Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 04:51 AM EDT

PDB ID	:	3OMX
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 (i) 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 (i)) were used in the production of this report:

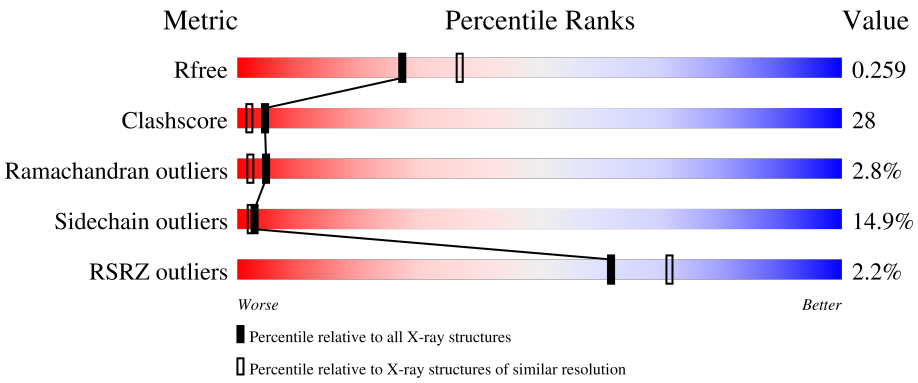
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	.% 51% 35% 11% •
1	B	190	52% 33% 12% •
1	C	190	.% 57% 32% 11% •
1	D	190	7% 38% 44% 15% •

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)

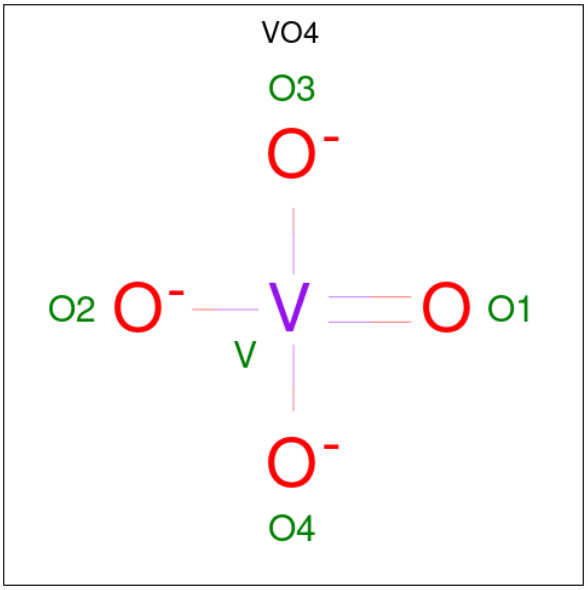
There are 3 unique types of molecules in this entry. The entry contains 6407 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	190	1554	975	268	298	13	0	0	0
1	B	190	1554	975	268	298	13	0	0	0
1	C	190	1554	975	268	298	13	0	0	0
1	D	190	1554	975	268	298	13	0	0	0

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O_4V).



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

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

- Molecule 3 is water.

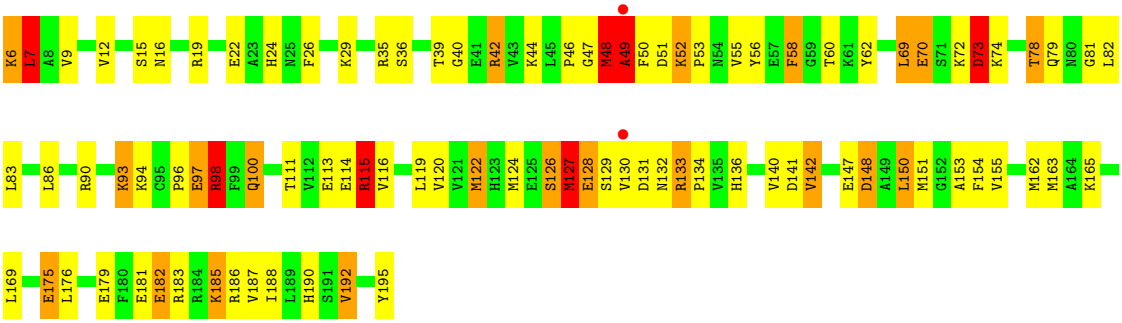
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	56	56	56	0	0
			Total	O		
3	B	49	49	49	0	0
			Total	O		
3	C	40	40	40	0	0
			Total	O		
3	D	26	26	26	0	0

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.

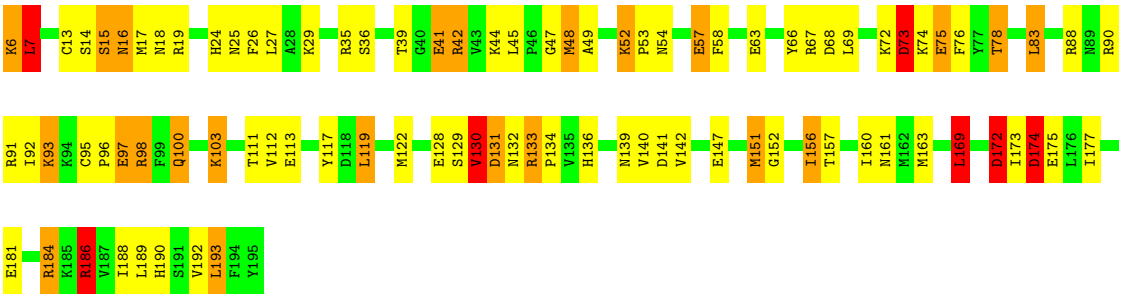
- Molecule 1: CG14216

Chain A:



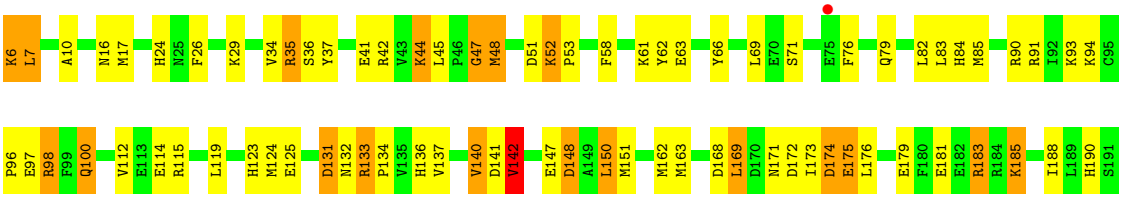
- Molecule 1: CG14216

Chain B:



- Molecule 1: CG14216

Chain C:



V192 L193 F194 Y195

- Molecule 1: CG14216

Chain D:

K6 L7 A8 V9 A10 V11 V12 C13 S14 S15 N16 M17 N18 R19 E22 A23 H24 N25 V34 R35 S36 Y37 G38 T39 G40 E41 R42 V43 K44 L45 P46 F50 D51 K52 P53 T60 E63 D64 I65 Y66 R67 D68 L69 E70 S71 K72 E75 Q79 L82 I92 K93

P96 E97 R98 F99 Q100 D101 T102 Q105 F106 D107 I108 I109 V110 T111 V112 E113 E114 R115 V116 Y117 D118 L119 V120 V121 M122 H123 M124 E125 S126 M127 E128 S129 V130 D131 N132 R133 P134 V135 H136 V137 L138 N139 V140 D141 V142 V143 D144 D148 M151 I156 M159 I160 N161 M162

M163 S166 T167 D168 L169 D170 N171 D172 I173 D174 E175 L176 I177 Q178 E179 F180 E181 E182 R183 R184 K185 R186 V187 I188 L189 H190 S191 V192 L193 F194 Y195

4 Data and refinement statistics (i)

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) 99.2 (48.66-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.205 , 0.267 0.197 , 0.259	Depositor DCC
R_{free} test set	2295 reflections (5.03%)	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 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.73	31/1579 (2.0%)	1.51	22/2121 (1.0%)
1	B	1.59	8/1579 (0.5%)	1.56	30/2121 (1.4%)
1	C	1.56	20/1579 (1.3%)	1.45	17/2121 (0.8%)
1	D	1.35	12/1579 (0.8%)	1.32	12/2121 (0.6%)
All	All	1.56	71/6316 (1.1%)	1.46	81/8484 (1.0%)

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 (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ALA	CA-CB	-9.49	1.32	1.52
1	A	182	GLU	CG-CD	9.36	1.66	1.51
1	C	175	GLU	CB-CG	9.01	1.69	1.52
1	C	175	GLU	CG-CD	8.97	1.65	1.51
1	A	182	GLU	CB-CG	8.62	1.68	1.52
1	A	97	GLU	CD-OE1	8.38	1.34	1.25
1	A	187	VAL	CB-CG2	8.11	1.69	1.52
1	A	26	PHE	CB-CG	-8.04	1.37	1.51
1	A	155	VAL	CB-CG2	7.77	1.69	1.52
1	C	125	GLU	CD-OE1	7.42	1.33	1.25
1	C	26	PHE	CB-CG	-7.24	1.39	1.51
1	C	147	GLU	CD-OE1	7.14	1.33	1.25
1	A	175	GLU	CG-CD	6.94	1.62	1.51
1	D	63	GLU	CB-CG	6.94	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	GLU	CD-OE1	6.87	1.33	1.25
1	D	22	GLU	CB-CG	-6.82	1.39	1.52
1	A	114	GLU	CG-CD	6.69	1.61	1.51
1	B	93	LYS	CB-CG	-6.69	1.34	1.52
1	D	63	GLU	CG-CD	6.62	1.61	1.51
1	A	148	ASP	CG-OD2	6.53	1.40	1.25
1	A	147	GLU	CG-CD	6.51	1.61	1.51
1	D	67	ARG	CA-CB	6.09	1.67	1.53
1	B	57	GLU	CG-CD	5.97	1.60	1.51
1	B	97	GLU	CG-CD	5.92	1.60	1.51
1	A	113	GLU	CG-CD	5.91	1.60	1.51
1	C	66	TYR	CD1-CE1	5.84	1.48	1.39
1	C	174	ASP	CG-OD1	5.83	1.38	1.25
1	C	58	PHE	CE2-CZ	5.71	1.48	1.37
1	D	51	ASP	CB-CG	5.69	1.63	1.51
1	A	58	PHE	CD1-CE1	5.67	1.50	1.39
1	B	63	GLU	CD-OE2	5.64	1.31	1.25
1	C	185	LYS	CD-CE	5.52	1.65	1.51
1	A	111	THR	CB-CG2	5.50	1.70	1.52
1	A	49	ALA	CA-CB	5.49	1.64	1.52
1	A	181	GLU	CG-CD	5.49	1.60	1.51
1	B	147	GLU	CD-OE2	5.48	1.31	1.25
1	A	179	GLU	CD-OE1	5.47	1.31	1.25
1	C	140	VAL	CB-CG1	-5.47	1.41	1.52
1	C	148	ASP	CG-OD2	5.46	1.38	1.25
1	A	154	PHE	CB-CG	-5.44	1.42	1.51
1	C	114	GLU	CB-CG	-5.43	1.41	1.52
1	C	26	PHE	CE2-CZ	5.42	1.47	1.37
1	A	175	GLU	CB-CG	5.41	1.62	1.52
1	A	114	GLU	CB-CG	-5.39	1.42	1.52
1	A	147	GLU	CD-OE1	5.36	1.31	1.25
1	A	12	VAL	CA-CB	5.33	1.66	1.54
1	C	142	VAL	CB-CG1	-5.32	1.41	1.52
1	A	35	ARG	CG-CD	5.31	1.65	1.51
1	C	29	LYS	CD-CE	5.30	1.64	1.51
1	C	37	TYR	CB-CG	-5.30	1.43	1.51
1	C	137	VAL	CB-CG2	5.24	1.63	1.52
1	C	181	GLU	CD-OE1	5.24	1.31	1.25
1	D	72	LYS	CE-NZ	5.24	1.62	1.49
1	C	63	GLU	CG-CD	5.23	1.59	1.51
1	A	116	VAL	CB-CG1	5.21	1.63	1.52
1	C	44	LYS	CD-CE	5.20	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	GLU	CD-OE2	5.20	1.31	1.25
1	B	41	GLU	CG-CD	5.20	1.59	1.51
1	D	70	GLU	CG-CD	5.19	1.59	1.51
1	A	179	GLU	CB-CG	-5.18	1.42	1.52
1	D	75	GLU	CD-OE2	5.16	1.31	1.25
1	D	12	VAL	CA-CB	5.15	1.65	1.54
1	D	66	TYR	CZ-OH	5.13	1.46	1.37
1	A	62	TYR	CE2-CZ	5.12	1.45	1.38
1	A	183	ARG	CZ-NH2	5.11	1.39	1.33
1	A	94	LYS	CD-CE	5.08	1.64	1.51
1	A	9	VAL	CB-CG1	-5.07	1.42	1.52
1	D	156	ILE	CB-CG2	-5.05	1.37	1.52
1	A	154	PHE	CD1-CE1	5.04	1.49	1.39
1	B	73	ASP	CB-CG	5.04	1.62	1.51
1	A	62	TYR	CG-CD1	5.03	1.45	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	67	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	C	148	ASP	CB-CG-OD1	-14.42	105.32	118.30
1	C	174	ASP	CB-CG-OD2	-13.98	105.72	118.30
1	A	148	ASP	CB-CG-OD1	-12.58	106.98	118.30
1	B	90	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	B	15	SER	C-N-CA	-9.59	97.73	121.70
1	B	186	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	B	7	LEU	CB-CG-CD1	-9.29	95.20	111.00
1	A	98	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	B	151	MET	CG-SD-CE	-8.80	86.11	100.20
1	A	186	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	172	ASP	CB-CG-OD1	-8.54	110.61	118.30
1	C	98	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	35	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	C	148	ASP	CB-CG-OD2	8.26	125.74	118.30
1	C	98	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	90	ARG	NE-CZ-NH1	-7.91	116.35	120.30
1	A	98	ARG	CG-CD-NE	-7.82	95.39	111.80
1	A	115	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	B	172	ASP	CB-CG-OD2	7.53	125.07	118.30
1	A	7	LEU	CB-CG-CD1	-7.47	98.29	111.00
1	D	68	ASP	CB-CG-OD2	7.43	124.98	118.30
1	B	133	ARG	NE-CZ-NH1	-7.33	116.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	15	SER	N-CA-C	-7.20	91.57	111.00
1	B	35	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	7	LEU	CA-CB-CG	7.03	131.46	115.30
1	B	88	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	7	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	98	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	B	184	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	141	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	90	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	148	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	B	68	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	133	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	C	163	MET	CA-CB-CG	-6.52	102.22	113.30
1	C	141	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	93	LYS	CB-CA-C	-6.38	97.64	110.40
1	B	15	SER	O-C-N	-6.35	112.54	122.70
1	B	119	LEU	CA-CB-CG	6.24	129.64	115.30
1	A	163	MET	CG-SD-CE	-6.21	90.26	100.20
1	B	163	MET	CA-CB-CG	-6.13	102.88	113.30
1	C	172	ASP	CB-CA-C	6.13	122.65	110.40
1	A	186	ARG	CG-CD-NE	-6.10	98.98	111.80
1	A	93	LYS	CD-CE-NZ	-6.07	97.75	111.70
1	B	7	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	A	115	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	130	VAL	N-CA-C	5.97	127.11	111.00
1	B	169	LEU	CB-CG-CD2	5.95	121.11	111.00
1	A	148	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	26	PHE	N-CA-CB	-5.86	100.05	110.60
1	C	85	MET	CG-SD-CE	-5.85	90.84	100.20
1	B	16	ASN	CB-CA-C	5.76	121.92	110.40
1	B	193	LEU	CA-CB-CG	5.74	128.51	115.30
1	C	183	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	D	98	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	17	MET	CG-SD-CE	-5.69	91.10	100.20
1	C	133	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	D	79	GLN	CA-CB-CG	5.54	125.60	113.40
1	B	68	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	D	142	VAL	CB-CA-C	5.49	121.83	111.40
1	B	131	ASP	N-CA-C	-5.42	96.37	111.00
1	B	83	LEU	CB-CG-CD2	5.41	120.20	111.00
1	D	15	SER	C-N-CA	-5.40	108.21	121.70
1	A	29	LYS	CD-CE-NZ	5.39	124.09	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	83	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	73	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	174	ASP	CB-CG-OD1	-5.36	113.47	118.30
1	B	98	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	D	67	ARG	CG-CD-NE	-5.33	100.61	111.80
1	A	179	GLU	CB-CA-C	-5.32	99.76	110.40
1	A	98	ARG	CD-NE-CZ	5.32	131.04	123.60
1	C	91	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	169	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	35	ARG	CG-CD-NE	-5.17	100.94	111.80
1	C	47	GLY	N-CA-C	5.10	125.86	113.10
1	D	13	CYS	CA-CB-SG	5.04	123.08	114.00
1	B	163	MET	CG-SD-CE	-5.02	92.17	100.20
1	D	67	ARG	NH1-CZ-NH2	5.02	124.92	119.40
1	C	174	ASP	OD1-CG-OD2	5.01	132.82	123.30
1	C	44	LYS	CD-CE-NZ	5.01	123.22	111.70

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	79	0
1	B	1554	0	1528	93	0
1	C	1554	0	1528	54	0
1	D	1554	0	1528	132	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	351	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 28.

All (351) 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: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: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: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: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:16:ASN:HD21	1:C:93:LYS:HZ1	1.27	0.81
1:C:175:GLU:HG3	3:C:5:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:124:MET:HE1	1:D:195:TYR:HE1	1.49	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: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:D:63:GLU:O	1:D:67:ARG:HG3	1.90	0.71
1:D:124:MET:HE1	1:D:195:TYR:CE1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:127:MET:HA	1:A:127:MET:CE	2.23	0.69
1:B:95:CYS:HB2	1:B:96:PRO:HD2	1.76	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: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: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:D:16:ASN:HD21	1:D:93:LYS:HZ3	1.40	0.67
1:B:16:ASN:HD21	1:B:93:LYS:HZ1	1.43	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:A:151:MET:HE1	1:C:151:MET:HB2	1.78	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:122:MET:O	1:D:123:HIS:C	2.32	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:D:98:ARG:HG2	1:D:100:GLN:NE2	2.14	0.63
1:D:162:MET:HE2	1:D:180:PHE:CD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASN:HD21	1:C:93:LYS:HZ3	1.46	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
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:A:22:GLU:OE2	1:A:150:LEU:HD13	2.00	0.61
1:D:162:MET:HE1	1:D:180:PHE:HB2	1.83	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:B:16:ASN:HD21	1:B:93:LYS:NZ	1.98	0.60
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:A:129:SER:OG	1:A:130:VAL:N	2.35	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:A:127:MET:HA	1:A:127:MET:HE3	1.84	0.59
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: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:24:HIS:HD2	1:C:36:SER:OG	1.86	0.59
1:D:75:GLU:HA	1:D:75:GLU:OE1	2.02	0.59
1:A:151:MET:HE2	1:C:151:MET:HB2	1.85	0.58
1:D:44:LYS:C	1:D:45:LEU:HD12	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:16:ASN:ND2	1:C:93:LYS:HZ1	2.00	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
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:192:VAL:C	1:C:193:LEU:HD22	2.24	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:111:THR:HB	1:D:116:VAL:HG12	1.88	0.55
1:B:141:ASP:O	1:B:186:ARG:NH2	2.39	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:D:16:ASN:HD21	1:D:93:LYS:HZ1	1.52	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: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:B:44:LYS:C	1:B:45:LEU:HD12	2.28	0.54
1:B:58:PHE:CG	1:B:98:ARG:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:180:PHE:C	1:D:182:GLU:H	2.12	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: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: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:B:57:GLU:OE1	1:B:57:GLU:HA	2.10	0.51
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: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:168:ASP:O	1:D:170:ASP:N	2.44	0.51
1:D:179:GLU:C	1:D:182:GLU:HB3	2.31	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:D:124:MET:HE3	1:D:124:MET:HA	1.93	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:B:52:LYS:HE2	1:B:53:PRO:O	2.12	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:C:7:LEU:H	1:C:7:LEU:HD22	1.75	0.49
1:D:108:ILE:C	1:D:109:ILE:HG13	2.33	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:CG	1:B:129:SER:N	2.75	0.48
1:C:162:MET:HE1	1:C:176:LEU:HB3	1.96	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:190:HIS:ND1	1:D:190:HIS:C	2.67	0.47
1:D:100:GLN:NE2	1:D:100:GLN:H	2.11	0.47
1:A:162:MET:HE3	1:A:176:LEU:HB3	1.95	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: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:D:140:VAL:O	1:D:141:ASP:C	2.54	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:D:180:PHE:C	1:D:182:GLU:N	2.67	0.46
1:A:15:SER:HB2	2:A:300:VO4:O2	2.16	0.46
1:A:127:MET:O	1:A:128:GLU:CB	2.64	0.46
1:B:66:TYR:CD1	1:B:66:TYR:C	2.89	0.46
1:D:168:ASP:O	1:D:169:LEU:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:MET:CE	1:A:176:LEU:HB3	2.46	0.45
1:B:54:ASN:HD22	1:B:72:LYS:HZ3	1.64	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:A:133:ARG:HG2	3:A:234:HOH:O	2.17	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:187:VAL:C	1:D:188:ILE:HD13	2.38	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:D:124:MET:HA	1:D:124:MET:CE	2.49	0.43
1:D:162:MET:HE1	1:D:180:PHE:CD2	2.52	0.43
1:D:190:HIS:ND1	1:D:191:SER:O	2.51	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: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
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:A:93:LYS:NZ	1:A:97:GLU:OE1	2.50	0.42
1:B:39:THR:HA	1:B:100:GLN:HE22	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:39:THR:HA	1:A:100:GLN:HE22	1.85	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:16:ASN:ND2	1:D:93:LYS:HZ3	2.12	0.41
1:A:192:VAL:O	1:A:192:VAL:CG2	2.67	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:C:61:LYS:O	1:C:62:TYR:C	2.56	0.41
1:A:122:MET:HE3	1:A:122:MET:HB3	1.58	0.41
1:B:133:ARG:HA	1:B:134:PRO:HD3	1.77	0.41
1:C:83:LEU:O	1:C:84:HIS:C	2.57	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:A:175:GLU:HG3	1:B:29:LYS:NZ	2.35	0.41
1:C:124:MET:HE3	1:C:195:TYR:CE1	2.56	0.41
1:D:114:GLU:HG3	1:D:189:LEU:HD11	2.02	0.41
1:D:122:MET:HE3	1:D:122:MET:HB3	1.96	0.41
1:D:173:ILE:CG2	1:D:174:ASP:N	2.80	0.41
1:D:128:GLU:CD	1:D:129:SER:N	2.75	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: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: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: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%)	7 4
1	B	188/190 (99%)	178 (95%)	7 (4%)	3 (2%)	9 7
1	C	188/190 (99%)	178 (95%)	8 (4%)	2 (1%)	14 13
1	D	188/190 (99%)	149 (79%)	27 (14%)	12 (6%)	1 0
All	All	752/760 (99%)	678 (90%)	53 (7%)	21 (3%)	5 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
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%)	150 (86%)	24 (14%)	3 3
1	C	174/174 (100%)	148 (85%)	26 (15%)	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	78	THR
1	A	79	GLN
1	A	98	ARG
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

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Mol	Chain	Res	Type
1	A	192	VAL
1	B	6	LYS
1	B	7	LEU
1	B	14	SER
1	B	26	PHE
1	B	42	ARG
1	B	48	MET
1	B	52	LYS
1	B	67	ARG
1	B	69	LEU
1	B	78	THR
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	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
1	C	7	LEU
1	C	34	VAL
1	C	35	ARG
1	C	42	ARG
1	C	44	LYS
1	C	52	LYS
1	C	69	LEU
1	C	71	SER
1	C	79	GLN
1	C	90	ARG
1	C	94	LYS
1	C	98	ARG
1	C	100	GLN
1	C	119	LEU
1	C	131	ASP
1	C	142	VAL

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Mol	Chain	Res	Type
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	93	LYS
1	D	100	GLN
1	D	107	ASP
1	D	115	ARG
1	D	124	MET
1	D	128	GLU
1	D	133	ARG
1	D	136	HIS
1	D	142	VAL
1	D	148	ASP
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	190	HIS
1	D	192	VAL
1	D	193	LEU

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	16	ASN
1	A	24	HIS
1	A	25	ASN
1	A	100	GLN
1	A	136	HIS
1	A	190	HIS
1	B	16	ASN
1	B	18	ASN
1	B	24	HIS
1	B	54	ASN
1	B	100	GLN
1	B	136	HIS
1	B	190	HIS
1	C	16	ASN
1	C	18	ASN
1	C	24	HIS
1	C	79	GLN
1	C	100	GLN
1	C	136	HIS
1	C	190	HIS
1	D	16	ASN
1	D	24	HIS
1	D	25	ASN
1	D	54	ASN
1	D	79	GLN
1	D	100	GLN
1	D	136	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	300	-	1,4,4	6.25	1 (100%)	-		
2	VO4	C	300	-	1,4,4	6.13	1 (100%)	-		
2	VO4	A	300	-	1,4,4	5.81	1 (100%)	-		
2	VO4	D	300	-	1,4,4	5.74	1 (100%)	-		

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	VO4	O1-V	6.25	1.99	1.63
2	C	300	VO4	O1-V	6.13	1.98	1.63
2	A	300	VO4	O1-V	5.81	1.97	1.63
2	D	300	VO4	O1-V	5.74	1.96	1.63

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	C	300	VO4	1	0
2	A	300	VO4	1	0
2	D	300	VO4	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.15	2 (1%) 80 86	38, 52, 81, 96	0
1	B	190/190 (100%)	-0.02	0 100 100	39, 53, 72, 84	0
1	C	190/190 (100%)	0.10	1 (0%) 91 95	41, 58, 79, 91	0
1	D	190/190 (100%)	0.46	14 (7%) 14 21	46, 72, 109, 121	0
All	All	760/760 (100%)	0.17	17 (2%) 62 71	38, 57, 96, 121	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130	VAL	5.1
1	A	130	VAL	4.3
1	D	195	TYR	3.8
1	D	135	VAL	3.4
1	A	49	ALA	3.3
1	D	180	PHE	3.2
1	D	183	ARG	3.0
1	D	50	PHE	3.0
1	D	132	ASN	2.9
1	D	137	VAL	2.8
1	D	186	ARG	2.8
1	D	121	VAL	2.7
1	D	138	LEU	2.5
1	D	187	VAL	2.5
1	D	127	MET	2.4
1	D	160	ILE	2.4
1	C	75	GLU	2.3

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 monosaccharides 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(Å^2)	Q<0.9
2	VO4	D	300	5/5	0.97	0.17	59,63,68,69	0
2	VO4	A	300	5/5	0.98	0.14	46,46,49,52	0
2	VO4	C	300	5/5	0.99	0.14	46,48,50,50	0
2	VO4	B	300	5/5	0.99	0.14	44,45,50,60	0

6.5 Other polymers (i)

There are no such residues in this entry.