:CB	2:F:370:GLU:HG3	2.28	0.63
2:O:367:ARG:CB	2:O:370:GLU:HG3	2.28	0.63
2:L:367:ARG:HB3	2:L:370:GLU:HG3	1.80	0.62
2:F:352:MET:HE1	2:F:546:VAL:HG11	1.82	0.62
2:I:367:ARG:HB3	2:I:370:GLU:HG3	1.82	0.62
2:I:443:VAL:HB	2:I:561:LEU:HB3	1.82	0.61
2:F:443:VAL:HB	2:F:561:LEU:HB3	1.82	0.60
2:C:367:ARG:HB3	2:C:370:GLU:HG3	1.83	0.59
2:F:461:ASP:HB3	2:F:464:ALA:HB2	1.85	0.59
2:R:335:GLN:O	2:R:339:ARG:HB2	2.02	0.59
2:L:335:GLN:O	2:L:339:ARG:HB2	2.02	0.59
2:C:352:MET:HE1	2:C:546:VAL:HG11	1.84	0.59
2:C:275:GLU:HA	2:C:286:ILE:HD12	1.84	0.59
2:F:367:ARG:HB3	2:F:370:GLU:HG3	1.83	0.59
2:F:335:GLN:O	2:F:339:ARG:HB2	2.03	0.59
2:O:352:MET:HE1	2:O:546:VAL:HG11	1.83	0.58
2:R:461:ASP:HB3	2:R:464:ALA:HB2	1.85	0.58
2:I:461:ASP:HB3	2:I:464:ALA:HB2	1.85	0.58
2:C:335:GLN:O	2:C:339:ARG:HB2	2.02	0.58
2:C:461:ASP:HB3	2:C:464:ALA:HB2	1.85	0.58
2:O:443:VAL:HB	2:O:561:LEU:HB3	1.85	0.58
2:R:443:VAL:HB	2:R:561:LEU:HB3	1.86	0.58
2:L:443:VAL:HB	2:L:561:LEU:HB3	1.85	0.57
2:F:162:PRO:HB3	2:I:459:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:461:ASP:HB3	2:L:464:ALA:HB2	1.87	0.57
2:I:335:GLN:O	2:I:339:ARG:HB2	2.04	0.57
2:O:335:GLN:O	2:O:339:ARG:HB2	2.04	0.57
2:C:443:VAL:HB	2:C:561:LEU:HB3	1.85	0.57
2:O:367:ARG:HB3	2:O:370:GLU:HG3	1.85	0.57
2:O:461:ASP:HB3	2:O:464:ALA:HB2	1.87	0.57
2:L:352:MET:HE1	2:L:546:VAL:HG11	1.87	0.56
2:I:352:MET:HE1	2:I:546:VAL:HG11	1.87	0.56
2:O:444:LYS:HD3	1:P:2:LYS:HB2	1.88	0.56
2:O:466:VAL:HG23	2:O:469:PRO:HD3	1.88	0.56
1:G:110:ILE:HG12	2:I:20:VAL:HG22	1.87	0.55
2:R:30:GLU:HB2	2:R:396:ASN:HB3	1.87	0.55
2:R:466:VAL:HG23	2:R:469:PRO:HD3	1.88	0.55
1:G:106:LYS:HB3	1:G:109:GLU:HB2	1.89	0.55
2:I:466:VAL:HG23	2:I:469:PRO:HD3	1.89	0.55
1:J:140:HIS:HB2	2:R:251:VAL:HB	1.88	0.55
1:M:120:LEU:HD12	2:O:1:MET:HE2	1.89	0.55
2:C:466:VAL:HG23	2:C:469:PRO:HD3	1.88	0.54
1:D:1:FME:HCN	1:D:2:LYS:HZ2	1.72	0.54
1:A:140:HIS:HB2	2:I:251:VAL:HB	1.90	0.54
2:I:298:SER:HB2	2:I:350:HIS:HE2	1.71	0.54
2:L:162:PRO:HB3	2:O:459:MET:HE1	1.90	0.54
2:L:466:VAL:HG23	2:L:469:PRO:HD3	1.89	0.54
2:C:169:THR:HB	2:C:171:ILE:HD12	1.89	0.53
2:L:298:SER:HB2	2:L:350:HIS:HE2	1.73	0.53
2:F:466:VAL:HG23	2:F:469:PRO:HD3	1.89	0.53
2:C:162:PRO:HB3	2:F:459:MET:HE1	1.90	0.53
2:L:464:ALA:HB1	2:L:469:PRO:HG2	1.91	0.53
2:F:464:ALA:HB1	2:F:469:PRO:HG2	1.91	0.52
2:L:459:MET:HE1	2:R:162:PRO:HB3	1.92	0.52
2:F:298:SER:HB2	2:F:350:HIS:HE2	1.73	0.52
1:J:110:ILE:HG12	2:L:20:VAL:HG22	1.92	0.52
2:I:537:VAL:HG22	2:I:544:VAL:HG22	1.90	0.52
2:C:464:ALA:HB1	2:C:469:PRO:HG2	1.92	0.51
1:P:113:ALA:HB2	2:R:17:GLY:C	2.36	0.51
2:L:275:GLU:OE2	2:L:339:ARG:NH2	2.44	0.51
2:O:464:ALA:HB1	2:O:469:PRO:HG2	1.92	0.51
2:R:464:ALA:HB1	2:R:469:PRO:HG2	1.93	0.51
2:C:459:MET:HE1	2:I:162:PRO:HB3	1.92	0.51
2:O:251:VAL:HB	1:P:140:HIS:HB2	1.94	0.50
1:J:2:LYS:HB2	2:R:444:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:GLY:HA2	2:I:21:ARG:O	2.12	0.49
1:A:2:LYS:HB2	2:I:444:LYS:HD3	1.94	0.49
2:O:162:PRO:HB3	2:R:459:MET:HE1	1.93	0.49
2:C:421:TYR:HB3	2:C:430:ILE:HD12	1.95	0.49
2:L:298:SER:CB	2:L:350:HIS:HE2	2.25	0.49
2:O:275:GLU:HG2	2:O:342:SER:HB2	1.94	0.49
2:O:367:ARG:HB2	2:O:370:GLU:HG3	1.95	0.48
2:O:421:TYR:HB3	2:O:430:ILE:HD12	1.95	0.48
2:R:328:ARG:HH11	2:R:333:PHE:HE1	1.62	0.48
2:R:274:ILE:HD11	2:R:288:MET:HB2	1.95	0.48
1:D:106:LYS:HB3	1:D:109:GLU:HB2	1.95	0.48
2:I:30:GLU:HB2	2:I:396:ASN:HB3	1.95	0.47
2:I:298:SER:CB	2:I:350:HIS:HE2	2.27	0.47
2:R:297:SER:HB3	2:R:357:MET:HB2	1.96	0.47
1:A:39:ILE:HD13	1:A:99:PRO:HB2	1.97	0.47
2:I:367:ARG:HB2	2:I:370:GLU:HG3	1.97	0.47
2:I:464:ALA:HB1	2:I:469:PRO:HG2	1.95	0.47
2:L:275:GLU:HA	2:L:286:ILE:HD12	1.95	0.47
2:O:328:ARG:HH11	2:O:333:PHE:HE1	1.62	0.47
2:F:301:PRO:HD3	2:F:366:GLY:HA2	1.96	0.47
1:D:39:ILE:HD13	1:D:99:PRO:HB2	1.97	0.47
2:F:367:ARG:HB2	2:F:370:GLU:HG3	1.97	0.47
2:O:186:GLU:HA	2:O:510:ARG:HD2	1.96	0.47
2:R:421:TYR:HB3	2:R:430:ILE:HD12	1.97	0.47
2:F:328:ARG:HH11	2:F:333:PHE:HE1	1.63	0.46
2:C:328:ARG:HH11	2:C:333:PHE:HE1	1.63	0.46
1:M:39:ILE:HD13	1:M:99:PRO:HB2	1.97	0.46
2:R:360:SER:O	2:R:366:GLY:HA3	2.15	0.46
2:I:275:GLU:HA	2:I:286:ILE:HD12	1.98	0.46
2:I:421:TYR:HB3	2:I:430:ILE:HD12	1.97	0.46
2:L:219:LEU:HB3	2:L:225:THR:HG23	1.98	0.46
2:F:421:TYR:HB3	2:F:430:ILE:HD12	1.96	0.46
2:I:135:HIS:HB3	2:I:359:SER:HB2	1.97	0.46
2:I:301:PRO:HD3	2:I:366:GLY:HA2	1.97	0.46
2:R:171:ILE:HG13	2:R:218:KCX:HB2	1.97	0.46
2:L:328:ARG:HH11	2:L:333:PHE:HE1	1.63	0.46
2:O:301:PRO:HD3	2:O:366:GLY:HA2	1.98	0.46
2:F:298:SER:CB	2:F:350:HIS:HE2	2.28	0.46
2:F:313:HIS:C	2:F:315:ASP:H	2.24	0.46
2:I:313:HIS:C	2:I:315:ASP:H	2.24	0.46
2:R:352:MET:HE1	2:R:546:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:537:VAL:HG22	2:L:544:VAL:HG22	1.97	0.46
2:C:98:ALA:HB2	2:C:111:MET:HE2	1.98	0.46
2:O:30:GLU:HB2	2:O:396:ASN:HB3	1.97	0.46
2:I:275:GLU:OE2	2:I:339:ARG:NH2	2.49	0.46
2:L:421:TYR:HB3	2:L:430:ILE:HD12	1.96	0.46
2:C:367:ARG:HB2	2:C:370:GLU:HG3	1.99	0.45
2:O:430:ILE:HD13	2:O:490:ILE:HD11	1.97	0.45
2:F:30:GLU:HB2	2:F:396:ASN:HB3	1.98	0.45
2:F:186:GLU:HA	2:F:510:ARG:HD2	1.97	0.45
2:C:169:THR:HG21	2:C:223:TRP:NE1	2.31	0.45
2:F:52:GLU:HG2	2:F:58:ASN:HD21	1.80	0.45
1:J:141:VAL:HA	2:R:253:GLU:HG3	1.98	0.45
2:C:169:THR:HG21	2:C:223:TRP:HE1	1.80	0.45
1:P:39:ILE:HD13	1:P:99:PRO:HB2	1.99	0.45
2:R:186:GLU:HA	2:R:510:ARG:HD2	1.99	0.45
2:I:186:GLU:HA	2:I:510:ARG:HD2	1.98	0.45
2:L:444:LYS:HD3	1:M:2:LYS:HB2	1.97	0.45
2:R:264:MET:HE2	2:R:269:ILE:HD13	1.99	0.45
2:L:301:PRO:HD3	2:L:366:GLY:HA2	1.99	0.45
2:F:264:MET:HE2	2:F:269:ILE:HD13	1.99	0.45
2:I:430:ILE:HD13	2:I:490:ILE:HD11	1.97	0.45
2:R:52:GLU:HG2	2:R:58:ASN:HD21	1.82	0.45
2:C:301:PRO:HD3	2:C:366:GLY:HA2	1.99	0.45
2:F:98:ALA:HB2	2:F:111:MET:HE2	1.98	0.45
2:I:328:ARG:HH11	2:I:333:PHE:HE1	1.64	0.45
2:O:313:HIS:C	2:O:315:ASP:H	2.25	0.45
2:C:444:LYS:HD3	1:D:2:LYS:HB2	1.98	0.45
1:J:48:ARG:HG3	1:P:23:ARG:CZ	2.47	0.45
2:L:237:ALA:O	2:L:519:ARG:HD3	2.17	0.45
1:J:39:ILE:HD13	1:J:99:PRO:HB2	1.99	0.44
2:L:186:GLU:HA	2:L:510:ARG:HD2	1.98	0.44
2:R:301:PRO:HD3	2:R:366:GLY:HA2	1.99	0.44
2:C:186:GLU:HA	2:C:510:ARG:HD2	1.99	0.44
2:L:98:ALA:HB2	2:L:111:MET:HE2	1.98	0.44
2:L:430:ILE:HD13	2:L:490:ILE:HD11	1.99	0.44
2:C:313:HIS:C	2:C:315:ASP:H	2.25	0.44
1:G:120:LEU:HD12	2:I:1:MET:HE2	1.98	0.44
2:F:251:VAL:HB	1:G:140:HIS:HB2	2.00	0.44
2:F:430:ILE:HD13	2:F:490:ILE:HD11	1.98	0.44
1:G:39:ILE:HD13	1:G:99:PRO:HB2	1.98	0.44
2:L:136:THR:O	2:L:157:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:98:ALA:HB2	2:O:111:MET:HE2	1.98	0.44
2:C:165:GLY:HA3	2:F:118:GLU:OE2	2.17	0.44
2:C:264:MET:HE2	2:C:269:ILE:HD13	2.00	0.44
2:F:292:VAL:CG1	1:J:205:ILE:HG21	2.48	0.44
2:I:264:MET:HE2	2:I:269:ILE:HD13	1.99	0.44
2:L:313:HIS:C	2:L:315:ASP:H	2.25	0.44
1:M:110:ILE:HG12	2:O:20:VAL:HG22	2.00	0.44
2:R:430:ILE:HD13	2:R:490:ILE:HD11	2.00	0.44
2:C:360:SER:O	2:C:366:GLY:HA3	2.17	0.44
2:F:237:ALA:O	2:F:519:ARG:HD3	2.18	0.44
2:R:313:HIS:C	2:R:315:ASP:H	2.24	0.44
2:R:367:ARG:HB2	2:R:370:GLU:HG3	2.00	0.44
2:R:98:ALA:HB2	2:R:111:MET:HE2	2.00	0.44
2:C:456:PHE:CE2	2:C:474:TYR:HB3	2.53	0.44
2:F:186:GLU:HG3	2:I:483:LYS:HD2	2.00	0.44
2:L:264:MET:HE2	2:L:269:ILE:HD13	2.00	0.44
2:F:62:GLU:HG2	2:L:516:LYS:HD2	2.00	0.43
2:O:264:MET:HE2	2:O:269:ILE:HD13	1.99	0.43
2:R:275:GLU:OE2	2:R:339:ARG:NH2	2.51	0.43
2:I:98:ALA:HB2	2:I:111:MET:HE2	2.00	0.43
2:C:251:VAL:HB	1:D:140:HIS:HB2	2.01	0.43
2:L:274:ILE:HG12	2:L:289:ALA:HB2	2.01	0.43
2:L:367:ARG:HB2	2:L:370:GLU:HG3	2.01	0.43
1:A:114:SER:OG	1:A:116:LYS:HB2	2.18	0.43
2:O:247:HIS:CE1	2:O:279:GLY:HA3	2.54	0.43
2:C:216:GLY:HA2	2:C:242:VAL:HB	2.01	0.43
2:L:360:SER:O	2:L:366:GLY:HA3	2.19	0.43
2:R:456:PHE:CE2	2:R:474:TYR:HB3	2.54	0.43
1:D:113:ALA:HB2	2:F:17:GLY:C	2.44	0.42
2:L:456:PHE:CE2	2:L:474:TYR:HB3	2.54	0.42
2:F:140:SER:HB2	2:I:459:MET:HE3	2.01	0.42
2:L:253:GLU:HG3	1:M:141:VAL:HA	2.01	0.42
2:O:150:ASN:O	2:O:372:ILE:HD12	2.19	0.42
2:I:354:VAL:HG11	2:I:535:ILE:HD11	1.99	0.42
2:C:150:ASN:O	2:C:372:ILE:HD12	2.18	0.42
2:C:312:GLU:OE2	2:C:367:ARG:NH2	2.53	0.42
2:F:150:ASN:O	2:F:372:ILE:HD12	2.19	0.42
2:L:354:VAL:HG11	2:L:535:ILE:HD11	2.02	0.42
2:R:150:ASN:O	2:R:372:ILE:HD12	2.19	0.42
1:D:108:GLY:HA2	2:F:21:ARG:O	2.20	0.42
2:O:535:ILE:HG12	2:O:546:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:72:PRO:HG2	2:R:564:ARG:HH12	1.84	0.42
2:I:456:PHE:CE2	2:I:474:TYR:HB3	2.55	0.42
2:L:169:THR:HG22	2:L:220:HIS:CG	2.55	0.42
2:O:312:GLU:OE2	2:O:367:ARG:NH2	2.52	0.42
2:C:275:GLU:OE2	2:C:339:ARG:NH2	2.52	0.42
2:C:354:VAL:HG11	2:C:535:ILE:HD11	2.02	0.42
2:C:430:ILE:HD13	2:C:490:ILE:HD11	2.02	0.42
1:G:194:LYS:HB3	2:I:102:ASP:HB3	2.02	0.42
1:M:108:GLY:HA2	2:O:21:ARG:O	2.19	0.42
2:F:261:LEU:HD21	2:F:288:MET:HG2	2.02	0.42
2:I:216:GLY:HA2	2:I:242:VAL:HB	2.01	0.42
2:L:251:VAL:HB	1:M:140:HIS:HB2	2.01	0.42
2:C:52:GLU:HG2	2:C:58:ASN:HD21	1.85	0.42
2:F:169:THR:HB	2:F:171:ILE:HD12	2.01	0.42
2:O:456:PHE:CE2	2:O:474:TYR:HB3	2.55	0.42
2:O:216:GLY:HA2	2:O:242:VAL:HB	2.01	0.41
2:F:169:THR:HG22	2:F:220:HIS:CG	2.55	0.41
2:R:298:SER:HB2	2:R:350:HIS:HE2	1.85	0.41
1:A:72:PRO:HG2	2:C:564:ARG:HH12	1.85	0.41
2:C:338:ILE:HG22	2:C:339:ARG:NH1	2.35	0.41
2:I:150:ASN:O	2:I:372:ILE:HD12	2.20	0.41
2:I:52:GLU:HG2	2:I:58:ASN:HD21	1.84	0.41
2:I:261:LEU:HD21	2:I:288:MET:HG2	2.03	0.41
2:F:338:ILE:HG22	2:F:339:ARG:NH1	2.35	0.41
1:M:113:ALA:HB2	2:O:17:GLY:C	2.46	0.41
1:A:48:ARG:HG3	1:G:23:ARG:CZ	2.51	0.41
2:F:456:PHE:CE2	2:F:474:TYR:HB3	2.56	0.41
2:L:163:VAL:HG12	2:O:120:LEU:HD13	2.02	0.41
2:L:338:ILE:HG22	2:L:339:ARG:NH1	2.35	0.41
2:I:338:ILE:HG22	2:I:339:ARG:NH1	2.36	0.41
2:L:52:GLU:HG2	2:L:58:ASN:HD21	1.86	0.41
1:P:1:FME:HCN	1:P:2:LYS:HZ3	1.85	0.41
2:R:338:ILE:HG22	2:R:339:ARG:NH1	2.36	0.41
2:L:150:ASN:O	2:L:372:ILE:HD12	2.21	0.41
2:C:44:PHE:HB2	2:C:50:ILE:HD12	2.03	0.40
2:C:294:ILE:O	2:C:296:PRO:HD3	2.21	0.40
2:I:137:HIS:CD2	2:I:364:ALA:HB3	2.56	0.40
2:I:316:MET:HE3	2:I:365:MET:HG2	2.02	0.40
1:J:53:THR:HG1	1:J:56:GLN:HG3	1.86	0.40
2:R:169:THR:HG22	2:R:220:HIS:CG	2.56	0.40
1:A:138:SER:HB2	1:A:177:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:139:LEU:HD11	2:I:167:ASN:HA	2.02	0.40
1:J:108:GLY:HA2	2:L:21:ARG:O	2.21	0.40
1:P:194:LYS:HB3	2:R:102:ASP:HB3	2.02	0.40
1:J:114:SER:OG	1:J:116:LYS:HB2	2.21	0.40
2:O:253:GLU:HG3	1:P:141:VAL:HA	2.02	0.40
2:F:312:GLU:OE2	2:F:367:ARG:NH2	2.55	0.40
2:F:354:VAL:HG11	2:F:535:ILE:HD11	2.03	0.40
1:G:114:SER:OG	1:G:116:LYS:HB2	2.21	0.40
1:M:32:GLN:HE22	1:P:1:FME:HCN	1.86	0.40
2:I:220:HIS:HA	2:I:247:HIS:HB3	2.03	0.40
2:R:354:VAL:HG11	2:R:535:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
1	D	223/225 (99%)	218 (98%)	5 (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%)	527 (94%)	29 (5%)	3 (0%)	24	60
2	F	559/568 (98%)	522 (93%)	32 (6%)	5 (1%)	14	48
2	I	559/568 (98%)	525 (94%)	31 (6%)	3 (0%)	24	60
2	L	559/568 (98%)	521 (93%)	36 (6%)	2 (0%)	30	65
2	O	559/568 (98%)	523 (94%)	32 (6%)	4 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	R	559/568 (98%)	526 (94%)	30 (5%)	3 (0%)	24 60
All	All	4692/4758 (99%)	4452 (95%)	220 (5%)	20 (0%)	30 65

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	365	MET
2	C	365	MET
2	C	464	ALA
2	F	365	MET
2	F	464	ALA
2	I	464	ALA
2	L	464	ALA
2	O	464	ALA
2	R	365	MET
2	R	464	ALA
2	O	249	ASP
2	F	281	HIS
2	I	365	MET
2	O	365	MET
2	C	314	LEU
2	F	199	ASN
2	F	314	LEU
2	I	314	LEU
2	O	314	LEU
2	R	314	LEU

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%)	175 (95%)	10 (5%)	20 53
1	D	185/185 (100%)	175 (95%)	10 (5%)	20 53
1	G	185/185 (100%)	173 (94%)	12 (6%)	15 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	185/185 (100%)	174 (94%)	11 (6%)	18	50
1	M	185/185 (100%)	175 (95%)	10 (5%)	20	53
1	P	185/185 (100%)	175 (95%)	10 (5%)	20	53
2	C	459/466 (98%)	443 (96%)	16 (4%)	32	65
2	F	459/466 (98%)	442 (96%)	17 (4%)	30	64
2	I	459/466 (98%)	442 (96%)	17 (4%)	30	64
2	L	459/466 (98%)	441 (96%)	18 (4%)	28	62
2	O	459/466 (98%)	441 (96%)	18 (4%)	28	62
2	R	459/466 (98%)	441 (96%)	18 (4%)	28	62
All	All	3864/3906 (99%)	3697 (96%)	167 (4%)	26	60

All (167) 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	152	ARG
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
2	C	210	VAL
2	C	298	SER
2	C	324	ASP
2	C	328	ARG
2	C	335	GLN
2	C	336	SER
2	C	339	ARG
2	C	502	ILE
2	C	510	ARG
2	C	521	VAL

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Mol	Chain	Res	Type
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	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	95	THR
1	G	104	ASP
1	G	114	SER
1	G	116	LYS
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

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Mol	Chain	Res	Type
2	I	49	THR
2	I	139	LEU
2	I	180	ARG
2	I	210	VAL
2	I	298	SER
2	I	324	ASP
2	I	328	ARG
2	I	335	GLN
2	I	336	SER
2	I	339	ARG
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	95	THR
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
2	L	180	ARG
2	L	210	VAL
2	L	247	HIS
2	L	298	SER
2	L	324	ASP
2	L	328	ARG
2	L	335	GLN
2	L	336	SER
2	L	339	ARG
2	L	502	ILE
2	L	510	ARG

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Mol	Chain	Res	Type
2	L	521	VAL
2	L	563	SER
1	M	51	LYS
1	M	83	VAL
1	M	104	ASP
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	134	SER
2	O	139	LEU
2	O	160	THR
2	O	169	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	502	ILE
2	O	510	ARG
2	O	521	VAL
2	O	563	SER
1	P	51	LYS
1	P	83	VAL
1	P	104	ASP
1	P	116	LYS
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

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Mol	Chain	Res	Type
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	258	ASP
2	R	324	ASP
2	R	328	ARG
2	R	335	GLN
2	R	336	SER
2	R	339	ARG
2	R	502	ILE
2	R	510	ARG
2	R	521	VAL
2	R	563	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	86	ASN
2	C	143	GLN
2	C	377	GLN
2	C	463	ASN
2	F	143	GLN
2	F	167	ASN
2	F	463	ASN
2	I	89	ASN
2	I	100	ASN
2	I	143	GLN
2	I	377	GLN
1	J	56	GLN
1	J	86	ASN
2	L	100	ASN
2	L	143	GLN
1	M	8	GLN
1	M	86	ASN
2	O	6	GLN
2	O	89	ASN
2	O	100	ASN
2	O	143	GLN

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Mol	Chain	Res	Type
2	O	321	HIS
2	O	463	ASN
2	R	6	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	F	218	3,2	10,11,12	0.99	1 (10%)	6,12,14	1.99	1 (16%)
1	FME	J	1	1	8,9,10	0.52	0	8,9,11	0.93	0
2	KCX	R	218	3,2	10,11,12	1.00	1 (10%)	6,12,14	2.26	1 (16%)
1	FME	G	1	1	8,9,10	0.44	0	8,9,11	1.07	1 (12%)
1	FME	A	1	1	8,9,10	0.54	0	8,9,11	0.96	1 (12%)
1	FME	M	1	1	8,9,10	0.53	0	8,9,11	1.02	1 (12%)
1	FME	P	1	1	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
1	FME	D	1	1	8,9,10	0.50	0	8,9,11	0.92	0
2	KCX	I	218	3,2	10,11,12	1.08	1 (10%)	6,12,14	1.97	1 (16%)
2	KCX	O	218	3,2	10,11,12	0.98	1 (10%)	6,12,14	2.02	1 (16%)
2	KCX	L	218	3,2	10,11,12	0.98	1 (10%)	6,12,14	2.07	1 (16%)
2	KCX	C	218	3,2	10,11,12	1.06	1 (10%)	6,12,14	1.93	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	F	218	3,2	-	1/9/10/12	-
1	FME	J	1	1	-	2/7/9/11	-
2	KCX	R	218	3,2	-	1/9/10/12	-
1	FME	G	1	1	-	2/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
1	FME	M	1	1	-	2/7/9/11	-
1	FME	P	1	1	-	2/7/9/11	-
1	FME	D	1	1	-	2/7/9/11	-
2	KCX	I	218	3,2	-	1/9/10/12	-
2	KCX	O	218	3,2	-	1/9/10/12	-
2	KCX	L	218	3,2	-	0/9/10/12	-
2	KCX	C	218	3,2	-	0/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	218	KCX	OQ1-CX	2.74	1.26	1.21
2	C	218	KCX	OQ1-CX	2.52	1.26	1.21
2	L	218	KCX	OQ1-CX	2.41	1.26	1.21
2	R	218	KCX	OQ1-CX	2.34	1.26	1.21
2	O	218	KCX	OQ1-CX	2.32	1.26	1.21
2	F	218	KCX	OQ1-CX	2.29	1.25	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	218	KCX	OQ1-CX-NZ	-5.20	117.02	124.92
2	L	218	KCX	OQ1-CX-NZ	-4.80	117.63	124.92
2	O	218	KCX	OQ1-CX-NZ	-4.72	117.75	124.92
2	I	218	KCX	OQ1-CX-NZ	-4.61	117.92	124.92
2	F	218	KCX	OQ1-CX-NZ	-4.61	117.92	124.92
2	C	218	KCX	OQ1-CX-NZ	-4.53	118.04	124.92
1	G	1	FME	O-C-CA	-2.24	119.00	124.77
1	M	1	FME	O-C-CA	-2.15	119.25	124.77
1	A	1	FME	O-C-CA	-2.11	119.34	124.77
1	P	1	FME	O-C-CA	-2.09	119.39	124.77

There are no chirality outliers.

All (16) 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
2	F	218	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	218	KCX	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%)	-0.36	0 100 100	17, 30, 49, 64	0
1	D	224/225 (99%)	-0.20	3 (1%) 75 53	21, 30, 51, 68	0
1	G	224/225 (99%)	-0.33	0 100 100	20, 30, 51, 65	0
1	J	224/225 (99%)	-0.26	2 (0%) 81 61	22, 35, 55, 73	0
1	M	224/225 (99%)	-0.29	2 (0%) 81 61	19, 32, 53, 72	0
1	P	224/225 (99%)	-0.28	1 (0%) 88 76	22, 34, 55, 70	0
2	C	563/568 (99%)	-0.35	24 (4%) 40 21	13, 24, 58, 105	0
2	F	563/568 (99%)	-0.36	22 (3%) 43 24	14, 24, 58, 103	0
2	I	563/568 (99%)	-0.36	20 (3%) 46 26	13, 24, 57, 102	0
2	L	563/568 (99%)	-0.31	21 (3%) 45 25	15, 26, 60, 106	0
2	O	563/568 (99%)	-0.32	23 (4%) 41 23	14, 26, 62, 110	0
2	R	563/568 (99%)	-0.30	26 (4%) 37 20	18, 28, 62, 109	0
All	All	4722/4758 (99%)	-0.32	144 (3%) 52 30	13, 27, 57, 110	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	319	THR	5.7
2	C	325	LYS	5.3
2	C	327	ILE	5.2
2	R	319	THR	5.2
2	O	328	ARG	5.1
2	R	328	ARG	4.9
2	O	462	SER	4.9
2	C	328	ARG	4.9
2	R	317	LEU	4.8
2	L	327	ILE	4.6
2	F	327	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
2	O	327	ILE	4.5
2	O	325	LYS	4.5
2	L	322	HIS	4.5
2	F	328	ARG	4.5
2	L	319	THR	4.4
2	L	328	ARG	4.3
2	R	327	ILE	4.2
2	F	325	LYS	4.1
2	I	325	LYS	4.1
2	R	321	HIS	4.1
2	O	317	LEU	4.0
2	I	328	ARG	4.0
2	C	326	ARG	3.9
2	C	321	HIS	3.9
2	O	319	THR	3.9
2	L	321	HIS	3.8
2	I	327	ILE	3.8
2	F	322	HIS	3.8
2	O	322	HIS	3.8
2	R	462	SER	3.7
2	I	319	THR	3.7
2	C	322	HIS	3.7
2	L	325	LYS	3.7
2	R	325	LYS	3.7
2	R	318	MET	3.6
2	C	364	ALA	3.6
2	I	322	HIS	3.5
1	J	6	LYS	3.5
2	L	323	LEU	3.5
2	O	318	MET	3.5
1	M	6	LYS	3.4
2	I	321	HIS	3.4
2	L	462	SER	3.4
2	R	333	PHE	3.4
2	L	317	LEU	3.4
2	C	368	ALA	3.3
2	C	317	LEU	3.3
2	I	313	HIS	3.3
2	R	323	LEU	3.3
2	F	323	LEU	3.2
2	F	321	HIS	3.2
2	R	322	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	6	LYS	3.2
2	I	320	CYS	3.1
2	I	317	LEU	3.1
2	C	333	PHE	3.1
2	L	318	MET	3.1
2	F	465	SER	3.1
2	F	319	THR	3.0
2	O	321	HIS	3.0
2	R	313	HIS	3.0
2	R	364	ALA	3.0
2	C	320	CYS	3.0
2	R	334	SER	2.9
1	D	104	ASP	2.9
2	L	460	GLY	2.9
2	O	326	ARG	2.9
2	I	338	ILE	2.9
2	L	320	CYS	2.9
2	C	318	MET	2.9
2	F	467	PRO	2.9
2	R	320	CYS	2.9
2	L	326	ARG	2.9
2	O	314	LEU	2.9
2	F	318	MET	2.8
2	L	335	GLN	2.8
2	F	462	SER	2.8
2	I	318	MET	2.8
2	O	333	PHE	2.7
2	O	320	CYS	2.7
2	I	326	ARG	2.7
2	F	313	HIS	2.7
2	C	314	LEU	2.7
2	I	333	PHE	2.7
2	F	26	ASP	2.7
2	O	465	SER	2.6
2	C	324	ASP	2.6
2	I	323	LEU	2.6
2	R	362	SER	2.6
2	I	335	GLN	2.6
2	O	335	GLN	2.6
2	O	324	ASP	2.6
2	R	326	ARG	2.6
2	C	315	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	324	ASP	2.5
2	I	314	LEU	2.5
2	R	466	VAL	2.5
2	L	364	ALA	2.5
2	O	461	ASP	2.5
2	F	460	GLY	2.5
2	R	335	GLN	2.5
2	O	323	LEU	2.4
2	C	335	GLN	2.4
2	C	362	SER	2.4
2	O	334	SER	2.4
2	F	333	PHE	2.4
2	L	333	PHE	2.4
2	O	313	HIS	2.4
2	C	365	MET	2.3
2	F	466	VAL	2.3
1	P	6	LYS	2.3
2	F	463	ASN	2.3
2	L	461	ASP	2.3
2	C	323	LEU	2.3
2	F	314	LEU	2.3
2	R	324	ASP	2.3
2	I	368	ALA	2.2
2	R	315	ASP	2.2
2	O	467	PRO	2.2
2	C	466	VAL	2.2
2	R	539	PRO	2.2
1	D	114	SER	2.2
2	F	335	GLN	2.2
2	F	317	LEU	2.2
2	L	314	LEU	2.2
1	J	7	GLU	2.2
2	L	324	ASP	2.2
2	R	393	LYS	2.1
2	C	313	HIS	2.1
2	R	365	MET	2.1
2	C	338	ILE	2.1
2	F	326	ARG	2.1
2	L	338	ILE	2.1
2	R	336	SER	2.1
2	R	461	ASP	2.1
2	O	368	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	467	PRO	2.1
1	M	7	GLU	2.0
2	I	465	SER	2.0
2	L	365	MET	2.0
2	I	468	THR	2.0
2	O	468	THR	2.0
2	F	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	0.11	49,50,55,55	0
1	FME	A	1	10/11	0.95	0.10	41,42,47,48	0
1	FME	M	1	10/11	0.95	0.13	49,51,55,55	0
1	FME	P	1	10/11	0.95	0.12	46,49,53,53	0
1	FME	D	1	10/11	0.96	0.10	44,46,50,50	0
2	KCX	I	218	12/13	0.97	0.07	18,20,26,27	0
1	FME	G	1	10/11	0.97	0.10	40,42,47,48	0
2	KCX	R	218	12/13	0.97	0.06	21,23,27,28	0
2	KCX	F	218	12/13	0.98	0.06	19,20,22,23	0
2	KCX	O	218	12/13	0.98	0.05	24,27,29,29	0
2	KCX	C	218	12/13	0.98	0.06	19,20,24,25	0
2	KCX	L	218	12/13	0.98	0.06	18,19,21,22	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	R	774	1/1	0.98	0.06	35,35,35,35	0
3	FE	C	775	1/1	0.99	0.03	31,31,31,31	0
3	FE	I	774	1/1	0.99	0.06	24,24,24,24	0
3	FE	I	775	1/1	0.99	0.03	28,28,28,28	0
3	FE	L	774	1/1	0.99	0.05	20,20,20,20	0
3	FE	O	774	1/1	0.99	0.03	29,29,29,29	0
3	FE	C	774	1/1	0.99	0.03	21,21,21,21	0
3	FE	R	775	1/1	0.99	0.02	31,31,31,31	0
3	FE	F	775	1/1	1.00	0.02	24,24,24,24	0
3	FE	O	775	1/1	1.00	0.02	27,27,27,27	0
3	FE	F	774	1/1	1.00	0.03	22,22,22,22	0
3	FE	L	775	1/1	1.00	0.03	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.