



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:29 PM UTC

PDB ID : 5JAW / pdb_00005jaw
Title : Structure of a beta galactosidase with inhibitor
Authors : Offen, W.; Davies, G.
Deposited on : 2016-04-12
Resolution : 1.60 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

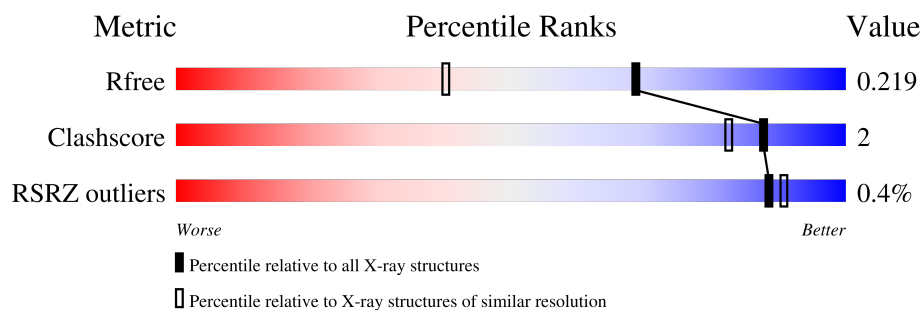
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	550	 90% 7% .
1	B	550	 90% 6% .
1	C	550	 90% 7% .
1	D	550	 89% 8% .
1	E	550	 91% 6% .
1	F	550	 89% 6% 5%
1	G	550	 91% 5% .

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Mol	Chain	Length	Quality of chain
1	H	550	% 90% 6% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35244 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 Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	6	0
			4212	2697	716	782	17			
1	B	528	Total	C	N	O	S	0	6	0
			4189	2686	710	777	16			
1	C	536	Total	C	N	O	S	0	8	0
			4240	2714	726	784	16			
1	D	532	Total	C	N	O	S	0	2	0
			4163	2667	707	774	15			
1	E	533	Total	C	N	O	S	0	6	0
			4204	2690	716	781	17			
1	F	525	Total	C	N	O	S	0	4	0
			4142	2653	704	769	16			
1	G	531	Total	C	N	O	S	0	4	0
			4178	2681	708	772	17			
1	H	527	Total	C	N	O	S	0	4	0
			4154	2663	703	772	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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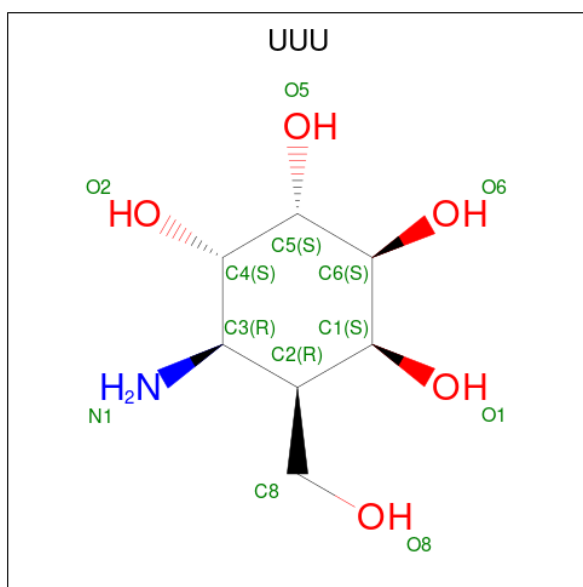
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is (1S,2S,3S,4S,5R,6R)-5-amino-6-(hydroxymethyl)cyclohexane-1,2,3,4-tetrol (CCD ID: UUU) (formula: C₇H₁₅NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	7	1	4		
2	B	1	Total	C	N	O	0	0
			12	7	1	4		
2	C	1	Total	C	N	O	0	0
			12	7	1	4		
2	D	1	Total	C	N	O	0	0
			12	7	1	4		
2	E	1	Total	C	N	O	0	0
			12	7	1	4		
2	F	1	Total	C	N	O	0	0
			12	7	1	4		
2	G	1	Total	C	N	O	0	0
			12	7	1	4		
2	H	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

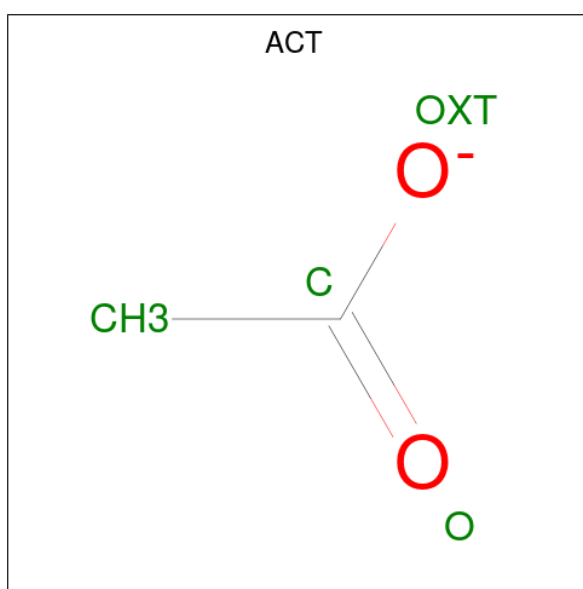
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	B	3	Total	Na	0	0
			3	3		
3	C	4	Total	Na	0	0
			4	4		
3	D	3	Total	Na	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	5	Total	Na	0	0
			5	5		
3	F	2	Total	Na	0	0
			2	2		
3	G	3	Total	Na	0	0
			3	3		
3	H	2	Total	Na	0	0
			2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total	O	0	0
			241	241		
5	B	210	Total	O	0	0
			210	210		
5	C	264	Total	O	0	0
			264	264		
5	D	214	Total	O	0	0
			214	214		

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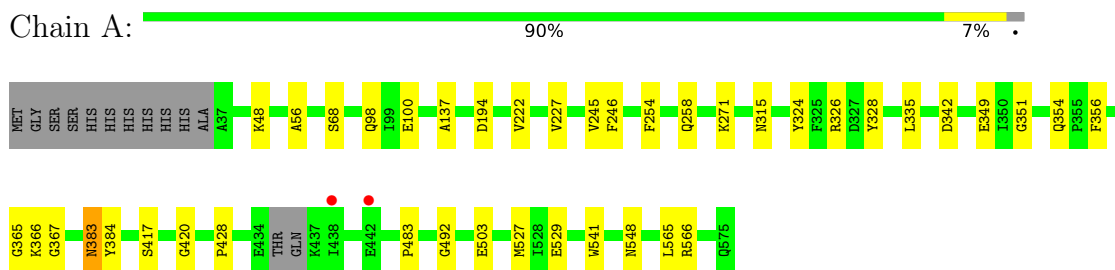
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	226	Total 226	O 226	0	0
5	F	165	Total 165	O 165	0	0
5	G	161	Total 161	O 161	0	0
5	H	155	Total 156	O 156	0	1

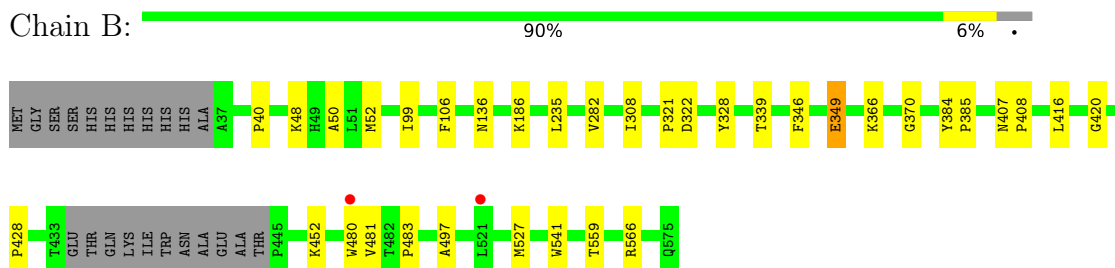
3 Residue-property plots

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.

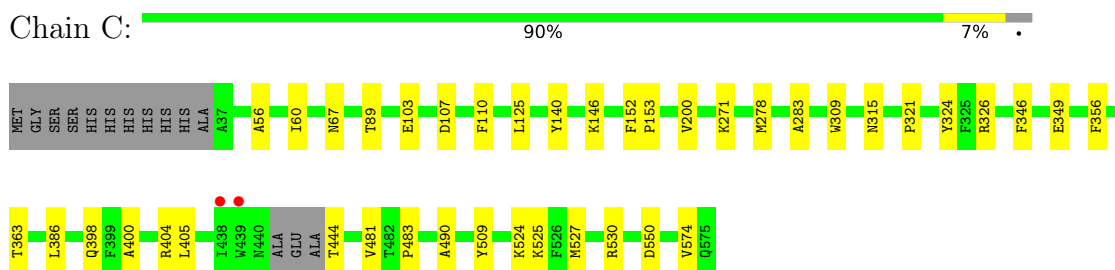
- Molecule 1: Beta-galactosidase, putative, bgl35A



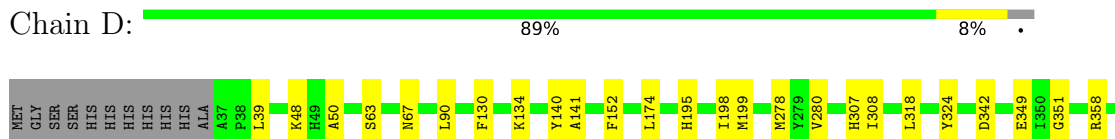
- Molecule 1: Beta-galactosidase, putative, bgl35A

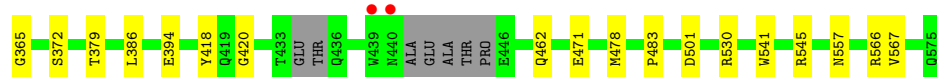


- Molecule 1: Beta-galactosidase, putative, bgl35A



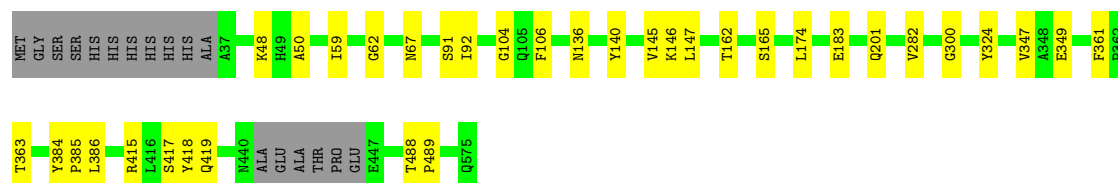
- Molecule 1: Beta-galactosidase, putative, bgl35A





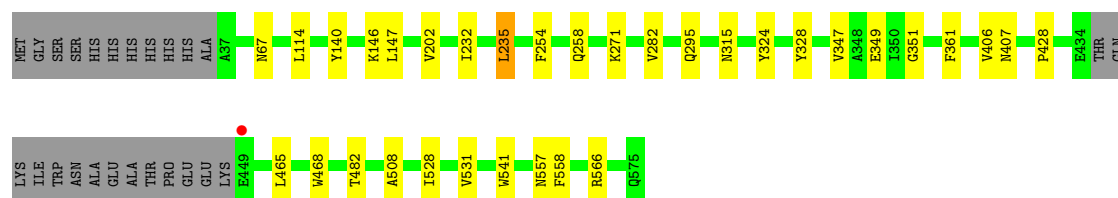
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain E: 91% 6% .



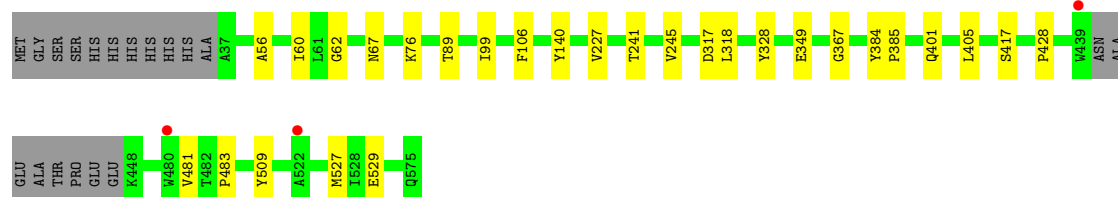
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain F: 89% 6% 5%



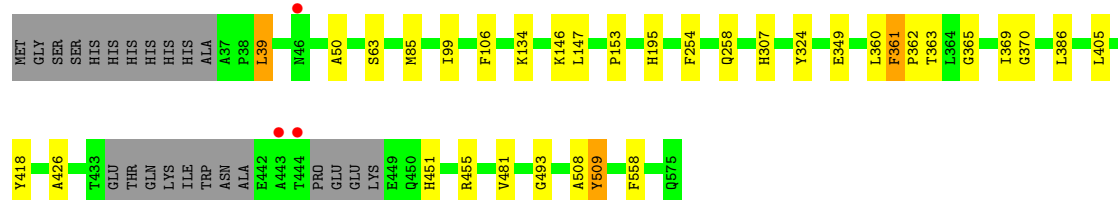
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain G: 91% 5% .



- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H: 90% 6% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.17Å 115.66Å 115.94Å 90.15° 90.11° 90.11°	Depositor
Resolution (Å)	81.99 – 1.60 81.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (81.99-1.60) 94.5 (81.99-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.197 , 0.214 (Not available) , 0.219	Depositor DCC
R_{free} test set	32570 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.207 for h,l,-k 0.207 for h,-l,k 0.155 for h,-k,-l 0.090 for -h,k,-l 0.088 for -h,-k,l 0.086 for -h,l,k 0.087 for -h,-l,-k	Xtriage
Reported twinning fraction	0.649 for H, K, L 0.052 for h,-k,-l 0.142 for H, L, -K 0.158 for H, -L, K	Depositor
Outliers	0 of 650569 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35244	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: NA, ACT, UUU

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	1.32	8/4328 (0.2%)	1.28	6/5898 (0.1%)
1	B	1.19	6/4310 (0.1%)	1.17	4/5873 (0.1%)
1	C	1.29	14/4359 (0.3%)	1.23	6/5938 (0.1%)
1	D	1.28	15/4275 (0.4%)	1.23	7/5826 (0.1%)
1	E	1.27	13/4320 (0.3%)	1.23	4/5888 (0.1%)
1	F	1.13	5/4258 (0.1%)	1.10	4/5802 (0.1%)
1	G	1.09	1/4296 (0.0%)	1.14	5/5854 (0.1%)
1	H	1.09	7/4270 (0.2%)	1.13	6/5818 (0.1%)
All	All	1.21	69/34416 (0.2%)	1.19	42/46897 (0.1%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CD-OE1	8.97	1.42	1.25
1	E	59	ILE	C-O	8.48	1.33	1.24
1	C	483	PRO	CA-C	7.29	1.55	1.51
1	C	349	GLU	CD-OE1	7.15	1.39	1.25
1	D	280	VAL	C-O	6.77	1.31	1.24
1	H	349	GLU	CD-OE1	6.76	1.38	1.25
1	B	483	PRO	CA-C	6.47	1.55	1.51
1	H	134	LYS	C-O	6.13	1.31	1.24
1	C	490	ALA	CA-CB	-6.09	1.43	1.53
1	F	557	ASN	N-CA	6.04	1.53	1.46
1	D	478	MET	N-CA	5.97	1.53	1.46
1	C	550	ASP	C-O	-5.94	1.17	1.24
1	E	300	GLY	C-O	5.93	1.30	1.23
1	B	349	GLU	CD-OE1	5.91	1.36	1.25
1	H	369	ILE	C-O	-5.88	1.17	1.24
1	C	125	LEU	N-CA	5.88	1.53	1.46
1	G	349	GLU	CD-OE1	5.86	1.36	1.25
1	E	363	THR	N-CA	5.80	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	ASP	C-O	-5.80	1.17	1.23
1	A	100	GLU	N-CA	5.78	1.53	1.46
1	B	186	LYS	C-O	-5.75	1.17	1.24
1	E	165	SER	C-O	5.74	1.30	1.23
1	B	50	ALA	C-O	5.72	1.30	1.23
1	E	201	GLN	C-O	-5.71	1.17	1.24
1	A	56	ALA	CA-C	5.70	1.58	1.52
1	E	361	PHE	N-CA	-5.68	1.42	1.46
1	C	309	TRP	C-O	-5.64	1.17	1.24
1	D	130	PHE	C-O	5.61	1.30	1.24
1	A	548	ASN	N-CA	-5.59	1.39	1.46
1	C	152	PHE	C-O	-5.55	1.18	1.24
1	F	202	VAL	CA-CB	5.44	1.60	1.53
1	H	509	TYR	C-O	5.43	1.30	1.23
1	E	349	GLU	CD-OE1	5.41	1.35	1.25
1	D	199	MET	N-CA	-5.40	1.39	1.46
1	D	198	ILE	N-CA	5.39	1.52	1.46
1	E	282	VAL	C-O	-5.39	1.18	1.24
1	D	134	LYS	C-O	5.38	1.30	1.24
1	H	363	THR	C-O	5.38	1.30	1.24
1	A	100	GLU	C-O	5.37	1.30	1.24
1	D	63	SER	N-CA	5.37	1.52	1.46
1	D	557	ASN	CA-CB	-5.36	1.45	1.53
1	C	398	GLN	N-CA	5.36	1.52	1.46
1	C	363	THR	C-O	5.35	1.30	1.24
1	D	567	VAL	C-O	-5.34	1.18	1.24
1	E	361	PHE	CA-CB	5.32	1.60	1.53
1	F	114	LEU	CA-C	5.30	1.59	1.52
1	H	360	LEU	C-O	-5.29	1.17	1.24
1	C	56	ALA	CA-CB	-5.28	1.46	1.53
1	D	349	GLU	CD-OE1	5.28	1.35	1.25
1	F	349	GLU	CD-OE1	5.22	1.35	1.25
1	D	379	THR	C-O	5.21	1.31	1.24
1	B	136	ASN	N-CA	5.20	1.52	1.46
1	B	559	THR	CA-C	-5.18	1.50	1.53
1	E	174	LEU	C-O	-5.17	1.18	1.24
1	A	483	PRO	CA-C	5.16	1.54	1.51
1	A	565	LEU	C-O	5.15	1.30	1.24
1	H	365	GLY	N-CA	5.15	1.52	1.45
1	C	146	LYS	N-CA	5.12	1.53	1.46
1	E	145	VAL	C-O	-5.11	1.18	1.24
1	D	90	LEU	N-CA	5.10	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	347	VAL	N-CA	-5.10	1.40	1.47
1	D	365	GLY	N-CA	5.09	1.52	1.45
1	C	110	PHE	N-CA	5.08	1.52	1.46
1	E	91	SER	N-CA	5.07	1.52	1.46
1	A	383	ASN	N-CA	5.07	1.52	1.46
1	C	103	GLU	C-O	5.06	1.29	1.23
1	F	361	PHE	CA-C	5.05	1.58	1.52
1	D	394	GLU	N-CA	5.03	1.52	1.46
1	D	174	LEU	N-CA	5.00	1.52	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	THR	CA-C-N	9.42	129.12	118.85
1	C	444	THR	C-N-CA	9.42	129.12	118.85
1	G	227	VAL	N-CA-C	-8.36	99.85	108.96
1	D	152	PHE	CA-C-N	7.47	127.23	119.76
1	D	152	PHE	C-N-CA	7.47	127.23	119.76
1	D	372	SER	O-C-N	6.83	126.73	121.27
1	D	483	PRO	O-C-N	6.79	124.43	121.31
1	H	39	LEU	CA-C-N	-6.45	113.14	119.78
1	H	39	LEU	C-N-CA	-6.45	113.14	119.78
1	A	492	GLY	N-CA-C	6.32	120.64	112.54
1	F	282	VAL	N-CA-C	5.97	116.70	107.99
1	F	235	LEU	N-CA-C	-5.96	102.50	110.55
1	G	62	GLY	N-CA-C	5.93	122.66	112.51
1	A	222	VAL	N-CA-C	-5.91	104.56	111.00
1	D	141	ALA	CA-C-O	-5.75	114.43	120.70
1	E	92	ILE	CB-CA-C	5.66	114.88	109.33
1	H	361	PHE	O-C-N	5.61	124.81	120.38
1	B	559	THR	O-C-N	5.54	125.63	121.47
1	B	282	VAL	N-CA-C	5.54	116.08	107.99
1	B	370	GLY	N-CA-C	5.52	118.65	110.42
1	E	62	GLY	N-CA-C	5.49	121.56	112.89
1	G	317	ASP	N-CA-C	5.43	117.28	111.36
1	F	347	VAL	CB-CA-C	5.35	118.78	112.68
1	G	483	PRO	O-C-N	5.30	123.75	121.31
1	H	307	HIS	N-CA-C	5.29	117.73	111.33
1	G	56	ALA	N-CA-C	5.28	114.38	108.25
1	E	136	ASN	N-CA-C	5.26	122.00	110.80
1	A	98	GLN	CA-C-O	-5.25	114.42	120.24
1	C	153	PRO	N-CA-C	5.23	120.42	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	358	ARG	CG-CD-NE	5.20	123.44	112.00
1	E	104	GLY	N-CA-C	5.19	122.26	115.47
1	B	559	THR	CB-CA-C	-5.18	109.62	117.07
1	A	194	ASP	N-CA-C	-5.16	106.76	113.16
1	H	370	GLY	N-CA-C	5.16	118.11	110.42
1	D	278	MET	O-C-N	-5.16	117.29	123.27
1	C	283	ALA	N-CA-C	-5.14	100.40	108.63
1	H	153	PRO	N-CA-C	5.14	119.26	111.19
1	C	483	PRO	O-C-N	5.10	123.66	121.31
1	C	483	PRO	N-CA-C	5.09	115.36	110.47
1	A	365	GLY	N-CA-C	5.09	120.04	113.27
1	A	137	ALA	N-CA-C	5.06	118.19	110.50
1	F	295	GLN	N-CA-C	-5.04	105.25	111.40

There are no chirality outliers.

There are no planarity outliers.

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	4212	0	4031	18	0
1	B	4189	0	4035	21	0
1	C	4240	0	4070	23	0
1	D	4163	0	3988	15	0
1	E	4204	0	4030	19	0
1	F	4142	0	3988	17	0
1	G	4178	0	4015	18	0
1	H	4154	0	3990	17	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
2	C	12	0	0	0	0
2	D	12	0	0	0	0
2	E	12	0	0	0	0
2	F	12	0	0	0	0
2	G	12	0	0	0	0
2	H	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	5	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
4	E	4	0	3	1	0
5	A	241	0	0	0	0
5	B	210	0	0	0	0
5	C	264	0	0	0	0
5	D	214	0	0	1	0
5	E	226	0	0	1	0
5	F	165	0	0	1	0
5	G	161	0	0	0	0
5	H	156	0	0	0	0
All	All	35244	0	32150	131	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 2.

All (131) 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:C:530[B]:ARG:HH11	1:C:530[B]:ARG:CG	1.65	1.07
1:C:530[B]:ARG:HG2	1:C:530[B]:ARG:NH1	1.51	0.96
1:D:530:ARG:NH1	5:D:701:HOH:O	1.93	0.92
1:B:48[A]:LYS:NZ	1:B:420:GLY:O	2.02	0.91
1:D:48:LYS:NZ	1:D:420:GLY:O	2.05	0.90
1:C:530[B]:ARG:HH11	1:C:530[B]:ARG:HG2	0.71	0.72
1:A:48[A]:LYS:NZ	1:A:420:GLY:O	2.22	0.71
1:A:245:VAL:HG23	1:A:246:PHE:CD2	2.27	0.70
1:E:48:LYS:NZ	1:E:417:SER:O	2.23	0.70
1:A:527[A]:MET:HE3	1:A:529:GLU:HA	1.74	0.69
1:F:482:THR:HG22	5:F:710:HOH:O	1.94	0.67
1:A:227:VAL:HG21	1:A:245:VAL:HG21	1.77	0.67
1:G:527[A]:MET:HE2	1:H:147:LEU:HD21	1.78	0.64
1:C:524:LYS:NZ	1:D:501:ASP:OD1	2.31	0.64
1:B:527[A]:MET:HE2	1:F:147:LEU:HD21	1.85	0.58
1:E:415[A]:ARG:HG3	1:E:419[A]:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527[A]:MET:HE1	1:F:146:LYS:HG3	1.86	0.56
1:F:508:ALA:HB3	1:F:558:PHE:CD1	2.42	0.55
1:E:384:TYR:CD1	1:E:385:PRO:HA	2.43	0.54
1:D:541:TRP:CD2	1:D:566:ARG:HD2	2.42	0.54
1:B:416:LEU:HD13	1:B:497:ALA:HB1	1.90	0.53
1:B:527[A]:MET:HE2	1:F:147:LEU:CD2	2.38	0.53
1:C:527[A]:MET:HE1	1:E:146:LYS:HG3	1.91	0.52
1:D:462:GLN:NE2	1:D:471:GLU:OE1	2.40	0.52
1:A:541:TRP:CE2	1:A:566:ARG:HD3	2.44	0.52
1:G:527[A]:MET:HE1	1:H:146:LYS:HE3	1.91	0.52
1:B:527[A]:MET:HE1	1:F:146:LYS:HE3	1.91	0.52
1:G:401:GLN:O	1:G:405:LEU:HD13	2.10	0.52
1:C:530[B]:ARG:CG	1:C:530[B]:ARG:NH1	2.36	0.51
1:G:99:ILE:O	1:G:106:PHE:HA	2.10	0.51
1:H:405:LEU:HD21	1:H:509:TYR:HB2	1.92	0.51
1:E:415[A]:ARG:HG3	1:E:419[A]:GLN:NE2	2.26	0.50
1:B:40:PRO:HA	1:B:52:MET:O	2.11	0.50
1:D:39:LEU:HD23	1:D:195:HIS:CE1	2.47	0.49
1:F:324:TYR:CE1	1:F:351:GLY:HA2	2.47	0.49
1:F:528:ILE:HG21	1:F:531:VAL:HG23	1.93	0.49
1:B:480:TRP:CG	1:B:481:VAL:H	2.31	0.49
1:C:525[A]:LYS:CE	1:E:162:THR:O	2.61	0.49
1:A:254:PHE:O	1:A:258:GLN:HG2	2.13	0.48
1:C:527[A]:MET:HE1	1:E:146:LYS:CG	2.43	0.48
1:G:405:LEU:HD21	1:G:509:TYR:HB2	1.95	0.48
1:F:67:ASN:HB3	1:F:140:TYR:OH	2.13	0.48
1:A:335:LEU:HB3	1:A:366:LYS:HD2	1.95	0.48
1:G:367:GLY:HA2	1:G:417:SER:OG	2.14	0.48
1:F:254:PHE:O	1:F:258:GLN:HG2	2.14	0.48
1:B:407:ASN:HB2	1:B:408:PRO:HD3	1.96	0.48
1:A:328:TYR:CD1	1:A:428:PRO:HA	2.49	0.47
1:B:99:ILE:O	1:B:106:PHE:HA	2.14	0.47
1:H:324:TYR:CE1	1:H:386:LEU:HB3	2.49	0.47
1:G:384:TYR:CD1	1:G:385:PRO:HA	2.49	0.47
1:A:271:LYS:HE3	1:A:315:ASN:O	2.15	0.46
1:E:415[B]:ARG:CZ	1:E:415[B]:ARG:CB	2.93	0.46
1:B:235:LEU:HD11	1:B:308:ILE:HD13	1.97	0.46
1:E:415[B]:ARG:HD2	1:E:419[B]:GLN:NE2	2.30	0.46
1:C:481:VAL:O	1:C:481:VAL:HG22	2.15	0.46
1:E:67:ASN:HB3	1:E:140:TYR:OH	2.15	0.46
1:H:254:PHE:O	1:H:258:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:527[A]:MET:HE1	1:H:146:LYS:CD	2.46	0.46
1:C:525[B]:LYS:HE3	1:C:574:VAL:HG11	1.97	0.46
1:F:328:TYR:CD1	1:F:428:PRO:HA	2.50	0.46
1:H:361:PHE:CD2	1:H:493:GLY:HA3	2.51	0.46
1:C:326[B]:ARG:HG2	1:C:356:PHE:CZ	2.51	0.45
1:C:525[A]:LYS:HD2	1:C:574:VAL:HG11	1.97	0.45
1:C:527[A]:MET:HE1	1:E:146:LYS:CD	2.45	0.45
1:G:481:VAL:HG22	1:G:481:VAL:O	2.16	0.45
1:C:324:TYR:CE1	1:C:386:LEU:HB3	2.52	0.45
1:D:318:LEU:HD12	1:D:318:LEU:C	2.42	0.45
1:A:245:VAL:HG23	1:A:246:PHE:CG	2.52	0.45
1:E:106:PHE:CE2	1:E:183:GLU:HG3	2.52	0.45
1:G:76[B]:LYS:HB3	1:G:76[B]:LYS:HE3	1.73	0.45
1:A:503:GLU:OE2	1:A:566:ARG:NH2	2.43	0.44
1:B:541:TRP:CD2	1:B:566:ARG:HD3	2.51	0.44
1:B:416:LEU:HD13	1:B:497:ALA:CB	2.47	0.44
1:H:63:SER:HB3	1:H:85:MET:SD	2.58	0.44
1:B:452[A]:LYS:HE3	1:B:452[A]:LYS:HB3	1.64	0.44
1:C:321:PRO:HD2	1:C:346:PHE:O	2.17	0.44
1:D:67:ASN:HB3	1:D:140:TYR:OH	2.18	0.44
1:G:527[A]:MET:HE1	1:H:146:LYS:CE	2.48	0.44
1:G:60:ILE:HG23	1:G:89:THR:HB	2.00	0.44
1:B:321:PRO:HD2	1:B:346:PHE:O	2.18	0.43
1:G:67:ASN:HB3	1:G:140:TYR:OH	2.18	0.43
1:C:525[A]:LYS:HE3	1:E:162:THR:O	2.18	0.43
1:D:342:ASP:OD1	1:D:342:ASP:C	2.61	0.43
1:D:324:TYR:CE1	1:D:386:LEU:HB3	2.54	0.43
1:E:415[B]:ARG:CD	1:E:419[B]:GLN:NE2	2.81	0.43
1:C:405:LEU:HD21	1:C:509:TYR:HB2	2.01	0.43
1:F:232:ILE:O	1:F:235:LEU:O	2.36	0.43
1:G:328:TYR:CD2	1:G:428:PRO:HA	2.54	0.43
1:B:322:ASP:HB3	1:B:349:GLU:OE2	2.19	0.42
1:H:481:VAL:HG22	1:H:481:VAL:O	2.19	0.42
1:D:324:TYR:CE1	1:D:351:GLY:HA2	2.55	0.42
1:G:527[A]:MET:HE2	1:H:147:LEU:CD2	2.47	0.42
1:G:527[A]:MET:HE3	1:G:529:GLU:HA	2.01	0.42
1:A:367:GLY:HA2	1:A:417[A]:SER:OG	2.19	0.42
1:A:383:ASN:O	1:A:384:TYR:C	2.62	0.42
1:B:328:TYR:CD2	1:B:428:PRO:HA	2.54	0.42
1:B:384:TYR:CG	1:B:385:PRO:HA	2.54	0.42
1:B:339:THR:CB	1:B:366:LYS:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:541:TRP:CE2	1:F:566:ARG:HD2	2.54	0.42
1:H:508:ALA:HB3	1:H:558:PHE:CD1	2.54	0.42
1:H:362:PRO:HD3	1:H:426:ALA:HB2	2.02	0.42
1:A:68:SER:O	1:D:545:ARG:HD2	2.19	0.42
1:C:60:ILE:HG23	1:C:89:THR:HB	2.02	0.42
1:H:451:HIS:CE1	1:H:455:ARG:HD2	2.55	0.42
1:F:271:LYS:HE3	1:F:315:ASN:O	2.20	0.42
1:H:39:LEU:HD23	1:H:195:HIS:CE1	2.54	0.42
1:D:307:HIS:CE1	1:D:308:ILE:HG12	2.54	0.41
1:C:400:ALA:O	1:C:404:ARG:HG3	2.21	0.41
1:D:50:ALA:HB2	1:D:418:TYR:CG	2.55	0.41
1:D:541:TRP:CG	1:D:566:ARG:HH11	2.39	0.41
1:G:318:LEU:C	1:G:318:LEU:HD12	2.46	0.41
1:C:271:LYS:HE3	1:C:315:ASN:O	2.21	0.41
4:E:607:ACT:H3	5:E:726:HOH:O	2.20	0.41
1:F:465:LEU:HB2	1:F:468:TRP:O	2.21	0.41
1:E:488:THR:HA	1:E:489:PRO:HA	1.94	0.41
1:A:324:TYR:CE1	1:A:351:GLY:HA2	2.56	0.41
1:C:527[A]:MET:HE2	1:E:147:LEU:CD2	2.50	0.41
1:E:147:LEU:HD23	1:E:147:LEU:HA	1.87	0.41
1:F:406:VAL:O	1:F:407:ASN:C	2.63	0.41
1:A:342:ASP:OD1	1:A:342:ASP:C	2.64	0.40
1:C:67:ASN:HB3	1:C:140:TYR:OH	2.22	0.40
1:E:324:TYR:CE1	1:E:386:LEU:HB3	2.56	0.40
1:G:241:THR:O	1:G:245:VAL:HG13	2.21	0.40
1:A:354:GLN:C	1:A:354:GLN:CD	2.89	0.40
1:B:48[B]:LYS:HE3	1:B:48[B]:LYS:HB2	1.09	0.40
1:A:326[B]:ARG:HG2	1:A:356:PHE:CZ	2.57	0.40
1:B:527[A]:MET:HE1	1:F:146:LYS:CD	2.52	0.40
1:C:200:VAL:O	1:C:278:MET:HA	2.21	0.40
1:E:50:ALA:HB2	1:E:418:TYR:HB2	2.02	0.40
1:H:50:ALA:HB2	1:H:418:TYR:CG	2.57	0.40
1:H:99:ILE:O	1:H:106:PHE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 25 are monoatomic - leaving 9 for Mogul analysis.

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	UUU	D	601	1	12,12,13	0.81	0	14,17,19	0.97	0
2	UUU	G	601	1	12,12,13	0.83	0	14,17,19	0.67	0
2	UUU	E	601	1	12,12,13	0.93	1 (8%)	14,17,19	1.03	1 (7%)
2	UUU	B	601	1	12,12,13	1.08	1 (8%)	14,17,19	1.17	1 (7%)
4	ACT	E	607	3	3,3,3	1.03	0	3,3,3	0.44	0
2	UUU	C	601	1	12,12,13	1.31	2 (16%)	14,17,19	1.15	1 (7%)
2	UUU	A	601	1	12,12,13	0.99	1 (8%)	14,17,19	0.73	0
2	UUU	F	601	1	12,12,13	1.10	1 (8%)	14,17,19	0.82	0
2	UUU	H	601	1	12,12,13	0.70	0	14,17,19	1.53	3 (21%)

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
2	UUU	D	601	1	-	0/2/22/26	0/1/1/1
2	UUU	G	601	1	-	0/2/22/26	0/1/1/1
2	UUU	E	601	1	-	0/2/22/26	0/1/1/1
2	UUU	B	601	1	-	0/2/22/26	0/1/1/1
2	UUU	C	601	1	-	0/2/22/26	0/1/1/1
2	UUU	A	601	1	-	0/2/22/26	0/1/1/1
2	UUU	F	601	1	-	0/2/22/26	0/1/1/1
2	UUU	H	601	1	-	0/2/22/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	UUU	C2-C1	3.16	1.56	1.53
2	F	601	UUU	C2-C1	3.14	1.56	1.53
2	B	601	UUU	C2-C1	2.96	1.56	1.53
2	A	601	UUU	C5-C6	2.67	1.56	1.52
2	C	601	UUU	C8-C2	-2.43	1.48	1.52
2	E	601	UUU	O1-C1	2.22	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	UUU	O5-C5-C4	3.01	117.35	109.86
2	H	601	UUU	C4-C5-C6	-2.63	106.87	110.67
2	H	601	UUU	C4-C3-C2	-2.59	108.43	111.67
2	E	601	UUU	C2-C1-C6	2.41	114.81	110.77
2	C	601	UUU	C4-C5-C6	-2.35	107.27	110.67
2	B	601	UUU	C4-C3-C2	-2.31	108.78	111.67

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
4	E	607	ACT	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	537/550 (97%)	-0.63	2 (0%) 88 91	11, 21, 37, 69	8 (1%)
1	B	528/550 (96%)	-0.53	2 (0%) 88 91	15, 23, 35, 65	9 (1%)
1	C	536/550 (97%)	-0.62	2 (0%) 88 91	10, 21, 35, 53	15 (2%)
1	D	532/550 (96%)	-0.55	2 (0%) 88 91	11, 23, 40, 58	3 (0%)
1	E	533/550 (96%)	-0.61	0 100 100	12, 22, 36, 65	6 (1%)
1	F	525/550 (95%)	-0.41	1 (0%) 91 92	14, 25, 37, 52	8 (1%)
1	G	531/550 (96%)	-0.37	3 (0%) 85 88	12, 25, 40, 58	7 (1%)
1	H	527/550 (95%)	-0.37	3 (0%) 85 88	15, 26, 40, 60	5 (0%)
All	All	4249/4400 (96%)	-0.51	15 (0%) 88 91	10, 23, 38, 69	61 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	439	TRP	5.2
1	G	439	TRP	4.0
1	F	449	GLU	3.5
1	B	521	LEU	3.1
1	B	480	TRP	2.6
1	C	438	ILE	2.5
1	G	522	ALA	2.5
1	G	480	TRP	2.3
1	A	442	GLU	2.3
1	H	443	ALA	2.2
1	H	46	ASN	2.1
1	H	444	THR	2.1
1	A	438	ILE	2.1
1	D	440	ASN	2.0
1	D	439	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	E	607	4/4	0.95	0.08	28,32,34,36	0
3	NA	E	605	1/1	0.97	0.09	27,27,27,27	0
3	NA	E	602	1/1	0.97	0.07	27,27,27,27	0
3	NA	C	603	1/1	0.98	0.04	24,24,24,24	0
3	NA	D	604	1/1	0.98	0.07	24,24,24,24	0
2	UUU	F	601	12/13	0.98	0.04	17,19,21,21	0
3	NA	E	603	1/1	0.98	0.05	23,23,23,23	0
3	NA	B	602	1/1	0.98	0.12	45,45,45,45	0
3	NA	F	603	1/1	0.98	0.09	24,24,24,24	0
3	NA	G	602	1/1	0.98	0.04	33,33,33,33	0
3	NA	B	603	1/1	0.98	0.06	34,34,34,34	0
2	UUU	B	601	12/13	0.99	0.04	15,18,20,22	0
2	UUU	C	601	12/13	0.99	0.03	13,15,16,19	0
3	NA	B	604	1/1	0.99	0.04	32,32,32,32	0
3	NA	C	602	1/1	0.99	0.03	22,22,22,22	0
2	UUU	D	601	12/13	0.99	0.04	16,17,19,20	0
3	NA	C	604	1/1	0.99	0.03	23,23,23,23	0
3	NA	C	605	1/1	0.99	0.05	25,25,25,25	0
3	NA	D	603	1/1	0.99	0.02	26,26,26,26	0
2	UUU	E	601	12/13	0.99	0.03	14,16,18,19	0
2	UUU	A	601	12/13	0.99	0.03	14,15,16,17	0
2	UUU	G	601	12/13	0.99	0.04	16,18,21,21	12
3	NA	E	604	1/1	0.99	0.03	25,25,25,25	0
2	UUU	H	601	12/13	0.99	0.04	18,20,24,25	0
3	NA	E	606	1/1	0.99	0.04	21,21,21,21	0
3	NA	F	602	1/1	0.99	0.03	32,32,32,32	0
3	NA	A	602	1/1	0.99	0.03	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	603	1/1	0.99	0.04	25,25,25,25	0
3	NA	G	603	1/1	0.99	0.05	27,27,27,27	0
3	NA	G	604	1/1	0.99	0.09	29,29,29,29	0
3	NA	H	602	1/1	0.99	0.05	25,25,25,25	0
3	NA	H	603	1/1	0.99	0.04	29,29,29,29	0
3	NA	A	604	1/1	0.99	0.09	26,26,26,26	0
3	NA	D	602	1/1	1.00	0.01	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.