



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:32 pm BST

PDB ID : 1DWK
Title : STRUCTURE OF CYANASE WITH THE DI-ANION OXALATE BOUND
AT THE ENZYME ACTIVE SITE
Authors : Walsh, M.A.; Otwinowski, Z.; Perrakis, A.; Anderson, P.M.; Joachimiak, A.
Deposited on : 1999-12-07
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

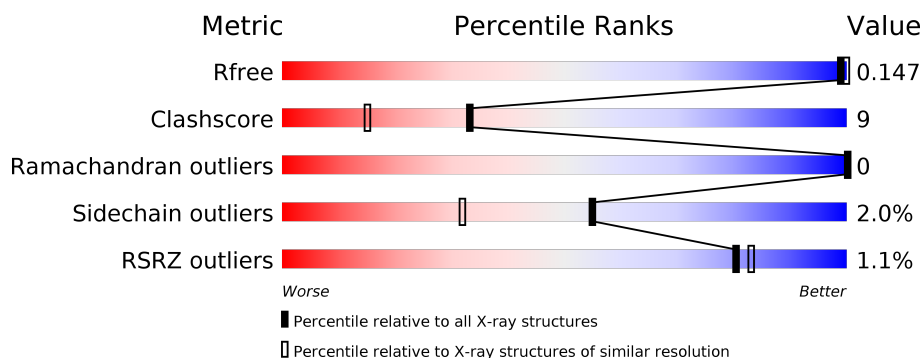
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 85% 12% . </div> </div>
1	B	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 83% 14% . </div> </div>
1	C	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 79% 17% .. </div> </div>
1	D	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 85% 12% . </div> </div>
1	E	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 83% 16% .. </div> </div>
1	F	156	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 12% . </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	156	<div><div><div>%</div><div><div></div><div>83%</div><div>15%</div><div></div></div><div>..</div></div></div>
1	H	156	<div><div><div>2%</div><div><div></div><div>82%</div><div>13%</div><div></div></div><div>. .</div></div></div>
1	I	156	<div><div><div>%</div><div><div></div><div>85%</div><div>13%</div><div></div></div><div>.</div></div></div>
1	J	156	<div><div><div>%</div><div><div></div><div>83%</div><div>14%</div><div></div></div><div>. .</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14777 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 CYANATE HYDRATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	Se	0	10	0
			1229	791	201	232	1	4			
1	B	156	Total	C	N	O	S	Se	0	6	0
			1219	787	199	228	1	4			
1	C	156	Total	C	N	O	S	Se	0	8	0
			1223	790	200	228	1	4			
1	D	156	Total	C	N	O	S	Se	0	5	0
			1212	782	199	226	1	4			
1	E	156	Total	C	N	O	S	Se	0	6	0
			1217	783	199	230	1	4			
1	F	156	Total	C	N	O	S	Se	0	4	0
			1210	780	199	226	1	4			
1	G	156	Total	C	N	O	S	Se	0	7	0
			1219	784	200	230	1	4			
1	H	156	Total	C	N	O	S	Se	0	4	0
			1211	779	199	228	1	4			
1	I	156	Total	C	N	O	S	Se	0	2	0
			1204	774	199	226	1	4			
1	J	156	Total	C	N	O	S	Se	0	6	0
			1219	785	199	230	1	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P00816
A	77	MSE	MET	modified residue	UNP P00816
A	94	MSE	MET	modified residue	UNP P00816
A	100	MSE	MET	modified residue	UNP P00816
B	1	MSE	MET	modified residue	UNP P00816
B	77	MSE	MET	modified residue	UNP P00816
B	94	MSE	MET	modified residue	UNP P00816
B	100	MSE	MET	modified residue	UNP P00816
C	1	MSE	MET	modified residue	UNP P00816

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MSE	MET	modified residue	UNP P00816
C	94	MSE	MET	modified residue	UNP P00816
C	100	MSE	MET	modified residue	UNP P00816
D	1	MSE	MET	modified residue	UNP P00816
D	77	MSE	MET	modified residue	UNP P00816
D	94	MSE	MET	modified residue	UNP P00816
D	100	MSE	MET	modified residue	UNP P00816
E	1	MSE	MET	modified residue	UNP P00816
E	77	MSE	MET	modified residue	UNP P00816
E	94	MSE	MET	modified residue	UNP P00816
E	100	MSE	MET	modified residue	UNP P00816
F	1	MSE	MET	modified residue	UNP P00816
F	77	MSE	MET	modified residue	UNP P00816
F	94	MSE	MET	modified residue	UNP P00816
F	100	MSE	MET	modified residue	UNP P00816
G	1	MSE	MET	modified residue	UNP P00816
G	77	MSE	MET	modified residue	UNP P00816
G	94	MSE	MET	modified residue	UNP P00816
G	100	MSE	MET	modified residue	UNP P00816
H	1	MSE	MET	modified residue	UNP P00816
H	77	MSE	MET	modified residue	UNP P00816
H	94	MSE	MET	modified residue	UNP P00816
H	100	MSE	MET	modified residue	UNP P00816
I	1	MSE	MET	modified residue	UNP P00816
I	77	MSE	MET	modified residue	UNP P00816
I	94	MSE	MET	modified residue	UNP P00816
I	100	MSE	MET	modified residue	UNP P00816
J	1	MSE	MET	modified residue	UNP P00816
J	77	MSE	MET	modified residue	UNP P00816
J	94	MSE	MET	modified residue	UNP P00816
J	100	MSE	MET	modified residue	UNP P00816

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



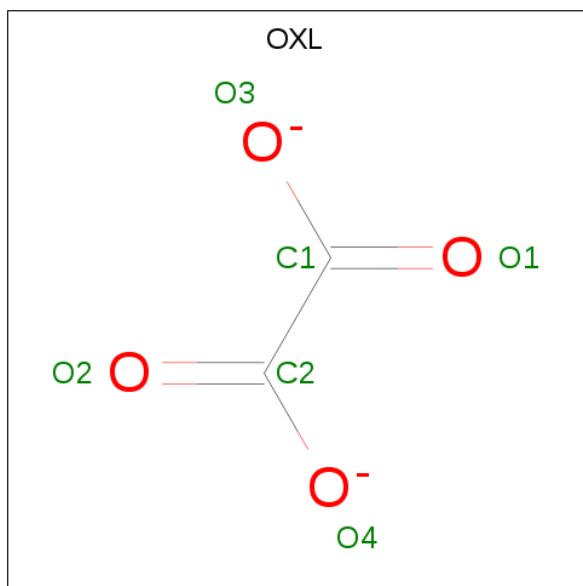
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	1
			10	8	2		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	J	1	Total	C	O	0	0
			6	2	4		

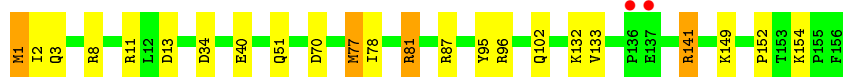
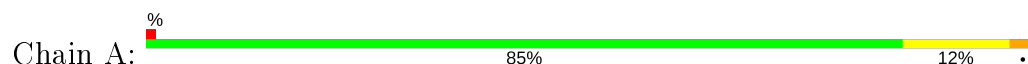
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	261	Total	O	0	0
			261	261		
4	B	266	Total	O	0	0
			266	266		
4	C	264	Total	O	0	0
			264	264		
4	D	245	Total	O	0	0
			245	245		
4	E	245	Total	O	0	0
			245	245		
4	F	238	Total	O	0	0
			238	238		
4	G	249	Total	O	0	0
			249	249		
4	H	220	Total	O	0	0
			220	220		
4	I	224	Total	O	0	0
			224	224		
4	J	252	Total	O	0	0
			252	252		

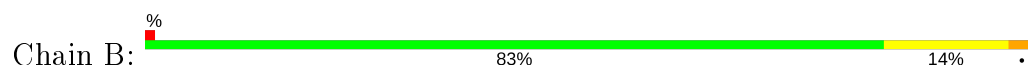
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

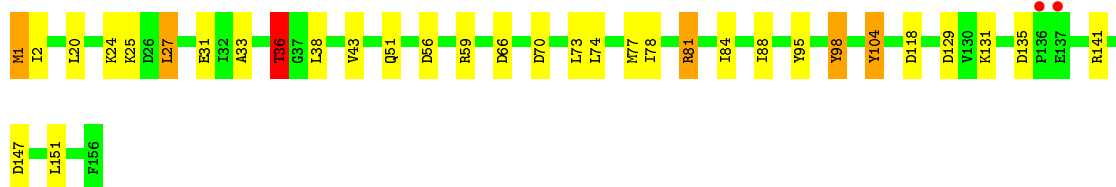
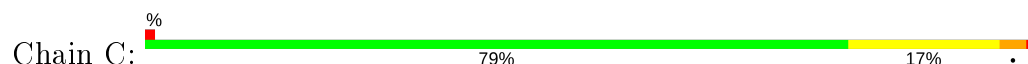
• Molecule 1: CYANATE HYDRATASE



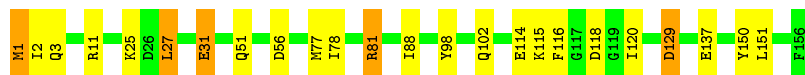
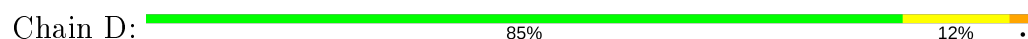
• Molecule 1: CYANATE HYDRATASE



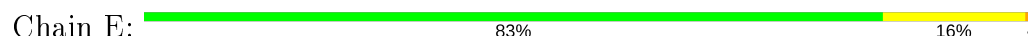
• Molecule 1: CYANATE HYDRATASE



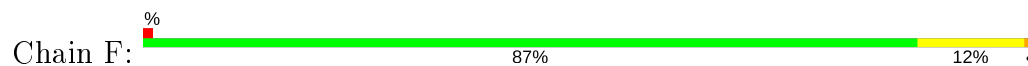
• Molecule 1: CYANATE HYDRATASE



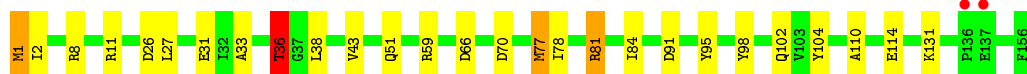
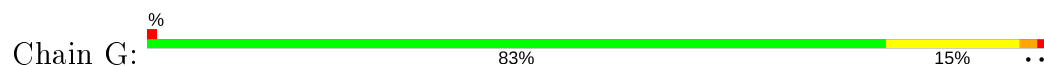
• Molecule 1: CYANATE HYDRATASE



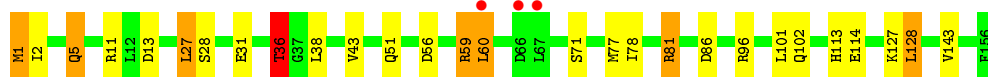
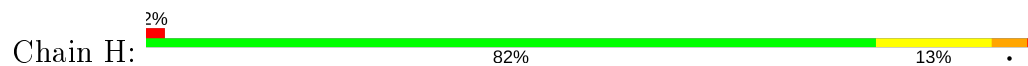
• Molecule 1: CYANATE HYDRATASE



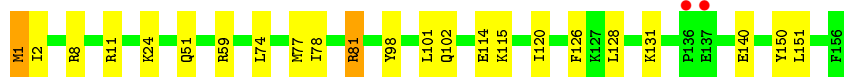
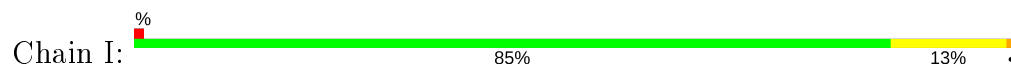
• Molecule 1: CYANATE HYDRATASE



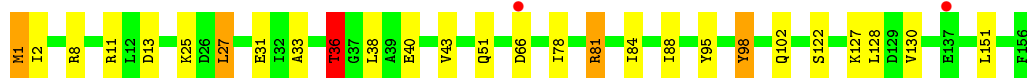
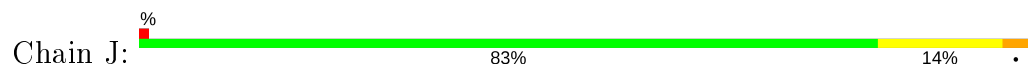
• Molecule 1: CYANATE HYDRATASE



• Molecule 1: CYANATE HYDRATASE



• Molecule 1: CYANATE HYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.33Å 80.93Å 82.13Å 70.10° 71.95° 66.42°	Depositor
Resolution (Å)	20.00 – 1.65 19.98 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-1.65) 95.1 (19.98-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.68 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.181 0.143 , 0.147	Depositor DCC
R_{free} test set	9561 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14777	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 5.75% 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: OXL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.83	2/1293 (0.2%)	1.37	13/1743 (0.7%)
1	B	0.86	2/1259 (0.2%)	1.35	15/1699 (0.9%)
1	C	0.85	2/1277 (0.2%)	1.47	17/1723 (1.0%)
1	D	0.86	1/1250 (0.1%)	1.40	13/1687 (0.8%)
1	E	0.85	0/1260	1.38	8/1700 (0.5%)
1	F	0.81	0/1243	1.36	8/1677 (0.5%)
1	G	0.84	2/1269 (0.2%)	1.38	15/1711 (0.9%)
1	H	0.90	1/1244 (0.1%)	1.58	17/1678 (1.0%)
1	I	0.83	1/1227 (0.1%)	1.31	8/1654 (0.5%)
1	J	0.82	2/1261 (0.2%)	1.40	9/1701 (0.5%)
All	All	0.84	13/12583 (0.1%)	1.40	123/16973 (0.7%)

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	C	1	0
1	H	0	1
All	All	1	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	MSE	CG-SE	-7.17	1.71	1.95
1	I	1	MSE	CG-SE	-7.12	1.71	1.95
1	B	1	MSE	CG-SE	-6.39	1.73	1.95
1	H	1	MSE	CG-SE	-6.06	1.74	1.95
1	C	1	MSE	SE-CE	-5.98	1.60	1.95
1	D	1	MSE	CG-SE	-5.90	1.75	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	77	MSE	SE-CE	-5.84	1.60	1.95
1	A	1	MSE	CG-SE	-5.67	1.76	1.95
1	B	69	GLU	CD-OE1	5.26	1.31	1.25
1	A	77	MSE	SE-CE	-5.22	1.64	1.95
1	G	1	MSE	CG-SE	-5.08	1.78	1.95
1	J	1	MSE	SE-CE	-5.05	1.65	1.95
1	J	1	MSE	CG-SE	-5.04	1.78	1.95

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	MSE	CG-SE-CE	24.67	153.18	98.90
1	H	59	ARG	NE-CZ-NH2	-17.99	111.31	120.30
1	E	81	ARG	NE-CZ-NH2	-11.97	114.31	120.30
1	E	81	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	D	137	GLU	OE1-CD-OE2	11.45	137.03	123.30
1	B	1	MSE	CG-SE-CE	10.75	122.56	98.90
1	I	1	MSE	CG-SE-CE	10.57	122.16	98.90
1	F	11	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	G	8	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	D	129	ASP	CB-CG-OD1	-10.14	109.17	118.30
1	I	8	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	J	1	MSE	CG-SE-CE	10.07	121.06	98.90
1	H	1	MSE	CG-SE-CE	9.46	119.71	98.90
1	H	11	ARG	NE-CZ-NH2	9.43	125.02	120.30
1	J	81	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	1	MSE	CG-SE-CE	9.07	118.86	98.90
1	A	8	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	D	81	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	G	81	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	I	8	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	34[A]	ASP	CB-CG-OD1	8.54	125.98	118.30
1	A	34[B]	ASP	CB-CG-OD1	8.54	125.98	118.30
1	I	11	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	E	36	THR	N-CA-CB	-8.35	94.44	110.30
1	H	13	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	56	ASP	CB-CG-OD1	8.23	125.70	118.30
1	J	11	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	H	56	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	J	36	THR	N-CA-CB	-8.14	94.84	110.30
1	J	13	ASP	CB-CG-OD1	8.00	125.50	118.30
1	F	8	ARG	NE-CZ-NH2	-7.96	116.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	H	59	ARG	NH1-CZ-NH2	7.72	127.89	119.40
1	G	36	THR	N-CA-CB	-7.68	95.70	110.30
1	G	59	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	66	ASP	CB-CG-OD1	7.50	125.05	118.30
1	E	36	THR	OG1-CB-CG2	7.42	127.06	110.00
1	J	36	THR	OG1-CB-CG2	7.38	126.97	110.00
1	F	141	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	F	8	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	31	GLU	CA-CB-CG	7.09	129.01	113.40
1	G	1	MSE	CG-SE-CE	7.08	114.48	98.90
1	C	36	THR	N-CA-CB	-7.06	96.88	110.30
1	D	81	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	C	36	THR	OG1-CB-CG2	6.99	126.09	110.00
1	G	8	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	I	11	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	F	81	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	D	137	GLU	CG-CD-OE2	-6.84	104.63	118.30
1	B	59	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	F	95	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	D	150	TYR	CB-CG-CD1	6.79	125.08	121.00
1	D	11	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	C	98	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	C	70	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	G	11	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	98	TYR	CB-CG-CD1	6.67	125.00	121.00
1	H	36	THR	O-C-N	-6.67	111.87	123.20
1	D	11	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	E	129	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	A	95	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	B	69	GLU	CB-CG-CD	6.50	131.76	114.20
1	C	56	ASP	CB-CG-OD1	6.37	124.03	118.30
1	D	1	MSE	CG-SE-CE	6.30	112.77	98.90
1	A	81	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	H	81	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	G	31	GLU	OE1-CD-OE2	6.25	130.80	123.30
1	G	36	THR	OG1-CB-CG2	6.21	124.28	110.00
1	B	59	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	141	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	141	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	13	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	E	69	GLU	OE1-CD-OE2	-5.95	116.16	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5	GLN	CB-CA-C	-5.94	98.52	110.40
1	G	26	ASP	CB-CG-OD1	5.91	123.62	118.30
1	H	11	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	H	86	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	150	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	B	116	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	I	150	TYR	CB-CG-CD1	5.75	124.45	121.00
1	H	59	ARG	CA-CB-CG	-5.74	100.77	113.40
1	B	87	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	95	TYR	CG-CD1-CE1	-5.68	116.76	121.30
1	B	150	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	H	36	THR	C-N-CA	5.64	134.14	122.30
1	F	59	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	F	98	TYR	CG-CD1-CE1	-5.60	116.82	121.30
1	G	81	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	H	36	THR	N-CA-CB	-5.59	99.68	110.30
1	J	8	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	98	TYR	CG-CD1-CE1	-5.55	116.86	121.30
1	E	8	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	11	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	H	71	SER	O-C-N	-5.53	113.86	122.70
1	C	81	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	8	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	95	TYR	CZ-CE2-CD2	-5.47	114.88	119.80
1	H	27	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	129	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	147	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	151	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	B	104	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	E	137	GLU	OE1-CD-OE2	-5.37	116.85	123.30
1	G	91	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	J	95	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	B	8	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	77	MSE	CG-SE-CE	-5.31	87.21	98.90
1	D	56	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	104	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	C	118	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	C	59	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	J	98	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	H	96	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	135	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	B	77	MSE	CG-SE-CE	-5.14	87.58	98.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	81	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	96	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	87	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	60	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	13	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	G	95	TYR	CG-CD1-CE1	-5.03	117.27	121.30
1	A	149	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	I	98	TYR	CB-CG-CD2	-5.01	117.99	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	36	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	143	VAL	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1229	0	1288	19	0
1	B	1219	0	1278	24	0
1	C	1223	0	1288	27	0
1	D	1212	0	1276	28	0
1	E	1217	0	1273	32	0
1	F	1210	0	1271	17	0
1	G	1219	0	1270	25	0
1	H	1211	0	1266	26	0
1	I	1204	0	1257	21	0
1	J	1219	0	1275	27	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	10	0	0	0	0
2	F	15	0	0	1	0
2	G	15	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	J	6	0	0	0	0
4	A	261	0	0	4	0
4	B	266	0	0	2	0
4	C	264	0	0	6	0
4	D	245	0	0	7	0
4	E	245	0	0	4	0
4	F	238	0	0	3	0
4	G	249	0	0	4	0
4	H	220	0	0	6	0
4	I	224	0	0	7	0
4	J	252	0	0	10	0
All	All	14777	0	12742	216	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 9.

All (216) 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:D:1:MSE:HE3	1:D:2:ILE:HG22	1.22	1.18
1:I:1:MSE:HE2	1:I:2:ILE:HG22	1.25	1.16
1:B:1:MSE:HE3	1:B:2:ILE:HG22	1.21	1.13
1:H:2:ILE:HD11	1:H:78[A]:ILE:HD11	1.31	1.13
1:G:1:MSE:HE3	1:G:2:ILE:HG22	1.21	1.13
1:D:2:ILE:HD11	1:D:78[A]:ILE:HD11	1.29	1.13
1:J:2:ILE:HD11	1:J:78[A]:ILE:HD11	1.31	1.12
1:I:2:ILE:HD11	1:I:78:ILE:HD11	1.32	1.11
1:F:2:ILE:HD11	1:F:78[A]:ILE:HD11	1.32	1.08
1:H:1:MSE:HE3	1:H:2:ILE:HG22	1.24	1.08
1:G:2:ILE:HD11	1:G:78[A]:ILE:HD11	1.31	1.06
1:C:1:MSE:HE3	1:I:114:GLU:HG3	1.39	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ILE:HD11	1:E:78[A]:ILE:HD11	1.39	1.05
1:C:2:ILE:HD11	1:C:78[A]:ILE:HD11	1.40	1.03
1:B:1:MSE:CE	1:B:2:ILE:HG22	1.92	1.00
1:A:2:ILE:HD11	1:A:78[B]:ILE:HD11	1.43	1.00
1:B:2:ILE:HD11	1:B:78[A]:ILE:HD11	1.42	0.99
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:CD	1.83	0.99
1:E:27[B]:LEU:HD23	1:E:31[B]:GLU:OE1	1.65	0.97
1:A:1:MSE:CE	1:A:2:ILE:HG22	1.98	0.94
1:J:25:LYS:HE2	4:J:398:HOH:O	1.68	0.92
1:A:1:MSE:HE2	1:A:2:ILE:HG22	1.49	0.92
1:J:1:MSE:HE3	1:J:2:ILE:HG22	1.49	0.92
1:E:114:GLU:HG3	1:F:1:MSE:HE1	1.50	0.91
1:H:1:MSE:CE	1:H:2:ILE:HG22	2.01	0.90
1:J:1:MSE:CE	1:J:2:ILE:HG22	2.02	0.88
1:I:1:MSE:CE	1:I:2:ILE:HG22	2.03	0.88
1:C:1:MSE:CE	1:I:114:GLU:HG3	2.05	0.87
1:D:1:MSE:CE	1:D:2:ILE:HG22	2.05	0.86
1:C:1:MSE:SE	4:J:538:HOH:O	2.44	0.84
1:D:115:LYS:HG3	4:D:453:HOH:O	1.78	0.82
1:D:1:MSE:HE3	1:D:2:ILE:CG2	2.08	0.81
4:C:538:HOH:O	1:G:1:MSE:SE	2.49	0.79
1:G:1:MSE:CE	1:G:2:ILE:HG22	2.10	0.78
1:E:24:LYS:HG3	4:E:301:HOH:O	1.84	0.78
1:C:25:LYS:HE2	4:C:359:HOH:O	1.85	0.77
4:A:532:HOH:O	1:B:1:MSE:SE	2.52	0.77
1:H:2:ILE:CD1	1:H:78[A]:ILE:HD11	2.12	0.77
1:G:1:MSE:CE	1:H:114:GLU:HG3	2.16	0.76
1:F:1:MSE:SE	4:G:526:HOH:O	2.54	0.76
4:H:515:HOH:O	1:I:1:MSE:SE	2.53	0.75
1:I:1:MSE:HE3	4:I:427:HOH:O	1.88	0.74
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:OE1	2.35	0.74
1:E:27[B]:LEU:HD22	1:E:31[B]:GLU:HG3	1.70	0.74
1:J:66:ASP:HB3	4:J:434:HOH:O	1.88	0.74
1:I:140:GLU:HG2	4:I:464:HOH:O	1.88	0.73
1:G:1:MSE:HE3	1:G:2:ILE:CG2	2.12	0.72
1:D:115:LYS:HE2	4:D:453:HOH:O	1.90	0.72
1:F:2:ILE:HD11	1:F:78[A]:ILE:CD1	2.17	0.72
4:C:491:HOH:O	1:I:151:LEU:HD13	1.92	0.70
1:C:131:LYS:HD2	4:C:497:HOH:O	1.90	0.70
1:D:1:MSE:SE	4:F:520:HOH:O	2.59	0.70
1:F:137:GLU:HG2	4:F:342:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78[A]:ILE:HD13	1:D:118:ASP:HB2	1.76	0.68
1:D:2:ILE:HD11	1:D:78[A]:ILE:CD1	2.16	0.68
1:H:59:ARG:HH11	1:H:59:ARG:HG2	1.61	0.66
1:A:1:MSE:SE	4:I:516:HOH:O	2.63	0.66
1:G:1:MSE:HE1	1:H:114:GLU:HG3	1.77	0.65
1:C:77:MSE:SE	4:C:498:HOH:O	2.65	0.65
1:E:114:GLU:HG3	1:F:1:MSE:CE	2.27	0.63
1:B:114:GLU:HG3	1:D:1:MSE:CE	2.30	0.61
1:A:133[A]:VAL:HG21	4:D:476:HOH:O	2.00	0.61
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CD	2.65	0.61
1:A:1:MSE:HE3	1:A:2:ILE:HG22	1.80	0.60
1:B:78[A]:ILE:HD13	1:D:118:ASP:CB	2.30	0.60
1:J:36:THR:CG2	1:J:38:LEU:H	2.15	0.60
1:F:1:MSE:HE3	1:F:2:ILE:HG22	1.84	0.60
1:C:27[A]:LEU:HD12	1:C:31:GLU:CD	2.22	0.60
1:E:36:THR:CG2	1:E:38:LEU:H	2.15	0.60
1:H:36:THR:CG2	1:H:38:LEU:H	2.15	0.60
1:C:36:THR:CG2	1:C:38:LEU:H	2.14	0.59
1:C:20:LEU:HG	1:C:24:LYS:HE3	1.82	0.59
1:E:151:LEU:HD23	4:E:390:HOH:O	2.03	0.59
1:B:2:ILE:HD11	1:B:78[A]:ILE:CD1	2.25	0.59
1:C:36:THR:HG23	1:C:38:LEU:H	1.66	0.59
1:B:1:MSE:HE1	4:D:378:HOH:O	2.03	0.59
1:G:1:MSE:HE2	1:H:114:GLU:HG3	1.82	0.59
1:D:27[A]:LEU:HD12	4:D:403:HOH:O	2.03	0.58
1:G:36:THR:HG21	1:G:43:VAL:HG21	1.84	0.58
1:D:120:ILE:HD11	1:D:151:LEU:HD12	1.87	0.57
1:G:2:ILE:CD1	1:G:78[A]:ILE:HD11	2.22	0.57
1:E:25:LYS:HB3	1:E:27[A]:LEU:HD13	1.87	0.56
1:H:59:ARG:NH1	1:H:59:ARG:HG2	2.19	0.56
1:E:25:LYS:HE2	4:E:425:HOH:O	2.05	0.56
1:G:131:LYS:HG3	4:G:336:HOH:O	2.05	0.56
1:C:25:LYS:HB2	1:C:27[A]:LEU:HD22	1.87	0.56
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:HG3	2.35	0.56
1:H:36:THR:HG22	4:H:304:HOH:O	2.06	0.56
1:E:51:GLN:NE2	1:E:81:ARG:HH21	2.05	0.55
1:J:151:LEU:HD22	4:J:363:HOH:O	2.07	0.55
1:I:131:LYS:HD2	4:I:480:HOH:O	2.07	0.55
1:F:51:GLN:NE2	1:F:81:ARG:HH21	2.04	0.55
1:J:40[B]:GLU:OE2	4:J:301:HOH:O	2.18	0.55
1:E:33:ALA:O	1:E:36:THR:HB	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:51:GLN:NE2	1:J:81:ARG:HH21	2.05	0.54
1:C:73:LEU:HD12	4:C:306:HOH:O	2.08	0.54
1:A:132[B]:LYS:HG3	1:D:116:PHE:CE1	2.43	0.54
1:J:151:LEU:HD13	4:J:363:HOH:O	2.07	0.54
1:J:130:VAL:O	4:J:301:HOH:O	2.19	0.54
1:J:36:THR:HG21	1:J:43:VAL:HG21	1.90	0.54
1:G:36:THR:CG2	1:G:38:LEU:H	2.22	0.53
1:J:2:ILE:HD11	1:J:78[A]:ILE:CD1	2.21	0.53
1:I:2:ILE:HD11	1:I:78:ILE:CD1	2.21	0.53
1:G:51:GLN:NE2	1:G:81:ARG:HH21	2.07	0.53
1:I:51:GLN:NE2	1:I:81:ARG:HH21	2.07	0.52
1:G:78[A]:ILE:HD12	1:H:113:HIS:HB3	1.91	0.52
1:E:88:ILE:HD12	1:E:98:TYR:CZ	2.45	0.51
1:B:25:LYS:HB2	1:B:27[B]:LEU:HD22	1.93	0.51
1:J:2:ILE:CD1	1:J:78[A]:ILE:HD11	2.22	0.51
1:E:27[B]:LEU:CD2	1:E:31[B]:GLU:CG	2.89	0.51
1:E:20:LEU:HD12	4:E:301:HOH:O	2.10	0.51
1:E:36:THR:HG22	1:E:38:LEU:H	1.75	0.51
1:B:88:ILE:HD12	1:B:98:TYR:CZ	2.45	0.51
1:H:36:THR:HG22	1:H:38:LEU:H	1.75	0.51
1:G:77:MSE:HG2	4:G:459:HOH:O	2.11	0.51
1:B:78[A]:ILE:CD1	1:D:118:ASP:HB2	2.41	0.50
1:C:51:GLN:NE2	1:C:81:ARG:HH21	2.10	0.50
1:D:25:LYS:HB3	1:D:27[A]:LEU:HD13	1.92	0.50
1:H:51:GLN:NE2	1:H:81:ARG:HH21	2.09	0.50
1:D:51:GLN:NE2	1:D:81:ARG:HH21	2.09	0.50
1:A:51:GLN:NE2	1:A:81:ARG:HH21	2.10	0.50
1:H:36:THR:HG21	1:H:43:VAL:HG21	1.93	0.50
1:A:1:MSE:HE3	4:A:449:HOH:O	2.12	0.50
1:E:151:LEU:HD13	4:F:477:HOH:O	2.12	0.50
1:B:1:MSE:CE	1:D:114:GLU:HG3	2.41	0.49
1:B:114:GLU:HG3	1:D:1:MSE:HE1	1.93	0.49
1:D:115:LYS:NZ	4:D:302:HOH:O	2.43	0.49
1:J:88:ILE:HD12	1:J:98:TYR:CZ	2.48	0.49
1:D:77:MSE:HG2	4:D:474:HOH:O	2.13	0.49
1:G:33:ALA:O	1:G:36:THR:HB	2.13	0.49
1:C:1:MSE:HE1	4:I:456:HOH:O	2.13	0.49
1:C:24:LYS:HE2	1:G:70:ASP:OD1	2.13	0.49
1:G:66:ASP:HB3	4:G:475:HOH:O	2.13	0.49
1:B:114:GLU:HG3	1:D:1:MSE:HE2	1.96	0.48
1:B:69:GLU:HG3	4:B:338:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MSE:HE3	1:F:2:ILE:CG2	2.43	0.48
1:E:77:MSE:HE2	1:E:77:MSE:HB3	1.52	0.48
1:J:36:THR:HG23	1:J:38:LEU:H	1.77	0.48
1:A:1:MSE:HE1	4:J:380:HOH:O	2.13	0.48
1:C:1:MSE:HE1	4:I:411:HOH:O	2.13	0.48
1:E:36:THR:HG23	1:E:38:LEU:HB2	1.96	0.48
1:B:74:LEU:HA	1:B:77:MSE:HG3	1.96	0.47
1:B:51:GLN:NE2	1:B:81:ARG:HH21	2.12	0.47
1:E:78[A]:ILE:HD12	1:F:113:HIS:HB3	1.95	0.47
1:G:36:THR:HG22	1:G:38:LEU:H	1.79	0.47
1:J:36:THR:HG22	1:J:38:LEU:H	1.78	0.47
1:A:77:MSE:HG2	4:A:475:HOH:O	2.14	0.47
1:G:114:GLU:HG3	1:H:1:MSE:CE	2.44	0.47
1:H:77:MSE:HE1	4:H:436:HOH:O	2.15	0.47
1:C:77:MSE:HE2	1:C:77:MSE:HB3	1.65	0.47
1:I:59:ARG:HD3	4:I:324:HOH:O	2.15	0.47
1:J:33:ALA:O	1:J:36:THR:HB	2.15	0.46
1:G:77:MSE:HE2	1:G:77:MSE:HB3	1.46	0.46
1:C:25:LYS:CB	1:C:27[A]:LEU:HD22	2.45	0.46
1:B:77:MSE:HE2	1:B:77:MSE:HB3	1.45	0.46
1:C:84:ILE:HD11	1:H:101[B]:LEU:HG	1.98	0.46
1:F:77:MSE:HE2	1:F:77:MSE:HB3	1.66	0.46
1:D:88:ILE:HD12	1:D:98:TYR:CZ	2.50	0.46
1:H:59:ARG:NH1	1:H:59:ARG:CG	2.78	0.46
1:H:28:SER:OG	1:H:31[A]:GLU:HG3	2.16	0.46
1:F:1:MSE:CE	1:F:2:ILE:HG22	2.46	0.46
1:I:74:LEU:HA	1:I:77:MSE:HG3	1.98	0.45
1:C:88[A]:ILE:HD12	1:C:98:TYR:CZ	2.52	0.45
1:B:135:ASP:HB2	1:B:141:ARG:HG3	1.98	0.45
1:H:36:THR:HG23	1:H:38:LEU:H	1.81	0.45
1:E:29:PHE:CE2	1:G:110:ALA:HB1	2.52	0.45
1:E:128[A]:LEU:HD21	1:G:104:TYR:CD1	2.51	0.45
1:H:5:GLN:HG3	4:H:382:HOH:O	2.17	0.45
1:E:36:THR:HG21	1:E:43:VAL:HG21	1.97	0.45
1:A:1:MSE:HE3	1:A:2:ILE:H	1.82	0.45
1:A:40:GLU:HG2	4:A:335:HOH:O	2.16	0.45
1:I:2:ILE:CD1	1:I:78:ILE:HD11	2.24	0.45
1:B:77:MSE:SE	4:B:498:HOH:O	2.85	0.44
1:F:25:LYS:HB2	1:F:27:LEU:HD22	1.98	0.44
1:D:77:MSE:HE2	1:D:77:MSE:HB3	1.72	0.44
1:E:101[B]:LEU:HG	1:G:84:ILE:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HA	1:C:77:MSE:HG3	2.00	0.44
1:H:127:LYS:NZ	4:H:302:HOH:O	2.50	0.44
1:A:77:MSE:HE2	1:A:77:MSE:HB3	1.57	0.44
1:B:113:HIS:HB3	1:D:78[A]:ILE:HD12	1.99	0.44
1:F:35:GLY:N	2:F:204:SO4:O4	2.39	0.44
1:J:1:MSE:HE2	1:J:2:ILE:HG22	1.91	0.44
1:A:2:ILE:CD1	1:A:78[B]:ILE:HD11	2.32	0.44
1:B:24:LYS:HE2	1:E:70:ASP:OD1	2.17	0.44
1:D:27[B]:LEU:CD2	1:D:31:GLU:HG3	2.48	0.43
1:B:1:MSE:HE2	1:D:114:GLU:HG3	2.00	0.43
1:I:115:LYS:NZ	4:J:301:HOH:O	2.51	0.43
1:C:2:ILE:HD11	1:C:78[A]:ILE:CD1	2.29	0.43
1:E:36:THR:HG23	1:E:38:LEU:H	1.80	0.43
1:I:120:ILE:HD11	1:I:151:LEU:HD12	2.00	0.43
1:H:60:LEU:HD22	4:H:464:HOH:O	2.17	0.43
1:J:122:SER:HB2	1:J:151:LEU:HD12	2.00	0.43
1:A:133[A]:VAL:CG2	1:A:141:ARG:HB2	2.49	0.42
1:I:101[B]:LEU:HG	1:J:84:ILE:HD11	2.00	0.42
1:C:33:ALA:O	1:C:36:THR:HG22	2.20	0.42
1:J:1:MSE:HE3	1:J:2:ILE:H	1.84	0.42
1:F:3:GLN:HB3	1:F:77:MSE:HE3	2.02	0.42
1:H:28:SER:HG	1:H:31[A]:GLU:HG3	1.84	0.42
1:C:129:ASP:OD2	1:C:131:LYS:HE2	2.20	0.41
1:E:25:LYS:CB	1:E:27[A]:LEU:HD13	2.49	0.41
1:J:151:LEU:HD21	4:J:488:HOH:O	2.20	0.41
1:C:104:TYR:CD1	1:H:128[A]:LEU:HD21	2.55	0.41
1:F:152:PRO:CG	1:F:154:LYS:HZ3	2.34	0.41
1:A:3:GLN:HB3	1:A:77:MSE:HE3	2.03	0.41
1:I:126:PHE:HE2	1:I:128[A]:LEU:HD22	1.86	0.41
1:E:114:GLU:CG	1:F:1:MSE:HE1	2.36	0.41
1:J:36:THR:HG23	1:J:38:LEU:HB2	2.03	0.41
1:A:152:PRO:CG	1:A:154:LYS:HE2	2.51	0.40
1:J:2:ILE:HD13	1:J:2:ILE:HG21	1.84	0.40
1:C:36:THR:HG21	1:C:43:VAL:HG21	2.03	0.40
1:A:70:ASP:OD1	1:I:24:LYS:HE2	2.21	0.40
1:D:3:GLN:HB3	1:D:77:MSE:HE3	2.03	0.40
1:J:27[B]:LEU:HD23	1:J:31[B]:GLU:CD	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	164/156 (105%)	161 (98%)	3 (2%)	0	100	100
1	B	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
1	C	162/156 (104%)	159 (98%)	3 (2%)	0	100	100
1	D	159/156 (102%)	156 (98%)	3 (2%)	0	100	100
1	E	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
1	F	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	G	161/156 (103%)	158 (98%)	3 (2%)	0	100	100
1	H	158/156 (101%)	155 (98%)	3 (2%)	0	100	100
1	I	156/156 (100%)	152 (97%)	4 (3%)	0	100	100
1	J	160/156 (103%)	157 (98%)	3 (2%)	0	100	100
All	All	1598/1560 (102%)	1567 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/123 (111%)	136 (99%)	1 (1%)	84	73
1	B	133/123 (108%)	131 (98%)	2 (2%)	65	44
1	C	135/123 (110%)	132 (98%)	3 (2%)	52	27
1	D	132/123 (107%)	128 (97%)	4 (3%)	41	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	133/123 (108%)	131 (98%)	2 (2%)	65	44
1	F	131/123 (106%)	129 (98%)	2 (2%)	65	44
1	G	134/123 (109%)	132 (98%)	2 (2%)	65	44
1	H	131/123 (106%)	125 (95%)	6 (5%)	27	6
1	I	129/123 (105%)	128 (99%)	1 (1%)	81	70
1	J	133/123 (108%)	126 (95%)	7 (5%)	22	4
All	All	1328/1230 (108%)	1298 (98%)	30 (2%)	55	25

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	B	60	LEU
1	B	102	GLN
1	C	27[A]	LEU
1	C	27[B]	LEU
1	C	36	THR
1	D	27[A]	LEU
1	D	27[B]	LEU
1	D	102	GLN
1	D	129	ASP
1	E	36	THR
1	E	102	GLN
1	F	27	LEU
1	F	102	GLN
1	G	36	THR
1	G	102	GLN
1	H	27	LEU
1	H	36	THR
1	H	60	LEU
1	H	102	GLN
1	H	128[A]	LEU
1	H	128[B]	LEU
1	I	102	GLN
1	J	27[A]	LEU
1	J	27[B]	LEU
1	J	36	THR
1	J	102	GLN
1	J	127	LYS
1	J	128[A]	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	128[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	102	GLN
1	B	51	GLN
1	B	102	GLN
1	C	51	GLN
1	C	102	GLN
1	D	51	GLN
1	D	102	GLN
1	E	51	GLN
1	E	102	GLN
1	F	51	GLN
1	F	102	GLN
1	G	51	GLN
1	G	102	GLN
1	H	51	GLN
1	H	76	GLN
1	H	102	GLN
1	I	51	GLN
1	I	102	GLN
1	J	51	GLN
1	J	102	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

29 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	SO4	G	202	-	4,4,4	0.56	0	6,6,6	0.74	0
2	SO4	A	201	-	4,4,4	0.49	0	6,6,6	0.86	0
2	SO4	F	201	-	4,4,4	0.52	0	6,6,6	0.85	0
2	SO4	G	201	-	4,4,4	0.55	0	6,6,6	0.97	1 (16%)
2	SO4	D	201	-	4,4,4	0.45	0	6,6,6	0.51	0
2	SO4	A	203[A]	-	4,4,4	1.05	1 (25%)	6,6,6	0.73	0
2	SO4	B	201	-	4,4,4	0.55	0	6,6,6	0.70	0
2	SO4	A	203[B]	-	4,4,4	0.73	0	6,6,6	0.31	0
3	OXL	G	204	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	F	203	-	4,4,4	0.57	0	6,6,6	0.60	0
2	SO4	E	202	-	4,4,4	0.64	0	6,6,6	0.57	0
2	SO4	F	204	-	4,4,4	0.49	0	6,6,6	0.87	0
2	SO4	C	201	-	4,4,4	0.69	0	6,6,6	1.32	0
2	SO4	E	201	-	4,4,4	0.66	0	6,6,6	0.91	0
2	SO4	B	202	-	4,4,4	0.60	0	6,6,6	0.95	0
2	SO4	D	203	-	4,4,4	0.45	0	6,6,6	1.10	0
3	OXL	C	202	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	J	203	-	4,4,4	0.52	0	6,6,6	0.85	0
2	SO4	A	202	-	4,4,4	0.45	0	6,6,6	1.07	0
3	OXL	J	201	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	I	202	-	4,4,4	0.50	0	6,6,6	0.44	0
2	SO4	D	202	-	4,4,4	0.84	0	6,6,6	0.55	0
2	SO4	J	202	-	4,4,4	0.63	0	6,6,6	0.91	0
2	SO4	H	202	-	4,4,4	0.51	0	6,6,6	0.39	0
2	SO4	I	201	-	4,4,4	0.59	0	6,6,6	1.06	0
2	SO4	H	201	-	4,4,4	0.76	0	6,6,6	0.73	0
3	OXL	F	202	-	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	B	203	-	0,5,5	0.00	-	0,6,6	0.00	-
2	SO4	G	203	-	4,4,4	0.53	0	6,6,6	0.72	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
3	OXL	C	202	-	-	0/0/4/4	-
3	OXL	B	203	-	-	0/0/4/4	-
3	OXL	G	204	-	-	0/0/4/4	-
3	OXL	J	201	-	-	0/0/4/4	-
3	OXL	F	202	-	-	0/0/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203[A]	SO4	O2-S	2.00	1.56	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	SO4	O4-S-O3	2.02	117.69	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	204	SO4	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	152/156 (97%)	-0.38	2 (1%) 77 80	6, 12, 20, 38	0
1	B	152/156 (97%)	-0.45	2 (1%) 77 80	7, 11, 20, 38	0
1	C	152/156 (97%)	-0.45	2 (1%) 77 80	7, 11, 21, 37	0
1	D	152/156 (97%)	-0.42	0 100 100	7, 12, 21, 26	0
1	E	152/156 (97%)	-0.44	0 100 100	7, 12, 21, 25	0
1	F	152/156 (97%)	-0.39	1 (0%) 87 89	7, 13, 23, 33	0
1	G	152/156 (97%)	-0.35	2 (1%) 77 80	7, 12, 22, 37	0
1	H	152/156 (97%)	-0.20	3 (1%) 65 67	6, 13, 28, 36	0
1	I	152/156 (97%)	-0.39	2 (1%) 77 80	7, 12, 24, 37	0
1	J	152/156 (97%)	-0.39	2 (1%) 77 80	7, 12, 21, 36	0
All	All	1520/1560 (97%)	-0.39	16 (1%) 80 83	6, 12, 22, 38	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	PRO	4.0
1	A	136	PRO	3.8
1	B	136	PRO	3.1
1	C	137	GLU	3.0
1	H	66	ASP	2.9
1	I	137	GLU	2.9
1	H	60	LEU	2.9
1	J	137	GLU	2.7
1	I	136	PRO	2.4
1	F	137	GLU	2.3
1	H	67	LEU	2.3
1	A	137	GLU	2.3
1	G	136	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	66	ASP	2.1
1	G	137	GLU	2.1
1	B	137	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	E	202	5/5	0.64	0.28	59,59,60,62	0
2	SO4	D	202	5/5	0.76	0.26	58,59,59,60	0
2	SO4	H	202	5/5	0.78	0.24	61,61,62,63	0
2	SO4	J	203	5/5	0.84	0.21	55,55,56,57	0
2	SO4	I	202	5/5	0.84	0.27	58,60,60,61	0
2	SO4	F	204	5/5	0.90	0.22	60,61,61,61	0
2	SO4	A	203[B]	5/5	0.91	0.17	21,21,23,23	5
2	SO4	A	203[A]	5/5	0.91	0.17	27,29,30,32	5
3	OXL	J	201	6/6	0.91	0.16	7,15,17,17	0
2	SO4	G	203	5/5	0.92	0.15	44,45,46,46	0
3	OXL	F	202	6/6	0.93	0.12	9,16,16,17	0
3	OXL	B	203	6/6	0.93	0.11	8,15,15,17	0
3	OXL	C	202	6/6	0.93	0.12	7,14,15,15	0
3	OXL	G	204	6/6	0.94	0.12	6,15,16,16	0
2	SO4	J	202	5/5	0.96	0.20	29,32,35,36	0
2	SO4	B	202	5/5	0.96	0.18	25,32,33,34	0
2	SO4	H	201	5/5	0.96	0.18	33,35,38,38	0
2	SO4	I	201	5/5	0.97	0.20	28,30,34,34	0
2	SO4	F	203	5/5	0.97	0.18	35,37,39,40	0
2	SO4	A	201	5/5	0.97	0.14	23,25,29,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	G	202	5/5	0.97	0.19	32,32,35,36	0
2	SO4	C	201	5/5	0.97	0.17	25,31,32,33	0
2	SO4	E	201	5/5	0.98	0.20	27,30,33,33	0
2	SO4	D	201	5/5	0.98	0.16	24,26,30,31	0
2	SO4	G	201	5/5	0.99	0.15	23,27,28,28	0
2	SO4	D	203	5/5	0.99	0.13	23,27,29,30	0
2	SO4	B	201	5/5	0.99	0.20	21,27,28,29	0
2	SO4	F	201	5/5	0.99	0.17	24,27,30,31	0
2	SO4	A	202	5/5	0.99	0.16	22,26,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.