



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:39 am BST

PDB ID : 1QHB
Title : VANADIUM BROMOPEROXIDASE FROM RED ALGA CORALLINA OF-
FICINALIS
Authors : Isupov, M.N.; Dalby, A.R.; Brindley, A.A.; Littlechild, J.A.
Deposited on : 1999-05-11
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

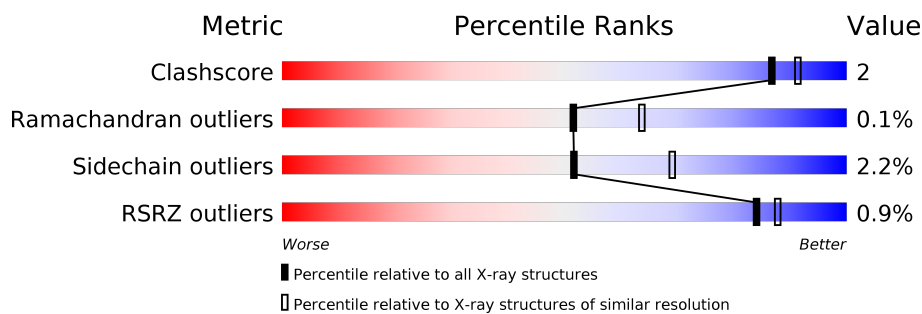
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	596	<div> <div>2%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
1	B	596	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	C	596	<div> <div>%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	D	596	<div> <div>90%</div> <div>9%</div> </div>
1	E	596	<div> <div>%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
1	F	596	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition [i](#)

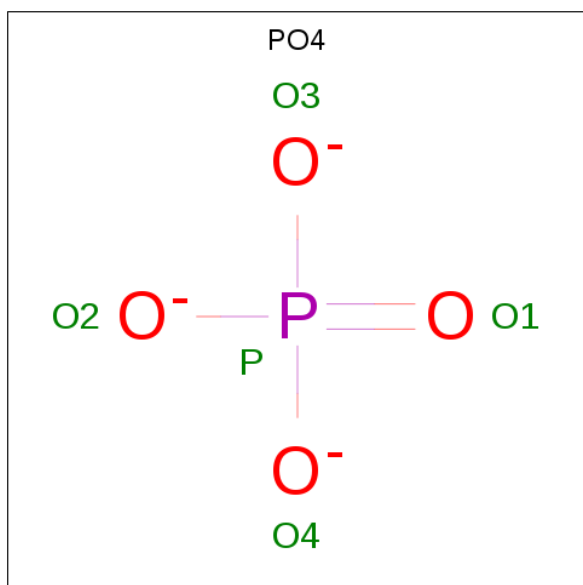
There are 4 unique types of molecules in this entry. The entry contains 29624 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HALOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4567	2900	766	893	8			
1	B	595	Total	C	N	O	S	0	0	0
			4567	2900	766	893	8			
1	C	595	Total	C	N	O	S	0	0	0
			4567	2900	766	893	8			
1	D	595	Total	C	N	O	S	0	0	0
			4567	2900	766	893	8			
1	E	595	Total	C	N	O	S	0	0	0
			4567	2900	766	893	8			
1	F	595	Total	C	N	O	S	0	0	0
			4567	2900	766	893	8			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

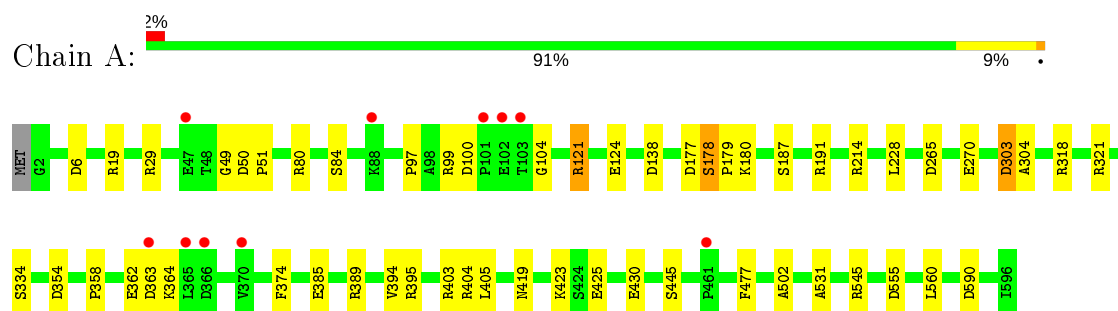
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	335	Total O 335 335	0	0
4	B	394	Total O 394 394	0	0
4	C	372	Total O 372 372	0	0
4	D	387	Total O 387 387	0	0
4	E	352	Total O 352 352	0	0
4	F	346	Total O 346 346	0	0

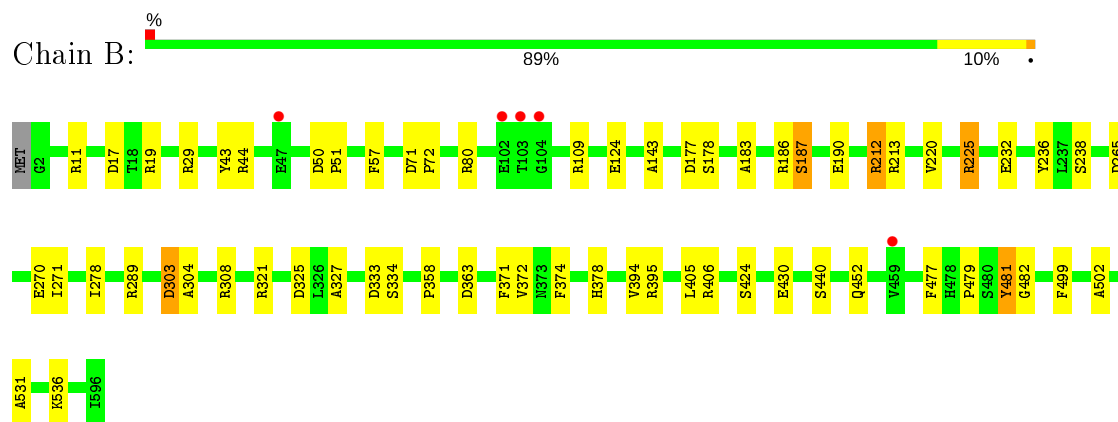
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

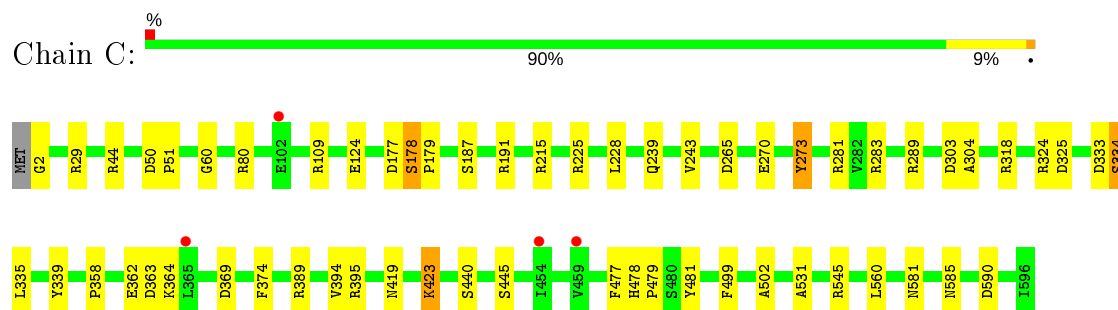
• Molecule 1: HALOPEROXIDASE



• Molecule 1: HALOPEROXIDASE

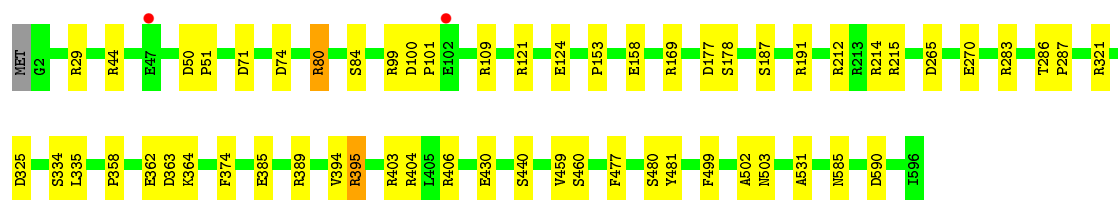


• Molecule 1: HALOPEROXIDASE

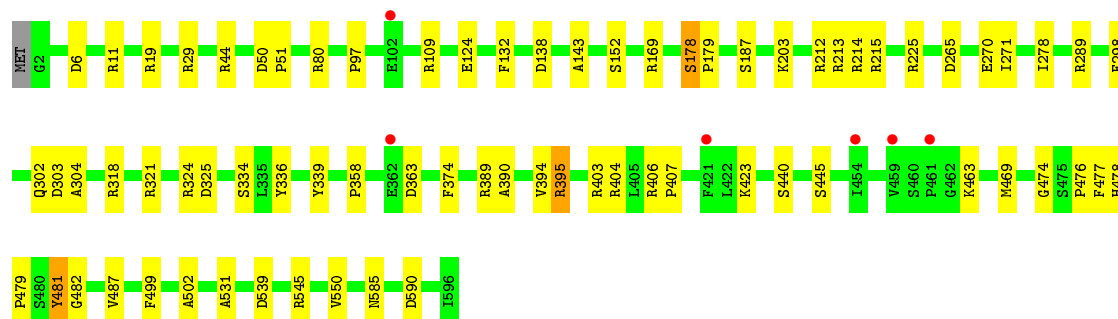
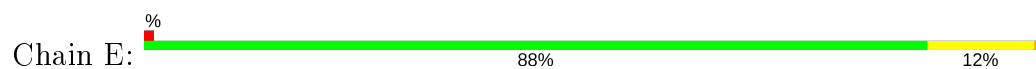


• Molecule 1: HALOPEROXIDASE

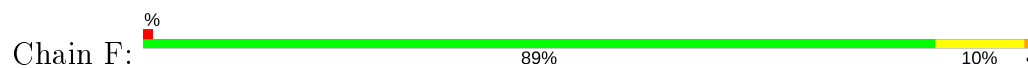




● Molecule 1: HALOPEROXIDASE



● Molecule 1: HALOPEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, α , β , γ	201.91Å 201.91Å 178.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-2.30) 96.8 (19.94-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.30Å)	Xtriage
Refinement program	REFMAC WITH INPUT DM PHASES	Depositor
R, R_{free}	0.172 , 0.227 0.155 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29624	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8834e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CA, PO4

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	0.64	0/4666	1.33	27/6339 (0.4%)
1	B	0.63	0/4666	1.31	37/6339 (0.6%)
1	C	0.62	0/4666	1.29	26/6339 (0.4%)
1	D	0.64	0/4666	1.30	36/6339 (0.6%)
1	E	0.61	0/4666	1.33	39/6339 (0.6%)
1	F	0.64	0/4666	1.29	30/6339 (0.5%)
All	All	0.63	0/27996	1.31	195/38034 (0.5%)

There are no bond length outliers.

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	29	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	A	29	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	A	321	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	D	503	ASN	OD1-CG-ND2	-12.95	92.12	121.90
1	C	389	ARG	NE-CZ-NH2	-12.58	114.01	120.30
1	D	29	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	A	321	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	C	191	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	C	318	ARG	NE-CZ-NH2	11.45	126.02	120.30
1	E	44	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	F	225	ARG	NE-CZ-NH1	10.81	125.71	120.30
1	D	503	ASN	CB-CG-OD1	10.78	143.16	121.60
1	D	403	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	F	29	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	B	44	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	E	403	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	C	44	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	325	ASP	CB-CG-OD2	-9.92	109.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ASP	CB-CG-OD1	9.78	127.10	118.30
1	B	212	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	E	324	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	D	363	ASP	CB-CG-OD2	9.52	126.86	118.30
1	E	389	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	E	321	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	225	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	E	169	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	E	29	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	121	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	E	395	ARG	NE-CZ-NH2	9.29	124.94	120.30
1	F	80	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	C	289	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	D	214	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	E	363	ASP	CB-CG-OD2	8.98	126.39	118.30
1	E	404	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	138	ASP	CB-CG-OD2	8.94	126.35	118.30
1	E	44	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	C	363	ASP	CB-CG-OD2	8.90	126.31	118.30
1	E	80	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	F	404	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	F	109	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	283	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	D	44	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	F	169	ARG	NE-CZ-NH1	-8.66	115.97	120.30
1	D	590	ASP	CB-CG-OD1	8.65	126.08	118.30
1	D	71	ASP	CB-CG-OD1	8.54	125.99	118.30
1	C	590	ASP	CB-CG-OD1	8.53	125.97	118.30
1	D	44	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	E	321	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	29	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	99	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	F	321	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	E	214	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	E	225	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	E	318	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	B	29	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	E	325	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	C	29	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	F	325	ASP	CB-CG-OD1	7.86	125.37	118.30
1	E	169	ARG	NH1-CZ-NH2	7.72	127.90	119.40
1	E	169	ARG	NE-CZ-NH1	-7.66	116.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	E	539	ASP	CB-CG-OD2	7.62	125.16	118.30
1	D	121	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	F	403	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	F	308	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	F	325	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	D	109	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	225	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	303	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	C	109	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	D	29	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	E	19	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	80	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	324	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	E	213	ARG	CD-NE-CZ	6.96	133.35	123.60
1	E	324	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	D	406	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	B	327	ALA	CA-C-O	6.92	134.64	120.10
1	B	321	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	80	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	D	99	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	B	17	ASP	CB-CG-OD2	6.71	124.34	118.30
1	C	481	TYR	N-CA-CB	-6.70	98.53	110.60
1	D	395	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	80	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	404	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	E	11	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	545	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	C	281	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	283	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	354	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	D	403	ARG	NH1-CZ-NH2	-6.53	112.22	119.40
1	B	19	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	C	80	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	F	80	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	F	363	ASP	CB-CG-OD2	6.44	124.10	118.30
1	E	389	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	430	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	E	289	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	430	GLU	OE1-CD-OE2	-6.37	115.65	123.30
1	D	389	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	321	ARG	NE-CZ-NH1	6.34	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASP	CB-CG-OD1	6.34	124.00	118.30
1	B	109	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	F	29	ARG	CD-NE-CZ	6.30	132.41	123.60
1	D	169	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	C	333	ASP	CB-CG-OD1	6.25	123.92	118.30
1	E	213	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	215	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	403	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	19	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	D	169	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	363	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	281	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	E	403	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	363	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	215	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	325	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	80	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	E	225	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	C	339	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	590	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	389	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	D	80	ARG	CD-NE-CZ	6.01	132.02	123.60
1	B	186	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	143	ALA	CB-CA-C	-6.00	101.11	110.10
1	B	212	ARG	CD-NE-CZ	5.98	131.97	123.60
1	E	109	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	545	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	F	198	PHE	CB-CG-CD2	-5.94	116.64	120.80
1	F	80	ARG	CD-NE-CZ	5.92	131.89	123.60
1	F	324	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	308	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	289	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	F	481	TYR	N-CA-CB	-5.81	100.14	110.60
1	B	327	ALA	O-C-N	-5.77	113.46	122.70
1	E	80	ARG	CD-NE-CZ	5.77	131.67	123.60
1	B	406	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	212	ARG	CD-NE-CZ	5.75	131.65	123.60
1	F	212	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	213	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	169	ARG	NH1-CZ-NH2	5.66	125.62	119.40
1	F	109	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	481	TYR	N-CA-CB	-5.61	100.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	481	TYR	N-CA-CB	-5.60	100.52	110.60
1	C	29	ARG	CD-NE-CZ	5.58	131.42	123.60
1	E	138	ASP	CB-CG-OD2	5.58	123.33	118.30
1	F	289	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	74	ASP	CB-CG-OD1	5.55	123.30	118.30
1	E	590	ASP	CB-CG-OD1	5.55	123.29	118.30
1	F	389	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	F	321	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	404	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	F	590	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	11	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	F	555	ASP	CB-CG-OD1	5.39	123.16	118.30
1	D	430	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	C	191	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	143	ALA	CB-CA-C	-5.33	102.10	110.10
1	D	321	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	19	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	F	11	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	19	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	186	ARG	CD-NE-CZ	5.31	131.03	123.60
1	B	333	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	212	ARG	CD-NE-CZ	5.31	131.03	123.60
1	B	225	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	555	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	A	80	ARG	CD-NE-CZ	5.26	130.96	123.60
1	F	547	MET	CA-CB-CG	-5.25	104.38	113.30
1	D	325	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	232	GLU	CA-CB-CG	-5.23	101.90	113.40
1	C	80	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	389	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	214	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	D	325	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	186	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	481	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	D	212	ARG	CD-NE-CZ	5.14	130.80	123.60
1	E	339	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	318	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	425	GLU	CA-CB-CG	5.11	124.64	113.40
1	D	109	ARG	CD-NE-CZ	5.11	130.75	123.60
1	C	273	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	E	481	TYR	N-CA-CB	-5.08	101.45	110.60
1	E	395	ARG	NH1-CZ-NH2	-5.08	113.81	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	354	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	335	LEU	CA-C-N	5.06	128.33	117.20
1	A	403	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
1	B	190	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	F	388	THR	CA-CB-CG2	-5.04	105.34	112.40
1	A	321	ARG	N-CA-CB	-5.04	101.53	110.60
1	B	43	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	D	158	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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	4567	0	4453	18	0
1	B	4567	0	4453	18	0
1	C	4567	0	4453	24	0
1	D	4567	0	4453	15	0
1	E	4567	0	4453	22	0
1	F	4567	0	4453	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	335	0	0	3	0
4	B	394	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	372	0	0	3	0
4	D	387	0	0	2	0
4	E	352	0	0	5	0
4	F	346	0	0	1	0
All	All	29624	0	26718	112	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 2.

All (112) 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:E:203:LYS:HG2	4:E:3321:HOH:O	1.77	0.84
1:A:49:GLY:HA2	4:A:3281:HOH:O	1.83	0.78
1:F:502:ALA:HB1	1:F:531:ALA:HB2	1.72	0.72
1:E:124:GLU:O	1:E:395:ARG:NH1	2.28	0.67
1:C:369:ASP:HB3	1:F:124:GLU:HG2	1.77	0.66
1:A:50:ASP:HB3	1:A:51:PRO:HD2	1.79	0.64
1:C:50:ASP:HB3	1:C:51:PRO:HD2	1.80	0.64
1:D:50:ASP:HB3	1:D:51:PRO:HD2	1.78	0.64
1:B:50:ASP:HB3	1:B:51:PRO:HD2	1.80	0.63
1:D:502:ALA:HB1	1:D:531:ALA:HB2	1.82	0.62
1:E:50:ASP:HB3	1:E:51:PRO:HD2	1.83	0.60
1:E:502:ALA:HB1	1:E:531:ALA:HB2	1.83	0.59
4:C:3373:HOH:O	1:D:80:ARG:HD3	2.00	0.59
1:B:502:ALA:HB1	1:B:531:ALA:HB2	1.84	0.59
1:E:469:MET:HE2	1:E:474:GLY:HA2	1.84	0.58
1:C:502:ALA:HB1	1:C:531:ALA:HB2	1.86	0.58
1:D:191:ARG:NH2	4:D:3201:HOH:O	2.37	0.57
1:C:419:ASN:O	1:C:423:LYS:HD2	2.04	0.57
1:D:124:GLU:O	1:D:395:ARG:NH1	2.38	0.57
1:C:124:GLU:O	1:C:395:ARG:NH1	2.39	0.56
1:A:265:ASP:HB3	1:A:270:GLU:HB2	1.87	0.55
1:B:124:GLU:O	1:B:395:ARG:NH1	2.40	0.55
1:A:358:PRO:HG2	1:A:374:PHE:CE2	2.42	0.55
1:E:358:PRO:HG2	1:E:374:PHE:CE2	2.41	0.54
1:A:124:GLU:O	1:A:395:ARG:NH1	2.40	0.54
1:A:502:ALA:HB1	1:A:531:ALA:HB2	1.88	0.54
1:C:358:PRO:HG2	1:C:374:PHE:CE2	2.42	0.54
1:D:358:PRO:HG2	1:D:374:PHE:CE2	2.41	0.54
1:A:121:ARG:HD3	4:A:3218:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:HG2	1:B:374:PHE:CE2	2.43	0.53
1:A:191:ARG:NH2	4:A:3225:HOH:O	2.38	0.53
1:B:358:PRO:HG2	1:B:374:PHE:CD2	2.43	0.53
1:E:358:PRO:HG2	1:E:374:PHE:CD2	2.44	0.52
1:F:239:GLN:O	1:F:243:VAL:HG22	2.08	0.52
1:A:303:ASP:O	1:A:304:ALA:HB3	2.09	0.52
1:E:463:LYS:NZ	4:E:3335:HOH:O	2.44	0.51
1:C:303:ASP:O	1:C:304:ALA:HB3	2.10	0.51
1:D:265:ASP:HB3	1:D:270:GLU:HB2	1.91	0.51
1:F:124:GLU:O	1:F:395:ARG:NH1	2.43	0.51
1:E:545:ARG:O	1:E:550:VAL:HG22	2.11	0.51
1:B:220:VAL:HG23	4:B:3194:HOH:O	2.11	0.50
1:B:303:ASP:O	1:B:304:ALA:HB3	2.11	0.50
1:C:60:GLY:HA2	1:C:304:ALA:HB2	1.93	0.50
1:C:124:GLU:HG2	1:F:369:ASP:HB3	1.94	0.50
1:D:358:PRO:HG2	1:D:374:PHE:CD2	2.46	0.50
1:C:239:GLN:O	1:C:243:VAL:HG22	2.11	0.49
1:F:271:ILE:HB	1:F:278:ILE:HB	1.94	0.49
1:A:419:ASN:O	1:A:423:LYS:HD3	2.13	0.48
1:F:183:ALA:O	1:F:187:SER:HB3	2.14	0.48
1:E:476:PRO:HA	4:E:3239:HOH:O	2.14	0.48
1:F:358:PRO:HG2	1:F:374:PHE:CE2	2.49	0.47
1:A:358:PRO:HG2	1:A:374:PHE:CD2	2.50	0.46
1:F:298:PHE:O	1:F:302:GLN:HG2	2.15	0.46
1:E:152:SER:HB2	4:E:3152:HOH:O	2.16	0.46
1:A:228:LEU:HD11	1:A:560:LEU:HD13	1.97	0.46
1:C:178:SER:HA	1:C:179:PRO:HD3	1.87	0.45
1:C:423:LYS:N	1:C:423:LYS:HD2	2.32	0.45
1:E:390:ALA:HB1	1:E:487:VAL:HG22	1.98	0.45
1:F:60:GLY:HA2	1:F:304:ALA:HB2	1.97	0.45
1:B:481:TYR:HA	1:B:482:GLY:HA2	1.71	0.45
1:B:271:ILE:HB	1:B:278:ILE:HB	1.97	0.45
1:C:228:LEU:HD11	1:C:560:LEU:HD13	1.99	0.45
1:B:372:VAL:O	1:B:378:HIS:HB2	2.17	0.44
1:D:286:THR:HA	1:D:287:PRO:HD3	1.86	0.44
1:D:459:VAL:HG12	1:D:460:SER:N	2.33	0.44
1:C:369:ASP:N	1:F:123:TRP:O	2.47	0.44
1:F:158:GLU:O	1:F:162:LEU:HG	2.18	0.44
1:B:452:GLN:HB2	4:B:3335:HOH:O	2.18	0.43
1:D:362:GLU:OE1	1:D:364:LYS:HE2	2.19	0.43
1:B:183:ALA:O	1:B:187:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLU:OE1	1:A:364:LYS:HE2	2.17	0.43
1:E:298:PHE:O	1:E:302:GLN:HG2	2.18	0.43
1:C:265:ASP:HB3	1:C:270:GLU:HB2	2.00	0.43
1:C:334:SER:HB2	1:F:380:LEU:HD13	1.99	0.43
1:C:335:LEU:N	4:C:3296:HOH:O	2.51	0.43
1:C:273:TYR:CZ	1:F:337:GLU:HG3	2.53	0.43
1:F:372:VAL:O	1:F:378:HIS:HB2	2.18	0.43
1:E:265:ASP:HB3	1:E:270:GLU:HB2	2.00	0.43
1:C:362:GLU:OE1	1:C:364:LYS:HE2	2.19	0.43
1:E:132:PHE:HB3	4:E:3294:HOH:O	2.19	0.42
1:B:265:ASP:HB3	1:B:270:GLU:HB2	2.01	0.42
1:F:178:SER:OG	1:F:180:LYS:HG2	2.19	0.42
1:F:303:ASP:O	1:F:304:ALA:HB3	2.19	0.42
1:C:50:ASP:HB3	1:C:51:PRO:CD	2.49	0.42
1:F:358:PRO:HG2	1:F:374:PHE:CD2	2.55	0.42
1:B:238:SER:HA	1:B:536:LYS:HD2	2.00	0.42
1:E:178:SER:HA	1:E:179:PRO:HD3	1.88	0.42
1:E:481:TYR:HA	1:E:482:GLY:HA2	1.68	0.42
1:F:481:TYR:HA	1:F:482:GLY:HA2	1.65	0.42
1:D:50:ASP:HB3	1:D:51:PRO:CD	2.47	0.42
1:F:212:ARG:HD3	4:F:3290:HOH:O	2.20	0.42
1:F:265:ASP:HB3	1:F:270:GLU:HB2	2.01	0.42
1:A:84:SER:HB3	1:F:581:ASN:ND2	2.35	0.42
1:E:303:ASP:O	1:E:304:ALA:HB3	2.19	0.41
1:B:57:PHE:CD2	1:B:479:PRO:HG3	2.55	0.41
1:A:178:SER:OG	1:A:180:LYS:HG2	2.20	0.41
1:B:212:ARG:NH2	4:B:3370:HOH:O	2.53	0.41
1:A:178:SER:HA	1:A:179:PRO:HD3	1.88	0.41
1:C:2:GLY:N	4:C:3102:HOH:O	2.54	0.41
1:A:6:ASP:OD2	1:E:6:ASP:OD2	2.39	0.41
1:C:358:PRO:HG2	1:C:374:PHE:CD2	2.56	0.41
1:E:478:HIS:HA	1:E:479:PRO:HD3	1.91	0.41
1:B:71:ASP:HA	1:B:72:PRO:HD2	1.80	0.41
1:C:581:ASN:ND2	1:D:84:SER:HB3	2.36	0.41
1:E:271:ILE:HB	1:E:278:ILE:HB	2.03	0.41
1:D:153:PRO:HD2	4:D:3112:HOH:O	2.21	0.41
1:E:406:ARG:HA	1:E:407:PRO:HD3	1.87	0.41
1:F:178:SER:HA	1:F:179:PRO:HD3	1.91	0.41
1:A:100:ASP:O	1:A:104:GLY:N	2.45	0.40
1:C:478:HIS:HA	1:C:479:PRO:HD3	1.87	0.40
1:B:225:ARG:HG2	1:B:236:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ASP:HA	1:D:101:PRO:HD3	1.93	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	593/596 (100%)	585 (99%)	8 (1%)	0	100	100
1	B	593/596 (100%)	583 (98%)	8 (1%)	2 (0%)	41	50
1	C	593/596 (100%)	587 (99%)	6 (1%)	0	100	100
1	D	593/596 (100%)	585 (99%)	8 (1%)	0	100	100
1	E	593/596 (100%)	586 (99%)	7 (1%)	0	100	100
1	F	593/596 (100%)	583 (98%)	9 (2%)	1 (0%)	47	58
All	All	3558/3576 (100%)	3509 (99%)	46 (1%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	424	SER
1	B	371	PHE
1	F	371	PHE

5.3.2 Protein sidechains [i](#)

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	487/488 (100%)	477 (98%)	10 (2%)	53	70
1	B	487/488 (100%)	478 (98%)	9 (2%)	59	75
1	C	487/488 (100%)	476 (98%)	11 (2%)	50	67
1	D	487/488 (100%)	476 (98%)	11 (2%)	50	67
1	E	487/488 (100%)	475 (98%)	12 (2%)	47	65
1	F	487/488 (100%)	476 (98%)	11 (2%)	50	67
All	All	2922/2928 (100%)	2858 (98%)	64 (2%)	52	69

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	PRO
1	A	177	ASP
1	A	178	SER
1	A	187	SER
1	A	334	SER
1	A	385	GLU
1	A	394	VAL
1	A	405	LEU
1	A	445	SER
1	A	477	PHE
1	B	177	ASP
1	B	178	SER
1	B	187	SER
1	B	334	SER
1	B	394	VAL
1	B	405	LEU
1	B	440	SER
1	B	477	PHE
1	B	499	PHE
1	C	177	ASP
1	C	178	SER
1	C	187	SER
1	C	334	SER
1	C	394	VAL
1	C	423	LYS
1	C	440	SER
1	C	445	SER
1	C	477	PHE
1	C	499	PHE
1	C	585	ASN

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Mol	Chain	Res	Type
1	D	177	ASP
1	D	178	SER
1	D	187	SER
1	D	334	SER
1	D	385	GLU
1	D	394	VAL
1	D	440	SER
1	D	477	PHE
1	D	480	SER
1	D	499	PHE
1	D	585	ASN
1	E	97	PRO
1	E	178	SER
1	E	187	SER
1	E	334	SER
1	E	336	TYR
1	E	394	VAL
1	E	423	LYS
1	E	440	SER
1	E	445	SER
1	E	477	PHE
1	E	499	PHE
1	E	585	ASN
1	F	72	PRO
1	F	103	THR
1	F	177	ASP
1	F	178	SER
1	F	187	SER
1	F	334	SER
1	F	394	VAL
1	F	440	SER
1	F	445	SER
1	F	477	PHE
1	F	499	PHE

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

Mol	Chain	Res	Type
1	A	66	ASN
1	A	341	ASN
1	A	505	GLN
1	A	585	ASN

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Mol	Chain	Res	Type
1	A	595	GLN
1	B	66	ASN
1	B	341	ASN
1	B	505	GLN
1	C	66	ASN
1	C	341	ASN
1	C	505	GLN
1	C	585	ASN
1	D	66	ASN
1	D	341	ASN
1	D	368	GLN
1	D	505	GLN
1	D	595	GLN
1	E	66	ASN
1	E	341	ASN
1	E	368	GLN
1	E	505	GLN
1	E	585	ASN
1	E	595	GLN
1	F	66	ASN
1	F	341	ASN
1	F	505	GLN
1	F	585	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	F	3010	-	4,4,4	1.46	1 (25%)	6,6,6	0.95	0
2	PO4	E	3008	-	4,4,4	1.39	0	6,6,6	0.26	0
2	PO4	B	3002	-	4,4,4	1.60	0	6,6,6	1.57	2 (33%)
2	PO4	A	3000	-	4,4,4	1.55	1 (25%)	6,6,6	0.74	0
2	PO4	C	3004	-	4,4,4	1.62	1 (25%)	6,6,6	1.19	0
2	PO4	D	3006	-	4,4,4	1.59	1 (25%)	6,6,6	0.57	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3004	PO4	P-O2	-2.43	1.47	1.54
2	A	3000	PO4	P-O3	-2.29	1.47	1.54
2	D	3006	PO4	P-O3	-2.24	1.47	1.54
2	F	3010	PO4	P-O2	-2.09	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3002	PO4	O3-P-O2	2.51	116.03	107.97
2	B	3002	PO4	O3-P-O1	-2.28	102.54	110.89

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 ⓘ

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	595/596 (99%)	-0.63	10 (1%) 70 76	7, 15, 40, 74	0
1	B	595/596 (99%)	-0.72	5 (0%) 86 89	7, 15, 39, 75	0
1	C	595/596 (99%)	-0.73	4 (0%) 87 91	7, 15, 38, 66	0
1	D	595/596 (99%)	-0.72	2 (0%) 94 96	7, 15, 39, 73	0
1	E	595/596 (99%)	-0.70	6 (1%) 82 86	7, 15, 38, 66	0
1	F	595/596 (99%)	-0.70	6 (1%) 82 86	7, 15, 39, 90	0
All	All	3570/3576 (99%)	-0.70	33 (0%) 84 88	7, 15, 39, 90	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	LEU	4.8
1	F	102	GLU	4.5
1	B	102	GLU	3.4
1	D	102	GLU	3.3
1	C	459	VAL	3.0
1	F	454	ILE	3.0
1	E	454	ILE	2.9
1	B	459	VAL	2.8
1	F	461	PRO	2.8
1	B	47	GLU	2.7
1	E	362	GLU	2.7
1	E	461	PRO	2.7
1	F	365	LEU	2.7
1	D	47	GLU	2.7
1	A	88	LYS	2.7
1	A	363	ASP	2.6
1	F	47	GLU	2.6
1	F	457	GLY	2.6
1	A	102	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	103	THR	2.5
1	C	102	GLU	2.5
1	E	459	VAL	2.5
1	C	365	LEU	2.5
1	A	47	GLU	2.4
1	B	103	THR	2.3
1	A	461	PRO	2.3
1	E	102	GLU	2.3
1	A	366	ASP	2.2
1	B	104	GLY	2.2
1	A	370	VAL	2.2
1	A	101	PRO	2.1
1	E	421	PHE	2.1
1	C	454	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
3	CA	C	3005	1/1	0.83	0.10	45,45,45,45	0
3	CA	F	3011	1/1	0.86	0.09	45,45,45,45	0
3	CA	D	3007	1/1	0.90	0.09	45,45,45,45	0
3	CA	B	3003	1/1	0.91	0.17	44,44,44,44	0
3	CA	A	3001	1/1	0.92	0.11	46,46,46,46	0
3	CA	E	3009	1/1	0.95	0.08	45,45,45,45	0
2	PO4	B	3002	5/5	0.99	0.07	11,13,16,17	0
2	PO4	A	3000	5/5	0.99	0.05	11,14,15,17	0
2	PO4	C	3004	5/5	0.99	0.06	12,14,15,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	D	3006	5/5	0.99	0.06	11,13,16,17	0
2	PO4	F	3010	5/5	0.99	0.05	13,13,15,17	0
2	PO4	E	3008	5/5	0.99	0.05	10,13,14,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.