



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:48 PM UTC

PDB ID : 3OMX / pdb_00003omx
Title : Crystal structure of Ssu72 with vanadate complex
Authors : Zhang, Y.; Zhang, M.; Zhang, Y.
Deposited on : 2010-08-27
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

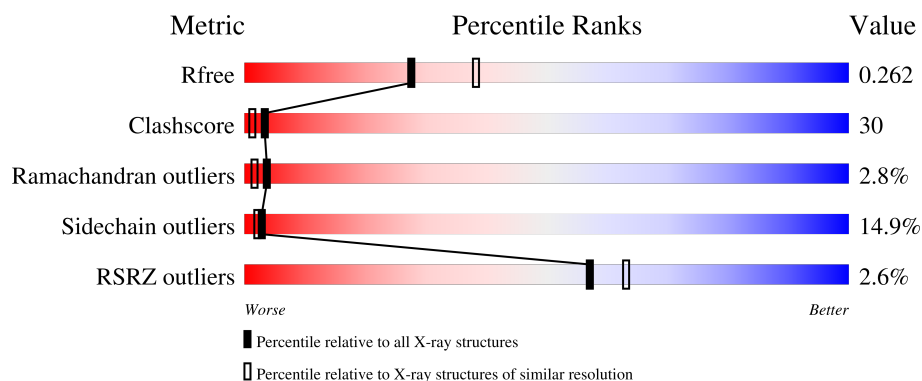
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	190	2% 39% 42% 17% .
1	B	190	% 44% 37% 15% .
1	C	190	2% 56% 29% 14% .
1	D	190	7% 33% 45% 18% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VO4	D	300	-	-	X	-

2 Entry composition [i](#)

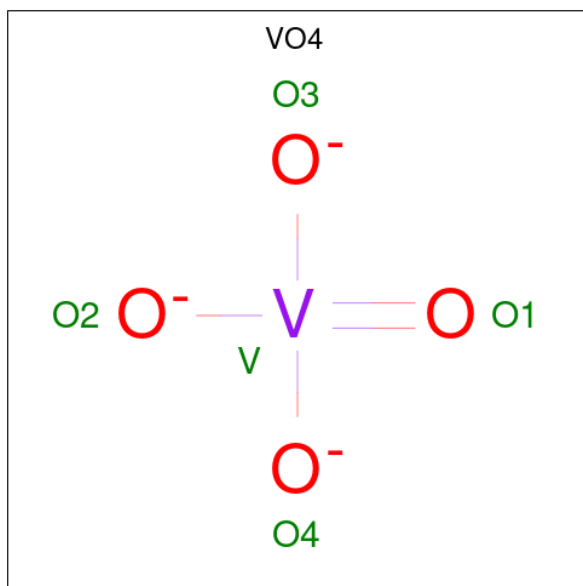
There are 3 unique types of molecules in this entry. The entry contains 6407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CG14216.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1554	975	268	298	13			
1	B	190	Total	C	N	O	S	0	0	0
			1554	975	268	298	13			
1	C	190	Total	C	N	O	S	0	0	0
			1554	975	268	298	13			
1	D	190	Total	C	N	O	S	0	0	0
			1554	975	268	298	13			

- Molecule 2 is VANADATE ION (CCD ID: VO4) (formula: O₄V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	V	0	0
			5	4	1		
2	B	1	Total	O	V	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	V	0	0
			5	4	1		
2	D	1	Total	O	V	0	0
			5	4	1		

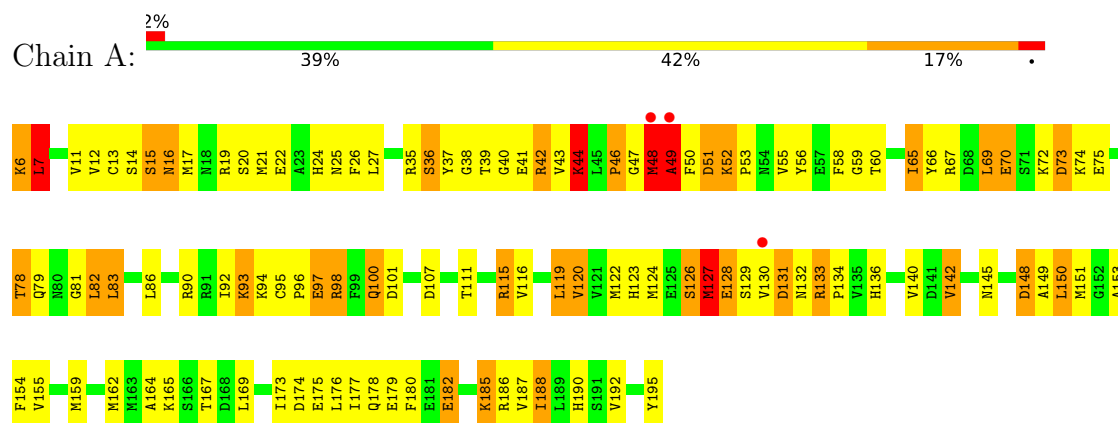
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	49	Total	O	0	0
			49	49		
3	C	40	Total	O	0	0
			40	40		
3	D	26	Total	O	0	0
			26	26		

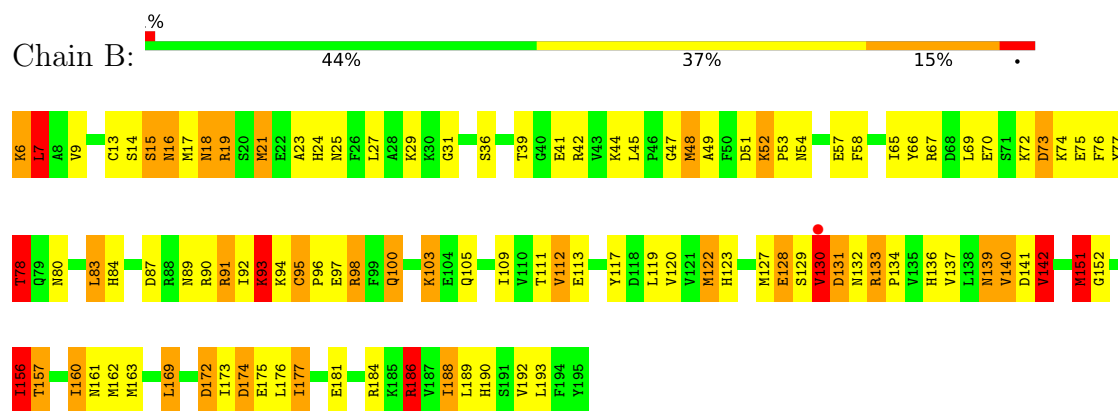
3 Residue-property plots [i](#)

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.

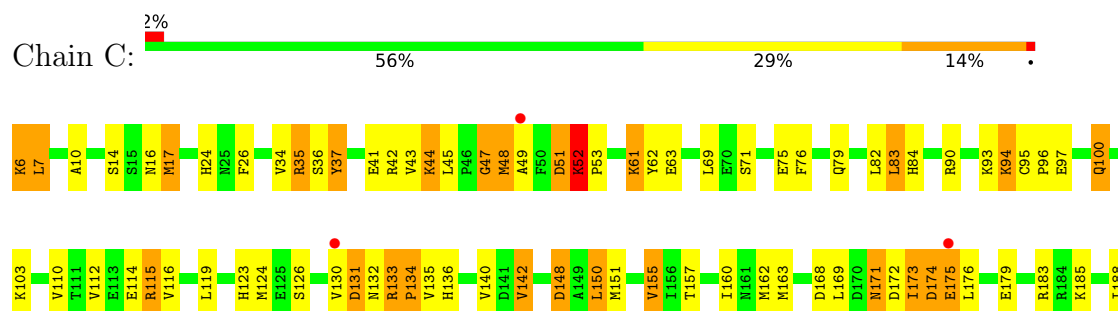
• Molecule 1: CG14216



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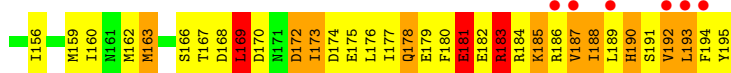


• Molecule 1: CG14216





• Molecule 1: CG14216



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.62Å 102.31Å 65.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 2.34 48.66 – 2.34	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.66-2.34) 99.3 (48.66-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.205 , 0.267 0.199 , 0.262	Depositor DCC
R_{free} test set	2295 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.8	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	0.96	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: VO4

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	2.01	38/1579 (2.4%)	1.80	37/2121 (1.7%)
1	B	1.91	24/1579 (1.5%)	1.84	37/2121 (1.7%)
1	C	1.75	18/1579 (1.1%)	1.74	37/2121 (1.7%)
1	D	1.61	13/1579 (0.8%)	1.68	25/2121 (1.2%)
All	All	1.83	93/6316 (1.5%)	1.77	136/8484 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ALA	CA-CB	-13.32	1.32	1.53
1	B	18	ASN	CA-C	13.04	1.60	1.52
1	C	17	MET	CA-C	9.43	1.61	1.52
1	D	67	ARG	CA-CB	8.94	1.67	1.53
1	A	12	VAL	CA-CB	8.87	1.66	1.54
1	A	11	VAL	N-CA	-8.57	1.36	1.46
1	D	12	VAL	CA-CB	8.33	1.65	1.54
1	B	91	ARG	CA-C	8.23	1.63	1.52
1	A	49	ALA	CA-CB	8.04	1.64	1.53
1	A	107	ASP	CA-C	7.97	1.63	1.52
1	A	148	ASP	CG-OD2	7.90	1.40	1.25
1	B	177	ILE	CA-CB	-7.54	1.45	1.54
1	A	177	ILE	CA-CB	-7.39	1.45	1.54
1	B	109	ILE	CA-CB	-7.31	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	ASN	CA-C	-7.26	1.43	1.53
1	A	116	VAL	CA-C	-7.24	1.43	1.52
1	B	84	HIS	CA-C	7.11	1.62	1.52
1	C	174	ASP	CG-OD1	7.06	1.38	1.25
1	A	149	ALA	C-O	-6.96	1.16	1.24
1	A	15	SER	CA-C	6.94	1.61	1.52
1	D	187	VAL	CA-CB	6.84	1.62	1.53
1	A	36	SER	N-CA	-6.63	1.37	1.45
1	C	148	ASP	CG-OD2	6.61	1.38	1.25
1	C	14	SER	C-O	6.59	1.32	1.23
1	D	14	SER	CA-C	6.58	1.60	1.52
1	A	164	ALA	C-O	-6.47	1.15	1.24
1	A	145	ASN	CA-C	6.46	1.60	1.52
1	B	16	ASN	N-CA	6.44	1.55	1.46
1	D	149	ALA	C-O	-6.29	1.16	1.24
1	B	112	VAL	CA-CB	-6.27	1.47	1.54
1	B	157	THR	N-CA	-6.24	1.38	1.46
1	B	15	SER	C-N	-6.13	1.25	1.33
1	A	14	SER	CA-C	6.07	1.61	1.52
1	D	85	MET	CA-C	6.01	1.60	1.52
1	B	93	LYS	CB-CG	-5.99	1.34	1.52
1	A	188	ILE	CA-CB	-5.96	1.46	1.53
1	C	173	ILE	C-O	-5.93	1.17	1.24
1	C	116	VAL	CA-CB	5.92	1.62	1.54
1	C	49	ALA	C-O	5.89	1.31	1.24
1	C	160	ILE	CA-CB	5.80	1.61	1.54
1	B	137	VAL	CA-CB	-5.78	1.47	1.54
1	C	43	VAL	C-O	-5.77	1.18	1.24
1	A	44	LYS	C-O	-5.75	1.16	1.23
1	D	120	VAL	CA-CB	-5.73	1.47	1.54
1	A	173	ILE	C-O	-5.67	1.17	1.24
1	B	105	GLN	CA-C	-5.64	1.45	1.52
1	A	26	PHE	CB-CG	-5.64	1.37	1.50
1	A	7	LEU	CA-C	-5.61	1.45	1.52
1	C	175	GLU	CB-CG	5.61	1.69	1.52
1	C	172	ASP	N-CA	-5.60	1.38	1.46
1	D	79	GLN	N-CA	5.59	1.53	1.46
1	B	98	ARG	CA-C	5.58	1.59	1.52
1	A	182	GLU	CG-CD	5.58	1.66	1.52
1	D	76	PHE	CA-C	-5.56	1.45	1.52
1	D	87	ASP	N-CA	-5.50	1.39	1.46
1	A	82	LEU	CA-C	5.47	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	GLU	C-O	-5.46	1.17	1.24
1	A	111	THR	CB-CG2	5.44	1.70	1.52
1	A	21	MET	CA-C	5.43	1.60	1.52
1	B	120	VAL	CA-C	5.41	1.59	1.52
1	B	9	VAL	C-O	-5.39	1.18	1.24
1	A	13	CYS	N-CA	-5.38	1.39	1.46
1	B	123	HIS	C-O	-5.37	1.18	1.24
1	A	182	GLU	CB-CG	5.36	1.68	1.52
1	C	175	GLU	CG-CD	5.34	1.65	1.52
1	A	178	GLN	C-O	-5.32	1.17	1.24
1	C	110	VAL	CA-CB	-5.32	1.47	1.54
1	B	139	ASN	C-O	-5.31	1.17	1.24
1	A	159	MET	CA-C	5.28	1.59	1.52
1	C	116	VAL	N-CA	-5.27	1.39	1.46
1	C	157	THR	CA-CB	5.26	1.61	1.53
1	A	187	VAL	CB-CG2	5.25	1.69	1.52
1	B	31	GLY	C-O	-5.25	1.17	1.24
1	D	75	GLU	N-CA	5.25	1.52	1.46
1	B	23	ALA	CA-CB	5.24	1.61	1.53
1	A	15	SER	C-O	-5.23	1.17	1.23
1	D	61	LYS	C-O	5.18	1.30	1.23
1	B	19	ARG	N-CA	5.16	1.52	1.46
1	B	95	CYS	C-O	-5.14	1.17	1.24
1	D	98	ARG	CA-C	5.13	1.59	1.52
1	A	43	VAL	CA-C	-5.12	1.46	1.52
1	A	27	LEU	CA-C	5.11	1.59	1.52
1	B	21	MET	C-O	-5.10	1.17	1.24
1	A	20	SER	C-O	-5.10	1.17	1.24
1	B	140	VAL	CA-CB	-5.09	1.48	1.54
1	C	43	VAL	CA-CB	-5.08	1.48	1.54
1	C	63	GLU	CA-C	5.07	1.59	1.52
1	A	43	VAL	CA-CB	5.06	1.60	1.54
1	C	26	PHE	CB-CG	-5.05	1.39	1.50
1	A	155	VAL	CB-CG2	5.04	1.69	1.52
1	A	93	LYS	CA-C	-5.01	1.46	1.52
1	A	97	GLU	CD-OE1	5.01	1.34	1.25
1	B	131	ASP	C-O	5.01	1.30	1.24

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	SER	CA-C-N	-15.63	97.73	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	SER	C-N-CA	-15.63	97.73	123.37
1	D	15	SER	N-CA-C	-12.76	91.57	110.46
1	A	37	TYR	CA-C-N	11.62	129.56	121.65
1	A	37	TYR	C-N-CA	11.62	129.56	121.65
1	B	131	ASP	N-CA-C	-11.09	96.37	113.89
1	D	15	SER	CA-C-N	-10.86	108.21	123.20
1	D	15	SER	C-N-CA	-10.86	108.21	123.20
1	A	95	CYS	N-CA-C	9.33	116.61	108.22
1	B	89	ASN	N-CA-C	8.78	120.85	111.28
1	B	77	TYR	N-CA-C	-8.76	102.33	113.72
1	B	130	VAL	N-CA-C	8.54	127.11	109.34
1	D	41	GLU	N-CA-C	-8.31	101.26	111.40
1	C	130	VAL	N-CA-C	-8.10	105.32	112.12
1	C	49	ALA	N-CA-C	8.02	122.64	113.01
1	C	52	LYS	CA-C-N	7.89	127.91	119.78
1	C	52	LYS	C-N-CA	7.89	127.91	119.78
1	C	163	MET	N-CA-C	7.84	120.91	111.82
1	C	95	CYS	N-CA-C	7.79	115.23	108.22
1	A	92	ILE	N-CA-C	-7.78	105.18	112.96
1	D	142	VAL	CB-CA-C	7.57	121.83	110.63
1	A	98	ARG	CG-CD-NE	-7.55	95.39	112.00
1	C	94	LYS	N-CA-C	7.41	119.00	111.07
1	C	172	ASP	CB-CA-C	7.39	122.65	110.17
1	C	95	CYS	CA-C-N	-7.31	112.46	119.85
1	C	95	CYS	C-N-CA	-7.31	112.46	119.85
1	D	67	ARG	NE-CZ-NH2	-7.24	112.68	119.20
1	B	15	SER	O-C-N	-7.23	112.54	122.81
1	A	26	PHE	N-CA-C	7.03	118.94	111.28
1	B	16	ASN	CB-CA-C	6.91	121.92	111.76
1	D	15	SER	O-C-N	-6.90	114.84	122.84
1	A	26	PHE	N-CA-CB	-6.85	100.05	110.12
1	D	93	LYS	CB-CA-C	-6.84	97.64	110.16
1	A	65	ILE	N-CA-C	-6.77	104.16	110.53
1	D	181	GLU	N-CA-C	-6.74	104.92	113.01
1	B	160	ILE	CB-CA-C	-6.73	103.22	112.04
1	B	151	MET	CG-SD-CE	-6.72	86.11	100.90
1	C	51	ASP	N-CA-C	6.69	120.72	109.76
1	A	179	GLU	CB-CA-C	-6.64	99.76	110.79
1	A	131	ASP	N-CA-C	-6.61	105.04	113.23
1	D	67	ARG	N-CA-C	-6.58	103.21	111.11
1	A	83	LEU	N-CA-C	-6.57	104.04	111.14
1	B	186	ARG	NE-CZ-NH2	6.54	125.08	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	ARG	CA-C-N	6.47	126.70	119.90
1	C	133	ARG	C-N-CA	6.47	126.70	119.90
1	A	119	LEU	CA-C-N	-6.47	112.41	120.56
1	A	119	LEU	C-N-CA	-6.47	112.41	120.56
1	A	46	PRO	CA-C-O	-6.42	114.10	122.19
1	B	131	ASP	CA-C-O	6.37	126.23	119.03
1	A	120	VAL	N-CA-C	6.36	116.53	110.42
1	D	19	ARG	N-CA-C	6.34	118.76	111.02
1	A	48	MET	CA-C-N	-6.30	113.78	123.17
1	A	48	MET	C-N-CA	-6.30	113.78	123.17
1	A	59	GLY	N-CA-C	-6.30	106.43	114.37
1	C	155	VAL	CB-CA-C	-6.28	103.93	111.97
1	C	83	LEU	N-CA-C	-6.23	104.02	111.69
1	C	103	LYS	N-CA-C	-6.15	104.39	113.61
1	B	133	ARG	CA-C-N	6.14	126.33	120.31
1	B	133	ARG	C-N-CA	6.14	126.33	120.31
1	C	37	TYR	CA-C-N	6.13	126.33	121.61
1	C	37	TYR	C-N-CA	6.13	126.33	121.61
1	B	51	ASP	CA-C-N	-6.07	114.67	122.98
1	B	51	ASP	C-N-CA	-6.07	114.67	122.98
1	D	111	THR	N-CA-C	-6.06	101.24	110.14
1	D	86	LEU	N-CA-C	-6.05	104.68	111.28
1	D	52	LYS	CA-C-N	6.03	125.99	119.78
1	D	52	LYS	C-N-CA	6.03	125.99	119.78
1	A	41	GLU	N-CA-C	-5.99	104.68	112.23
1	A	67	ARG	N-CA-C	-5.99	104.67	111.14
1	D	79	GLN	CB-CA-C	-5.96	100.90	110.79
1	C	163	MET	CA-CB-CG	-5.94	102.22	114.10
1	C	171	ASN	CA-C-N	-5.93	113.30	122.49
1	C	171	ASN	C-N-CA	-5.93	113.30	122.49
1	A	186	ARG	CG-CD-NE	-5.92	98.98	112.00
1	B	95	CYS	N-CA-C	5.86	113.49	108.22
1	C	75	GLU	N-CA-C	5.83	118.13	111.02
1	A	38	GLY	N-CA-C	-5.81	101.29	111.46
1	A	167	THR	N-CA-C	-5.81	105.50	112.59
1	A	16	ASN	CB-CA-C	-5.80	103.75	111.63
1	C	190	HIS	N-CA-C	5.76	117.82	108.26
1	D	79	GLN	CA-CB-CG	5.75	125.60	114.10
1	B	65	ILE	N-CA-C	-5.72	104.94	110.72
1	C	148	ASP	CB-CG-OD1	-5.68	105.32	118.40
1	A	25	ASN	CA-C-O	5.68	126.98	120.90
1	B	70	GLU	N-CA-C	-5.67	105.19	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	HIS	N-CA-C	5.63	118.14	111.33
1	B	163	MET	CA-CB-CG	-5.61	102.88	114.10
1	C	173	ILE	N-CA-C	5.58	115.77	110.53
1	A	154	PHE	N-CA-CB	5.54	118.04	110.01
1	B	93	LYS	N-CA-CB	-5.54	102.93	111.46
1	B	188	ILE	CB-CA-C	-5.54	104.62	111.32
1	C	174	ASP	CB-CG-OD2	-5.51	105.72	118.40
1	D	116	VAL	N-CA-C	-5.51	105.16	110.72
1	D	148	ASP	N-CA-C	5.50	117.36	111.36
1	C	126	SER	N-CA-C	-5.48	106.55	113.18
1	C	114	GLU	N-CA-C	5.47	116.92	111.07
1	D	194	PHE	N-CA-C	5.45	117.47	109.24
1	C	134	PRO	CA-C-N	-5.45	115.37	122.94
1	C	134	PRO	C-N-CA	-5.45	115.37	122.94
1	B	177	ILE	CB-CG1-CD1	-5.42	102.42	113.80
1	C	26	PHE	N-CA-C	5.40	117.59	111.11
1	D	16	ASN	N-CA-C	-5.40	100.92	108.54
1	C	47	GLY	N-CA-C	5.35	125.86	113.18
1	D	89	ASN	CA-C-N	5.32	127.40	120.28
1	D	89	ASN	C-N-CA	5.32	127.40	120.28
1	C	44	LYS	N-CA-C	5.30	118.05	109.40
1	C	160	ILE	CB-CA-C	-5.28	104.94	112.22
1	A	94	LYS	N-CA-C	5.27	117.03	111.28
1	B	127	MET	CA-C-N	-5.27	112.64	121.75
1	B	127	MET	C-N-CA	-5.27	112.64	121.75
1	C	115	ARG	CA-CB-CG	-5.26	103.57	114.10
1	A	44	LYS	N-CA-C	5.26	117.81	109.50
1	A	51	ASP	N-CA-C	5.22	118.52	110.42
1	A	35	ARG	CB-CG-CD	5.21	123.29	111.30
1	B	156	ILE	CA-CB-CG2	5.20	119.34	110.50
1	B	94	LYS	N-CA-C	5.20	119.71	112.90
1	A	101	ASP	N-CA-C	5.19	119.30	112.92
1	B	15	SER	N-CA-C	-5.18	102.23	109.69
1	C	42	ARG	N-CA-C	5.18	116.53	109.18
1	D	67	ARG	CG-CD-NE	-5.17	100.61	112.00
1	B	128	GLU	N-CA-C	5.17	116.93	109.07
1	B	7	LEU	CB-CG-CD1	-5.17	95.20	110.70
1	D	94	LYS	N-CA-C	5.17	118.74	112.23
1	A	90	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	95	CYS	CA-C-N	-5.14	114.46	119.76
1	A	95	CYS	C-N-CA	-5.14	114.46	119.76
1	B	127	MET	N-CA-C	-5.14	101.89	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	B	93	LYS	N-CA-C	-5.11	101.13	108.60
1	C	130	VAL	CB-CA-C	5.08	115.89	110.91
1	B	83	LEU	N-CA-C	-5.03	105.46	112.45
1	A	35	ARG	CG-CD-NE	-5.03	100.94	112.00
1	B	87	ASP	N-CA-CB	-5.02	102.71	110.20
1	B	78	THR	CB-CA-C	5.02	119.89	110.70
1	A	164	ALA	N-CA-C	-5.01	107.00	113.01
1	B	142	VAL	CB-CA-C	5.01	117.64	110.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	MET	Peptide
1	A	49	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1554	0	1528	83	0
1	B	1554	0	1528	101	0
1	C	1554	0	1528	59	0
1	D	1554	0	1528	138	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	2	0
3	A	56	0	0	18	0
3	B	49	0	0	10	0
3	C	40	0	0	11	0
3	D	26	0	0	15	0
All	All	6407	0	6112	374	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 30.

All (374) 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:B:186:ARG:CB	1:B:186:ARG:HH11	1.57	1.16
1:B:186:ARG:HH11	1:B:186:ARG:HB3	1.06	1.11
1:D:172:ASP:O	1:D:175:GLU:HB3	1.56	1.06
1:B:186:ARG:HB3	1:B:186:ARG:NH1	1.74	1.01
1:C:100:GLN:HE21	1:C:100:GLN:N	1.61	0.99
1:A:128:GLU:OE1	1:A:129:SER:N	1.95	0.99
1:C:123:HIS:HD2	3:C:213:HOH:O	1.45	0.98
1:C:16:ASN:HD21	1:C:93:LYS:NZ	1.62	0.97
1:D:99:PHE:O	1:D:102:THR:HG22	1.66	0.96
1:A:151:MET:HE2	1:C:151:MET:HB2	1.49	0.95
1:A:6:LYS:HG3	3:A:225:HOH:O	1.65	0.94
1:C:100:GLN:H	1:C:100:GLN:NE2	1.65	0.94
1:A:127:MET:HE3	1:A:127:MET:HA	1.49	0.93
1:D:136:HIS:HB3	3:D:204:HOH:O	1.67	0.92
1:A:100:GLN:HE21	1:A:100:GLN:N	1.67	0.92
1:B:100:GLN:H	1:B:100:GLN:HE21	0.92	0.91
1:D:117:TYR:O	1:D:121:VAL:HG23	1.68	0.91
1:A:162:MET:HE3	1:A:176:LEU:HB3	1.50	0.91
1:A:100:GLN:HE21	1:A:100:GLN:H	0.91	0.91
1:B:100:GLN:HE21	1:B:100:GLN:N	1.70	0.89
1:A:127:MET:SD	3:A:246:HOH:O	2.31	0.88
1:A:7:LEU:H	1:A:7:LEU:HD23	1.36	0.88
1:A:7:LEU:H	1:A:7:LEU:CD2	1.86	0.87
1:D:115:ARG:O	1:D:119:LEU:HD13	1.73	0.87
1:B:186:ARG:HH11	1:B:186:ARG:CG	1.88	0.85
1:A:100:GLN:H	1:A:100:GLN:NE2	1.75	0.85
1:D:52:LYS:HB2	3:D:209:HOH:O	1.75	0.84
1:C:41:GLU:HG3	3:C:228:HOH:O	1.75	0.84
1:C:16:ASN:HD21	1:C:93:LYS:HZ3	1.23	0.83
1:C:7:LEU:H	1:C:7:LEU:CD2	1.92	0.83
1:A:115:ARG:CZ	1:A:115:ARG:HB3	2.07	0.81
1:B:48:MET:CE	1:B:48:MET:HA	2.10	0.81
1:C:175:GLU:HG3	3:C:5:HOH:O	1.80	0.81
1:D:16:ASN:HD21	1:D:93:LYS:NZ	1.78	0.81
1:B:7:LEU:HD23	1:B:7:LEU:H	1.45	0.81
1:D:46:PRO:HD2	1:D:82:LEU:HD11	1.63	0.81
1:D:16:ASN:HD21	1:D:93:LYS:HZ1	1.26	0.79
1:A:133:ARG:HB3	3:A:234:HOH:O	1.81	0.79
1:A:151:MET:CE	1:C:151:MET:HB2	2.12	0.79
1:B:74:LYS:O	1:B:78:THR:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:LEU:HD23	1:D:7:LEU:H	1.47	0.79
1:A:133:ARG:CB	3:A:234:HOH:O	2.31	0.78
1:B:27:LEU:HD11	1:B:156:ILE:HD11	1.65	0.78
1:D:7:LEU:H	1:D:7:LEU:CD2	1.95	0.78
1:D:173:ILE:HG23	1:D:174:ASP:H	1.49	0.78
1:B:136:HIS:CD2	1:B:190:HIS:HE1	2.01	0.78
1:D:190:HIS:CE1	3:D:204:HOH:O	2.37	0.78
1:B:100:GLN:H	1:B:100:GLN:NE2	1.77	0.77
1:C:193:LEU:N	1:C:193:LEU:HD22	1.97	0.77
1:C:7:LEU:H	1:C:7:LEU:HD23	1.48	0.76
1:B:136:HIS:HD2	1:B:190:HIS:HE1	1.32	0.76
1:A:136:HIS:CD2	1:A:190:HIS:HE1	2.03	0.76
1:A:46:PRO:HD2	1:A:82:LEU:HD11	1.69	0.75
1:B:129:SER:O	1:B:130:VAL:HG13	1.86	0.75
1:B:16:ASN:HD22	1:B:97:GLU:H	1.35	0.74
1:D:124:MET:HE1	1:D:195:TYR:CE1	2.23	0.74
1:D:52:LYS:CB	3:D:209:HOH:O	2.32	0.74
1:B:186:ARG:CB	1:B:186:ARG:NH1	2.41	0.73
1:A:50:PHE:N	3:A:244:HOH:O	2.21	0.72
1:D:25:ASN:HB2	1:D:92:ILE:HD11	1.70	0.72
1:D:181:GLU:HB3	1:D:186:ARG:O	1.89	0.72
1:D:106:PHE:CD2	3:D:220:HOH:O	2.43	0.71
1:B:6:LYS:HD3	3:B:217:HOH:O	1.89	0.71
1:B:7:LEU:H	1:B:7:LEU:CD2	2.03	0.71
1:A:48:MET:N	3:A:216:HOH:O	2.23	0.71
1:B:129:SER:HB3	3:B:237:HOH:O	1.90	0.71
1:C:151:MET:HE3	1:C:155:VAL:CG2	2.20	0.71
1:D:63:GLU:O	1:D:67:ARG:HG3	1.90	0.71
1:D:136:HIS:N	1:D:136:HIS:CD2	2.59	0.70
1:B:52:LYS:CB	3:B:222:HOH:O	2.40	0.70
1:D:16:ASN:HD22	1:D:97:GLU:H	1.40	0.70
1:A:16:ASN:HD22	1:A:97:GLU:H	1.37	0.70
1:B:24:HIS:HE1	3:B:219:HOH:O	1.73	0.69
1:A:42:ARG:NH1	1:A:55:VAL:HG11	2.07	0.69
1:A:136:HIS:HD2	1:A:190:HIS:HE1	1.38	0.69
1:C:112:VAL:HB	1:C:142:VAL:HG13	1.74	0.69
1:D:106:PHE:HD2	3:D:220:HOH:O	1.73	0.69
1:B:48:MET:HA	1:B:48:MET:HE3	1.74	0.69
1:D:99:PHE:HB3	3:D:203:HOH:O	1.91	0.69
1:D:122:MET:O	1:D:123:HIS:C	2.32	0.69
1:B:95:CYS:HB2	1:B:96:PRO:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:MET:HE1	1:D:195:TYR:HE1	1.54	0.68
1:D:128:GLU:HB2	3:D:208:HOH:O	1.94	0.68
1:D:179:GLU:O	1:D:182:GLU:HB3	1.93	0.68
1:A:127:MET:HA	1:A:127:MET:CE	2.23	0.68
1:C:7:LEU:HD23	1:C:7:LEU:N	2.09	0.68
1:A:74:LYS:O	1:A:78:THR:HG23	1.93	0.68
1:D:107:ASP:OD1	1:D:107:ASP:N	2.25	0.67
1:D:162:MET:HE1	1:D:180:PHE:CD2	2.29	0.67
1:C:136:HIS:CD2	1:C:190:HIS:HE1	2.13	0.67
1:A:7:LEU:CD2	1:A:7:LEU:N	2.57	0.67
1:D:190:HIS:CE1	1:D:191:SER:O	2.48	0.67
1:A:78:THR:HG22	1:A:83:LEU:HD12	1.76	0.67
1:C:162:MET:HE2	1:C:176:LEU:HB3	1.75	0.66
1:D:64:ASP:HA	1:D:67:ARG:HD3	1.77	0.66
1:D:108:ILE:O	1:D:109:ILE:HG13	1.96	0.66
1:B:172:ASP:N	1:B:172:ASP:OD1	2.26	0.66
1:D:184:ARG:O	1:D:185:LYS:HB2	1.95	0.66
1:D:173:ILE:HG23	1:D:174:ASP:N	2.11	0.65
1:A:52:LYS:HD3	1:A:53:PRO:HD2	1.78	0.65
1:B:52:LYS:HB3	3:B:222:HOH:O	1.95	0.65
1:B:78:THR:HG22	1:B:83:LEU:HD12	1.78	0.65
1:B:128:GLU:CG	1:B:129:SER:H	2.09	0.65
1:C:47:GLY:O	1:C:48:MET:HB2	1.97	0.65
1:D:79:GLN:HA	1:D:79:GLN:HE21	1.61	0.65
1:A:74:LYS:O	1:A:78:THR:CG2	2.45	0.65
1:D:119:LEU:CD1	1:D:119:LEU:N	2.59	0.65
1:D:162:MET:HE1	1:D:180:PHE:HD2	1.62	0.64
1:B:157:THR:O	1:B:161:ASN:HB2	1.98	0.64
1:B:136:HIS:HD2	1:B:190:HIS:CE1	2.13	0.64
1:C:192:VAL:C	1:C:193:LEU:HD22	2.24	0.63
1:D:98:ARG:HG2	1:D:100:GLN:NE2	2.14	0.63
1:D:44:LYS:C	1:D:45:LEU:HD12	2.23	0.63
1:A:175:GLU:HG2	1:B:29:LYS:HD3	1.81	0.63
1:C:136:HIS:HD2	1:C:190:HIS:CE1	2.17	0.63
1:A:127:MET:O	1:A:128:GLU:HB2	1.99	0.62
1:B:75:GLU:HA	1:B:75:GLU:OE1	1.99	0.62
1:D:119:LEU:N	1:D:119:LEU:HD12	2.13	0.62
1:B:48:MET:HA	1:B:48:MET:HE2	1.82	0.62
1:C:136:HIS:CD2	1:C:190:HIS:CE1	2.87	0.62
1:B:129:SER:CB	3:B:237:HOH:O	2.46	0.62
1:B:72:LYS:O	1:B:73:ASP:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HD2	3:B:235:HOH:O	1.99	0.62
1:B:186:ARG:NH1	1:B:186:ARG:CG	2.53	0.62
1:D:192:VAL:O	1:D:193:LEU:HD22	2.00	0.61
1:B:16:ASN:HD21	1:B:93:LYS:NZ	1.98	0.61
1:A:22:GLU:OE2	1:A:150:LEU:HD13	2.00	0.61
1:A:48:MET:O	1:A:51:ASP:HB2	1.99	0.61
1:D:136:HIS:CD2	1:D:136:HIS:H	2.19	0.61
1:A:195:TYR:HB2	3:A:234:HOH:O	1.99	0.61
1:B:24:HIS:HD2	1:B:36:SER:OG	1.84	0.61
1:A:52:LYS:HD3	1:A:53:PRO:CD	2.32	0.60
1:D:131:ASP:OD1	1:D:133:ARG:HG2	2.01	0.60
1:D:113:GLU:O	1:D:139:ASN:OD1	2.19	0.60
1:D:190:HIS:ND1	1:D:191:SER:N	2.49	0.60
1:D:190:HIS:HB2	3:D:207:HOH:O	2.01	0.60
1:D:39:THR:HG22	3:D:203:HOH:O	2.01	0.60
1:D:162:MET:CE	1:D:180:PHE:CD2	2.85	0.60
1:B:74:LYS:O	1:B:78:THR:CG2	2.49	0.60
1:B:136:HIS:CD2	1:B:190:HIS:CE1	2.87	0.59
1:D:162:MET:CE	1:D:180:PHE:HD2	2.15	0.59
1:A:128:GLU:OE1	1:A:129:SER:O	2.20	0.59
1:B:54:ASN:HD22	1:B:72:LYS:NZ	2.00	0.59
1:D:162:MET:HE1	1:D:180:PHE:HB2	1.85	0.59
1:A:58:PHE:CD2	1:A:98:ARG:HB2	2.38	0.59
1:D:178:GLN:HA	1:D:181:GLU:OE1	2.03	0.59
1:C:16:ASN:HD21	1:C:93:LYS:HZ1	1.50	0.59
1:C:24:HIS:HD2	1:C:36:SER:OG	1.86	0.59
1:D:75:GLU:HA	1:D:75:GLU:OE1	2.02	0.58
1:B:44:LYS:C	1:B:45:LEU:HD12	2.28	0.58
1:D:177:ILE:O	1:D:181:GLU:OE1	2.21	0.58
1:B:48:MET:HE3	1:B:76:PHE:CE2	2.37	0.58
1:D:8:ALA:HB1	3:D:220:HOH:O	2.02	0.58
1:D:111:THR:HG21	1:D:117:TYR:HA	1.86	0.58
1:A:49:ALA:N	3:A:244:HOH:O	2.36	0.58
1:A:58:PHE:CG	1:A:98:ARG:HB2	2.39	0.58
1:C:48:MET:N	3:C:230:HOH:O	2.01	0.57
1:D:177:ILE:HG21	3:D:207:HOH:O	2.03	0.57
1:D:79:GLN:HE21	1:D:79:GLN:CA	2.17	0.57
1:C:16:ASN:HD22	1:C:97:GLU:H	1.52	0.57
1:A:40:GLY:O	1:A:98:ARG:HD2	2.05	0.57
1:D:7:LEU:HD23	1:D:7:LEU:N	2.18	0.57
1:D:117:TYR:HE1	1:D:137:VAL:HG12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:SER:OG	1:A:130:VAL:N	2.35	0.57
1:B:7:LEU:HD23	1:B:7:LEU:N	2.12	0.57
1:C:47:GLY:O	1:C:48:MET:CB	2.53	0.57
1:D:119:LEU:CD1	1:D:119:LEU:H	2.17	0.57
1:C:124:MET:HE1	1:C:135:VAL:HG11	1.88	0.56
1:D:112:VAL:HB	1:D:142:VAL:HG13	1.87	0.56
1:D:117:TYR:CE1	1:D:137:VAL:HG12	2.39	0.56
1:A:16:ASN:ND2	1:A:97:GLU:H	2.03	0.56
1:A:56:TYR:OH	1:A:69:LEU:HD13	2.05	0.56
1:C:6:LYS:HE2	3:C:3:HOH:O	2.06	0.56
1:C:131:ASP:CB	3:C:215:HOH:O	2.53	0.56
1:A:115:ARG:HB3	1:A:115:ARG:NH1	2.19	0.56
1:D:169:LEU:O	1:D:173:ILE:HB	2.06	0.56
1:C:193:LEU:N	1:C:193:LEU:CD2	2.66	0.56
1:D:108:ILE:HD12	1:D:108:ILE:N	2.21	0.56
1:D:179:GLU:C	1:D:182:GLU:HB3	2.31	0.56
1:D:111:THR:HB	1:D:116:VAL:HG12	1.88	0.55
1:D:180:PHE:C	1:D:182:GLU:H	2.12	0.55
1:B:141:ASP:O	1:B:186:ARG:NH2	2.39	0.55
1:D:21:MET:HE2	1:D:62:TYR:OH	2.06	0.55
1:B:128:GLU:HG3	1:B:129:SER:H	1.71	0.55
1:B:19:ARG:NH1	1:B:113:GLU:OE1	2.36	0.55
1:C:100:GLN:HE21	1:C:100:GLN:H	0.79	0.55
1:D:24:HIS:HD2	1:D:36:SER:OG	1.89	0.55
1:B:112:VAL:HA	1:B:140:VAL:O	2.05	0.55
1:B:54:ASN:ND2	1:B:72:LYS:HZ2	2.05	0.55
1:A:140:VAL:HG22	1:A:188:ILE:HD12	1.88	0.54
1:D:122:MET:O	1:D:124:MET:N	2.40	0.54
1:D:110:VAL:HG11	1:D:156:ILE:HG12	1.89	0.54
1:A:70:GLU:HG2	3:A:204:HOH:O	2.07	0.54
1:D:52:LYS:HE3	1:D:53:PRO:HD2	1.90	0.54
1:C:7:LEU:CD2	1:C:7:LEU:N	2.60	0.54
1:C:151:MET:HE3	1:C:155:VAL:HG23	1.88	0.54
1:B:7:LEU:CD2	1:B:7:LEU:N	2.64	0.54
1:B:18:ASN:ND2	3:B:201:HOH:O	2.37	0.54
1:D:108:ILE:C	1:D:109:ILE:HG13	2.33	0.54
1:D:127:MET:HE1	1:D:129:SER:HB3	1.88	0.54
1:B:58:PHE:CG	1:B:98:ARG:HB2	2.43	0.54
1:B:54:ASN:ND2	1:B:72:LYS:NZ	2.55	0.53
1:A:47:GLY:CA	3:A:216:HOH:O	2.57	0.53
1:B:41:GLU:O	1:B:42:ARG:HD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:MET:O	1:D:162:MET:HB3	2.08	0.53
1:A:136:HIS:HD2	1:A:190:HIS:CE1	2.24	0.52
1:B:16:ASN:HD21	1:B:93:LYS:HZ1	1.56	0.52
1:B:48:MET:HE3	1:B:76:PHE:CZ	2.44	0.52
1:D:184:ARG:O	1:D:185:LYS:CB	2.56	0.52
1:D:190:HIS:ND1	1:D:190:HIS:C	2.67	0.52
1:A:136:HIS:CD2	1:A:190:HIS:CE1	2.93	0.52
1:B:19:ARG:CD	1:B:142:VAL:HG22	2.40	0.52
1:C:16:ASN:ND2	1:C:93:LYS:HZ3	2.00	0.52
1:D:122:MET:O	1:D:125:GLU:N	2.38	0.52
1:D:187:VAL:O	1:D:188:ILE:HD13	2.10	0.52
1:D:52:LYS:HD3	1:D:53:PRO:O	2.10	0.51
1:A:115:ARG:CZ	1:A:115:ARG:CB	2.80	0.51
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.10	0.51
1:B:169:LEU:HD22	1:B:173:ILE:HB	1.92	0.51
1:A:175:GLU:CG	1:B:29:LYS:HD3	2.41	0.51
1:D:136:HIS:H	1:D:136:HIS:HD2	1.57	0.51
1:D:140:VAL:O	1:D:141:ASP:C	2.54	0.51
1:D:168:ASP:O	1:D:170:ASP:N	2.44	0.51
1:A:131:ASP:HB2	3:A:234:HOH:O	2.11	0.51
1:A:120:VAL:O	1:A:124:MET:HG3	2.11	0.51
1:C:6:LYS:HA	1:C:6:LYS:HE3	1.93	0.51
1:B:66:TYR:CD1	1:B:66:TYR:C	2.89	0.50
1:D:10:ALA:HB3	1:D:109:ILE:HG12	1.93	0.50
1:D:44:LYS:O	1:D:45:LEU:HD12	2.11	0.50
1:D:168:ASP:O	1:D:169:LEU:C	2.54	0.50
1:B:52:LYS:HE2	1:B:53:PRO:O	2.12	0.50
1:D:180:PHE:C	1:D:182:GLU:N	2.67	0.50
1:B:152:GLY:O	1:B:156:ILE:HG23	2.12	0.50
1:A:82:LEU:O	1:A:86:LEU:HD12	2.12	0.50
1:D:51:ASP:OD2	1:D:52:LYS:HB2	2.11	0.50
1:B:100:GLN:O	3:B:213:HOH:O	2.19	0.49
1:D:190:HIS:NE2	3:D:204:HOH:O	2.35	0.49
1:C:131:ASP:HB2	3:C:215:HOH:O	2.13	0.49
1:B:21:MET:HE3	1:B:92:ILE:HD12	1.94	0.49
1:C:7:LEU:H	1:C:7:LEU:HD22	1.75	0.49
1:B:19:ARG:HD2	1:B:142:VAL:HG22	1.93	0.49
1:B:184:ARG:O	1:B:186:ARG:HG3	2.13	0.49
1:D:187:VAL:C	1:D:188:ILE:HD13	2.38	0.48
1:D:52:LYS:HE3	1:D:53:PRO:HG2	1.95	0.48
1:A:115:ARG:HG3	3:A:196:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:TYR:CE1	1:C:96:PRO:HD3	2.48	0.48
1:A:24:HIS:HD2	1:A:36:SER:OG	1.96	0.48
1:C:124:MET:HE3	1:C:195:TYR:CE1	2.49	0.48
1:A:7:LEU:H	1:A:7:LEU:HD22	1.77	0.48
1:D:24:HIS:CD2	1:D:36:SER:HB3	2.48	0.48
1:A:133:ARG:CG	3:A:234:HOH:O	2.61	0.48
1:D:137:VAL:O	1:D:138:LEU:HD23	2.14	0.48
1:B:111:THR:HG21	1:B:117:TYR:HA	1.95	0.47
1:D:160:ILE:HD12	1:D:160:ILE:N	2.29	0.47
1:D:19:ARG:N	2:D:300:VO4:O4	2.47	0.47
1:D:180:PHE:O	1:D:184:ARG:HB2	2.15	0.47
1:D:100:GLN:NE2	1:D:100:GLN:H	2.11	0.47
1:B:52:LYS:HE3	1:B:53:PRO:HD2	1.96	0.47
1:C:123:HIS:CD2	3:C:213:HOH:O	2.35	0.47
1:B:6:LYS:HE3	3:B:223:HOH:O	2.14	0.47
1:D:114:GLU:O	1:D:117:TYR:HB3	2.14	0.47
1:B:52:LYS:HA	1:B:53:PRO:HD2	1.69	0.47
1:D:52:LYS:HA	1:D:53:PRO:HD2	1.48	0.47
1:C:168:ASP:OD2	1:C:171:ASN:HB2	2.14	0.46
1:D:7:LEU:HD12	1:D:108:ILE:HD11	1.97	0.46
1:C:52:LYS:HA	1:C:53:PRO:HD3	1.72	0.46
1:B:151:MET:HE3	1:B:151:MET:C	2.40	0.46
1:D:119:LEU:HD13	1:D:119:LEU:H	1.80	0.46
1:D:136:HIS:CG	3:D:204:HOH:O	2.67	0.46
1:A:60:THR:O	1:A:96:PRO:HD2	2.15	0.46
1:C:47:GLY:CA	3:C:230:HOH:O	2.62	0.46
1:C:133:ARG:HA	1:C:134:PRO:HD3	1.62	0.46
1:D:106:PHE:HA	3:D:220:HOH:O	2.15	0.46
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.75	0.46
1:A:165:LYS:HD3	1:B:151:MET:HG2	1.97	0.46
1:A:182:GLU:O	1:A:185:LYS:HE2	2.16	0.46
1:C:61:LYS:O	1:C:62:TYR:C	2.56	0.46
1:B:17:MET:HB3	1:B:17:MET:HE3	1.50	0.46
1:A:15:SER:HB2	2:A:300:VO4:O2	2.16	0.46
1:C:83:LEU:O	1:C:84:HIS:C	2.57	0.46
1:A:127:MET:O	1:A:128:GLU:CB	2.64	0.46
1:D:129:SER:OG	1:D:130:VAL:N	2.49	0.46
1:D:173:ILE:HG13	1:D:177:ILE:HD11	1.98	0.46
1:B:47:GLY:O	1:B:49:ALA:N	2.48	0.45
1:A:133:ARG:HA	1:A:134:PRO:HD3	1.70	0.45
1:C:17:MET:HE3	1:C:17:MET:HB3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASN:HD22	1:B:72:LYS:HZ3	1.64	0.45
1:D:128:GLU:CD	1:D:129:SER:N	2.75	0.45
1:A:127:MET:HE3	1:A:127:MET:CA	2.35	0.45
1:D:173:ILE:CG2	1:D:174:ASP:H	2.22	0.45
1:C:6:LYS:HB3	3:C:202:HOH:O	2.16	0.45
1:B:103:LYS:HA	1:B:103:LYS:HD3	1.61	0.45
1:B:25:ASN:HB2	1:B:92:ILE:HD11	1.99	0.45
1:C:10:ALA:HA	1:C:35:ARG:O	2.16	0.45
1:B:19:ARG:CG	1:B:142:VAL:HG22	2.47	0.45
1:B:128:GLU:CG	1:B:129:SER:N	2.75	0.45
1:D:122:MET:HE3	1:D:122:MET:HB3	1.77	0.45
1:A:133:ARG:HG2	3:A:234:HOH:O	2.17	0.44
1:A:162:MET:HE1	1:A:180:PHE:HB2	1.99	0.44
1:B:19:ARG:HG2	1:B:142:VAL:HG22	1.98	0.44
1:D:163:MET:HB3	1:D:169:LEU:HD21	1.99	0.44
1:D:182:GLU:HG3	1:D:183:ARG:N	2.32	0.44
1:A:133:ARG:N	3:A:234:HOH:O	2.49	0.44
1:D:177:ILE:HD13	1:D:190:HIS:HD2	1.83	0.44
1:C:115:ARG:HG3	3:C:203:HOH:O	2.18	0.44
1:D:105:GLN:HB3	1:D:195:TYR:CE2	2.53	0.44
1:A:7:LEU:HD22	3:A:202:HOH:O	2.18	0.43
1:A:81:GLY:HA2	3:A:240:HOH:O	2.18	0.43
1:A:124:MET:HB3	1:A:124:MET:HE2	1.65	0.43
1:D:124:MET:CE	1:D:124:MET:HA	2.49	0.43
1:D:190:HIS:ND1	1:D:191:SER:O	2.51	0.43
1:B:73:ASP:O	1:B:74:LYS:C	2.59	0.43
1:D:131:ASP:HB3	1:D:195:TYR:O	2.18	0.43
1:D:166:SER:OG	1:D:167:THR:N	2.50	0.43
1:A:19:ARG:CD	1:A:142:VAL:HG22	2.49	0.43
1:B:45:LEU:HD12	1:B:45:LEU:N	2.31	0.43
1:C:17:MET:HB2	2:C:300:VO4:O2	2.19	0.43
1:D:17:MET:HE1	1:D:86:LEU:CD2	2.49	0.43
1:D:75:GLU:O	1:D:76:PHE:C	2.62	0.43
1:A:93:LYS:NZ	1:A:97:GLU:OE1	2.50	0.43
1:D:175:GLU:O	1:D:178:GLN:N	2.52	0.43
1:B:139:ASN:HB3	1:B:189:LEU:HB2	2.01	0.42
1:B:173:ILE:HG23	1:B:174:ASP:N	2.34	0.42
1:D:52:LYS:HE3	1:D:53:PRO:CD	2.49	0.42
1:D:107:ASP:HB2	1:D:108:ILE:HD12	2.01	0.42
1:D:169:LEU:O	1:D:169:LEU:HD13	2.19	0.42
1:A:190:HIS:HD2	3:A:206:HOH:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:VAL:HG22	1:C:188:ILE:HD12	2.01	0.42
1:B:13:CYS:SG	1:B:15:SER:O	2.77	0.42
1:B:39:THR:HA	1:B:100:GLN:HE22	1.84	0.42
1:B:122:MET:HB3	1:B:122:MET:HE3	1.46	0.42
1:B:181:GLU:HG2	1:B:188:ILE:HG12	2.02	0.42
1:D:82:LEU:HD23	1:D:82:LEU:HA	1.85	0.42
1:B:160:ILE:HD13	1:B:160:ILE:HA	1.74	0.42
1:B:80:ASN:OD1	1:B:80:ASN:C	2.62	0.42
1:C:151:MET:HE3	1:C:155:VAL:HG22	2.02	0.42
1:D:176:LEU:HD23	1:D:176:LEU:HA	1.87	0.42
1:A:42:ARG:HH11	1:A:55:VAL:HG11	1.84	0.42
1:A:44:LYS:HD2	1:A:44:LYS:C	2.45	0.42
1:B:103:LYS:HZ2	1:B:103:LYS:HG2	1.65	0.42
1:B:177:ILE:HG21	1:B:177:ILE:HD13	1.59	0.42
1:A:17:MET:HB3	1:A:17:MET:HE3	1.55	0.42
1:A:39:THR:HA	1:A:100:GLN:HE22	1.85	0.42
1:C:16:ASN:HB2	1:C:37:TYR:C	2.45	0.42
1:C:150:LEU:HD13	1:C:150:LEU:HA	1.81	0.42
1:A:72:LYS:O	1:A:73:ASP:HB2	2.18	0.41
1:D:17:MET:HB2	2:D:300:VO4:O2	2.20	0.41
1:C:45:LEU:HD23	1:C:82:LEU:HD13	2.01	0.41
1:A:65:ILE:O	1:A:66:TYR:C	2.62	0.41
1:B:133:ARG:HA	1:B:134:PRO:HD3	1.77	0.41
1:B:16:ASN:ND2	1:B:97:GLU:H	2.10	0.41
1:C:48:MET:HG3	1:C:76:PHE:CZ	2.55	0.41
1:C:48:MET:O	1:C:51:ASP:HB2	2.21	0.41
1:D:24:HIS:HD2	1:D:36:SER:CB	2.33	0.41
1:D:139:ASN:C	1:D:140:VAL:HG23	2.45	0.41
1:A:175:GLU:HG3	1:B:29:LYS:NZ	2.35	0.41
1:D:172:ASP:C	1:D:175:GLU:HB3	2.38	0.41
1:A:174:ASP:CG	1:D:94:LYS:HZ1	2.28	0.41
1:D:114:GLU:HG3	1:D:189:LEU:HD11	2.02	0.41
1:D:173:ILE:CG2	1:D:174:ASP:N	2.80	0.41
1:A:128:GLU:OE1	1:A:128:GLU:C	2.60	0.41
1:B:48:MET:CE	1:B:76:PHE:CE2	3.02	0.40
1:D:34:VAL:O	1:D:35:ARG:HG3	2.21	0.40
1:B:16:ASN:HD22	1:B:97:GLU:N	2.12	0.40
1:B:76:PHE:CD1	1:B:76:PHE:C	2.99	0.40
1:B:93:LYS:HE3	1:B:95:CYS:O	2.21	0.40
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.93	0.40
1:D:21:MET:HE2	1:D:62:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:MET:HE3	1:B:176:LEU:HB3	2.04	0.40
1:D:11:VAL:HG11	1:D:23:ALA:HB3	2.03	0.40
1:D:37:TYR:CB	1:D:99:PHE:HB2	2.51	0.40
1:D:159:MET:O	1:D:163:MET:HG3	2.21	0.40
1:D:16:ASN:HD21	1:D:93:LYS:HZ3	1.66	0.40
1:D:60:THR:O	1:D:96:PRO:HD2	2.22	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	188/190 (99%)	173 (92%)	11 (6%)	4 (2%)	5	3
1	B	188/190 (99%)	178 (95%)	7 (4%)	3 (2%)	7	5
1	C	188/190 (99%)	178 (95%)	8 (4%)	2 (1%)	11	10
1	D	188/190 (99%)	149 (79%)	27 (14%)	12 (6%)	1	0
All	All	752/760 (99%)	678 (90%)	53 (7%)	21 (3%)	4	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	126	SER
1	B	73	ASP
1	D	122	MET
1	D	132	ASN
1	D	140	VAL
1	A	132	ASN
1	B	130	VAL
1	D	169	LEU

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Mol	Chain	Res	Type
1	D	173	ILE
1	C	48	MET
1	D	40	GLY
1	D	123	HIS
1	D	185	LYS
1	C	132	ASN
1	D	183	ARG
1	A	48	MET
1	D	131	ASP
1	D	144	ASP
1	B	132	ASN
1	D	126	SER

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	174/174 (100%)	149 (86%)	25 (14%)	3	2
1	B	174/174 (100%)	149 (86%)	25 (14%)	3	2
1	C	174/174 (100%)	149 (86%)	25 (14%)	3	2
1	D	174/174 (100%)	145 (83%)	29 (17%)	2	1
All	All	696/696 (100%)	592 (85%)	104 (15%)	3	2

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	7	LEU
1	A	42	ARG
1	A	44	LYS
1	A	48	MET
1	A	52	LYS
1	A	69	LEU
1	A	70	GLU
1	A	75	GLU

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Mol	Chain	Res	Type
1	A	78	THR
1	A	79	GLN
1	A	100	GLN
1	A	115	ARG
1	A	119	LEU
1	A	122	MET
1	A	126	SER
1	A	127	MET
1	A	128	GLU
1	A	133	ARG
1	A	142	VAL
1	A	148	ASP
1	A	150	LEU
1	A	169	LEU
1	A	185	LYS
1	A	192	VAL
1	B	6	LYS
1	B	7	LEU
1	B	14	SER
1	B	48	MET
1	B	52	LYS
1	B	67	ARG
1	B	69	LEU
1	B	78	THR
1	B	93	LYS
1	B	100	GLN
1	B	103	LYS
1	B	119	LEU
1	B	122	MET
1	B	130	VAL
1	B	131	ASP
1	B	142	VAL
1	B	151	MET
1	B	156	ILE
1	B	169	LEU
1	B	172	ASP
1	B	174	ASP
1	B	175	GLU
1	B	186	ARG
1	B	192	VAL
1	B	193	LEU
1	C	6	LYS

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Mol	Chain	Res	Type
1	C	7	LEU
1	C	34	VAL
1	C	35	ARG
1	C	44	LYS
1	C	52	LYS
1	C	61	LYS
1	C	69	LEU
1	C	71	SER
1	C	79	GLN
1	C	90	ARG
1	C	94	LYS
1	C	100	GLN
1	C	119	LEU
1	C	131	ASP
1	C	142	VAL
1	C	148	ASP
1	C	150	LEU
1	C	169	LEU
1	C	173	ILE
1	C	174	ASP
1	C	179	GLU
1	C	183	ARG
1	C	185	LYS
1	C	192	VAL
1	D	6	LYS
1	D	7	LEU
1	D	35	ARG
1	D	42	ARG
1	D	50	PHE
1	D	51	ASP
1	D	52	LYS
1	D	69	LEU
1	D	79	GLN
1	D	98	ARG
1	D	100	GLN
1	D	107	ASP
1	D	115	ARG
1	D	124	MET
1	D	128	GLU
1	D	136	HIS
1	D	142	VAL
1	D	148	ASP

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Mol	Chain	Res	Type
1	D	151	MET
1	D	163	MET
1	D	169	LEU
1	D	172	ASP
1	D	178	GLN
1	D	181	GLU
1	D	183	ARG
1	D	188	ILE
1	D	190	HIS
1	D	192	VAL
1	D	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	24	HIS
1	A	25	ASN
1	A	54	ASN
1	A	79	GLN
1	A	100	GLN
1	A	136	HIS
1	A	161	ASN
1	A	190	HIS
1	B	16	ASN
1	B	24	HIS
1	B	54	ASN
1	B	100	GLN
1	B	136	HIS
1	B	139	ASN
1	B	190	HIS
1	C	16	ASN
1	C	24	HIS
1	C	79	GLN
1	C	100	GLN
1	C	132	ASN
1	C	136	HIS
1	C	161	ASN
1	C	190	HIS
1	D	16	ASN
1	D	24	HIS
1	D	54	ASN

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Mol	Chain	Res	Type
1	D	79	GLN
1	D	100	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	VO4	D	300	-	0,4,4	-	-	-		
2	VO4	A	300	-	0,4,4	-	-	-		
2	VO4	B	300	-	0,4,4	-	-	-		
2	VO4	C	300	-	0,4,4	-	-	-		

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	VO4	2	0
2	A	300	VO4	1	0
2	C	300	VO4	1	0

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	190/190 (100%)	0.09	3 (1%) 70 75	38, 52, 81, 96	0
1	B	190/190 (100%)	-0.01	1 (0%) 87 89	39, 53, 72, 84	0
1	C	190/190 (100%)	0.13	3 (1%) 70 75	41, 58, 79, 91	0
1	D	190/190 (100%)	0.71	13 (6%) 23 27	46, 72, 109, 121	0
All	All	760/760 (100%)	0.23	20 (2%) 57 63	38, 57, 96, 121	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	ALA	5.1
1	D	130	VAL	4.3
1	D	192	VAL	3.4
1	D	187	VAL	3.1
1	B	130	VAL	2.8
1	D	193	LEU	2.8
1	C	49	ALA	2.8
1	A	130	VAL	2.7
1	D	50	PHE	2.6
1	C	175	GLU	2.5
1	D	134	PRO	2.5
1	D	6	LYS	2.4
1	C	130	VAL	2.4
1	D	137	VAL	2.4
1	D	189	LEU	2.4
1	D	194	PHE	2.2
1	D	186	ARG	2.1
1	A	48	MET	2.1
1	D	142	VAL	2.1
1	D	127	MET	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 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
2	VO4	D	300	5/5	0.96	0.08	59,63,68,69	0
2	VO4	C	300	5/5	0.98	0.06	46,48,50,50	0
2	VO4	A	300	5/5	0.99	0.06	46,46,49,52	0
2	VO4	B	300	5/5	0.99	0.06	44,45,50,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.