W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:19 AM GMT

PDB ID	:	2MEV
Title	:	STRUCTURAL REFINEMENT AND ANALYSIS OF MENGO VIRUS
Authors	:	Rossmann, M.G.
Deposited on	:	1989-04-21
Resolution	:	3.00 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
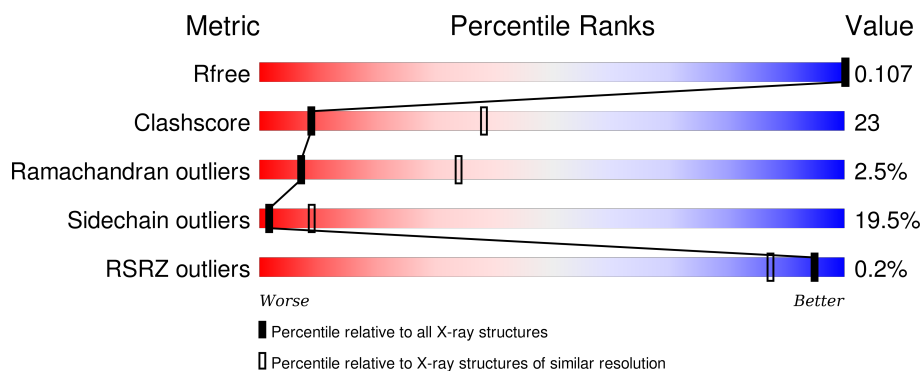
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1	277	45% 32% 14% 6% •
2	2	256	55% 24% 11% 7% •
3	3	231	55% 29% 12% •
4	4	70	% 27% 30% 17% 9% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6507 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 MENGO VIRUS COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	268	Total	C	N	O	S	0	0	0
			2091	1345	342	397	7			

- Molecule 2 is a protein called MENGO VIRUS COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	249	Total	C	N	O	S	0	0	0
			1973	1247	349	372	5			

- Molecule 3 is a protein called MENGO VIRUS COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	231	Total	C	N	O	S	0	0	0
			1772	1153	283	326	10			

- Molecule 4 is a protein called MENGO VIRUS COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	58	Total	C	N	O	S	0	0	0
			433	270	71	91	1			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	2	1	Total 5	O 4	P 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	106	Total 106	O 106	0	0
6	2	69	Total 69	O 69	0	0
6	3	49	Total 49	O 49	0	0
6	4	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 qua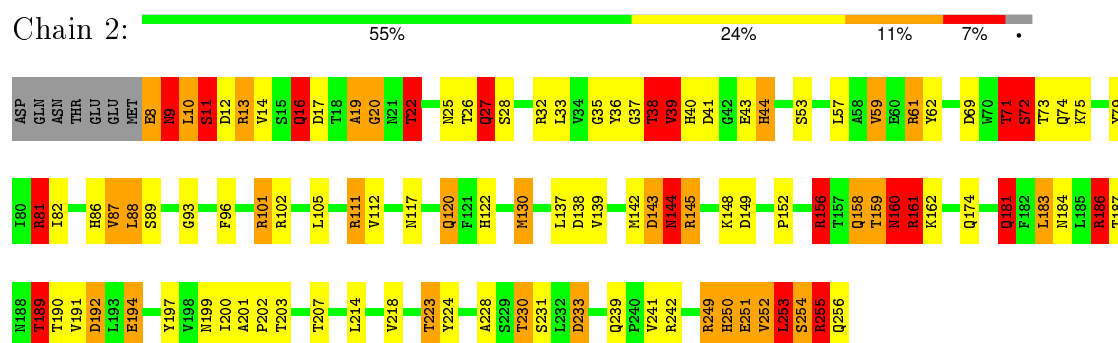lity criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MENGO VIRUS COAT PROTEIN (SUBUNIT VP1)
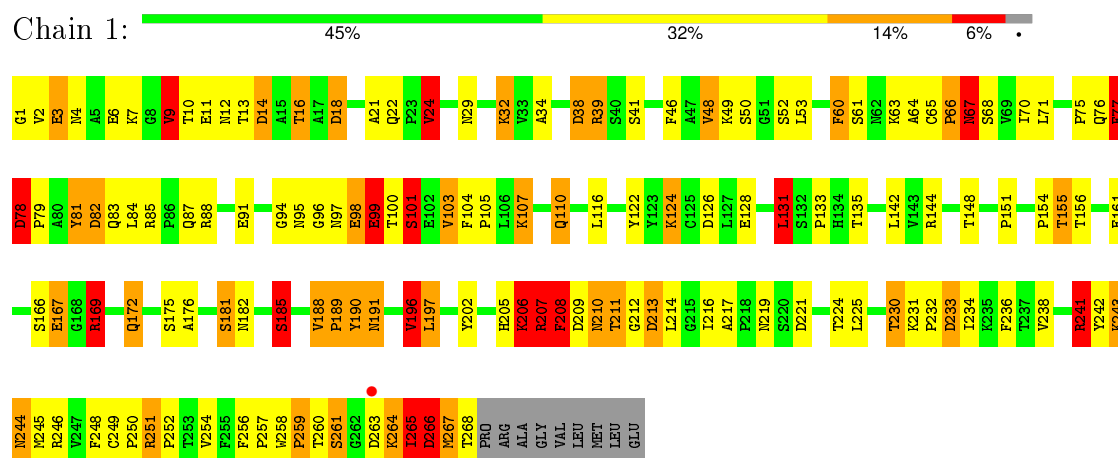
• Molecule 2: MENGO VIRUS COAT PROTEIN (SUBUNIT VP2)

• Molecule 3: MENGO VIRUS COAT PROTEIN (SUBUNIT VP3)

D176 Q177 A178 N179 I180 T181 N182 V183 D184 G185 W186 V187 T188 Q191 Y197 P198 C201 P202 T203 K206 I207 L208 V211 K215 D216 F217 S218 L219 K220 M221 P222 I223 S224 Q231
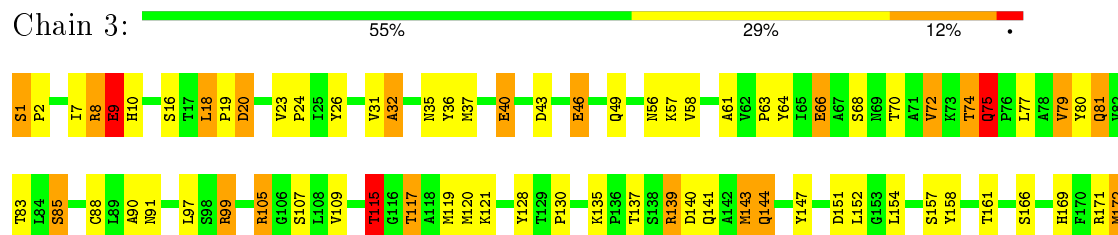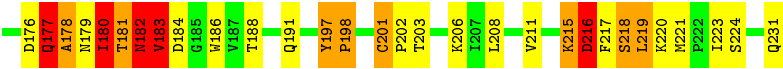
• Molecule 4: MENGO VIRUS COAT PROTEIN (SUBUNIT VP4)

Chain 4:

%

27% 30% 17% 9% 17%

GLY ASN SER THR SER SER ASP LYS ASN ASN SER SER S13 E14 E17 I20 I21 N22 Y25 S26 N27 Q28 Y29 Q30 N31 S32 I33 D34 L35 S36 A37 N38 A39 D43 P44 P45 K46 T47 Q50 N53 L54 L55 S56 V59 N60 A61 F62 S63 N64 M65 L66 P67 L68

L69 A70
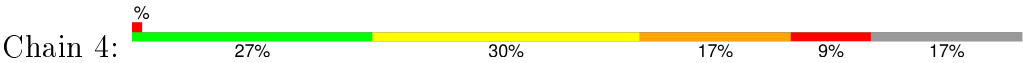
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	441.42Å 427.31Å 421.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 49.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 41.3 (49.94-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.61Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.221 , (Not available) 0.200 , 0.107	Depositor DCC
R_{free} test set	873 reflections (0.10%)	DCC
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 174.2	EDS
Estimated twinning fraction	0.055 for k,h,-l 0.050 for -l,-k,-h 0.049 for -h,l,k 0.049 for l,h,k 0.049 for k,l,h	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.40, < L^2 > = 0.22$	Xtriage
Outliers	1 of 991793 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.09	EDS
Total number of atoms	6507	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	1	1.14	2/2159 (0.1%)	2.35	115/2952 (3.9%)
2	2	1.13	6/2028 (0.3%)	2.60	122/2776 (4.4%)
3	3	1.07	3/1829 (0.2%)	2.13	73/2512 (2.9%)
4	4	1.34	1/441 (0.2%)	2.99	52/600 (8.7%)
All	All	1.14	12/6457 (0.2%)	2.42	362/8840 (4.1%)

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
2	2	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	20	GLY	N-CA	8.56	1.58	1.46
2	2	11	SER	CB-OG	7.89	1.52	1.42
2	2	254	SER	CB-OG	6.83	1.51	1.42
1	1	211	THR	CB-OG1	6.46	1.56	1.43
2	2	43	GLU	CD-OE2	6.13	1.32	1.25
3	3	68	SER	CB-OG	5.99	1.50	1.42
2	2	255	ARG	CZ-NH2	5.64	1.40	1.33
4	4	70	ALA	C-O	5.57	1.33	1.23
3	3	40	GLU	CD-OE2	5.53	1.31	1.25
3	3	58	VAL	C-N	5.18	1.44	1.34
1	1	6	GLU	CD-OE1	-5.06	1.20	1.25
2	2	145	ARG	CZ-NH2	5.00	1.39	1.33

All (362) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	102	ARG	NE-CZ-NH2	-21.77	109.42	120.30
2	2	61	ARG	NE-CZ-NH1	20.67	130.63	120.30
1	1	267	MET	C-N-CA	20.41	172.73	121.70
3	3	216	ASP	CB-CG-OD2	-19.35	100.88	118.30
2	2	161	ARG	CD-NE-CZ	18.62	149.67	123.60
1	1	233	ASP	CB-CG-OD2	-18.42	101.72	118.30
2	2	32	ARG	NE-CZ-NH2	18.30	129.45	120.30
2	2	10	LEU	C-N-CA	18.28	167.41	121.70
2	2	145	ARG	NE-CZ-NH1	18.12	129.36	120.30
2	2	255	ARG	NE-CZ-NH1	17.92	129.26	120.30
2	2	145	ARG	CD-NE-CZ	16.76	147.06	123.60
2	2	186	ARG	NE-CZ-NH1	16.25	128.42	120.30
1	1	207	ARG	NE-CZ-NH1	15.88	128.24	120.30
2	2	186	ARG	CD-NE-CZ	15.63	145.49	123.60
2	2	102	ARG	NE-CZ-NH1	15.57	128.08	120.30
2	2	255	ARG	NE-CZ-NH2	-15.47	112.57	120.30
2	2	101	ARG	NE-CZ-NH2	14.98	127.79	120.30
1	1	241	ARG	NE-CZ-NH1	14.90	127.75	120.30
2	2	223	THR	CA-CB-CG2	14.83	133.16	112.40
1	1	3	GLU	OE1-CD-OE2	13.90	139.98	123.30
3	3	151	ASP	CB-CG-OD1	13.81	130.73	118.30
2	2	254	SER	N-CA-CB	13.52	130.78	110.50
2	2	32	ARG	NE-CZ-NH1	-13.00	113.80	120.30
3	3	180	ILE	C-N-CA	12.88	153.89	121.70
4	4	34	ASP	CB-CG-OD1	12.61	129.65	118.30
2	2	161	ARG	NE-CZ-NH1	12.61	126.60	120.30
2	2	249	ARG	NE-CZ-NH1	-12.50	114.05	120.30
4	4	14	GLU	N-CA-CB	12.40	132.93	110.60
1	1	38	ASP	CB-CG-OD1	12.19	129.27	118.30
1	1	263	ASP	CB-CG-OD2	12.12	129.21	118.30
2	2	242	ARG	NE-CZ-NH1	11.99	126.30	120.30
2	2	255	ARG	N-CA-CB	11.81	131.86	110.60
4	4	64	ASN	CA-CB-CG	11.66	139.06	113.40
2	2	253	LEU	O-C-N	11.61	141.28	122.70
3	3	99	ARG	CA-CB-CG	11.52	138.74	113.40
1	1	124	LYS	CA-CB-CG	11.35	138.36	113.40
4	4	65	MET	C-N-CA	11.17	149.64	121.70
1	1	266	ASP	CA-CB-CG	10.95	137.49	113.40
2	2	32	ARG	CD-NE-CZ	-10.75	108.56	123.60
2	2	61	ARG	NE-CZ-NH2	-10.62	114.99	120.30
3	3	216	ASP	CB-CG-OD1	10.61	127.85	118.30
2	2	13	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	1	207	ARG	CD-NE-CZ	10.56	138.39	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	183	VAL	CA-CB-CG2	10.51	126.66	110.90
1	1	266	ASP	CB-CG-OD2	10.41	127.67	118.30
1	1	266	ASP	C-N-CA	10.34	147.55	121.70
1	1	66	PRO	C-N-CA	10.22	147.24	121.70
4	4	29	TYR	CB-CG-CD2	10.16	127.09	121.00
1	1	78	ASP	N-CA-CB	10.11	128.79	110.60
2	2	254	SER	CA-C-N	-10.07	95.03	117.20
4	4	63	SER	CA-CB-OG	10.03	138.27	111.20
3	3	171	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	2	255	ARG	CD-NE-CZ	9.83	137.36	123.60
2	2	36	TYR	CB-CG-CD1	-9.81	115.11	121.00
1	1	11	GLU	CA-CB-CG	9.63	134.59	113.40
4	4	65	MET	CA-C-N	-9.49	96.31	117.20
2	2	255	ARG	C-N-CA	9.45	145.32	121.70
3	3	58	VAL	CB-CA-C	9.43	129.32	111.40
2	2	181	GLN	CB-CA-C	9.43	129.26	110.40
1	1	24	VAL	N-CA-CB	-9.38	90.88	111.50
3	3	46	GLU	OE1-CD-OE2	-9.37	112.06	123.30
2	2	223	THR	CA-CB-OG1	-9.35	89.37	109.00
2	2	254	SER	CA-C-O	9.30	139.63	120.10
2	2	111	ARG	CD-NE-CZ	-9.28	110.61	123.60
2	2	130	MET	CA-CB-CG	-9.23	97.62	113.30
4	4	60	ASN	C-N-CA	9.20	144.71	121.70
2	2	17	ASP	CB-CG-OD1	9.15	126.54	118.30
1	1	233	ASP	CB-CG-OD1	9.11	126.50	118.30
4	4	65	MET	CA-C-O	9.08	139.17	120.10
1	1	221	ASP	CB-CG-OD1	9.03	126.43	118.30
3	3	183	VAL	CB-CA-C	9.01	128.51	111.40
3	3	178	ALA	N-CA-CB	8.98	122.67	110.10
1	1	267	MET	CA-C-O	8.95	138.89	120.10
1	1	267	MET	O-C-N	-8.93	108.42	122.70
2	2	19	ALA	CA-C-N	8.89	133.99	116.20
2	2	81	ARG	CD-NE-CZ	-8.87	111.18	123.60
2	2	255	ARG	N-CA-C	-8.83	87.16	111.00
3	3	140	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	1	88	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	1	87	GLN	CA-CB-CG	-8.70	94.26	113.40
3	3	158	TYR	CB-CG-CD1	8.70	126.22	121.00
1	1	18	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	1	221	ASP	CB-CG-OD2	-8.62	110.54	118.30
2	2	71	THR	CA-CB-OG1	-8.59	90.95	109.00
2	2	144	ASN	N-CA-CB	-8.59	95.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	255	ARG	CA-C-N	-8.58	98.33	117.20
2	2	186	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	2	20	GLY	N-CA-C	-8.43	92.03	113.10
1	1	81	TYR	O-C-N	8.31	136.00	122.70
3	3	151	ASP	CB-CG-OD2	-8.26	110.87	118.30
2	2	130	MET	CG-SD-CE	-8.10	87.24	100.20
2	2	120	GLN	CG-CD-OE1	-8.08	105.44	121.60
3	3	80	TYR	CB-CG-CD1	8.04	125.83	121.00
1	1	263	ASP	CA-CB-CG	7.99	130.97	113.40
3	3	74	THR	CA-CB-OG1	-7.97	92.25	109.00
1	1	211	THR	N-CA-CB	7.96	125.43	110.30
1	1	190	TYR	CB-CA-C	7.95	126.31	110.40
3	3	105	ARG	NE-CZ-NH1	7.92	124.26	120.30
4	4	27	ASN	CB-CA-C	-7.92	94.57	110.40
1	1	211	THR	CA-C-N	-7.85	100.49	116.20
2	2	249	ARG	CD-NE-CZ	-7.81	112.66	123.60
2	2	36	TYR	CB-CG-CD2	7.81	125.69	121.00
2	2	20	GLY	O-C-N	7.79	135.17	122.70
4	4	25	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	1	98	GLU	OE1-CD-OE2	7.74	132.59	123.30
4	4	14	GLU	CA-C-N	-7.73	100.73	116.20
3	3	66	GLU	CG-CD-OE2	-7.63	103.04	118.30
2	2	249	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	2	139	VAL	N-CA-CB	-7.62	94.73	111.50
1	1	144	ARG	NE-CZ-NH1	7.61	124.10	120.30
2	2	149	ASP	CB-CG-OD2	-7.58	111.48	118.30
2	2	230	THR	CA-CB-OG1	-7.53	93.18	109.00
2	2	81	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	1	67	ASN	CA-CB-CG	-7.50	96.91	113.40
4	4	70	ALA	CA-C-O	7.48	135.81	120.10
4	4	27	ASN	CA-CB-CG	-7.48	96.94	113.40
1	1	155	THR	CA-CB-OG1	-7.46	93.33	109.00
4	4	32	SER	CB-CA-C	7.46	124.27	110.10
4	4	54	LEU	N-CA-CB	-7.46	95.48	110.40
3	3	105	ARG	NE-CZ-NH2	7.43	124.02	120.30
4	4	14	GLU	O-C-N	7.42	135.81	123.20
1	1	185	SER	N-CA-CB	-7.41	99.38	110.50
2	2	10	LEU	CA-CB-CG	-7.40	98.28	115.30
4	4	21	ILE	CA-C-N	-7.40	100.93	117.20
2	2	19	ALA	C-N-CA	-7.38	106.81	122.30
1	1	32	LYS	N-CA-CB	7.36	123.86	110.60
2	2	101	ARG	NE-CZ-NH1	-7.36	116.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	10	LEU	O-C-N	-7.35	110.94	122.70
4	4	29	TYR	CB-CG-CD1	-7.31	116.62	121.00
2	2	181	GLN	CA-CB-CG	7.30	129.47	113.40
3	3	46	GLU	CG-CD-OE1	7.28	132.85	118.30
1	1	206	LYS	O-C-N	-7.27	111.07	122.70
1	1	190	TYR	N-CA-C	-7.24	91.45	111.00
2	2	22	THR	N-CA-CB	-7.24	96.55	110.30
2	2	255	ARG	CA-C-O	7.23	135.28	120.10
3	3	182	ASN	CB-CG-ND2	7.20	133.97	116.70
1	1	169	ARG	CB-CG-CD	7.18	130.27	111.60
2	2	16	GLN	CA-CB-CG	7.14	129.10	113.40
3	3	216	ASP	CA-CB-CG	-7.12	97.75	113.40
2	2	156	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	1	188	VAL	N-CA-CB	-7.09	95.89	111.50
3	3	218	SER	N-CA-CB	-7.08	99.88	110.50
2	2	43	GLU	CA-CB-CG	7.06	128.93	113.40
3	3	105	ARG	NH1-CZ-NH2	-7.03	111.67	119.40
1	1	13	THR	N-CA-CB	-7.03	96.95	110.30
2	2	189	THR	CA-CB-CG2	7.00	122.19	112.40
2	2	22	THR	CA-CB-OG1	-6.99	94.33	109.00
3	3	172	MET	N-CA-CB	-6.98	98.04	110.60
1	1	250	PRO	O-C-N	6.91	133.76	122.70
2	2	53	SER	N-CA-C	-6.89	92.40	111.00
2	2	144	ASN	OD1-CG-ND2	6.87	137.70	121.90
2	2	8	GLU	O-C-N	-6.85	111.73	122.70
1	1	167	GLU	CG-CD-OE2	6.82	131.94	118.30
1	1	213	ASP	O-C-N	6.81	133.60	122.70
1	1	266	ASP	CA-C-O	6.80	134.37	120.10
1	1	213	ASP	CB-CA-C	6.79	123.97	110.40
2	2	53	SER	N-CA-CB	6.77	120.66	110.50
1	1	210	ASN	N-CA-CB	6.77	122.78	110.60
3	3	183	VAL	N-CA-C	-6.72	92.85	111.00
4	4	63	SER	N-CA-CB	6.72	120.58	110.50
2	2	19	ALA	N-CA-CB	6.68	119.45	110.10
1	1	3	GLU	CG-CD-OE1	-6.67	104.97	118.30
4	4	67	PRO	C-N-CA	6.67	138.37	121.70
2	2	38	THR	CB-CA-C	-6.65	93.64	111.60
3	3	177	GLN	O-C-N	-6.64	112.08	122.70
2	2	111	ARG	CB-CG-CD	-6.62	94.38	111.60
4	4	70	ALA	N-CA-CB	-6.61	100.85	110.10
2	2	102	ARG	CD-NE-CZ	-6.60	114.36	123.60
2	2	12	ASP	CB-CG-OD1	-6.59	112.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	151	PRO	O-C-N	6.58	133.23	122.70
4	4	64	ASN	CA-C-O	6.58	133.92	120.10
1	1	196	VAL	CB-CA-C	6.58	123.90	111.40
2	2	192	ASP	CB-CG-OD2	-6.57	112.39	118.30
3	3	177	GLN	CB-CA-C	6.57	123.53	110.40
3	3	177	GLN	CB-CG-CD	6.54	128.62	111.60
1	1	207	ARG	NH1-CZ-NH2	-6.52	112.23	119.40
4	4	63	SER	C-N-CA	6.49	137.92	121.70
4	4	21	ILE	CA-C-O	6.45	133.65	120.10
3	3	139	ARG	CD-NE-CZ	-6.45	114.57	123.60
3	3	182	ASN	O-C-N	6.40	132.94	122.70
2	2	72	SER	N-CA-CB	-6.40	100.90	110.50
4	4	59	VAL	CA-C-O	6.40	133.54	120.10
3	3	182	ASN	CA-C-N	-6.39	103.14	117.20
2	2	81	ARG	CG-CD-NE	6.39	125.21	111.80
1	1	266	ASP	CB-CG-OD1	-6.37	112.57	118.30
4	4	50	GLN	CA-CB-CG	-6.34	99.46	113.40
1	1	52	SER	N-CA-CB	-6.33	101.00	110.50
4	4	27	ASN	N-CA-C	6.32	128.07	111.00
3	3	8	ARG	CD-NE-CZ	-6.32	114.75	123.60
3	3	99	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	3	184	ASP	O-C-N	6.30	133.92	123.20
3	3	58	VAL	N-CA-CB	-6.29	97.66	111.50
1	1	78	ASP	O-C-N	6.28	133.04	121.10
3	3	216	ASP	N-CA-CB	-6.28	99.29	110.60
1	1	196	VAL	N-CA-CB	-6.27	97.71	111.50
3	3	220	LYS	CA-CB-CG	6.25	127.15	113.40
4	4	68	LEU	N-CA-CB	-6.24	97.92	110.40
3	3	74	THR	N-CA-CB	-6.24	98.45	110.30
2	2	130	MET	CB-CA-C	6.23	122.86	110.40
3	3	32	ALA	N-CA-CB	6.22	118.80	110.10
2	2	138	ASP	CB-CG-OD1	-6.20	112.72	118.30
4	4	64	ASN	CB-CA-C	6.20	122.80	110.40
2	2	144	ASN	CA-CB-CG	-6.16	99.86	113.40
1	1	189	PRO	CA-C-N	6.14	130.70	117.20
2	2	197	TYR	CB-CG-CD1	6.13	124.68	121.00
3	3	201	CYS	N-CA-CB	-6.13	99.57	110.60
1	1	207	ARG	CG-CD-NE	6.12	124.66	111.80
3	3	180	ILE	O-C-N	-6.12	112.91	122.70
4	4	43	ASP	CB-CG-OD1	-6.12	112.79	118.30
3	3	197	TYR	CB-CG-CD2	-6.12	117.33	121.00
2	2	251	GLU	O-C-N	6.11	132.48	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	149	ASP	CB-CG-OD1	6.11	123.80	118.30
1	1	246	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	2	145	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	1	181	SER	O-C-N	6.08	132.42	122.70
3	3	26	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	1	41	SER	N-CA-CB	6.07	119.61	110.50
1	1	241	ARG	NH1-CZ-NH2	-6.06	112.74	119.40
4	4	36	SER	CB-CA-C	6.05	121.59	110.10
1	1	10	THR	CA-CB-CG2	6.03	120.84	112.40
1	1	188	VAL	CB-CA-C	6.01	122.83	111.40
2	2	59	VAL	N-CA-CB	-6.01	98.27	111.50
3	3	75	GLN	N-CA-CB	-6.01	99.79	110.60
3	3	180	ILE	CA-CB-CG2	6.00	122.91	110.90
1	1	81	TYR	CA-CB-CG	-5.99	102.03	113.40
3	3	166	SER	N-CA-CB	-5.97	101.55	110.50
2	2	20	GLY	CA-C-N	-5.96	104.09	117.20
3	3	80	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	1	39	ARG	CD-NE-CZ	-5.95	115.27	123.60
2	2	138	ASP	CA-C-N	-5.94	104.12	117.20
1	1	126	ASP	CB-CG-OD1	-5.93	112.96	118.30
2	2	233	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	1	246	ARG	CG-CD-NE	5.92	124.23	111.80
4	4	43	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	1	169	ARG	CD-NE-CZ	-5.91	115.33	123.60
3	3	183	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	1	251	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	1	82	ASP	O-C-N	5.89	132.13	122.70
1	1	267	MET	CA-CB-CG	5.89	123.31	113.30
2	2	69	ASP	CB-CG-OD1	-5.88	113.01	118.30
2	2	230	THR	N-CA-CB	-5.88	99.14	110.30
1	1	99	GLU	C-N-CA	5.87	136.38	121.70
1	1	219	ASN	O-C-N	5.87	132.09	122.70
1	1	81	TYR	CB-CG-CD2	-5.86	117.48	121.00
3	3	26	TYR	CB-CG-CD2	5.85	124.51	121.00
1	1	211	THR	CA-C-O	5.84	132.36	120.10
4	4	37	ALA	O-C-N	5.84	132.04	122.70
1	1	213	ASP	CA-CB-CG	-5.83	100.56	113.40
3	3	177	GLN	C-N-CA	5.83	136.28	121.70
1	1	208	PHE	N-CA-CB	5.81	121.06	110.60
1	1	14	ASP	CB-CG-OD2	-5.81	113.07	118.30
3	3	20	ASP	CB-CG-OD2	-5.81	113.08	118.30
2	2	139	VAL	CB-CA-C	5.80	122.42	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	143	ASP	CA-C-O	5.80	132.28	120.10
4	4	39	ALA	N-CA-CB	-5.79	101.99	110.10
2	2	138	ASP	N-CA-CB	-5.77	100.22	110.60
3	3	75	GLN	CB-CA-C	-5.77	98.87	110.40
2	2	253	LEU	CA-C-N	-5.77	104.51	117.20
2	2	9	ASN	CA-CB-CG	5.76	126.07	113.40
4	4	43	ASP	OD1-CG-OD2	5.75	134.23	123.30
2	2	138	ASP	CA-C-O	5.75	132.17	120.10
2	2	72	SER	CA-CB-OG	-5.75	95.69	111.20
3	3	7	ILE	CA-CB-CG1	-5.72	100.12	111.00
1	1	9	VAL	CB-CA-C	5.72	122.27	111.40
1	1	29	ASN	CB-CA-C	-5.71	98.97	110.40
3	3	181	THR	CA-C-O	5.70	132.07	120.10
4	4	62	PHE	C-N-CA	5.70	135.95	121.70
1	1	230	THR	CA-C-O	-5.69	108.14	120.10
3	3	9	GLU	CA-CB-CG	5.68	125.91	113.40
1	1	260	THR	N-CA-CB	5.68	121.09	110.30
2	2	242	ARG	CA-CB-CG	-5.67	100.92	113.40
4	4	14	GLU	N-CA-C	-5.67	95.69	111.00
1	1	32	LYS	CB-CA-C	-5.67	99.07	110.40
1	1	29	ASN	O-C-N	5.66	131.76	122.70
3	3	176	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	1	101	SER	CB-CA-C	5.63	120.80	110.10
3	3	184	ASP	CB-CG-OD2	-5.62	113.24	118.30
3	3	144	GLN	OE1-CD-NE2	5.62	134.83	121.90
1	1	211	THR	C-N-CA	5.60	134.06	122.30
2	2	250	HIS	O-C-N	5.59	131.64	122.70
2	2	224	TYR	CA-CB-CG	-5.57	102.83	113.40
1	1	167	GLU	CG-CD-OE1	-5.56	107.17	118.30
4	4	69	LEU	CA-C-N	-5.55	105.00	117.20
4	4	27	ASN	O-C-N	5.50	131.50	122.70
1	1	68	SER	N-CA-CB	5.49	118.73	110.50
4	4	68	LEU	CA-CB-CG	5.48	127.90	115.30
3	3	88	CYS	CA-CB-SG	5.48	123.86	114.00
3	3	49	GLN	CG-CD-OE1	-5.46	110.67	121.60
3	3	147	TYR	CB-CG-CD1	5.46	124.28	121.00
1	1	182	ASN	CB-CG-OD1	-5.46	110.69	121.60
1	1	208	PHE	CB-CG-CD1	-5.43	117.00	120.80
2	2	138	ASP	CB-CA-C	-5.43	99.54	110.40
1	1	254	VAL	CA-C-N	-5.42	105.27	117.20
2	2	189	THR	CA-CB-OG1	-5.42	97.61	109.00
4	4	54	LEU	CB-CG-CD1	-5.42	101.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	68	LEU	C-N-CA	5.41	135.23	121.70
1	1	21	ALA	N-CA-CB	-5.41	102.53	110.10
2	2	112	VAL	N-CA-CB	-5.39	99.64	111.50
4	4	64	ASN	CA-C-N	-5.38	105.35	117.20
3	3	40	GLU	CA-CB-CG	5.38	125.23	113.40
4	4	21	ILE	CA-CB-CG2	5.38	121.66	110.90
1	1	259	PRO	N-CA-CB	5.37	109.75	103.30
2	2	183	LEU	CB-CA-C	5.36	120.38	110.20
4	4	17	GLU	CG-CD-OE1	5.35	129.01	118.30
1	1	246	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	2	36	TYR	CG-CD1-CE1	-5.35	117.02	121.30
1	1	208	PHE	O-C-N	5.34	131.24	122.70
1	1	14	ASP	CB-CA-C	5.34	121.07	110.40
2	2	252	VAL	CA-C-N	-5.34	105.46	117.20
1	1	213	ASP	N-CA-C	-5.33	96.59	111.00
2	2	27	GLN	CA-CB-CG	-5.33	101.67	113.40
2	2	19	ALA	CA-C-O	-5.31	108.94	120.10
3	3	70	THR	O-C-N	5.31	131.20	122.70
3	3	128	TYR	CB-CG-CD1	5.31	124.19	121.00
1	1	103	VAL	CB-CA-C	5.30	121.47	111.40
1	1	11	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	1	197	LEU	N-CA-CB	-5.28	99.83	110.40
1	1	67	ASN	N-CA-CB	-5.27	101.11	110.60
3	3	8	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	1	38	ASP	CB-CG-OD2	-5.27	113.56	118.30
4	4	45	PRO	C-N-CA	5.27	134.87	121.70
3	3	180	ILE	CA-C-O	5.26	131.16	120.10
2	2	41	ASP	CA-C-N	5.26	126.72	116.20
1	1	11	GLU	CG-CD-OE1	5.25	128.80	118.30
2	2	230	THR	N-CA-C	5.25	125.17	111.00
1	1	259	PRO	O-C-N	5.23	131.06	122.70
3	3	154	LEU	N-CA-CB	-5.23	99.94	110.40
1	1	167	GLU	CA-CB-CG	5.22	124.89	113.40
2	2	160	ASN	CA-CB-CG	-5.21	101.93	113.40
2	2	13	ARG	CA-CB-CG	-5.20	101.95	113.40
1	1	107	LYS	O-C-N	5.19	131.01	122.70
1	1	88	ARG	N-CA-CB	5.18	119.93	110.60
2	2	11	SER	N-CA-CB	5.18	118.27	110.50
2	2	69	ASP	O-C-N	5.17	130.98	122.70
2	2	44	HIS	CB-CA-C	-5.16	100.07	110.40
4	4	69	LEU	C-N-CA	5.16	134.61	121.70
2	2	9	ASN	OD1-CG-ND2	-5.16	110.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	156	THR	O-C-N	5.15	130.94	122.70
1	1	264	LYS	O-C-N	5.15	130.94	122.70
1	1	211	THR	N-CA-C	-5.14	97.12	111.00
1	1	131	LEU	N-CA-CB	-5.14	100.12	110.40
4	4	38	ASN	CB-CA-C	5.13	120.66	110.40
2	2	72	SER	CB-CA-C	-5.13	100.36	110.10
2	2	156	ARG	NE-CZ-NH2	-5.13	117.74	120.30
4	4	45	PRO	N-CA-C	-5.12	98.80	112.10
1	1	261	SER	N-CA-CB	-5.11	102.84	110.50
1	1	242	TYR	CB-CG-CD1	-5.10	117.94	121.00
2	2	38	THR	O-C-N	5.09	130.85	122.70
3	3	115	THR	CA-CB-OG1	-5.09	98.32	109.00
1	1	154	PRO	CA-C-O	5.07	132.36	120.20
3	3	91	ASN	CB-CG-OD1	-5.07	111.46	121.60
1	1	104	PHE	CB-CG-CD1	-5.07	117.25	120.80
3	3	66	GLU	CG-CD-OE1	5.06	128.41	118.30
1	1	244	ASN	N-CA-CB	5.05	119.68	110.60
3	3	144	GLN	CB-CA-C	-5.04	100.32	110.40
2	2	194	GLU	OE1-CD-OE2	5.03	129.34	123.30
2	2	152	PRO	N-CA-CB	-5.02	97.08	102.60
2	2	39	VAL	N-CA-CB	-5.02	100.45	111.50
2	2	143	ASP	C-N-CA	5.01	134.24	121.70
4	4	27	ASN	CB-CG-OD1	-5.01	111.58	121.60
4	4	64	ASN	N-CA-C	-5.01	97.48	111.00
3	3	85	SER	CB-CA-C	-5.00	100.59	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	255	ARG	Sidechain
2	2	81	ARG	Sidechain

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	1	2091	0	2008	104	0
2	2	1973	0	1899	98	0
3	3	1772	0	1760	88	0
4	4	433	0	404	28	0
5	2	5	0	0	0	0
6	1	106	0	0	0	0
6	2	69	0	0	3	0
6	3	49	0	0	0	0
6	4	9	0	0	0	0
All	All	6507	0	6071	289	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 23.

All (289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:10:LEU:O	2:2:13:ARG:HB2	1.38	1.22
3:3:179:ASN:HB3	3:3:183:VAL:HG13	1.39	1.04
2:2:101:ARG:HD3	2:2:255:ARG:HB2	1.36	1.04
1:1:14:ASP:OD2	1:1:16:THR:HB	1.58	1.03
1:1:32:LYS:HE2	4:4:13:SER:HB2	1.41	1.02
4:4:46:LYS:HD2	4:4:46:LYS:H	1.26	0.99
2:2:22:THR:HG21	2:2:62:TYR:H	1.23	0.98
1:1:70:ILE:H	1:1:76:GLN:HE22	1.03	0.97
2:2:10:LEU:O	2:2:13:ARG:CB	2.19	0.91
4:4:21:ILE:HG23	4:4:22:ASN:O	1.72	0.89
2:2:19:ALA:HB1	2:2:61:ARG:HA	1.53	0.88
2:2:252:VAL:O	2:2:253:LEU:HB2	1.70	0.88
2:2:14:VAL:HG22	2:2:27:GLN:HG2	1.53	0.88
1:1:49:LYS:HG2	1:1:50:SER:N	1.89	0.87
2:2:19:ALA:HB3	2:2:22:THR:CG2	2.05	0.86
3:3:179:ASN:CB	3:3:183:VAL:HG13	2.06	0.86
2:2:19:ALA:HB3	2:2:22:THR:HG22	1.58	0.86
4:4:61:ALA:O	4:4:62:PHE:HB3	1.77	0.84
1:1:265:ILE:HG23	1:1:266:ASP:H	1.44	0.83
2:2:255:ARG:C	2:2:255:ARG:HD2	2.00	0.82
1:1:206:LYS:N	1:1:206:LYS:HD2	1.93	0.82
3:3:197:TYR:CZ	3:3:203:THR:HG22	2.13	0.82
2:2:10:LEU:HG	2:2:11:SER:N	1.96	0.81
2:2:181:GLN:HG2	2:2:191:VAL:HG22	1.60	0.80
1:1:207:ARG:CD	3:3:180:ILE:HD13	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:249:ARG:HH11	2:2:249:ARG:HG3	1.48	0.79
3:3:177:GLN:HG2	3:3:178:ALA:H	1.47	0.79
1:1:95:ASN:HB2	1:1:105:PRO:O	1.83	0.79
3:3:75:GLN:HE21	3:3:75:GLN:CA	1.98	0.77
3:3:143:MET:HG2	3:3:143:MET:O	1.83	0.77
2:2:72:SER:HB2	6:2:321:HOH:O	1.83	0.77
3:3:79:VAL:HB	3:3:188:THR:HG22	1.65	0.77
2:2:101:ARG:HD3	2:2:255:ARG:CB	2.11	0.77
4:4:65:MET:HA	4:4:67:PRO:CD	2.15	0.77
1:1:207:ARG:NE	3:3:180:ILE:HD13	2.00	0.76
2:2:181:GLN:CG	2:2:191:VAL:HG22	2.16	0.75
4:4:46:LYS:HD2	4:4:46:LYS:N	2.02	0.75
2:2:252:VAL:O	2:2:253:LEU:CB	2.35	0.75
3:3:117:THR:HG22	3:3:120:MET:H	1.50	0.74
1:1:79:PRO:HG3	1:1:107:LYS:HB3	1.69	0.74
2:2:186:ARG:NH1	2:2:187:THR:OG1	2.20	0.74
2:2:10:LEU:HG	2:2:11:SER:HB2	1.69	0.72
3:3:31:VAL:HG13	3:3:32:ALA:N	2.04	0.71
2:2:101:ARG:O	2:2:252:VAL:HG23	1.92	0.70
1:1:63:LYS:H	1:1:65:CYS:HB2	1.56	0.70
2:2:10:LEU:CG	2:2:11:SER:N	2.55	0.70
2:2:19:ALA:CB	2:2:61:ARG:HA	2.22	0.69
3:3:117:THR:HG23	3:3:119:MET:H	1.57	0.69
3:3:18:LEU:HD22	3:3:19:PRO:HD2	1.74	0.69
4:4:60:ASN:HD21	4:4:65:MET:CE	2.03	0.69
2:2:158:GLN:NE2	2:2:158:GLN:HA	2.07	0.69
2:2:59:VAL:HG22	2:2:96:PHE:HA	1.75	0.69
1:1:3:GLU:HG3	1:1:4:ASN:N	2.06	0.68
4:4:59:VAL:HG22	4:4:60:ASN:H	1.57	0.68
3:3:75:GLN:NE2	3:3:75:GLN:CA	2.56	0.68
2:2:22:THR:HG21	2:2:62:TYR:N	2.02	0.68
1:1:209:ASP:CG	1:1:211:THR:HG23	2.14	0.68
4:4:65:MET:HA	4:4:67:PRO:HD2	1.76	0.68
4:4:65:MET:HA	4:4:67:PRO:HD3	1.76	0.68
2:2:71:THR:CG2	2:2:73:THR:HB	2.24	0.67
1:1:205:HIS:CE1	1:1:210:ASN:HB3	2.29	0.67
1:1:208:PHE:HE1	3:3:182:ASN:CB	2.08	0.67
2:2:10:LEU:HG	2:2:11:SER:CB	2.25	0.67
3:3:117:THR:HG22	3:3:120:MET:N	2.09	0.66
3:3:75:GLN:NE2	3:3:75:GLN:HA	2.10	0.66
2:2:71:THR:HG23	2:2:73:THR:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:205:HIS:NE2	1:1:212:GLY:HA2	2.12	0.64
3:3:137:THR:H	3:3:141:GLN:NE2	1.96	0.64
4:4:66:LEU:N	4:4:67:PRO:CD	2.61	0.64
2:2:249:ARG:NH1	2:2:249:ARG:HG3	2.12	0.64
2:2:87:VAL:HG12	2:2:88:LEU:HD13	1.78	0.64
2:2:249:ARG:NH1	2:2:249:ARG:CG	2.59	0.63
2:2:81:ARG:HD3	2:2:143:ASP:OD1	1.99	0.63
3:3:179:ASN:O	3:3:182:ASN:HB2	1.99	0.62
1:1:208:PHE:CE1	3:3:182:ASN:HA	2.34	0.62
2:2:255:ARG:O	2:2:255:ARG:HD2	1.99	0.62
1:1:205:HIS:ND1	1:1:210:ASN:HA	2.14	0.62
3:3:105:ARG:HH12	3:3:169:HIS:CD2	2.18	0.62
2:2:39:VAL:HG22	2:2:194:GLU:OE2	2.00	0.61
1:1:96:GLY:HA3	1:1:101:SER:HB3	1.83	0.61
1:1:96:GLY:O	2:2:162:LYS:HG2	2.01	0.61
2:2:255:ARG:HH11	2:2:255:ARG:HB3	1.66	0.61
1:1:205:HIS:CD2	1:1:212:GLY:HA2	2.35	0.61
1:1:91:GLU:OE1	2:2:156:ARG:HB2	2.01	0.61
2:2:9:ASN:HB3	2:2:27:GLN:O	2.01	0.60
1:1:135:THR:HB	1:1:234:ILE:HG12	1.83	0.60
1:1:181:SER:HB2	3:3:9:GLU:O	2.02	0.60
3:3:180:ILE:CG2	3:3:181:THR:HG23	2.32	0.60
2:2:249:ARG:HH11	2:2:249:ARG:CG	2.04	0.60
1:1:265:ILE:O	1:1:266:ASP:HB2	2.02	0.60
2:2:158:GLN:HE21	2:2:158:GLN:HA	1.67	0.60
2:2:44:HIS:HB3	6:2:270:HOH:O	2.01	0.60
3:3:43:ASP:O	3:3:46:GLU:HB2	2.01	0.60
2:2:255:ARG:HB3	2:2:255:ARG:NH1	2.17	0.59
2:2:253:LEU:O	2:2:255:ARG:N	2.35	0.59
2:2:82:ILE:HG12	2:2:142:MET:HG3	1.85	0.59
3:3:105:ARG:HH12	3:3:169:HIS:HD2	1.51	0.59
3:3:56:ASN:O	3:3:61:ALA:HA	2.02	0.59
3:3:75:GLN:HE21	3:3:75:GLN:HA	1.66	0.58
1:1:63:LYS:O	1:1:64:ALA:HB3	2.03	0.58
1:1:207:ARG:NH1	3:3:182:ASN:OD1	2.36	0.58
1:1:81:TYR:HB3	1:1:84:LEU:HB2	1.84	0.58
1:1:71:LEU:HD21	1:1:225:LEU:HD22	1.85	0.58
3:3:177:GLN:HG2	3:3:178:ALA:N	2.19	0.58
3:3:179:ASN:CB	3:3:183:VAL:CG1	2.81	0.58
2:2:19:ALA:HB3	2:2:22:THR:HG21	1.84	0.57
1:1:265:ILE:CG2	1:1:266:ASP:H	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:202:PRO:HG3	3:3:169:HIS:CE1	2.40	0.57
3:3:72:VAL:HB	3:3:75:GLN:HB2	1.87	0.57
1:1:210:ASN:O	1:1:212:GLY:N	2.38	0.57
1:1:39:ARG:C	1:1:241:ARG:HG3	2.25	0.57
1:1:7:LYS:HE3	1:1:9:VAL:O	2.05	0.56
1:1:49:LYS:HG2	1:1:50:SER:H	1.66	0.56
1:1:61:SER:HA	1:1:66:PRO:HA	1.87	0.56
2:2:251:GLU:HG2	2:2:253:LEU:H	1.70	0.56
1:1:230:THR:O	1:1:232:PRO:HD3	2.06	0.56
1:1:98:GLU:O	1:1:101:SER:N	2.38	0.56
2:2:10:LEU:HG	2:2:11:SER:CA	2.36	0.56
3:3:31:VAL:CG1	3:3:32:ALA:N	2.67	0.55
1:1:24:VAL:HG13	1:1:24:VAL:O	2.05	0.55
3:3:179:ASN:HB3	3:3:183:VAL:CG1	2.27	0.55
2:2:159:THR:O	2:2:161:ARG:N	2.40	0.55
2:2:71:THR:HG22	2:2:73:THR:HB	1.87	0.55
3:3:107:SER:H	3:3:216:ASP:HB3	1.70	0.55
2:2:9:ASN:HB2	2:2:27:GLN:HB3	1.89	0.55
3:3:180:ILE:HG23	3:3:181:THR:HG23	1.90	0.54
3:3:182:ASN:O	3:3:183:VAL:HG23	2.06	0.54
1:1:77:PHE:CZ	1:1:82:ASP:HA	2.42	0.54
1:1:208:PHE:HE1	3:3:182:ASN:HA	1.71	0.54
3:3:182:ASN:O	3:3:183:VAL:CG2	2.55	0.54
1:1:207:ARG:CD	3:3:180:ILE:CD1	2.84	0.54
3:3:36:TYR:CE1	3:3:37:MET:HE2	2.43	0.54
1:1:122:TYR:HB3	1:1:196:VAL:HG13	1.90	0.53
1:1:185:SER:HB2	3:3:10:HIS:HB3	1.91	0.53
1:1:148:THR:H	1:1:191:ASN:ND2	2.07	0.53
3:3:215:LYS:HB2	4:4:44:PRO:HG3	1.89	0.53
1:1:32:LYS:CE	4:4:13:SER:HB2	2.27	0.53
1:1:206:LYS:N	1:1:206:LYS:CD	2.69	0.53
1:1:96:GLY:HA3	1:1:101:SER:CB	2.38	0.53
1:1:202:TYR:CG	1:1:217:ALA:HB2	2.43	0.53
1:1:248:PHE:CD2	1:1:248:PHE:N	2.77	0.53
3:3:217:PHE:HE2	3:3:219:LEU:HD22	1.74	0.52
1:1:60:PHE:O	1:1:67:ASN:HB2	2.09	0.52
1:1:169:ARG:HD2	3:3:223:ILE:O	2.09	0.52
3:3:197:TYR:CE2	3:3:203:THR:HG22	2.44	0.52
4:4:21:ILE:CG2	4:4:22:ASN:O	2.54	0.52
4:4:67:PRO:CD	4:4:68:LEU:H	2.23	0.52
4:4:60:ASN:HD21	4:4:65:MET:HE3	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:180:ILE:CG2	3:3:182:ASN:ND2	2.73	0.51
3:3:81:GLN:NE2	3:3:183:VAL:HG21	2.25	0.51
2:2:10:LEU:HD12	2:2:11:SER:N	2.25	0.51
4:4:65:MET:CA	4:4:67:PRO:HD3	2.40	0.51
1:1:208:PHE:HE1	3:3:182:ASN:CA	2.23	0.51
2:2:181:GLN:HG3	2:2:191:VAL:HG22	1.93	0.51
2:2:16:GLN:HE21	2:2:25:ASN:HD21	1.58	0.50
2:2:71:THR:CG2	2:2:73:THR:H	2.24	0.50
3:3:8:ARG:NH1	3:3:9:GLU:OE1	2.45	0.50
1:1:98:GLU:H	1:1:101:SER:HB2	1.76	0.50
1:1:61:SER:HB3	1:1:82:ASP:O	2.11	0.50
4:4:66:LEU:N	4:4:67:PRO:HD3	2.26	0.50
1:1:205:HIS:CE1	1:1:210:ASN:CB	2.95	0.50
4:4:60:ASN:CG	4:4:61:ALA:H	2.14	0.49
2:2:189:THR:HG22	2:2:190:THR:HG23	1.93	0.49
1:1:207:ARG:HD2	3:3:180:ILE:CD1	2.42	0.49
2:2:10:LEU:CD1	2:2:11:SER:N	2.76	0.49
3:3:117:THR:CG2	3:3:119:MET:HB2	2.42	0.49
1:1:24:VAL:CG1	1:1:24:VAL:O	2.61	0.49
2:2:26:THR:HB	2:2:190:THR:HG21	1.93	0.49
1:1:208:PHE:N	1:1:208:PHE:CD1	2.79	0.49
3:3:135:LYS:HB3	3:3:186:TRP:CE2	2.48	0.49
2:2:88:LEU:O	2:2:93:GLY:HA3	2.13	0.48
2:2:181:GLN:HE21	2:2:191:VAL:HA	1.78	0.48
2:2:249:ARG:HB3	3:3:130:PRO:HD2	1.95	0.48
1:1:77:PHE:O	1:1:78:ASP:CB	2.61	0.48
1:1:256:PHE:HA	1:1:257:PRO:HD3	1.63	0.48
2:2:181:GLN:NE2	2:2:192:ASP:H	2.11	0.48
4:4:21:ILE:HD12	4:4:21:ILE:HA	1.19	0.48
2:2:38:THR:HG22	2:2:39:VAL:H	1.79	0.48
3:3:23:VAL:HA	3:3:24:PRO:HD3	1.81	0.47
2:2:19:ALA:CB	2:2:22:THR:HG22	2.37	0.47
2:2:79:TYR:C	2:2:79:TYR:CD2	2.88	0.47
4:4:65:MET:HE2	4:4:65:MET:HB3	1.51	0.47
1:1:252:PRO:HB3	2:2:174:GLN:HB2	1.96	0.47
3:3:197:TYR:HB2	3:3:198:PRO:HD2	1.97	0.47
1:1:207:ARG:HB3	3:3:182:ASN:HD21	1.80	0.47
1:1:81:TYR:CD2	1:1:84:LEU:HD12	2.49	0.47
3:3:37:MET:HE2	3:3:37:MET:HA	1.97	0.47
4:4:14:GLU:N	4:4:14:GLU:OE1	2.47	0.47
1:1:148:THR:H	1:1:191:ASN:HD22	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:139:ARG:HH11	3:3:139:ARG:HD3	1.51	0.47
1:1:210:ASN:C	1:1:212:GLY:N	2.68	0.47
3:3:83:THR:C	3:3:85:SER:H	2.18	0.47
3:3:180:ILE:HG22	3:3:181:THR:HG23	1.97	0.46
3:3:117:THR:CG2	3:3:120:MET:HG3	2.45	0.46
1:1:128:GLU:HB3	1:1:241:ARG:HB3	1.96	0.46
2:2:38:THR:HG22	2:2:39:VAL:N	2.30	0.46
1:1:98:GLU:O	1:1:98:GLU:HG3	2.16	0.46
1:1:1:GLY:N	1:1:18:ASP:OD2	2.49	0.46
3:3:115:THR:HB	3:3:206:LYS:O	2.15	0.46
2:2:130:MET:HG3	2:2:214:LEU:HA	1.96	0.46
1:1:94:GLY:HA3	2:2:162:LYS:HB2	1.97	0.46
1:1:142:LEU:HD21	1:1:166:SER:HB2	1.98	0.46
1:1:224:THR:HG22	1:1:225:LEU:N	2.31	0.46
2:2:74:GLN:HB3	2:2:218:VAL:HG21	1.98	0.46
2:2:20:GLY:H	2:2:22:THR:HB	1.81	0.46
3:3:36:TYR:CE1	3:3:37:MET:CE	2.98	0.46
1:1:81:TYR:CD1	1:1:81:TYR:N	2.84	0.45
2:2:10:LEU:O	2:2:13:ARG:CA	2.64	0.45
3:3:1:SER:N	3:3:2:PRO:CD	2.79	0.45
1:1:46:PHE:N	1:1:46:PHE:CD1	2.85	0.45
1:1:53:LEU:HD12	1:1:53:LEU:HA	1.70	0.45
1:1:98:GLU:HA	2:2:161:ARG:HG2	1.99	0.45
1:1:169:ARG:HD2	1:1:169:ARG:HH11	1.43	0.45
2:2:79:TYR:CE2	2:2:81:ARG:HD2	2.51	0.45
3:3:64:TYR:CZ	3:3:206:LYS:HD3	2.52	0.45
1:1:207:ARG:HD3	3:3:182:ASN:OD1	2.16	0.45
3:3:215:LYS:H	3:3:215:LYS:HG3	1.42	0.45
3:3:201:CYS:HA	3:3:202:PRO:HD3	1.87	0.45
1:1:75:PRO:HA	1:1:110:GLN:HB3	1.99	0.45
2:2:162:LYS:HA	2:2:162:LYS:HE3	1.99	0.44
2:2:253:LEU:C	2:2:255:ARG:N	2.70	0.44
3:3:179:ASN:HB2	3:3:183:VAL:CG1	2.47	0.44
1:1:206:LYS:HE2	1:1:216:ILE:O	2.17	0.44
2:2:161:ARG:HD3	2:2:161:ARG:HA	1.72	0.44
1:1:131:LEU:HD12	1:1:238:VAL:HG22	2.00	0.44
3:3:180:ILE:HG22	3:3:182:ASN:ND2	2.33	0.44
2:2:144:ASN:HA	2:2:144:ASN:HD22	1.20	0.44
1:1:207:ARG:HD3	3:3:180:ILE:HD13	1.97	0.44
3:3:117:THR:HG23	3:3:119:MET:N	2.31	0.44
1:1:231:LYS:HA	1:1:231:LYS:HD2	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:105:LEU:HD13	2:2:203:THR:HG21	2.00	0.44
2:2:22:THR:HG23	2:2:62:TYR:HB2	2.00	0.44
2:2:28:SER:OG	2:2:189:THR:HB	2.18	0.44
1:1:39:ARG:HD3	1:1:39:ARG:HH11	1.58	0.43
3:3:217:PHE:CE2	3:3:219:LEU:HD22	2.53	0.43
2:2:122:HIS:CE1	2:2:228:ALA:HB1	2.53	0.43
2:2:33:LEU:C	2:2:33:LEU:HD13	2.39	0.43
3:3:182:ASN:C	3:3:183:VAL:O	2.52	0.43
3:3:144:GLN:NE2	3:3:144:GLN:CA	2.81	0.43
3:3:179:ASN:HB2	3:3:183:VAL:HG13	1.98	0.43
1:1:4:ASN:O	1:1:7:LYS:HE2	2.18	0.43
2:2:16:GLN:HB2	2:2:25:ASN:ND2	2.33	0.43
1:1:38:ASP:OD2	1:1:241:ARG:HD3	2.18	0.43
2:2:183:LEU:HD23	2:2:183:LEU:C	2.38	0.43
1:1:231:LYS:HB3	1:1:234:ILE:HD13	1.99	0.43
1:1:34:ALA:O	1:1:38:ASP:HB2	2.19	0.43
3:3:107:SER:HB3	3:3:161:THR:CG2	2.48	0.43
2:2:86:HIS:H	2:2:86:HIS:CD2	2.36	0.43
1:1:96:GLY:CA	1:1:101:SER:HB3	2.48	0.43
2:2:200:ILE:HD13	2:2:200:ILE:HG21	1.75	0.43
1:1:97:ASN:HD22	1:1:97:ASN:HA	1.55	0.43
2:2:9:ASN:CB	2:2:27:GLN:O	2.67	0.42
2:2:35:GLY:C	2:2:37:GLY:H	2.21	0.42
3:3:109:VAL:O	3:3:211:VAL:HA	2.19	0.42
4:4:53:ASN:HA	4:4:53:ASN:HD22	1.35	0.42
2:2:82:ILE:HG23	2:2:87:VAL:HG21	2.01	0.42
3:3:117:THR:HG22	3:3:120:MET:HG3	2.01	0.42
1:1:243:LYS:HA	1:1:243:LYS:HD2	1.48	0.42
1:1:208:PHE:CE1	3:3:182:ASN:CB	2.96	0.42
3:3:19:PRO:HB3	4:4:29:TYR:CD2	2.54	0.42
1:1:208:PHE:HE1	3:3:182:ASN:CG	2.22	0.42
3:3:182:ASN:C	3:3:183:VAL:CG2	2.88	0.42
1:1:48:VAL:HG12	1:1:232:PRO:HA	2.02	0.42
1:1:258:TRP:HA	1:1:259:PRO:HD3	1.92	0.42
3:3:18:LEU:HD13	3:3:20:ASP:HB3	2.01	0.42
2:2:156:ARG:HD3	6:2:305:HOH:O	2.18	0.42
1:1:3:GLU:HG3	1:1:4:ASN:H	1.80	0.42
1:1:205:HIS:CD2	1:1:214:LEU:HD23	2.55	0.42
4:4:59:VAL:HG22	4:4:60:ASN:N	2.32	0.41
1:1:205:HIS:HD1	1:1:210:ASN:HA	1.82	0.41
2:2:160:ASN:HD22	2:2:160:ASN:HA	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:133:PRO:HA	1:1:236:PHE:HB3	2.03	0.41
4:4:14:GLU:OE1	4:4:14:GLU:CA	2.67	0.41
1:1:67:ASN:HA	1:1:67:ASN:HD22	0.88	0.41
1:1:32:LYS:HA	1:1:32:LYS:HD2	1.94	0.41
2:2:111:ARG:NH1	2:2:194:GLU:OE1	2.53	0.41
1:1:172:GLN:O	3:3:16:SER:HB3	2.20	0.41
2:2:249:ARG:NH1	2:2:250:HIS:O	2.54	0.41
1:1:49:LYS:CG	1:1:50:SER:N	2.71	0.41
3:3:197:TYR:CZ	3:3:203:THR:CG2	2.96	0.41
2:2:158:GLN:NE2	2:2:158:GLN:CA	2.80	0.41
4:4:30:GLN:O	4:4:30:GLN:HG3	2.21	0.41
1:1:205:HIS:ND1	1:1:210:ASN:OD1	2.43	0.40
3:3:35:ASN:HD22	3:3:35:ASN:H	1.68	0.40
2:2:201:ALA:HB1	2:2:202:PRO:HD2	2.02	0.40
2:2:199:ASN:OD1	2:2:200:ILE:N	2.51	0.40
1:1:99:GLU:HB2	1:1:100:THR:HG23	2.03	0.40
2:2:40:HIS:HB3	2:2:241:VAL:HG12	2.04	0.40
4:4:55:LEU:HA	4:4:55:LEU:HD12	1.96	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	1	266/277 (96%)	238 (90%)	20 (8%)	8 (3%)	5	29
2	2	247/256 (96%)	227 (92%)	17 (7%)	3 (1%)	16	56
3	3	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	8	38
4	4	56/70 (80%)	46 (82%)	6 (11%)	4 (7%)	1	7
All	All	798/834 (96%)	719 (90%)	59 (7%)	20 (2%)	7	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	77	PHE
1	1	99	GLU
1	1	266	ASP
2	2	11	SER
2	2	253	LEU
3	3	183	VAL
4	4	66	LEU
1	1	265	ILE
3	3	90	ALA
3	3	177	GLN
4	4	59	VAL
4	4	62	PHE
4	4	63	SER
1	1	189	PRO
3	3	180	ILE
1	1	78	ASP
1	1	176	ALA
1	1	249	CYS
2	2	160	ASN
3	3	221	MET

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	1	233/240 (97%)	187 (80%)	46 (20%)	1	9
2	2	217/224 (97%)	177 (82%)	40 (18%)	2	10
3	3	195/195 (100%)	162 (83%)	33 (17%)	2	13
4	4	48/59 (81%)	32 (67%)	16 (33%)	0	1
All	All	693/718 (96%)	558 (80%)	135 (20%)	2	9

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	VAL
1	1	9	VAL

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Mol	Chain	Res	Type
1	1	12	ASN
1	1	16	THR
1	1	22	GLN
1	1	24	VAL
1	1	48	VAL
1	1	60	PHE
1	1	67	ASN
1	1	77	PHE
1	1	83	GLN
1	1	85	ARG
1	1	99	GLU
1	1	101	SER
1	1	103	VAL
1	1	110	GLN
1	1	116	LEU
1	1	124	LYS
1	1	131	LEU
1	1	155	THR
1	1	161	GLU
1	1	167	GLU
1	1	169	ARG
1	1	172	GLN
1	1	175	SER
1	1	185	SER
1	1	188	VAL
1	1	190	TYR
1	1	191	ASN
1	1	196	VAL
1	1	197	LEU
1	1	206	LYS
1	1	207	ARG
1	1	208	PHE
1	1	213	ASP
1	1	233	ASP
1	1	241	ARG
1	1	243	LYS
1	1	244	ASN
1	1	245	MET
1	1	251	ARG
1	1	261	SER
1	1	264	LYS
1	1	265	ILE

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Mol	Chain	Res	Type
1	1	267	MET
1	1	268	THR
2	2	8	GLU
2	2	9	ASN
2	2	11	SER
2	2	16	GLN
2	2	22	THR
2	2	27	GLN
2	2	38	THR
2	2	39	VAL
2	2	57	LEU
2	2	71	THR
2	2	72	SER
2	2	75	LYS
2	2	87	VAL
2	2	88	LEU
2	2	89	SER
2	2	117	ASN
2	2	120	GLN
2	2	137	LEU
2	2	144	ASN
2	2	145	ARG
2	2	148	LYS
2	2	156	ARG
2	2	158	GLN
2	2	159	THR
2	2	160	ASN
2	2	161	ARG
2	2	181	GLN
2	2	184	ASN
2	2	186	ARG
2	2	189	THR
2	2	207	THR
2	2	223	THR
2	2	230	THR
2	2	231	SER
2	2	233	ASP
2	2	239	GLN
2	2	253	LEU
2	2	254	SER
2	2	255	ARG
2	2	256	GLN

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Mol	Chain	Res	Type
3	3	1	SER
3	3	9	GLU
3	3	18	LEU
3	3	40	GLU
3	3	57	LYS
3	3	63	PRO
3	3	66	GLU
3	3	72	VAL
3	3	74	THR
3	3	75	GLN
3	3	77	LEU
3	3	79	VAL
3	3	81	GLN
3	3	97	LEU
3	3	99	ARG
3	3	115	THR
3	3	117	THR
3	3	121	LYS
3	3	143	MET
3	3	152	LEU
3	3	157	SER
3	3	172	MET
3	3	177	GLN
3	3	182	ASN
3	3	191	GLN
3	3	198	PRO
3	3	208	LEU
3	3	215	LYS
3	3	216	ASP
3	3	218	SER
3	3	219	LEU
3	3	224	SER
3	3	231	GLN
4	4	13	SER
4	4	14	GLU
4	4	20	ILE
4	4	21	ILE
4	4	22	ASN
4	4	27	ASN
4	4	34	ASP
4	4	35	LEU
4	4	38	ASN

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Mol	Chain	Res	Type
4	4	46	LYS
4	4	47	THR
4	4	54	LEU
4	4	56	SER
4	4	62	PHE
4	4	65	MET
4	4	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	67	ASN
1	1	76	GLN
1	1	83	GLN
1	1	97	ASN
1	1	110	GLN
1	1	157	GLN
1	1	172	GLN
1	1	182	ASN
1	1	191	ASN
2	2	25	ASN
2	2	86	HIS
2	2	144	ASN
2	2	158	GLN
2	2	160	ASN
2	2	181	GLN
2	2	184	ASN
2	2	250	HIS
3	3	35	ASN
3	3	75	GLN
3	3	81	GLN
3	3	141	GLN
3	3	144	GLN
3	3	169	HIS
4	4	27	ASN
4	4	30	GLN
4	4	50	GLN
4	4	53	ASN
4	4	60	ASN

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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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	#$|Z| > 2$
5	PO4	2	257	-	4,4,4	2.07	3 (75%)	6,6,6	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PO4	2	257	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	257	PO4	P-O4	-2.21	1.45	1.53
5	2	257	PO4	P-O3	-2.21	1.45	1.53
5	2	257	PO4	P-O2	-2.21	1.45	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	1	268/277 (96%)	-0.65	1 (0%)	93	80	2, 9, 57, 77	0
2	2	249/256 (97%)	-0.84	0	100	100	2, 7, 44, 62	0
3	3	231/231 (100%)	-0.75	0	100	100	2, 7, 40, 82	0
4	4	58/70 (82%)	0.28	1 (1%)	73	45	13, 38, 60, 61	0
All	All	806/834 (96%)	-0.67	2 (0%)	95	87	2, 8, 52, 82	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	4	64	ASN	2.7
1	1	263	ASP	2.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
5	PO4	2	257	5/5	0.98	0.13	0.50	43,56,64,66	0

6.5 Other polymers (i)

There are no such residues in this entry.