



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:17 PM UTC

PDB ID : 2QL3 / pdb_00002ql3
Title : Crystal structure of the C-terminal domain of a probable LysR family transcriptional regulator from *Rhodococcus* sp. RHA1
Authors : Tan, K.; Skarina, T.; Kagen, O.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-07-12
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

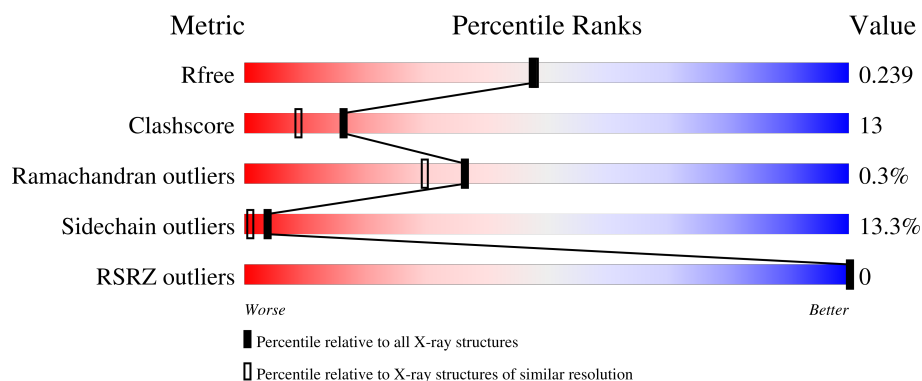
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

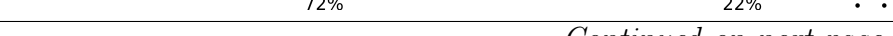
The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	209	
1	B	209	
1	C	209	
1	D	209	
1	E	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	209	 74%18%6% .
1	G	209	 65%23%9% ..
1	H	209	 70%21%5% ..
1	I	209	 74%20% ..
1	J	209	 72%22% . .
1	K	209	 71%20%6% ..
1	L	209	 70%24% . .

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	PO4	B	1670	-	-	X	-
2	PO4	H	1631	-	-	X	-
2	PO4	K	1669	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20701 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 Probable transcriptional regulator, LysR family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	Se	0	0	0
			1574	1009	274	284	2	5			
1	B	205	Total	C	N	O	S	Se	0	1	0
			1578	1013	274	284	2	5			
1	C	205	Total	C	N	O	S	Se	0	3	0
			1588	1022	274	284	2	6			
1	D	205	Total	C	N	O	S	Se	0	2	0
			1583	1018	274	284	2	5			
1	E	205	Total	C	N	O	S	Se	0	5	0
			1599	1030	277	284	2	6			
1	F	205	Total	C	N	O	S	Se	0	2	0
			1584	1019	274	284	2	5			
1	G	205	Total	C	N	O	S	Se	0	0	0
			1574	1009	274	284	2	5			
1	H	205	Total	C	N	O	S	Se	0	1	0
			1579	1013	274	284	2	6			
1	I	205	Total	C	N	O	S	Se	0	0	0
			1574	1009	274	284	2	5			
1	J	205	Total	C	N	O	S	Se	0	1	0
			1578	1013	274	284	2	5			
1	K	205	Total	C	N	O	S	Se	0	1	0
			1579	1013	274	284	2	6			
1	L	205	Total	C	N	O	S	Se	0	1	0
			1582	1015	275	285	2	5			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	GLY	-	cloning artifact	UNP Q0SFM8
A	98	HIS	-	cloning artifact	UNP Q0SFM8
A	119	MSE	MET	modified residue	UNP Q0SFM8
A	171	MSE	MET	modified residue	UNP Q0SFM8
A	176	MSE	MET	modified residue	UNP Q0SFM8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MSE	MET	modified residue	UNP Q0SFM8
A	215	MSE	MET	modified residue	UNP Q0SFM8
A	304	GLY	-	cloning artifact	UNP Q0SFM8
A	305	SER	-	cloning artifact	UNP Q0SFM8
B	97	GLY	-	cloning artifact	UNP Q0SFM8
B	98	HIS	-	cloning artifact	UNP Q0SFM8
B	119	MSE	MET	modified residue	UNP Q0SFM8
B	171	MSE	MET	modified residue	UNP Q0SFM8
B	176	MSE	MET	modified residue	UNP Q0SFM8
B	202	MSE	MET	modified residue	UNP Q0SFM8
B	215	MSE	MET	modified residue	UNP Q0SFM8
B	304	GLY	-	cloning artifact	UNP Q0SFM8
B	305	SER	-	cloning artifact	UNP Q0SFM8
C	97	GLY	-	cloning artifact	UNP Q0SFM8
C	98	HIS	-	cloning artifact	UNP Q0SFM8
C	119	MSE	MET	modified residue	UNP Q0SFM8
C	171	MSE	MET	modified residue	UNP Q0SFM8
C	176	MSE	MET	modified residue	UNP Q0SFM8
C	202	MSE	MET	modified residue	UNP Q0SFM8
C	215	MSE	MET	modified residue	UNP Q0SFM8
C	304	GLY	-	cloning artifact	UNP Q0SFM8
C	305	SER	-	cloning artifact	UNP Q0SFM8
D	97	GLY	-	cloning artifact	UNP Q0SFM8
D	98	HIS	-	cloning artifact	UNP Q0SFM8
D	119	MSE	MET	modified residue	UNP Q0SFM8
D	171	MSE	MET	modified residue	UNP Q0SFM8
D	176	MSE	MET	modified residue	UNP Q0SFM8
D	202	MSE	MET	modified residue	UNP Q0SFM8
D	215	MSE	MET	modified residue	UNP Q0SFM8
D	304	GLY	-	cloning artifact	UNP Q0SFM8
D	305	SER	-	cloning artifact	UNP Q0SFM8
E	97	GLY	-	cloning artifact	UNP Q0SFM8
E	98	HIS	-	cloning artifact	UNP Q0SFM8
E	119	MSE	MET	modified residue	UNP Q0SFM8
E	171	MSE	MET	modified residue	UNP Q0SFM8
E	176	MSE	MET	modified residue	UNP Q0SFM8
E	202	MSE	MET	modified residue	UNP Q0SFM8
E	215	MSE	MET	modified residue	UNP Q0SFM8
E	304	GLY	-	cloning artifact	UNP Q0SFM8
E	305	SER	-	cloning artifact	UNP Q0SFM8
F	97	GLY	-	cloning artifact	UNP Q0SFM8
F	98	HIS	-	cloning artifact	UNP Q0SFM8

Continued on next page...

Continued from previous page...

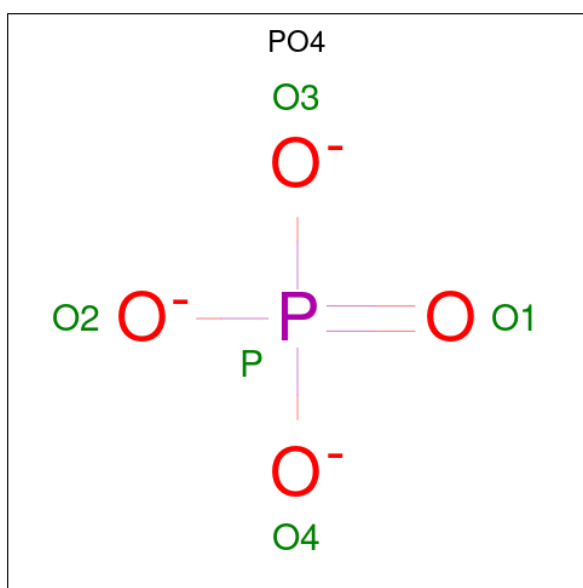
Chain	Residue	Modelled	Actual	Comment	Reference
F	119	MSE	MET	modified residue	UNP Q0SFM8
F	171	MSE	MET	modified residue	UNP Q0SFM8
F	176	MSE	MET	modified residue	UNP Q0SFM8
F	202	MSE	MET	modified residue	UNP Q0SFM8
F	215	MSE	MET	modified residue	UNP Q0SFM8
F	304	GLY	-	cloning artifact	UNP Q0SFM8
F	305	SER	-	cloning artifact	UNP Q0SFM8
G	97	GLY	-	cloning artifact	UNP Q0SFM8
G	98	HIS	-	cloning artifact	UNP Q0SFM8
G	119	MSE	MET	modified residue	UNP Q0SFM8
G	171	MSE	MET	modified residue	UNP Q0SFM8
G	176	MSE	MET	modified residue	UNP Q0SFM8
G	202	MSE	MET	modified residue	UNP Q0SFM8
G	215	MSE	MET	modified residue	UNP Q0SFM8
G	304	GLY	-	cloning artifact	UNP Q0SFM8
G	305	SER	-	cloning artifact	UNP Q0SFM8
H	97	GLY	-	cloning artifact	UNP Q0SFM8
H	98	HIS	-	cloning artifact	UNP Q0SFM8
H	119	MSE	MET	modified residue	UNP Q0SFM8
H	171	MSE	MET	modified residue	UNP Q0SFM8
H	176	MSE	MET	modified residue	UNP Q0SFM8
H	202	MSE	MET	modified residue	UNP Q0SFM8
H	215	MSE	MET	modified residue	UNP Q0SFM8
H	304	GLY	-	cloning artifact	UNP Q0SFM8
H	305	SER	-	cloning artifact	UNP Q0SFM8
I	97	GLY	-	cloning artifact	UNP Q0SFM8
I	98	HIS	-	cloning artifact	UNP Q0SFM8
I	119	MSE	MET	modified residue	UNP Q0SFM8
I	171	MSE	MET	modified residue	UNP Q0SFM8
I	176	MSE	MET	modified residue	UNP Q0SFM8
I	202	MSE	MET	modified residue	UNP Q0SFM8
I	215	MSE	MET	modified residue	UNP Q0SFM8
I	304	GLY	-	cloning artifact	UNP Q0SFM8
I	305	SER	-	cloning artifact	UNP Q0SFM8
J	97	GLY	-	cloning artifact	UNP Q0SFM8
J	98	HIS	-	cloning artifact	UNP Q0SFM8
J	119	MSE	MET	modified residue	UNP Q0SFM8
J	171	MSE	MET	modified residue	UNP Q0SFM8
J	176	MSE	MET	modified residue	UNP Q0SFM8
J	202	MSE	MET	modified residue	UNP Q0SFM8
J	215	MSE	MET	modified residue	UNP Q0SFM8
J	304	GLY	-	cloning artifact	UNP Q0SFM8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	305	SER	-	cloning artifact	UNP Q0SFM8
K	97	GLY	-	cloning artifact	UNP Q0SFM8
K	98	HIS	-	cloning artifact	UNP Q0SFM8
K	119	MSE	MET	modified residue	UNP Q0SFM8
K	171	MSE	MET	modified residue	UNP Q0SFM8
K	176	MSE	MET	modified residue	UNP Q0SFM8
K	202	MSE	MET	modified residue	UNP Q0SFM8
K	215	MSE	MET	modified residue	UNP Q0SFM8
K	304	GLY	-	cloning artifact	UNP Q0SFM8
K	305	SER	-	cloning artifact	UNP Q0SFM8
L	97	GLY	-	cloning artifact	UNP Q0SFM8
L	98	HIS	-	cloning artifact	UNP Q0SFM8
L	119	MSE	MET	modified residue	UNP Q0SFM8
L	171	MSE	MET	modified residue	UNP Q0SFM8
L	176	MSE	MET	modified residue	UNP Q0SFM8
L	202	MSE	MET	modified residue	UNP Q0SFM8
L	215	MSE	MET	modified residue	UNP Q0SFM8
L	304	GLY	-	cloning artifact	UNP Q0SFM8
L	305	SER	-	cloning artifact	UNP Q0SFM8

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	118	Total	O	0	0
			118	118		
3	C	67	Total	O	0	0
			67	67		
3	D	90	Total	O	0	0
			90	90		
3	E	122	Total	O	0	0
			122	122		
3	F	109	Total	O	0	0
			109	109		
3	G	81	Total	O	0	0
			81	81		
3	H	93	Total	O	0	0
			93	93		

Continued on next page...

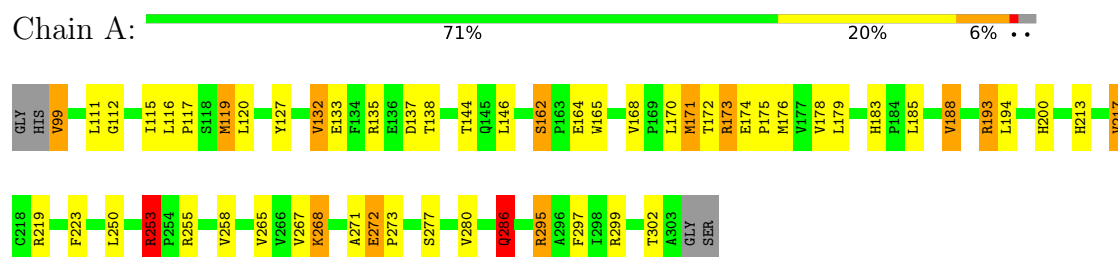
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	135	Total 135	O 135	0	0
3	J	130	Total 130	O 130	0	0
3	K	121	Total 121	O 121	0	0
3	L	167	Total 167	O 167	0	0

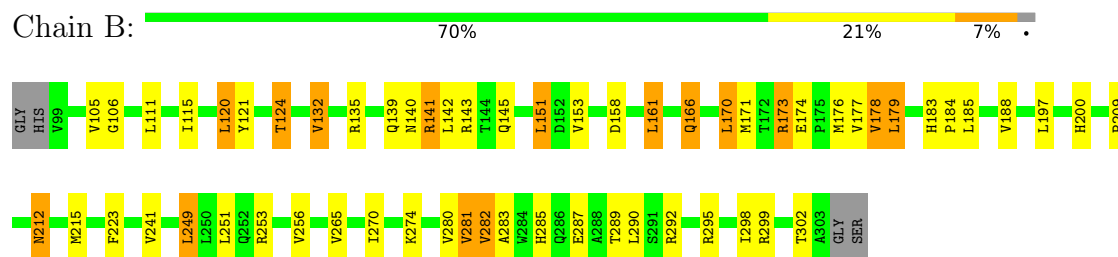
3 Residue-property plots

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.

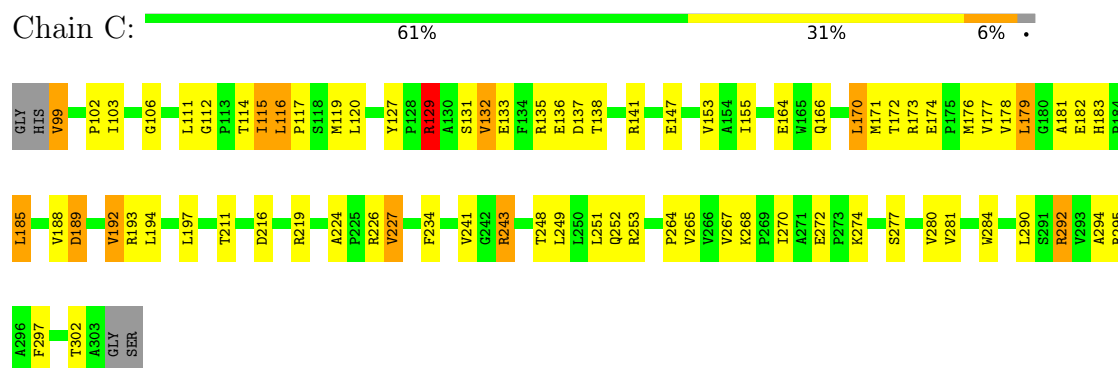
- Molecule 1: Probable transcriptional regulator, LysR family protein



- Molecule 1: Probable transcriptional regulator, LysR family protein



- Molecule 1: Probable transcriptional regulator, LysR family protein



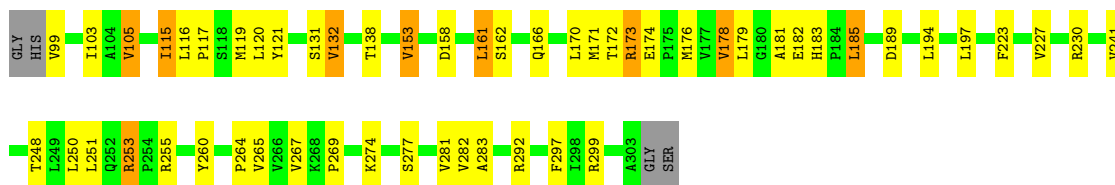
- Molecule 1: Probable transcriptional regulator, LysR family protein





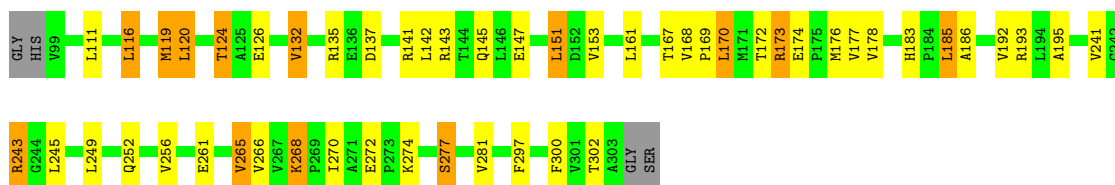
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain E: 72% 22% . .



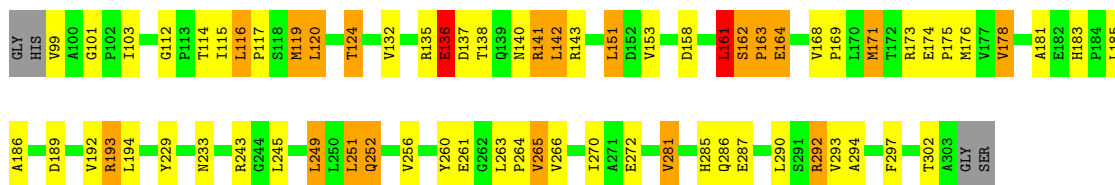
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain F: 74% 18% 6% .



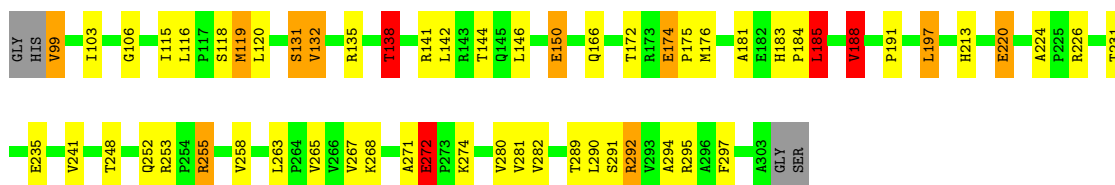
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain G: 65% 23% 9% . .



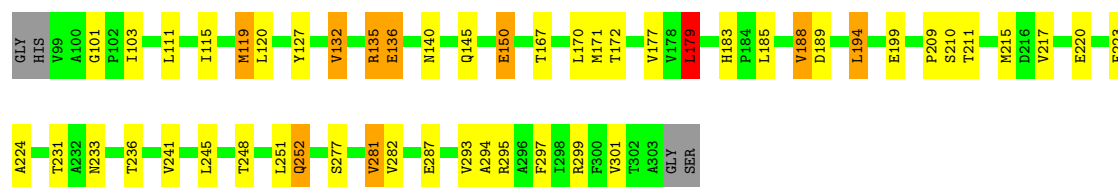
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain H: 70% 21% 5% . .



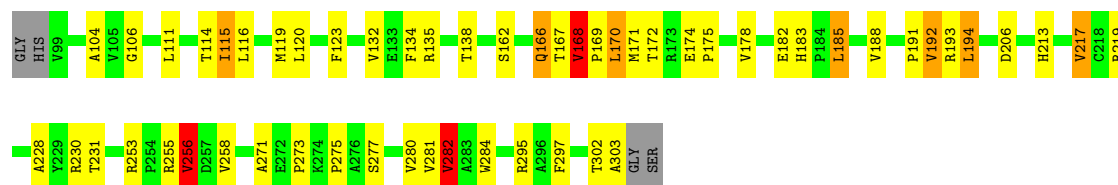
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain I:  74% 20% ..



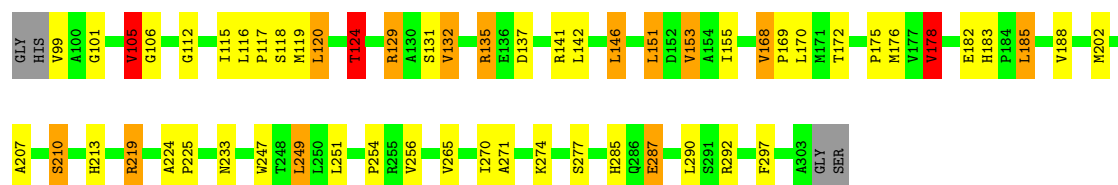
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain J:  72% 22% ...



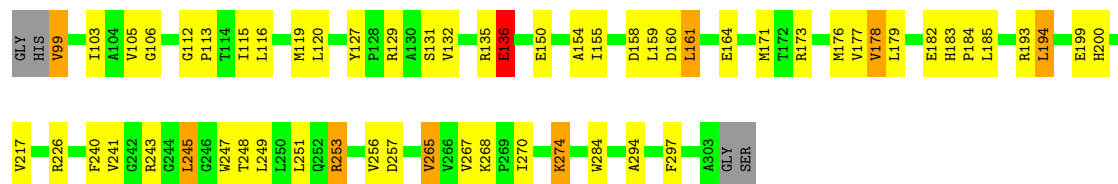
- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain K:  71% 20% 6% ..



- Molecule 1: Probable transcriptional regulator, LysR family protein

Chain L:  70% 24% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	114.28Å 114.28Å 175.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.60 – 2.05 36.60 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.60-2.05) 99.3 (36.60-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.239 0.177 , 0.239	Depositor DCC
R_{free} test set	7989 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.036 for h,-h-k,-l 0.059 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20701	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.15	0/1610	1.18	2/2199 (0.1%)
1	B	1.13	3/1617 (0.2%)	1.20	5/2209 (0.2%)
1	C	1.06	0/1633	1.18	7/2230 (0.3%)
1	D	1.08	1/1625 (0.1%)	1.23	13/2220 (0.6%)
1	E	1.17	2/1650 (0.1%)	1.19	4/2254 (0.2%)
1	F	1.16	1/1626 (0.1%)	1.20	5/2221 (0.2%)
1	G	1.05	1/1610 (0.1%)	1.22	8/2199 (0.4%)
1	H	1.13	1/1618 (0.1%)	1.22	10/2209 (0.5%)
1	I	1.25	0/1610	1.31	16/2199 (0.7%)
1	J	1.20	5/1617 (0.3%)	1.17	6/2209 (0.3%)
1	K	1.19	2/1618 (0.1%)	1.31	13/2209 (0.6%)
1	L	1.24	4/1618 (0.2%)	1.27	8/2210 (0.4%)
All	All	1.15	20/19452 (0.1%)	1.22	97/26568 (0.4%)

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	0	1
1	G	0	3
All	All	0	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	115	ILE	CA-CB	7.49	1.63	1.55
1	G	178	VAL	CA-CB	6.83	1.63	1.54
1	E	227	VAL	CA-CB	6.68	1.61	1.53
1	J	228	ALA	CA-CB	6.32	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	VAL	CA-CB	6.19	1.61	1.54
1	L	178	VAL	CA-CB	6.13	1.62	1.54
1	K	105	VAL	CA-CB	6.04	1.61	1.54
1	J	282	VAL	CA-CB	5.68	1.61	1.54
1	J	138	THR	CA-CB	5.66	1.62	1.53
1	J	192	VAL	CA-CB	5.66	1.61	1.54
1	K	178	VAL	CA-CB	5.65	1.61	1.54
1	J	104	ALA	CA-CB	5.65	1.61	1.53
1	L	257	ASP	N-CA	5.60	1.54	1.46
1	H	282	VAL	CA-CB	5.46	1.61	1.54
1	B	132	VAL	CA-CB	5.36	1.60	1.54
1	L	150	GLU	C-O	-5.22	1.17	1.24
1	F	241	VAL	CA-C	5.19	1.59	1.52
1	E	297	PHE	C-O	-5.11	1.18	1.24
1	B	105	VAL	CA-CB	5.05	1.60	1.54
1	B	253	ARG	C-O	-5.02	1.21	1.25

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	271	ALA	CA-C-N	-9.76	111.16	123.16
1	K	271	ALA	C-N-CA	-9.76	111.16	123.16
1	K	101	GLY	CA-C-N	9.40	129.16	119.76
1	K	101	GLY	C-N-CA	9.40	129.16	119.76
1	F	132	VAL	N-CA-C	7.54	119.14	108.36
1	I	132	VAL	N-CA-C	7.46	119.31	108.58
1	E	162	SER	CA-C-N	7.19	127.52	119.32
1	E	162	SER	C-N-CA	7.19	127.52	119.32
1	G	178	VAL	CB-CA-C	6.99	120.54	110.33
1	G	101	GLY	CA-C-N	6.87	126.83	119.76
1	G	101	GLY	C-N-CA	6.87	126.83	119.76
1	L	178	VAL	CB-CA-C	6.82	120.29	110.33
1	F	195	ALA	CA-C-N	-6.81	110.84	122.56
1	F	195	ALA	C-N-CA	-6.81	110.84	122.56
1	G	136	GLU	CB-CA-C	6.71	120.76	109.48
1	C	132	VAL	N-CA-C	6.71	117.70	107.77
1	I	210	SER	N-CA-C	6.69	119.43	111.33
1	K	115	ILE	N-CA-C	-6.58	106.57	111.90
1	I	136	GLU	CB-CA-C	6.52	120.67	109.51
1	C	127	TYR	CA-C-N	-6.47	113.63	120.03
1	C	127	TYR	C-N-CA	-6.47	113.63	120.03
1	H	185	LEU	N-CA-C	6.46	120.48	112.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	136	GLU	CB-CA-C	6.39	120.88	109.38
1	D	100	ALA	N-CA-C	6.32	118.47	108.79
1	H	181	ALA	CA-C-N	6.32	131.27	120.72
1	H	181	ALA	C-N-CA	6.32	131.27	120.72
1	K	210	SER	N-CA-C	6.30	118.95	111.33
1	D	227	VAL	N-CA-C	6.21	117.36	107.98
1	L	105	VAL	CA-C-N	-6.20	116.96	122.47
1	L	105	VAL	C-N-CA	-6.20	116.96	122.47
1	J	255	ARG	CA-C-N	-6.19	115.52	123.19
1	J	255	ARG	C-N-CA	-6.19	115.52	123.19
1	G	265	VAL	CB-CA-C	6.17	120.00	110.50
1	H	138	THR	N-CA-CB	-6.16	100.99	110.04
1	B	170	LEU	N-CA-C	-6.15	105.81	113.55
1	H	255	ARG	N-CA-C	6.14	118.77	111.71
1	D	211	THR	N-CA-C	6.03	117.55	110.97
1	L	265	VAL	CB-CA-C	6.00	119.51	110.63
1	H	224	ALA	CA-C-N	-5.99	113.51	119.92
1	H	224	ALA	C-N-CA	-5.99	113.51	119.92
1	I	189	ASP	CA-C-N	-5.98	112.48	121.87
1	I	189	ASP	C-N-CA	-5.98	112.48	121.87
1	B	212	ASN	N-CA-CB	5.91	120.20	110.39
1	B	282	VAL	CB-CA-C	-5.85	103.65	110.91
1	D	262	GLY	N-CA-C	-5.77	107.21	115.64
1	K	131	SER	CA-C-N	-5.76	114.94	122.37
1	K	131	SER	C-N-CA	-5.76	114.94	122.37
1	I	127	TYR	CA-C-N	5.74	125.42	119.56
1	I	127	TYR	C-N-CA	5.74	125.42	119.56
1	J	256	VAL	CB-CA-C	5.74	119.38	110.83
1	F	116	LEU	CA-C-N	-5.74	113.00	118.97
1	F	116	LEU	C-N-CA	-5.74	113.00	118.97
1	D	173	ARG	N-CA-C	5.71	117.95	108.99
1	A	253	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	170	LEU	N-CA-C	-5.67	106.50	113.41
1	A	132	VAL	N-CA-C	5.62	116.67	108.58
1	D	116	LEU	CA-C-N	-5.60	113.14	118.97
1	D	116	LEU	C-N-CA	-5.60	113.14	118.97
1	L	193	ARG	CB-CA-C	5.54	119.47	110.22
1	L	253	ARG	CA-C-N	-5.53	114.09	119.78
1	L	253	ARG	C-N-CA	-5.53	114.09	119.78
1	I	220	GLU	CA-CB-CG	5.52	125.14	114.10
1	K	271	ALA	N-CA-C	5.50	121.55	114.56
1	H	188	VAL	N-CA-C	5.49	116.14	108.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	101	GLY	CA-C-N	5.48	125.24	119.76
1	I	101	GLY	C-N-CA	5.48	125.24	119.76
1	H	116	LEU	N-CA-C	5.47	120.93	113.16
1	C	116	LEU	CA-C-N	-5.44	113.31	118.97
1	C	116	LEU	C-N-CA	-5.44	113.31	118.97
1	J	168	VAL	CB-CA-C	5.43	116.54	110.52
1	J	162	SER	CA-C-N	-5.42	114.43	120.45
1	J	162	SER	C-N-CA	-5.42	114.43	120.45
1	D	189	ASP	N-CA-C	5.41	122.32	110.80
1	E	223	PHE	N-CA-C	5.40	117.28	109.07
1	I	281	VAL	N-CA-CB	-5.38	101.97	111.93
1	K	124	THR	OG1-CB-CG2	5.38	120.05	109.30
1	G	192	VAL	N-CA-C	5.37	115.69	108.17
1	E	260	TYR	N-CA-C	5.36	117.81	111.33
1	D	212	ASN	N-CA-C	-5.35	105.45	111.28
1	D	265	VAL	N-CA-CB	-5.34	104.04	111.41
1	K	132	VAL	CB-CA-C	5.29	117.47	110.91
1	C	227	VAL	CB-CA-C	5.25	117.31	110.96
1	D	265	VAL	CB-CA-C	5.24	118.39	110.63
1	K	178	VAL	CB-CA-C	5.19	117.91	110.33
1	D	203	VAL	N-CA-C	-5.17	100.44	107.99
1	B	281	VAL	N-CA-CB	-5.16	102.99	111.45
1	I	233	ASN	CA-C-N	5.14	127.48	120.54
1	I	233	ASN	C-N-CA	5.14	127.48	120.54
1	G	116	LEU	CA-C-N	-5.10	113.66	118.97
1	G	116	LEU	C-N-CA	-5.10	113.66	118.97
1	I	179	LEU	CA-C-N	5.10	125.75	120.60
1	I	179	LEU	C-N-CA	5.10	125.75	120.60
1	K	219	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	H	272	GLU	N-CA-C	5.03	120.92	109.81
1	B	223	PHE	N-CA-C	5.03	116.63	109.14
1	I	140	ASN	N-CA-C	5.03	116.76	111.28
1	D	115	ILE	N-CA-C	5.00	118.46	113.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	129	ARG	Peptide
1	G	161	LEU	Peptide
1	G	162	SER	Peptide
1	G	163	PRO	Peptide

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	1574	0	1580	49	0
1	B	1578	0	1589	42	0
1	C	1588	0	1609	47	0
1	D	1583	0	1600	56	0
1	E	1599	0	1629	37	0
1	F	1584	0	1602	38	0
1	G	1574	0	1580	54	0
1	H	1579	0	1589	47	0
1	I	1574	0	1580	32	0
1	J	1578	0	1589	41	0
1	K	1579	0	1589	50	0
1	L	1582	0	1590	35	0
2	A	30	0	0	2	0
2	B	25	0	0	4	0
2	C	30	0	0	3	0
2	D	25	0	0	2	0
2	E	15	0	0	2	0
2	F	70	0	0	3	0
2	G	15	0	0	1	0
2	H	20	0	0	4	0
2	I	35	0	0	0	0
2	J	35	0	0	1	0
2	K	50	0	0	5	0
2	L	30	0	0	1	0
3	A	116	0	0	7	0
3	B	118	0	0	0	0
3	C	67	0	0	1	0
3	D	90	0	0	0	0
3	E	122	0	0	1	0
3	F	109	0	0	3	0
3	G	81	0	0	3	0
3	H	93	0	0	2	0
3	I	135	0	0	7	0
3	J	130	0	0	0	0
3	K	121	0	0	2	0
3	L	167	0	0	2	0
All	All	20701	0	19126	499	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 13.

All (499) 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:K:202:MSE:HE2	1:K:247:TRP:CH2	1.75	1.20
1:H:119:MSE:HE3	1:H:297:PHE:HZ	1.18	1.06
1:E:170:LEU:HD11	1:E:282:VAL:CG2	1.87	1.05
1:D:219:ARG:HG2	1:D:219:ARG:HH11	0.88	1.04
1:C:119:MSE:HE3	1:C:297:PHE:HZ	1.21	1.04
1:D:173:ARG:NH1	2:D:1660:PO4:O3	1.94	1.01
1:H:119:MSE:HE3	1:H:297:PHE:CZ	1.95	1.01
1:D:119:MSE:HE1	1:D:155:ILE:HG13	1.39	1.00
1:G:162:SER:OG	1:G:164:GLU:HB3	1.59	1.00
1:K:202:MSE:HE3	1:K:225:PRO:HB3	1.42	0.99
1:E:170:LEU:HD11	1:E:282:VAL:HG23	1.42	0.99
1:K:183:HIS:HD2	1:K:185:LEU:H	1.10	0.97
1:K:202:MSE:HE3	1:K:225:PRO:CB	1.94	0.96
1:E:176[A]:MSE:SE	1:E:253[A]:ARG:HG3	2.17	0.95
1:J:167:THR:HB	1:J:281[A]:VAL:HG21	1.48	0.94
1:D:219:ARG:HH11	1:D:219:ARG:CG	1.80	0.93
1:A:193:ARG:HE	1:A:272:GLU:HG3	1.34	0.93
1:D:219:ARG:HG2	1:D:219:ARG:NH1	1.67	0.93
1:K:116:LEU:HD13	1:K:119:MSE:HE2	1.49	0.92
1:G:161:LEU:HD22	1:G:161:LEU:H	1.32	0.92
1:A:183:HIS:HD2	1:A:185:LEU:H	1.22	0.88
1:C:119:MSE:HE3	1:C:297:PHE:CZ	2.08	0.87
1:H:119:MSE:CE	1:H:297:PHE:HZ	1.88	0.86
1:E:170:LEU:CD1	1:E:282:VAL:HG23	2.05	0.86
1:D:119:MSE:HE1	1:D:155:ILE:CG1	2.04	0.86
1:K:202:MSE:CE	1:K:225:PRO:HB3	2.07	0.84
1:H:191:PRO:HB2	1:H:271:ALA:HB2	1.61	0.83
1:J:167:THR:HB	1:J:281[A]:VAL:CG2	2.09	0.82
1:A:119:MSE:HE3	1:A:297:PHE:HZ	1.45	0.82
1:E:183:HIS:HD2	1:E:185:LEU:H	1.25	0.82
1:B:178:VAL:HG23	1:B:265[A]:VAL:HG13	1.62	0.81
1:K:119:MSE:HE3	1:K:297:PHE:HZ	1.44	0.81
1:E:194:LEU:HD12	1:E:197:LEU:HD12	1.61	0.81
1:F:176:MSE:HG2	3:F:1719:HOH:O	1.81	0.80
1:K:202:MSE:HE2	1:K:247:TRP:HH2	1.41	0.80
1:K:183:HIS:CD2	1:K:185:LEU:H	1.98	0.80
1:H:183:HIS:CD2	1:H:185:LEU:HD22	2.17	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:MSE:CE	1:K:225:PRO:CB	2.60	0.79
1:F:268:LYS:NZ	2:F:1675:PO4:O1	2.16	0.78
1:J:183:HIS:HD2	1:J:185:LEU:H	1.32	0.78
1:E:178[A]:VAL:HG22	1:E:248:THR:HG22	1.66	0.77
1:I:183:HIS:HD2	1:I:185:LEU:H	1.30	0.77
1:C:189:ASP:OD2	1:C:189:ASP:N	2.16	0.77
1:B:183:HIS:HD2	1:B:185:LEU:H	1.30	0.77
1:G:158:ASP:HA	1:G:161:LEU:HD11	1.67	0.77
1:B:173:ARG:NH1	2:B:1670:PO4:P	2.58	0.76
1:K:119:MSE:HE1	1:K:155:ILE:HG13	1.67	0.76
1:D:119:MSE:HE3	1:D:297:PHE:CZ	2.21	0.76
1:F:173:ARG:HD2	1:F:176:MSE:HE2	1.68	0.75
1:B:173:ARG:HH12	2:B:1670:PO4:P	2.09	0.75
1:D:162:SER:OG	1:D:164:GLU:HG3	1.87	0.75
1:D:191:PRO:HB2	1:D:271:ALA:HB2	1.66	0.75
1:K:202:MSE:CE	1:K:247:TRP:CH2	2.65	0.75
1:B:302:THR:HG23	1:J:273:PRO:HB3	1.69	0.74
1:E:172:THR:HG22	1:E:277:SER:HB3	1.69	0.74
1:J:166:GLN:HG2	1:J:284:TRP:CZ2	2.23	0.74
1:D:198:ALA:O	1:D:199:GLU:HB2	1.86	0.74
1:F:126:GLU:HG3	1:F:300:PHE:CE1	2.23	0.74
1:B:173:ARG:NH1	2:B:1670:PO4:O1	2.21	0.74
1:H:183:HIS:HD2	1:H:185:LEU:HD22	1.52	0.73
1:G:119:MSE:HE3	1:G:297:PHE:CZ	2.23	0.73
1:F:120:LEU:O	1:F:124:THR:HB	1.88	0.73
1:C:174:GLU:OE2	1:C:274:LYS:HE2	1.88	0.72
1:B:111:LEU:HD22	1:B:115:ILE:HD12	1.69	0.72
1:B:183:HIS:CD2	1:B:185:LEU:H	2.07	0.72
1:F:183:HIS:HD2	1:F:185:LEU:H	1.38	0.72
1:L:183:HIS:HD2	1:L:185:LEU:H	1.35	0.72
1:D:119:MSE:HE1	1:D:155:ILE:CD1	2.19	0.72
1:H:99:VAL:HA	1:H:292:ARG:HD2	1.72	0.72
1:C:99:VAL:HA	1:C:292:ARG:HH11	1.55	0.71
1:A:119:MSE:HE3	1:A:297:PHE:CZ	2.25	0.71
1:B:111:LEU:HD22	1:B:115:ILE:CD1	2.20	0.71
1:J:119:MSE:HE3	1:J:297:PHE:CZ	2.25	0.71
1:E:115:ILE:HG13	1:E:119:MSE:HE3	1.71	0.71
1:I:119:MSE:HE1	1:I:297:PHE:HZ	1.54	0.71
1:H:174:GLU:OE1	1:H:274:LYS:CE	2.39	0.71
1:H:295:ARG:NH1	2:H:1631:PO4:P	2.64	0.71
1:K:292:ARG:N	2:K:1673:PO4:O3	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:MSE:HE3	1:L:297:PHE:CZ	2.26	0.70
1:G:233:ASN:HB2	3:G:1722:HOH:O	1.91	0.70
1:J:119:MSE:HE3	1:J:297:PHE:HZ	1.56	0.69
1:D:119:MSE:CE	1:D:155:ILE:HG13	2.20	0.69
1:H:99:VAL:HB	1:H:292:ARG:HD2	1.75	0.69
1:C:183:HIS:HD2	1:C:185:LEU:H	1.40	0.69
1:E:178[A]:VAL:HG23	1:E:241:VAL:HG11	1.74	0.69
1:I:183:HIS:HE1	3:I:1696:HOH:O	1.76	0.69
1:I:224:ALA:O	1:K:219:ARG:NH1	2.25	0.69
1:A:175:PRO:HG3	1:A:213:HIS:HE1	1.58	0.68
1:D:183:HIS:HD2	1:D:185:LEU:H	1.40	0.68
1:K:120:LEU:O	1:K:124:THR:HB	1.92	0.68
1:L:99:VAL:HG13	1:L:127:TYR:CE2	2.28	0.68
1:I:119:MSE:CE	1:I:297:PHE:HZ	2.06	0.68
1:E:138:THR:OG1	2:E:1644:PO4:O3	2.12	0.68
1:C:174:GLU:O	1:C:176[A]:MSE:HE2	1.94	0.68
1:A:183:HIS:CD2	1:A:185:LEU:H	2.07	0.67
1:E:115:ILE:HG13	1:E:119:MSE:CE	2.24	0.67
1:K:112:GLY:O	1:K:117:PRO:HD3	1.94	0.67
1:H:103:ILE:HG22	1:H:131:SER:O	1.95	0.67
1:D:173:ARG:NH2	1:D:176:MSE:HE3	2.08	0.67
1:D:168:VAL:HG22	1:D:302:THR:HG21	1.77	0.67
1:H:138:THR:HG22	1:H:141:ARG:H	1.59	0.67
1:H:295:ARG:NH1	2:H:1631:PO4:O1	2.28	0.67
1:B:178:VAL:HG23	1:B:265[A]:VAL:CG1	2.25	0.67
1:E:170:LEU:HD11	1:E:282:VAL:HG22	1.77	0.67
1:G:261:GLU:O	1:H:255:ARG:HD2	1.95	0.66
1:D:100:ALA:O	1:D:293[A]:VAL:HG11	1.95	0.66
1:G:183:HIS:HD2	1:G:185:LEU:H	1.44	0.66
1:G:120:LEU:O	1:G:124:THR:HB	1.96	0.66
1:H:115:ILE:CD1	1:H:280:VAL:HG11	2.26	0.66
1:F:193:ARG:HG2	1:F:272:GLU:OE1	1.96	0.66
1:B:115:ILE:HD13	1:B:280:VAL:HG11	1.78	0.65
1:D:173:ARG:HH21	1:D:176:MSE:CE	2.09	0.65
1:C:99:VAL:HA	1:C:292:ARG:NH1	2.11	0.65
1:H:174:GLU:OE1	1:H:274:LYS:HE2	1.97	0.65
1:L:119:MSE:CE	1:L:297:PHE:HZ	2.09	0.65
1:L:119:MSE:HE3	1:L:297:PHE:HZ	1.60	0.65
1:J:183:HIS:CD2	1:J:185:LEU:H	2.15	0.64
1:B:298:ILE:O	1:B:302:THR:HG22	1.98	0.64
1:H:295:ARG:HH11	2:H:1631:PO4:P	2.21	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:O	1:D:124:THR:HB	1.98	0.63
1:F:170:LEU:CD1	1:F:302:THR:HG22	2.27	0.63
1:A:138:THR:OG1	2:A:1626:PO4:O2	2.15	0.63
1:G:119:MSE:HE3	1:G:297:PHE:HZ	1.63	0.63
1:G:161:LEU:H	1:G:161:LEU:CD2	2.04	0.63
1:D:173:ARG:NH2	1:D:176:MSE:CE	2.61	0.62
1:C:138:THR:OG1	2:C:1607:PO4:O3	2.13	0.62
1:H:185:LEU:HD21	1:H:197:LEU:HD11	1.80	0.62
1:A:188:VAL:O	1:A:268:LYS:HE2	1.99	0.62
1:C:176[A]:MSE:SE	1:C:253:ARG:HB2	2.50	0.62
1:A:175:PRO:HG3	1:A:213:HIS:CE1	2.35	0.62
1:C:177:VAL:HG12	1:C:179:LEU:HD13	1.82	0.62
1:J:119:MSE:CE	1:J:297:PHE:HZ	2.11	0.62
1:G:115:ILE:HD12	1:G:252:GLN:HE22	1.65	0.61
1:K:119:MSE:HE3	1:K:297:PHE:CZ	2.31	0.61
1:K:202:MSE:HE3	1:K:225:PRO:HB2	1.79	0.61
1:A:119:MSE:CE	1:A:297:PHE:HZ	2.13	0.61
1:B:120:LEU:O	1:B:124:THR:HB	2.00	0.61
1:E:170:LEU:CD1	1:E:282:VAL:CG2	2.70	0.61
1:H:174:GLU:OE1	1:H:274:LYS:HE3	1.99	0.61
1:G:175:PRO:HB3	1:G:251:LEU:HD12	1.82	0.61
1:D:173:ARG:HH21	1:D:176:MSE:HE3	1.66	0.61
1:E:178[A]:VAL:HG22	1:E:248:THR:CG2	2.29	0.60
1:L:284:TRP:NE1	2:L:1656:PO4:O1	2.32	0.60
1:D:119:MSE:HE3	1:D:297:PHE:HZ	1.65	0.60
1:H:103:ILE:HD12	1:H:294:ALA:HA	1.82	0.60
1:L:116:LEU:HD13	1:L:119:MSE:HE2	1.84	0.60
1:G:186:ALA:HB1	1:G:266:VAL:HG21	1.84	0.60
1:C:102:PRO:HA	1:C:131:SER:HB3	1.83	0.60
1:I:295:ARG:NH2	1:I:299:ARG:HE	1.99	0.60
1:D:297:PHE:O	1:D:301:VAL:HB	2.01	0.60
1:K:249:LEU:HD21	1:K:270:ILE:HD11	1.84	0.60
1:L:194:LEU:HD13	1:L:270:ILE:HG23	1.84	0.60
1:K:142:LEU:HD23	1:K:142:LEU:C	2.27	0.60
1:E:183:HIS:CD2	1:E:185:LEU:H	2.14	0.59
1:J:302:THR:O	1:J:303:ALA:CB	2.50	0.59
1:K:129:ARG:HD2	1:K:129:ARG:N	2.17	0.59
1:K:105:VAL:HB	1:K:153:VAL:HG12	1.83	0.59
1:K:175:PRO:HG3	1:K:213:HIS:HE1	1.68	0.59
1:I:119:MSE:CE	1:I:297:PHE:CZ	2.85	0.59
1:L:177:VAL:HG22	1:L:249[B]:LEU:HD12	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:HG12	1:B:179:LEU:HD13	1.85	0.59
1:C:115:ILE:HD12	1:C:280:VAL:HG11	1.83	0.59
1:G:229:TYR:HE1	1:H:132:VAL:HG22	1.68	0.59
1:H:176[A]:MSE:SE	1:H:253:ARG:HB2	2.52	0.59
1:B:158:ASP:HA	1:B:161:LEU:HD12	1.84	0.59
1:A:219:ARG:NH2	1:C:226:ARG:HD3	2.19	0.58
1:F:119:MSE:HE3	1:F:297:PHE:CZ	2.38	0.58
1:G:136:GLU:OE1	1:H:231:THR:OG1	2.19	0.58
1:G:119:MSE:CE	1:G:297:PHE:HZ	2.16	0.58
1:A:183:HIS:HE1	3:A:1729:HOH:O	1.85	0.58
1:I:231:THR:HG21	1:I:236:THR:HG22	1.86	0.58
1:C:177:VAL:HG23	1:C:270:ILE:HG12	1.86	0.57
1:F:170:LEU:HD12	1:F:302:THR:HG22	1.83	0.57
1:H:188:VAL:O	1:H:268:LYS:NZ	2.36	0.57
1:I:183:HIS:CD2	1:I:185:LEU:H	2.18	0.57
1:H:106:GLY:HA2	1:H:135:ARG:O	2.04	0.57
1:I:231:THR:HG22	1:J:134:PHE:HE1	1.68	0.57
1:K:116:LEU:HD13	1:K:119:MSE:CE	2.31	0.57
1:F:119:MSE:CE	1:F:297:PHE:HZ	2.17	0.57
1:G:103:ILE:HD12	1:G:294:ALA:HA	1.86	0.57
1:I:103:ILE:HD12	1:I:294:ALA:HA	1.85	0.57
1:G:114:THR:HG21	1:G:252:GLN:HG2	1.87	0.57
1:B:140:ASN:OD1	1:B:143:ARG:NH2	2.38	0.57
1:L:171:MSE:HE1	3:L:1754:HOH:O	2.05	0.56
1:A:172:THR:CG2	1:A:277:SER:HB3	2.35	0.56
1:I:135:ARG:HG3	3:I:1790:HOH:O	2.04	0.56
1:A:168:VAL:HG11	1:A:302:THR:HG21	1.87	0.56
1:I:119:MSE:HE3	1:I:297:PHE:CZ	2.40	0.56
1:J:168:VAL:HG13	1:J:282:VAL:HG13	1.87	0.56
1:L:99:VAL:HG13	1:L:127:TYR:CD2	2.40	0.56
1:A:115:ILE:HD11	1:A:171:MSE:SE	2.55	0.56
1:A:172:THR:HG22	1:A:277:SER:HB3	1.87	0.56
1:G:164:GLU:HG3	1:G:285:HIS:HE1	1.69	0.56
1:B:197:LEU:HA	1:B:200:HIS:HD2	1.70	0.56
1:G:302:THR:O	1:G:302:THR:HG22	2.04	0.56
1:C:193:ARG:HD3	1:C:272:GLU:OE2	2.04	0.56
1:K:146:LEU:HD12	1:K:151:LEU:HB3	1.88	0.56
1:L:199:GLU:O	1:L:226:ARG:NH1	2.39	0.56
1:H:99:VAL:HA	1:H:292:ARG:CD	2.35	0.56
1:A:173:ARG:NH2	1:A:253:ARG:H	2.04	0.55
1:G:164:GLU:CG	1:G:285:HIS:CE1	2.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:NH2	2:B:1651:PO4:O1	2.40	0.55
1:F:126:GLU:HG3	1:F:300:PHE:HE1	1.71	0.55
1:E:178[A]:VAL:CG2	1:E:248:THR:HG22	2.34	0.55
1:G:249:LEU:HD21	1:G:270:ILE:HD11	1.89	0.55
1:A:213:HIS:O	1:A:217:VAL:HG13	2.06	0.55
1:J:114:THR:OG1	1:J:115:ILE:HD12	2.07	0.55
1:J:302:THR:O	1:J:303:ALA:HB2	2.07	0.55
1:K:142:LEU:HD23	1:K:142:LEU:O	2.06	0.55
1:F:183:HIS:CD2	1:F:185:LEU:H	2.21	0.55
1:E:176[B]:MSE:HG2	1:E:269:PRO:HA	1.89	0.54
1:L:183:HIS:CD2	1:L:185:LEU:H	2.21	0.54
1:K:141:ARG:NH2	2:K:1669:PO4:O3	2.40	0.54
1:K:202:MSE:HE1	1:K:225:PRO:HG3	1.89	0.54
1:D:178:VAL:HG22	1:D:241:VAL:HG11	1.88	0.54
1:E:153[A]:VAL:CG1	1:E:282:VAL:HG12	2.38	0.54
1:F:119:MSE:HE3	1:F:297:PHE:HZ	1.73	0.54
1:F:176:MSE:SE	3:F:1719:HOH:O	2.75	0.54
1:L:158:ASP:HA	1:L:161:LEU:HD22	1.89	0.54
1:B:178:VAL:HG22	1:B:241:VAL:HG11	1.89	0.54
1:F:256:VAL:HG22	1:G:256:VAL:HG22	1.90	0.54
1:G:260:TYR:OH	1:H:235:GLU:OE2	2.24	0.54
1:J:167:THR:CB	1:J:281[A]:VAL:HG21	2.31	0.54
1:G:194:LEU:HD13	1:G:270:ILE:HG23	1.89	0.53
1:F:274:LYS:HG2	2:K:1608:PO4:O2	2.07	0.53
1:H:252:GLN:NE2	2:H:1617:PO4:O2	2.39	0.53
1:E:172:THR:CG2	1:E:277:SER:HB3	2.38	0.53
1:G:164:GLU:HG2	1:G:285:HIS:CE1	2.43	0.53
1:I:295:ARG:CZ	1:I:299:ARG:HE	2.22	0.53
1:A:99:VAL:HG12	1:A:127:TYR:CD1	2.44	0.53
1:C:137:ASP:OD1	1:C:141:ARG:HD3	2.09	0.53
1:F:174:GLU:HG2	2:F:1650:PO4:O4	2.09	0.53
1:C:103:ILE:HD12	1:C:294:ALA:HA	1.90	0.52
1:C:114:THR:HG21	1:C:252:GLN:HG2	1.91	0.52
1:E:116:LEU:N	1:E:117:PRO:HD3	2.24	0.52
1:C:216:ASP:OD1	1:C:219:ARG:NH2	2.30	0.52
1:C:119:MSE:HE1	1:C:155:ILE:HG13	1.92	0.52
1:H:115:ILE:HD13	1:H:280:VAL:HG11	1.90	0.52
1:A:193:ARG:NE	1:A:272:GLU:HG3	2.16	0.52
1:K:188:VAL:HG23	3:K:1711:HOH:O	2.09	0.52
1:D:197:LEU:HA	1:D:200:HIS:HD2	1.75	0.52
1:L:176:MSE:HG3	1:L:267:VAL:HG13	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:HD21	1:B:270:ILE:CD1	2.40	0.51
1:G:193:ARG:HD2	1:J:166:GLN:NE2	2.24	0.51
1:A:164:GLU:O	1:A:286:GLN:HB2	2.10	0.51
1:K:172:THR:OG1	1:K:277:SER:HB2	2.08	0.51
1:K:207:ALA:O	1:K:210:SER:HB2	2.10	0.51
1:B:111:LEU:CD2	1:B:115:ILE:HD12	2.40	0.51
1:B:249:LEU:CD2	1:B:270:ILE:HD11	2.41	0.51
1:G:171:MSE:CE	1:G:173:ARG:HG3	2.40	0.51
1:J:169:PRO:HA	1:J:281[B]:VAL:HG12	1.93	0.51
1:A:219:ARG:NE	1:C:226:ARG:HG2	2.25	0.51
1:F:193:ARG:CG	1:F:272:GLU:OE1	2.58	0.51
1:H:176[A]:MSE:HG3	1:H:267:VAL:HG13	1.92	0.51
1:I:136:GLU:OE1	1:J:231:THR:OG1	2.26	0.51
1:E:189:ASP:HB2	2:E:1624:PO4:O4	2.11	0.51
1:D:198:ALA:O	1:D:199:GLU:CB	2.54	0.51
1:K:116:LEU:CD1	1:K:119:MSE:HE2	2.34	0.51
1:J:256:VAL:HG22	1:J:258:VAL:HG12	1.92	0.50
1:B:178:VAL:CG2	1:B:265[A]:VAL:CG1	2.89	0.50
1:G:256:VAL:HG21	1:H:258:VAL:HG11	1.94	0.50
1:H:183:HIS:HD2	1:H:185:LEU:H	1.59	0.50
1:L:106:GLY:HA2	1:L:135:ARG:O	2.11	0.50
1:I:145:GLN:HA	1:I:150:GLU:HG3	1.94	0.50
1:E:116:LEU:N	1:E:117:PRO:CD	2.75	0.50
1:K:118:SER:OG	1:L:243:ARG:NH1	2.45	0.50
1:A:223:PHE:C	1:C:224:ALA:HB2	2.36	0.50
1:C:182:GLU:N	2:C:1619:PO4:O3	2.36	0.50
1:C:181:ALA:HB2	1:C:264:PRO:HG2	1.94	0.49
1:C:194:LEU:HD12	1:C:197:LEU:HD12	1.94	0.49
1:A:135:ARG:NH2	3:A:1786:HOH:O	2.45	0.49
1:J:172:THR:HB	1:J:277:SER:HB3	1.94	0.49
1:F:111:LEU:HD23	1:F:252:GLN:HE22	1.77	0.49
1:F:143:ARG:O	1:F:147:GLU:HG2	2.13	0.49
1:F:176:MSE:CG	3:F:1719:HOH:O	2.51	0.49
1:D:174:GLU:OE1	1:D:274:LYS:HE2	2.13	0.49
1:L:194:LEU:CD2	1:L:217:VAL:HG12	2.42	0.49
1:C:234:PHE:CZ	1:C:252:GLN:HB3	2.47	0.49
1:H:241:VAL:HG21	1:H:248:THR:HG22	1.94	0.49
1:A:162:SER:HB2	1:A:164:GLU:H	1.78	0.48
1:K:249:LEU:HD21	1:K:270:ILE:CD1	2.42	0.48
1:K:185:LEU:O	1:K:188:VAL:HG22	2.14	0.48
1:L:194:LEU:HD21	1:L:217:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:MSE:HE2	1:E:173:ARG:HD3	1.94	0.48
1:A:299:ARG:NH2	3:A:1775:HOH:O	2.46	0.48
1:D:99:VAL:HG13	1:D:129:ARG:HH22	1.77	0.48
1:A:173:ARG:NH1	3:A:1764:HOH:O	2.45	0.48
1:F:116:LEU:HD13	1:F:119:MSE:HE2	1.95	0.48
1:G:138:THR:OG1	1:G:141:ARG:HG3	2.14	0.48
1:I:293:VAL:HG12	3:I:1738:HOH:O	2.12	0.48
1:J:166:GLN:HG3	1:J:167:THR:N	2.28	0.48
1:D:241:VAL:HG21	1:D:248:THR:HG22	1.96	0.48
1:I:223:PHE:C	1:K:224:ALA:HB2	2.38	0.48
1:K:106:GLY:HA2	1:K:135:ARG:O	2.13	0.48
1:K:141:ARG:HH22	2:K:1669:PO4:P	2.37	0.48
1:K:175:PRO:HG3	1:K:213:HIS:CE1	2.47	0.48
1:K:256:VAL:HG12	3:K:1777:HOH:O	2.13	0.48
1:H:99:VAL:CA	1:H:292:ARG:HD2	2.42	0.48
1:A:146:LEU:HD23	1:A:165:TRP:CE2	2.49	0.48
1:A:223:PHE:O	1:C:224:ALA:HB2	2.13	0.47
1:F:177:VAL:HG23	1:F:270:ILE:CG1	2.44	0.47
1:C:183:HIS:CD2	1:C:185:LEU:H	2.25	0.47
1:D:164:GLU:HG3	1:D:164:GLU:H	1.59	0.47
1:G:164:GLU:HG3	1:G:285:HIS:CE1	2.47	0.47
1:L:241:VAL:HG21	1:L:248:THR:HG22	1.95	0.47
1:A:116:LEU:HD13	1:A:119:MSE:HE2	1.97	0.47
1:D:145:GLN:HG2	1:D:150:GLU:OE2	2.14	0.47
1:D:285:HIS:HD2	1:D:287:GLU:HB2	1.78	0.47
1:H:99:VAL:CB	1:H:292:ARG:HD2	2.42	0.47
1:I:177:VAL:CG1	1:I:179:LEU:HD13	2.44	0.47
1:J:166:GLN:HG2	1:J:284:TRP:CE2	2.48	0.47
1:A:115:ILE:HD13	1:A:280:VAL:HG11	1.96	0.47
1:E:173:ARG:HH11	1:E:253[A]:ARG:H	1.60	0.47
1:J:175:PRO:HG2	1:J:275:PRO:HB2	1.96	0.47
1:J:168:VAL:C	1:J:281[A]:VAL:HG23	2.39	0.47
1:L:183:HIS:CE1	1:L:200:HIS:HD2	2.31	0.47
1:E:255:ARG:HD3	1:F:261:GLU:O	2.15	0.47
1:K:137:ASP:OD2	1:K:141:ARG:NH1	2.47	0.47
1:B:174:GLU:OE1	1:B:274:LYS:HD2	2.15	0.46
1:I:177:VAL:HG12	1:I:179:LEU:HD13	1.98	0.46
1:B:183:HIS:CD2	1:B:184:PRO:HD2	2.50	0.46
1:F:111:LEU:HD23	1:F:252:GLN:NE2	2.30	0.46
1:G:164:GLU:CG	1:G:285:HIS:HE1	2.28	0.46
1:K:233:ASN:HD22	1:L:136:GLU:CD	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASP:HA	1:B:161:LEU:CD1	2.45	0.46
1:D:138:THR:OG1	2:D:1657:PO4:O2	2.20	0.46
1:A:258:VAL:HG11	1:B:256:VAL:HG21	1.98	0.46
1:D:173:ARG:HH21	1:D:176:MSE:HE1	1.81	0.46
1:E:158:ASP:HA	1:E:161:LEU:HD22	1.96	0.46
1:C:103:ILE:HG22	1:C:131:SER:O	2.16	0.46
1:K:182:GLU:N	2:K:1620:PO4:O1	2.41	0.46
1:B:285:HIS:HD2	1:B:287:GLU:H	1.64	0.46
1:D:119:MSE:CE	1:D:297:PHE:HZ	2.29	0.46
1:D:256:VAL:HG13	1:D:256:VAL:O	2.16	0.46
1:J:194:LEU:HD21	1:J:217:VAL:HG23	1.98	0.46
1:F:161:LEU:HD12	1:F:167:THR:HG21	1.98	0.46
1:C:112:GLY:O	1:C:117:PRO:HD3	2.16	0.46
1:C:192:VAL:HG12	1:C:268:LYS:HD3	1.98	0.46
1:C:241:VAL:HG21	1:C:248:THR:HG22	1.97	0.46
1:E:173:ARG:HH11	1:E:253[B]:ARG:H	1.62	0.46
1:F:169:PRO:HA	1:F:281:VAL:HG12	1.97	0.46
1:L:240:PHE:O	1:L:245:LEU:HB2	2.15	0.46
1:E:178[B]:VAL:HG21	1:E:250:LEU:HD12	1.98	0.46
1:F:137:ASP:OD1	1:F:141:ARG:HD3	2.16	0.46
1:A:271:ALA:C	1:A:272:GLU:HG2	2.41	0.45
1:B:139:GLN:NE2	1:B:209:PRO:HB3	2.31	0.45
1:G:135:ARG:HD2	1:G:151:LEU:HD13	1.98	0.45
1:D:119:MSE:HE1	1:D:155:ILE:HD11	1.96	0.45
1:B:173:ARG:HD2	1:B:176:MSE:HE2	1.98	0.45
1:D:119:MSE:HG3	1:D:301:VAL:HG22	1.97	0.45
1:D:219:ARG:CG	1:D:219:ARG:NH1	2.52	0.45
1:C:116:LEU:HD13	1:C:119:MSE:HE2	1.98	0.45
1:I:241:VAL:HG21	1:I:248:THR:HG22	1.97	0.45
1:A:219:ARG:HG3	1:C:224:ALA:HB3	1.98	0.45
1:B:178:VAL:CG2	1:B:265[A]:VAL:HG11	2.46	0.45
1:H:142:LEU:C	1:H:142:LEU:HD23	2.41	0.45
1:C:302:THR:O	1:C:302:THR:HG22	2.17	0.45
1:E:174:GLU:OE1	1:E:274:LYS:HE3	2.17	0.45
1:G:183:HIS:CD2	1:G:185:LEU:H	2.28	0.45
1:A:213:HIS:O	1:A:217:VAL:CG1	2.65	0.45
1:C:129:ARG:HB3	1:C:129:ARG:NH2	2.32	0.45
1:I:150:GLU:H	1:I:150:GLU:HG2	1.53	0.45
1:L:177:VAL:HG22	1:L:249[B]:LEU:CD1	2.47	0.45
1:C:106:GLY:HA2	1:C:135:ARG:O	2.17	0.45
1:G:173:ARG:HB2	3:G:1723:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:VAL:HG22	1:G:292:ARG:HD3	1.98	0.45
1:A:200:HIS:HB3	3:A:1729:HOH:O	2.17	0.44
1:I:209:PRO:HG3	3:I:1705:HOH:O	2.17	0.44
1:F:173:ARG:HD2	1:F:176:MSE:CE	2.43	0.44
1:I:172:THR:HG23	3:I:1759:HOH:O	2.17	0.44
1:J:111:LEU:CD2	1:J:115:ILE:HD13	2.47	0.44
1:F:142:LEU:HA	1:F:145:GLN:HE21	1.82	0.44
1:H:175:PRO:HG3	1:H:213:HIS:HE1	1.83	0.44
1:H:183:HIS:CD2	1:H:184:PRO:HD2	2.52	0.44
1:I:111:LEU:HD23	1:I:252:GLN:OE1	2.17	0.44
1:I:194:LEU:HD11	1:I:217:VAL:HG12	1.98	0.44
1:J:123:PHE:CE1	1:J:297:PHE:HA	2.52	0.44
1:A:295:ARG:NH2	1:A:299:ARG:NH2	2.66	0.44
1:F:145:GLN:HB2	1:F:151:LEU:HD22	2.00	0.44
1:G:171:MSE:HE3	1:G:173:ARG:CG	2.48	0.44
1:G:169:PRO:HA	1:G:281:VAL:HA	1.99	0.44
1:B:177:VAL:HG23	1:B:270:ILE:HD11	1.98	0.44
1:K:285:HIS:CE1	1:K:287:GLU:HB2	2.53	0.44
1:L:247:TRP:HZ3	1:L:249[B]:LEU:HD13	1.83	0.44
1:L:274:LYS:HE2	3:L:1780:HOH:O	2.18	0.44
1:A:272:GLU:HA	1:A:273:PRO:HA	1.78	0.44
1:G:162:SER:OG	1:G:164:GLU:OE1	2.30	0.44
1:G:243:ARG:HD3	1:G:263:LEU:CD1	2.46	0.44
1:I:183:HIS:CE1	3:I:1696:HOH:O	2.60	0.44
1:J:206:ASP:HB3	2:J:1668:PO4:O1	2.17	0.44
1:C:114:THR:HG21	1:C:252:GLN:CG	2.47	0.44
1:D:105:VAL:HG13	1:D:132:VAL:HG13	2.00	0.44
1:K:168:VAL:HA	1:K:169:PRO:HD3	1.88	0.44
1:F:186:ALA:HB1	1:F:266:VAL:HG21	2.00	0.43
1:K:183:HIS:HD2	1:K:185:LEU:N	1.94	0.43
1:D:213:HIS:CE1	1:D:251[A]:LEU:HD21	2.52	0.43
1:L:183:HIS:CD2	1:L:184:PRO:HD2	2.53	0.43
1:C:176[B]:MSE:HE2	1:C:267:VAL:HG12	1.98	0.43
1:C:295:ARG:NH1	2:C:1663:PO4:O1	2.50	0.43
1:I:167:THR:HA	1:I:282:VAL:O	2.18	0.43
1:D:285:HIS:CD2	1:D:287:GLU:H	2.36	0.43
1:E:253[B]:ARG:HD2	1:E:267:VAL:HG11	2.00	0.43
1:G:140:ASN:HB2	2:G:1678:PO4:O3	2.18	0.43
1:J:116:LEU:HD13	1:J:119:MSE:HE2	2.00	0.43
1:F:172:THR:OG1	1:F:277:SER:HB3	2.18	0.43
1:J:191:PRO:HB2	1:J:271:ALA:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:HIS:HE1	3:H:1679:HOH:O	2.01	0.43
1:I:231:THR:HG21	1:I:236:THR:CG2	2.48	0.43
1:D:290:LEU:HD13	1:D:298:ILE:CD1	2.48	0.43
1:F:192:VAL:HG23	1:F:268:LYS:HG2	2.01	0.43
1:G:243:ARG:HD3	1:G:263:LEU:HD11	2.00	0.43
1:B:106:GLY:HA2	1:B:135:ARG:O	2.18	0.43
3:A:1713:HOH:O	1:B:124:THR:HG21	2.17	0.43
1:D:173:ARG:NH2	1:D:176:MSE:HE1	2.32	0.43
1:E:105:VAL:HG13	1:E:132[B]:VAL:HG13	2.01	0.43
1:E:121:TYR:HB2	1:F:243:ARG:HG3	2.01	0.43
1:F:178:VAL:HG13	1:F:265:VAL:HG13	1.99	0.43
1:H:220:GLU:HG2	3:H:1686:HOH:O	2.18	0.43
1:C:166:GLN:HB2	1:C:284:TRP:CE2	2.53	0.42
1:B:166:GLN:O	1:B:283:ALA:HA	2.20	0.42
1:C:177:VAL:HG23	1:C:270:ILE:CG1	2.49	0.42
1:G:116:LEU:HD13	1:G:119:MSE:HE2	2.01	0.42
1:J:167:THR:HB	1:J:281[A]:VAL:HG22	1.97	0.42
1:L:116:LEU:HD13	1:L:119:MSE:CE	2.48	0.42
1:A:183:HIS:HD2	1:A:185:LEU:N	2.03	0.42
1:A:299:ARG:NE	3:A:1768:HOH:O	2.52	0.42
1:G:112:GLY:O	1:G:117:PRO:HD3	2.20	0.42
1:J:174:GLU:HA	1:J:175:PRO:HD3	1.92	0.42
1:J:185:LEU:O	1:J:188:VAL:HG12	2.19	0.42
1:J:213:HIS:O	1:J:217:VAL:HG13	2.19	0.42
1:G:164:GLU:HG2	1:G:285:HIS:ND1	2.35	0.42
1:I:115:ILE:HG12	1:I:171:MSE:HE1	1.99	0.42
1:L:176:MSE:SE	1:L:253:ARG:HB2	2.70	0.42
1:A:112:GLY:O	1:A:117:PRO:HD3	2.19	0.42
1:B:249:LEU:HD21	1:B:270:ILE:HD11	2.00	0.42
1:K:249:LEU:CD2	1:K:270:ILE:HD11	2.50	0.42
1:A:176:MSE:SE	1:A:253:ARG:HB2	2.70	0.42
1:H:150:GLU:H	1:H:150:GLU:HG2	1.62	0.42
1:D:116:LEU:N	1:D:117:PRO:CD	2.82	0.42
1:E:181:ALA:HB2	1:E:264:PRO:HG2	2.01	0.42
1:D:253:ARG:HG3	1:D:267:VAL:HG11	2.02	0.42
1:A:253:ARG:HD3	1:A:267:VAL:HG11	2.02	0.42
1:C:243:ARG:O	1:C:243:ARG:HD3	2.19	0.41
1:D:112:GLY:O	1:D:117:PRO:HD3	2.20	0.41
1:L:106:GLY:O	1:L:154:ALA:HA	2.20	0.41
1:C:174:GLU:OE1	1:H:289:THR:OG1	2.35	0.41
1:D:167:THR:HA	1:D:282:VAL:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:TYR:HE1	1:H:132:VAL:CG2	2.32	0.41
1:L:159:LEU:O	1:L:160:ASP:HB2	2.20	0.41
1:A:173:ARG:HH22	1:A:253:ARG:H	1.68	0.41
1:G:137:ASP:HB3	1:G:142:LEU:HD13	2.01	0.41
1:H:291:SER:O	1:H:295:ARG:HG3	2.19	0.41
1:I:215:MSE:HE1	3:I:1681:HOH:O	2.19	0.41
1:A:172:THR:N	2:A:1674:PO4:O3	2.37	0.41
1:D:119:MSE:HE3	1:D:297:PHE:CE2	2.55	0.41
1:D:219:ARG:O	1:D:222:GLY:N	2.43	0.41
1:G:163:PRO:O	1:G:164:GLU:CB	2.68	0.41
1:L:112:GLY:N	1:L:113:PRO:CD	2.84	0.41
1:D:175:PRO:HG3	1:D:213:HIS:CE1	2.55	0.41
1:G:181:ALA:HB2	1:G:264:PRO:HG2	2.02	0.41
1:G:243:ARG:NH1	1:H:118:SER:HB3	2.35	0.41
1:A:219:ARG:HD3	3:C:1716:HOH:O	2.20	0.41
1:B:302:THR:HG23	1:J:273:PRO:CB	2.45	0.41
1:D:272:GLU:HA	1:D:273:PRO:HA	1.97	0.41
1:C:302:THR:O	1:C:302:THR:CG2	2.68	0.41
1:G:193:ARG:HD2	1:J:166:GLN:CD	2.46	0.41
1:E:166:GLN:O	1:E:283:ALA:HA	2.21	0.41
1:H:272:GLU:O	1:H:272:GLU:HG3	2.21	0.41
1:I:103:ILE:HB	1:I:293:VAL:HG22	2.01	0.41
1:L:119:MSE:HE1	1:L:297:PHE:HZ	1.85	0.41
1:B:145:GLN:HB3	1:B:151:LEU:HD22	2.03	0.41
1:D:191:PRO:CB	1:D:271:ALA:HB2	2.43	0.41
1:D:243:ARG:HA	1:D:243:ARG:HD3	1.90	0.41
1:E:153[A]:VAL:HG11	1:E:282:VAL:HG12	2.03	0.41
1:F:173:ARG:HH12	2:F:1628:PO4:P	2.43	0.41
1:J:170:LEU:HD13	1:J:282:VAL:HG12	2.02	0.41
1:K:178:VAL:HG23	1:K:265:VAL:HB	2.03	0.41
1:K:202:MSE:HE1	1:K:225:PRO:CB	2.49	0.41
1:L:103:ILE:HD12	1:L:294:ALA:HA	2.03	0.41
1:D:100:ALA:O	1:D:293[A]:VAL:CG1	2.64	0.41
1:G:135:ARG:HD2	1:G:151:LEU:CD1	2.51	0.41
1:J:106:GLY:HA2	1:J:135:ARG:O	2.21	0.41
1:K:202:MSE:HE1	1:K:225:PRO:CG	2.51	0.41
1:A:178:VAL:HG21	1:A:250:LEU:HD12	2.02	0.40
1:B:289:THR:O	1:C:147:GLU:OE2	2.39	0.40
1:D:106:GLY:HA2	1:D:135:ARG:O	2.21	0.40
1:E:299:ARG:HD2	3:E:1711:HOH:O	2.21	0.40
1:G:171:MSE:CE	1:G:173:ARG:CG	2.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:C	1:A:173:ARG:HG2	2.45	0.40
1:B:121:TYR:CD2	1:B:121:TYR:C	2.99	0.40
1:D:100:ALA:O	1:D:293[B]:VAL:CG2	2.70	0.40
1:A:295:ARG:NH2	1:A:299:ARG:HH21	2.20	0.40
1:B:178:VAL:HG21	1:B:265[A]:VAL:HG11	2.03	0.40
1:B:274:LYS:HE3	1:B:274:LYS:HB3	1.91	0.40
1:G:272:GLU:OE1	1:J:295:ARG:NH1	2.49	0.40
3:G:1717:HOH:O	1:J:295:ARG:HD3	2.21	0.40
1:H:263:LEU:HD23	1:H:263:LEU:HA	1.89	0.40
1:J:171:MSE:HG2	1:J:280:VAL:HB	2.03	0.40
1:L:249[A]:LEU:CD2	1:L:270:ILE:HD11	2.52	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	203/209 (97%)	198 (98%)	3 (2%)	2 (1%)	12	6
1	B	204/209 (98%)	203 (100%)	1 (0%)	0	100	100
1	C	206/209 (99%)	203 (98%)	2 (1%)	1 (0%)	24	16
1	D	205/209 (98%)	198 (97%)	6 (3%)	1 (0%)	24	16
1	E	208/209 (100%)	206 (99%)	2 (1%)	0	100	100
1	F	205/209 (98%)	203 (99%)	2 (1%)	0	100	100
1	G	203/209 (97%)	199 (98%)	3 (2%)	1 (0%)	24	16
1	H	204/209 (98%)	201 (98%)	2 (1%)	1 (0%)	24	16
1	I	203/209 (97%)	199 (98%)	3 (2%)	1 (0%)	24	16
1	J	204/209 (98%)	202 (99%)	2 (1%)	0	100	100
1	K	204/209 (98%)	202 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	204/209 (98%)	197 (97%)	6 (3%)	1 (0%)	24	16
All	All	2453/2508 (98%)	2411 (98%)	34 (1%)	8 (0%)	36	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	VAL
1	A	188	VAL
1	G	164	GLU
1	I	188	VAL
1	A	286	GLN
1	H	272	GLU
1	C	171	MSE
1	L	256	VAL

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	165/162 (102%)	141 (86%)	24 (14%)	3	1
1	B	166/162 (102%)	141 (85%)	25 (15%)	3	0
1	C	168/162 (104%)	138 (82%)	30 (18%)	2	0
1	D	167/162 (103%)	144 (86%)	23 (14%)	3	1
1	E	170/162 (105%)	146 (86%)	24 (14%)	3	1
1	F	167/162 (103%)	149 (89%)	18 (11%)	6	2
1	G	165/162 (102%)	136 (82%)	29 (18%)	2	0
1	H	166/162 (102%)	145 (87%)	21 (13%)	4	1
1	I	165/162 (102%)	147 (89%)	18 (11%)	6	2
1	J	166/162 (102%)	148 (89%)	18 (11%)	6	2
1	K	166/162 (102%)	144 (87%)	22 (13%)	4	1
1	L	166/162 (102%)	147 (89%)	19 (11%)	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1997/1944 (103%)	1726 (86%)	271 (14%)	4 1

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	A	111	LEU
1	A	119	MSE
1	A	120	LEU
1	A	132	VAL
1	A	133	GLU
1	A	137	ASP
1	A	144	THR
1	A	162	SER
1	A	170	LEU
1	A	171	MSE
1	A	173	ARG
1	A	174	GLU
1	A	179	LEU
1	A	193	ARG
1	A	194	LEU
1	A	217	VAL
1	A	253	ARG
1	A	255	ARG
1	A	265	VAL
1	A	268	LYS
1	A	272	GLU
1	A	286	GLN
1	A	295	ARG
1	B	120	LEU
1	B	124	THR
1	B	132	VAL
1	B	141	ARG
1	B	142	LEU
1	B	151	LEU
1	B	153	VAL
1	B	161	LEU
1	B	166	GLN
1	B	170	LEU
1	B	171	MSE
1	B	173	ARG
1	B	178	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	179	LEU
1	B	188	VAL
1	B	212	ASN
1	B	215	MSE
1	B	249	LEU
1	B	251	LEU
1	B	281	VAL
1	B	282	VAL
1	B	290	LEU
1	B	292	ARG
1	B	295	ARG
1	B	299	ARG
1	C	99	VAL
1	C	111	LEU
1	C	115	ILE
1	C	120	LEU
1	C	129	ARG
1	C	132	VAL
1	C	133	GLU
1	C	136	GLU
1	C	153	VAL
1	C	164	GLU
1	C	170	LEU
1	C	172	THR
1	C	173	ARG
1	C	178	VAL
1	C	179	LEU
1	C	185	LEU
1	C	188	VAL
1	C	189	ASP
1	C	192	VAL
1	C	211	THR
1	C	227	VAL
1	C	243	ARG
1	C	249	LEU
1	C	251[A]	LEU
1	C	251[B]	LEU
1	C	265	VAL
1	C	277	SER
1	C	281	VAL
1	C	290	LEU
1	C	292	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	103	ILE
1	D	105	VAL
1	D	120	LEU
1	D	124	THR
1	D	164	GLU
1	D	168	VAL
1	D	170	LEU
1	D	171	MSE
1	D	173	ARG
1	D	178	VAL
1	D	188	VAL
1	D	204	LEU
1	D	211	THR
1	D	219	ARG
1	D	227	VAL
1	D	251[A]	LEU
1	D	251[B]	LEU
1	D	265	VAL
1	D	274	LYS
1	D	281	VAL
1	D	282	VAL
1	D	289	THR
1	D	301	VAL
1	E	99	VAL
1	E	103	ILE
1	E	105	VAL
1	E	115	ILE
1	E	120	LEU
1	E	131	SER
1	E	132[A]	VAL
1	E	132[B]	VAL
1	E	153[A]	VAL
1	E	153[B]	VAL
1	E	161	LEU
1	E	173	ARG
1	E	178[A]	VAL
1	E	178[B]	VAL
1	E	179	LEU
1	E	182	GLU
1	E	185	LEU
1	E	230	ARG
1	E	251	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	253[A]	ARG
1	E	253[B]	ARG
1	E	265	VAL
1	E	281	VAL
1	E	292	ARG
1	F	119	MSE
1	F	120	LEU
1	F	124	THR
1	F	132	VAL
1	F	135	ARG
1	F	151	LEU
1	F	153	VAL
1	F	168	VAL
1	F	170	LEU
1	F	173	ARG
1	F	185	LEU
1	F	243	ARG
1	F	245	LEU
1	F	249[A]	LEU
1	F	249[B]	LEU
1	F	265	VAL
1	F	268	LYS
1	F	277	SER
1	G	119	MSE
1	G	120	LEU
1	G	124	THR
1	G	132	VAL
1	G	136	GLU
1	G	141	ARG
1	G	142	LEU
1	G	143	ARG
1	G	151	LEU
1	G	153	VAL
1	G	161	LEU
1	G	168	VAL
1	G	171	MSE
1	G	174	GLU
1	G	176	MSE
1	G	178	VAL
1	G	189	ASP
1	G	193	ARG
1	G	245	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	249	LEU
1	G	251	LEU
1	G	252	GLN
1	G	265	VAL
1	G	281	VAL
1	G	286	GLN
1	G	287	GLU
1	G	290	LEU
1	G	292	ARG
1	G	293	VAL
1	H	99	VAL
1	H	119	MSE
1	H	120	LEU
1	H	131	SER
1	H	132	VAL
1	H	138	THR
1	H	144	THR
1	H	146	LEU
1	H	150	GLU
1	H	166	GLN
1	H	172	THR
1	H	174	GLU
1	H	185	LEU
1	H	188	VAL
1	H	197	LEU
1	H	220	GLU
1	H	226	ARG
1	H	265	VAL
1	H	281	VAL
1	H	290	LEU
1	H	292	ARG
1	I	119	MSE
1	I	120	LEU
1	I	132	VAL
1	I	135	ARG
1	I	150	GLU
1	I	170	LEU
1	I	179	LEU
1	I	188	VAL
1	I	194	LEU
1	I	199	GLU
1	I	211	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	245	LEU
1	I	251	LEU
1	I	252	GLN
1	I	277	SER
1	I	281	VAL
1	I	287	GLU
1	I	301	VAL
1	J	115	ILE
1	J	120	LEU
1	J	132	VAL
1	J	166	GLN
1	J	168	VAL
1	J	170	LEU
1	J	178	VAL
1	J	182	GLU
1	J	185	LEU
1	J	192	VAL
1	J	193	ARG
1	J	194	LEU
1	J	217	VAL
1	J	219	ARG
1	J	230	ARG
1	J	253	ARG
1	J	256	VAL
1	J	282	VAL
1	K	99	VAL
1	K	105	VAL
1	K	120	LEU
1	K	124	THR
1	K	129	ARG
1	K	132	VAL
1	K	135	ARG
1	K	146	LEU
1	K	151	LEU
1	K	153	VAL
1	K	168	VAL
1	K	170	LEU
1	K	176[A]	MSE
1	K	176[B]	MSE
1	K	178	VAL
1	K	185	LEU
1	K	249	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	251	LEU
1	K	254	PRO
1	K	274	LYS
1	K	287	GLU
1	K	290	LEU
1	L	99	VAL
1	L	120	LEU
1	L	129	ARG
1	L	131	SER
1	L	132	VAL
1	L	136	GLU
1	L	155	ILE
1	L	161	LEU
1	L	164	GLU
1	L	173	ARG
1	L	178	VAL
1	L	179	LEU
1	L	182	GLU
1	L	194	LEU
1	L	245	LEU
1	L	251	LEU
1	L	265	VAL
1	L	268	LYS
1	L	274	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	HIS
1	A	213	HIS
1	A	252	GLN
1	B	139	GLN
1	B	145	GLN
1	B	183	HIS
1	B	200	HIS
1	B	285	HIS
1	C	139	GLN
1	C	183	HIS
1	C	286	GLN
1	D	166	GLN
1	D	183	HIS
1	D	200	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	285	HIS
1	E	183	HIS
1	E	252	GLN
1	E	286	GLN
1	F	183	HIS
1	F	200	HIS
1	F	212	ASN
1	F	252	GLN
1	F	286	GLN
1	G	145	GLN
1	G	183	HIS
1	G	212	ASN
1	G	252	GLN
1	G	286	GLN
1	H	183	HIS
1	H	233	ASN
1	H	286	GLN
1	I	139	GLN
1	I	183	HIS
1	J	183	HIS
1	J	252	GLN
1	K	183	HIS
1	K	200	HIS
1	K	213	HIS
1	K	233	ASN
1	K	252	GLN
1	K	286	GLN
1	L	183	HIS
1	L	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

76 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	PO4	B	1670	-	4,4,4	0.89	0	6,6,6	0.71	0
2	PO4	E	1644	-	4,4,4	0.94	0	6,6,6	0.69	0
2	PO4	I	1665	-	4,4,4	0.96	0	6,6,6	0.33	0
2	PO4	D	1657	-	4,4,4	0.84	0	6,6,6	0.71	0
2	PO4	J	1613	-	4,4,4	0.95	0	6,6,6	0.76	0
2	PO4	F	1650	-	4,4,4	0.89	0	6,6,6	0.58	0
2	PO4	F	1647	-	4,4,4	0.84	0	6,6,6	0.69	0
2	PO4	C	1623	-	4,4,4	1.01	0	6,6,6	0.60	0
2	PO4	C	1648	-	4,4,4	0.87	0	6,6,6	0.66	0
2	PO4	A	1615	-	4,4,4	0.90	0	6,6,6	0.61	0
2	PO4	K	1669	-	4,4,4	0.82	0	6,6,6	0.71	0
2	PO4	F	1611	-	4,4,4	0.59	0	6,6,6	1.15	0
2	PO4	J	1603	-	4,4,4	0.62	0	6,6,6	0.87	0
2	PO4	J	1614	-	4,4,4	0.72	0	6,6,6	0.51	0
2	PO4	H	1676	-	4,4,4	0.68	0	6,6,6	0.89	0
2	PO4	D	1660	-	4,4,4	0.98	0	6,6,6	0.65	0
2	PO4	I	1621	-	4,4,4	0.85	0	6,6,6	1.39	1 (16%)
2	PO4	B	1638	-	4,4,4	1.02	0	6,6,6	0.59	0
2	PO4	L	1622	-	4,4,4	1.12	0	6,6,6	1.08	1 (16%)
2	PO4	I	1655	-	4,4,4	0.55	0	6,6,6	1.34	1 (16%)
2	PO4	I	1662	-	4,4,4	0.79	0	6,6,6	0.79	0
2	PO4	D	1659	-	4,4,4	0.79	0	6,6,6	0.77	0
2	PO4	F	1640	-	4,4,4	0.82	0	6,6,6	0.51	0
2	PO4	B	1651	-	4,4,4	0.97	0	6,6,6	0.75	0
2	PO4	L	1656	-	4,4,4	0.44	0	6,6,6	1.41	1 (16%)
2	PO4	F	1628	-	4,4,4	1.07	0	6,6,6	1.10	1 (16%)
2	PO4	C	1619	-	4,4,4	0.83	0	6,6,6	1.59	1 (16%)
2	PO4	I	1632	-	4,4,4	0.83	0	6,6,6	1.04	0
2	PO4	K	1661	-	4,4,4	0.82	0	6,6,6	0.75	0
2	PO4	K	1620	-	4,4,4	0.33	0	6,6,6	1.27	0
2	PO4	D	1629	-	4,4,4	0.88	0	6,6,6	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	E	1624	-	4,4,4	0.97	0	6,6,6	0.31	0
2	PO4	J	1668	-	4,4,4	0.73	0	6,6,6	0.75	0
2	PO4	K	1672	-	4,4,4	0.73	0	6,6,6	0.93	0
2	PO4	K	1625	-	4,4,4	0.83	0	6,6,6	0.43	0
2	PO4	A	1674	-	4,4,4	0.94	0	6,6,6	0.71	0
2	PO4	H	1631	-	4,4,4	0.89	0	6,6,6	0.55	0
2	PO4	F	1605	-	4,4,4	0.95	0	6,6,6	0.87	0
2	PO4	C	1612	-	4,4,4	1.02	0	6,6,6	0.32	0
2	PO4	L	1666	-	4,4,4	0.86	0	6,6,6	0.59	0
2	PO4	F	1639	-	4,4,4	0.93	0	6,6,6	0.63	0
2	PO4	L	1609	-	4,4,4	0.90	0	6,6,6	0.65	0
2	PO4	K	1610	-	4,4,4	0.88	0	6,6,6	0.65	0
2	PO4	I	1606	-	4,4,4	1.04	0	6,6,6	1.38	1 (16%)
2	PO4	J	1633	-	4,4,4	0.69	0	6,6,6	0.87	0
2	PO4	F	1636	-	4,4,4	0.85	0	6,6,6	0.71	0
2	PO4	D	1658	-	4,4,4	0.98	0	6,6,6	0.80	0
2	PO4	B	1677	-	4,4,4	0.69	0	6,6,6	0.88	0
2	PO4	F	1652	-	4,4,4	0.88	0	6,6,6	0.60	0
2	PO4	L	1643	-	4,4,4	0.83	0	6,6,6	0.65	0
2	PO4	K	1673	-	4,4,4	1.04	0	6,6,6	1.07	0
2	PO4	K	1634	-	4,4,4	0.91	0	6,6,6	0.63	0
2	PO4	J	1653	-	4,4,4	0.64	0	6,6,6	0.57	0
2	PO4	A	1664	-	4,4,4	0.72	0	6,6,6	0.46	0
2	PO4	A	1626	-	4,4,4	0.95	0	6,6,6	0.93	0
2	PO4	H	1604	-	4,4,4	0.99	0	6,6,6	1.19	1 (16%)
2	PO4	C	1663	-	4,4,4	0.72	0	6,6,6	0.59	0
2	PO4	B	1630	-	4,4,4	1.00	0	6,6,6	0.86	0
2	PO4	I	1645	-	4,4,4	0.70	0	6,6,6	0.83	0
2	PO4	C	1607	-	4,4,4	0.66	0	6,6,6	1.16	1 (16%)
2	PO4	J	1667	-	4,4,4	0.87	0	6,6,6	0.72	0
2	PO4	K	1601	-	4,4,4	0.83	0	6,6,6	1.59	1 (16%)
2	PO4	H	1617	-	4,4,4	0.90	0	6,6,6	0.82	0
2	PO4	A	1641	-	4,4,4	0.91	0	6,6,6	1.13	1 (16%)
2	PO4	A	1616	-	4,4,4	0.88	0	6,6,6	0.55	0
2	PO4	G	1637	-	4,4,4	0.54	0	6,6,6	1.14	1 (16%)
2	PO4	K	1608	-	4,4,4	0.98	0	6,6,6	0.52	0
2	PO4	F	1618	-	4,4,4	0.87	0	6,6,6	0.71	0
2	PO4	F	1627	-	4,4,4	0.71	0	6,6,6	0.76	0
2	PO4	F	1675	-	4,4,4	0.50	0	6,6,6	0.82	0
2	PO4	F	1635	-	4,4,4	0.46	0	6,6,6	0.62	0
2	PO4	G	1654	-	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	E	1642	-	4,4,4	0.90	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	L	1602	-	4,4,4	1.29	0	6,6,6	1.51	1 (16%)
2	PO4	F	1646	-	4,4,4	0.65	0	6,6,6	0.73	0
2	PO4	G	1678	-	4,4,4	1.10	0	6,6,6	0.74	0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1619	PO4	O4-P-O2	3.06	117.44	107.91
2	L	1602	PO4	O3-P-O2	2.78	116.57	107.91
2	I	1621	PO4	O2-P-O1	-2.63	101.64	110.95
2	H	1604	PO4	O4-P-O3	2.63	116.10	107.91
2	L	1656	PO4	O2-P-O1	-2.63	101.66	110.95
2	G	1637	PO4	O3-P-O2	2.41	115.42	107.91
2	K	1601	PO4	O3-P-O2	2.31	115.09	107.91
2	A	1641	PO4	O4-P-O3	2.24	114.87	107.91
2	C	1607	PO4	O4-P-O3	-2.23	100.96	107.91
2	I	1655	PO4	O4-P-O3	2.20	114.74	107.91
2	I	1606	PO4	O3-P-O2	2.13	114.52	107.91
2	L	1622	PO4	O4-P-O2	2.06	114.33	107.91
2	F	1628	PO4	O3-P-O2	2.01	114.17	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1670	PO4	3	0
2	E	1644	PO4	1	0
2	D	1657	PO4	1	0
2	F	1650	PO4	1	0
2	K	1669	PO4	2	0
2	D	1660	PO4	1	0
2	B	1651	PO4	1	0
2	L	1656	PO4	1	0
2	F	1628	PO4	1	0
2	C	1619	PO4	1	0
2	K	1620	PO4	1	0
2	E	1624	PO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1668	PO4	1	0
2	A	1674	PO4	1	0
2	H	1631	PO4	3	0
2	K	1673	PO4	1	0
2	A	1626	PO4	1	0
2	C	1663	PO4	1	0
2	C	1607	PO4	1	0
2	H	1617	PO4	1	0
2	K	1608	PO4	1	0
2	F	1675	PO4	1	0
2	G	1678	PO4	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 [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	200/209 (95%)	-1.52	0 100 100	23, 30, 39, 44	0
1	B	200/209 (95%)	-1.48	0 100 100	18, 32, 46, 49	1 (0%)
1	C	200/209 (95%)	-1.41	0 100 100	21, 36, 47, 53	2 (1%)
1	D	200/209 (95%)	-1.43	0 100 100	18, 33, 44, 52	2 (1%)
1	E	200/209 (95%)	-1.52	0 100 100	15, 29, 41, 49	4 (2%)
1	F	200/209 (95%)	-1.49	0 100 100	16, 30, 40, 45	2 (1%)
1	G	200/209 (95%)	-1.37	0 100 100	25, 37, 53, 58	0
1	H	200/209 (95%)	-1.48	0 100 100	22, 32, 45, 51	0
1	I	200/209 (95%)	-1.58	0 100 100	20, 26, 38, 46	0
1	J	200/209 (95%)	-1.52	0 100 100	17, 29, 40, 48	1 (0%)
1	K	200/209 (95%)	-1.51	0 100 100	21, 29, 42, 47	0
1	L	200/209 (95%)	-1.56	0 100 100	13, 27, 38, 50	1 (0%)
All	All	2400/2508 (95%)	-1.49	0 100 100	13, 31, 45, 58	13 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	PO4	G	1678	5/5	0.96	0.06	45,46,47,51	0
2	PO4	C	1663	5/5	0.97	0.06	93,93,94,94	0
2	PO4	D	1657	5/5	0.97	0.05	93,94,94,94	0
2	PO4	D	1658	5/5	0.97	0.09	45,46,47,48	0
2	PO4	D	1659	5/5	0.97	0.04	76,76,77,77	0
2	PO4	E	1624	5/5	0.97	0.04	92,93,93,94	0
2	PO4	E	1642	5/5	0.97	0.05	104,104,105,106	0
2	PO4	F	1652	5/5	0.97	0.05	128,128,128,128	0
2	PO4	G	1654	5/5	0.97	0.06	134,135,135,135	0
2	PO4	C	1648	5/5	0.97	0.03	85,85,86,87	0
2	PO4	J	1633	5/5	0.97	0.05	90,91,91,92	0
2	PO4	J	1653	5/5	0.97	0.06	112,112,113,113	0
2	PO4	J	1667	5/5	0.97	0.04	92,92,93,93	0
2	PO4	K	1625	5/5	0.97	0.04	88,88,89,89	0
2	PO4	K	1634	5/5	0.97	0.04	91,92,92,93	0
2	PO4	L	1666	5/5	0.97	0.04	86,86,86,87	0
2	PO4	F	1640	5/5	0.98	0.05	92,92,93,94	0
2	PO4	F	1646	5/5	0.98	0.04	75,76,78,78	0
2	PO4	F	1647	5/5	0.98	0.05	77,77,78,78	0
2	PO4	F	1650	5/5	0.98	0.05	96,96,97,97	0
2	PO4	A	1615	5/5	0.98	0.05	71,71,72,73	0
2	PO4	F	1675	5/5	0.98	0.05	75,76,78,78	0
2	PO4	G	1637	5/5	0.98	0.04	65,66,69,69	0
2	PO4	A	1664	5/5	0.98	0.04	91,91,92,92	0
2	PO4	A	1674	5/5	0.98	0.04	78,78,79,79	0
2	PO4	H	1617	5/5	0.98	0.06	55,56,57,58	0
2	PO4	H	1676	5/5	0.98	0.04	81,81,83,83	0
2	PO4	I	1621	5/5	0.98	0.03	60,60,61,64	0
2	PO4	I	1662	5/5	0.98	0.04	66,69,69,70	0
2	PO4	B	1638	5/5	0.98	0.05	76,78,78,80	0
2	PO4	B	1651	5/5	0.98	0.05	91,92,93,94	0
2	PO4	B	1670	5/5	0.98	0.05	71,73,74,74	0
2	PO4	B	1677	5/5	0.98	0.06	88,89,90,91	0
2	PO4	F	1611	5/5	0.98	0.05	64,65,67,68	0
2	PO4	K	1661	5/5	0.98	0.05	90,90,90,90	0
2	PO4	K	1669	5/5	0.98	0.04	81,82,82,83	0
2	PO4	K	1672	5/5	0.98	0.04	59,61,62,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	L	1643	5/5	0.98	0.05	113,113,114,114	0
2	PO4	L	1656	5/5	0.98	0.05	71,75,77,77	0
2	PO4	F	1639	5/5	0.98	0.04	91,91,92,92	0
2	PO4	C	1619	5/5	0.99	0.06	49,49,51,53	0
2	PO4	E	1644	5/5	0.99	0.03	68,68,70,70	0
2	PO4	H	1604	5/5	0.99	0.04	53,54,56,56	0
2	PO4	F	1605	5/5	0.99	0.06	47,49,51,52	0
2	PO4	H	1631	5/5	0.99	0.04	61,64,66,66	0
2	PO4	C	1623	5/5	0.99	0.04	77,78,79,80	0
2	PO4	I	1606	5/5	0.99	0.04	46,49,53,56	0
2	PO4	F	1618	5/5	0.99	0.06	86,87,88,88	0
2	PO4	I	1632	5/5	0.99	0.04	77,78,79,80	0
2	PO4	I	1645	5/5	0.99	0.04	64,66,67,67	0
2	PO4	I	1655	5/5	0.99	0.05	66,68,70,73	0
2	PO4	F	1627	5/5	0.99	0.04	46,47,49,50	0
2	PO4	I	1665	5/5	0.99	0.05	90,90,90,90	0
2	PO4	J	1613	5/5	0.99	0.03	69,70,71,73	0
2	PO4	J	1614	5/5	0.99	0.04	59,60,61,62	0
2	PO4	F	1628	5/5	0.99	0.06	54,54,57,58	0
2	PO4	F	1635	5/5	0.99	0.06	46,47,51,53	0
2	PO4	F	1636	5/5	0.99	0.08	54,55,57,58	0
2	PO4	J	1668	5/5	0.99	0.04	78,78,79,80	0
2	PO4	K	1601	5/5	0.99	0.04	29,29,32,33	0
2	PO4	K	1608	5/5	0.99	0.03	83,83,83,84	0
2	PO4	K	1610	5/5	0.99	0.04	61,63,64,65	0
2	PO4	K	1620	5/5	0.99	0.03	55,58,58,60	0
2	PO4	A	1641	5/5	0.99	0.06	67,67,70,74	0
2	PO4	A	1616	5/5	0.99	0.04	72,72,74,74	0
2	PO4	D	1629	5/5	0.99	0.04	67,68,72,72	0
2	PO4	A	1626	5/5	0.99	0.06	27,34,41,42	0
2	PO4	B	1630	5/5	0.99	0.03	58,58,59,60	0
2	PO4	K	1673	5/5	0.99	0.04	68,68,71,71	0
2	PO4	L	1602	5/5	0.99	0.03	44,45,46,48	0
2	PO4	L	1609	5/5	0.99	0.06	54,56,59,59	0
2	PO4	L	1622	5/5	0.99	0.05	77,79,81,81	0
2	PO4	C	1607	5/5	0.99	0.06	34,42,45,45	0
2	PO4	D	1660	5/5	0.99	0.04	66,67,70,70	0
2	PO4	C	1612	5/5	0.99	0.03	62,62,63,63	0
2	PO4	J	1603	5/5	1.00	0.06	36,38,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.