



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:28 AM UTC

PDB ID : 5L2O / pdb_00005l2o
Title : Crystal Structure of ALDH1A1 in complex with BUC22
Authors : Buchman, C.D.; Hurley, T.D.
Deposited on : 2016-08-02
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

i

X-RAY DIFFRACTION

A.

Metric	Percentile Rank	Value
Mean	50	1.00
Median	50	1.00
Mode	50	1.00
Standard Deviation	50	0.00
Variance	50	0.00
Skewness	50	0.00
Kurtosis	50	0.00
Minimum	50	0.00
Maximum	50	1.00
Range	50	1.00
Interquartile Range	50	0.00
Five-Number Summary	50	0.00, 1.00, 1.00, 1.00, 1.00
Box Plot	50	0.00, 1.00, 1.00, 1.00, 1.00
Normal Q-Q Plot	50	0.00, 1.00, 1.00, 1.00, 1.00
Shapiro-Wilk Test	50	0.00
Anderson-Darling Test	50	0.00
Kolmogorov-Smirnov Test	50	0.00
Chi-Square Test	50	0.00
F-Test	50	0.00
T-Test	50	0.00
Z-Test	50	0.00
Correlation Coefficient	50	0.00
Covariance	50	0.00
Regression Line	50	0.00
Residuals	50	0.00
ANOVA	50	0.00
MANOVA	50	0.00
Discriminant Analysis	50	0.00
Logistic Regression	50	0.00
Decision Tree	50	0.00
Random Forest	50	0.00
Support Vector Machine	50	0.00
Neural Network	50	0.00
Bayesian Network	50	0.00
Markov Chain Monte Carlo	50	0.00
Monte Carlo Simulation	50	0.00
Stochastic Process	50	0.00
Time Series Analysis	50	0.00
Survival Analysis	50	0.00
Healthcare Data Analysis	50	0.00
Financial Data Analysis	50	0.00
Marketing Data Analysis	50	0.00
Operational Data Analysis	50	0.00
Manufacturing Data Analysis	50	0.00
Energy Data Analysis	50	0.00
Environmental Data Analysis	50	0.00
Transportation Data Analysis	50	0.00
Telecommunications Data Analysis	50	0.00
Government Data Analysis	50	0.00
Academic Data Analysis	50	0.00
Biological Data Analysis	50	0.00
Astronomical Data Analysis	50	0.00
Geological Data Analysis	50	0.00
Archaeological Data Analysis	50	0.00
Historical Data Analysis	50	0.00
Legal Data Analysis	50	0.00
Medical Data Analysis	50	0.00
Psychological Data Analysis	50	0.00
Sociological Data Analysis	50	0.00
Economic Data Analysis	50	0.00
Political Data Analysis	50	0.00
Environmental Data Analysis	50	0.00
Energy Data Analysis	50	0.00
Transportation Data Analysis	50	0.00
Telecommunications Data Analysis	50	0.00
Government Data Analysis	50	0.00
Academic Data Analysis	50	0.00
Biological Data Analysis	50	0.00
Astronomical Data Analysis	50	0.00
Geological Data Analysis	50	0.00
Archaeological Data Analysis	50	0.00
Historical Data Analysis	50	0.00
Legal Data Analysis	50	0.00
Medical Data Analysis	50	0.00
Psychological Data Analysis	50	0.00
Sociological Data Analysis	50	0.00
Economic Data Analysis	50	0.00
Political Data Analysis	50	0.00
Environmental Data Analysis	50	0.00
Energy Data Analysis	50	0.00
Transportation Data Analysis	50	0.00
Telecommunications Data Analysis	50	0.00
Government Data Analysis	50	0.00
Academic Data Analysis	50	0.00
Biological Data Analysis	50	0.00
Astronomical Data Analysis	50	0.00
Geological Data Analysis	50	0.00
Archaeological Data Analysis	50	0.00
Historical Data Analysis	50	0.00
Legal Data Analysis	50	0.00
Medical Data Analysis	50	0.00
Psychological Data Analysis	50	0.00
Sociological Data Analysis	50	0.00
Economic Data Analysis	50	0.00
Political Data Analysis	50	0.00
Environmental Data Analysis	50	0.00
Energy Data Analysis	50	0.00
Transportation Data Analysis	50	0.00
Telecommunications Data Analysis	50	0.00
Government Data Analysis	50	0.00
Academic Data Analysis	50	0.00
Biological Data Analysis	50	0.00
Astronomical Data Analysis	50	0.00
Geological Data Analysis	50	0.00
Archaeological Data Analysis	50	0.00
Historical Data Analysis	50	0.00
Legal Data Analysis	50	0.00
Medical Data Analysis	50	0.00
Psychological Data Analysis	50	0.00
Sociological Data Analysis	50	0.00
Economic Data Analysis	50	0.00
Political Data Analysis	50	0.00
Environmental Data Analysis	50	0.00
Energy Data Analysis	50	0.00
Transportation Data Analysis	50	0.00
Telecommunications Data Analysis	50	



■ Percentile relative to all X-ray structures

Percentile relative to X-ray structures of similar resolution

MetricWhole archive
(#Entries)

Similar resolution
(#Entries, resolution range(Å))

 R_{free}

Clashscore

Ramachandran outliers

Sidechain outliers

RSRZ outliers

180053

190562

187476

187428

180081

2260 (2.04-2.04)

2333 (2.04-2.04)

2318 (2.04-2.04)

2318 (2.04-2.04)

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.

Quality of chain

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Mol	Chain	Length	Quality of chain
1	F	501	5% 93% 5%
1	G	501	% 93% 5%
1	H	501	% 93%

2 Entry composition

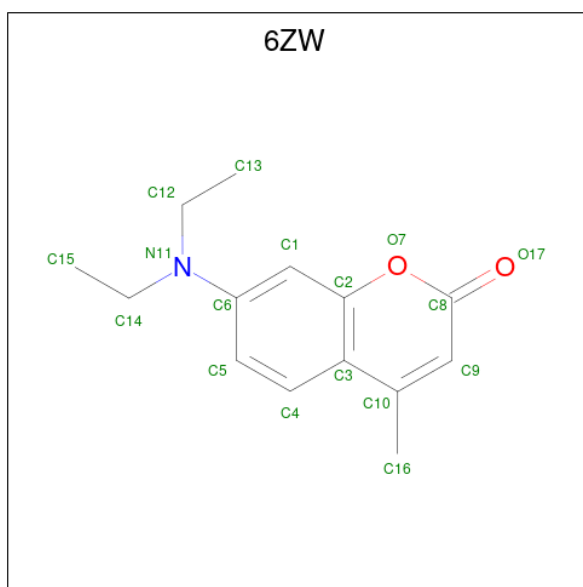
There are 5 unique types of molecules in this entry. The entry contains 33056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinal dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3828	2445	644	719	20			
1	B	494	Total	C	N	O	S	0	2	0
			3828	2445	644	719	20			
1	C	493	Total	C	N	O	S	0	2	0
			3820	2441	643	716	20			
1	D	493	Total	C	N	O	S	0	3	0
			3823	2443	643	716	21			
1	E	493	Total	C	N	O	S	0	3	0
			3823	2443	643	716	21			
1	F	493	Total	C	N	O	S	0	2	0
			3820	2441	643	716	20			
1	G	494	Total	C	N	O	S	0	2	0
			3822	2439	644	718	21			
1	H	493	Total	C	N	O	S	0	2	0
			3814	2435	643	715	21			

- Molecule 2 is 7-(diethylamino)-4-methyl-2H-1-benzopyran-2-one (CCD ID: 6ZW) (formula: C₁₄H₁₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	1	2		
2	B	1	Total	C	N	O	0	0
			17	14	1	2		
2	C	1	Total	C	N	O	0	0
			17	14	1	2		
2	D	1	Total	C	N	O	0	0
			17	14	1	2		
2	E	1	Total	C	N	O	0	0
			17	14	1	2		
2	F	1	Total	C	N	O	0	0
			17	14	1	2		
2	G	1	Total	C	N	O	0	0
			17	14	1	2		
2	H	1	Total	C	N	O	0	0
			17	14	1	2		

- Molecule 3 is YTTERBIUM (III) ION (CCD ID: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Yb	0	0
			1	1		
3	B	1	Total	Yb	0	0
			1	1		
3	D	1	Total	Yb	0	0
			1	1		
3	E	2	Total	Yb	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Yb 1	0	0
3	G	1	Total 1	Yb 1	0	0
3	H	1	Total 1	Yb 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	G	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total 303	O 303	0	0
5	B	287	Total 287	O 287	0	0
5	C	312	Total 312	O 312	0	0
5	D	325	Total 325	O 325	0	0
5	E	292	Total 292	O 292	0	0
5	F	236	Total 236	O 236	0	0

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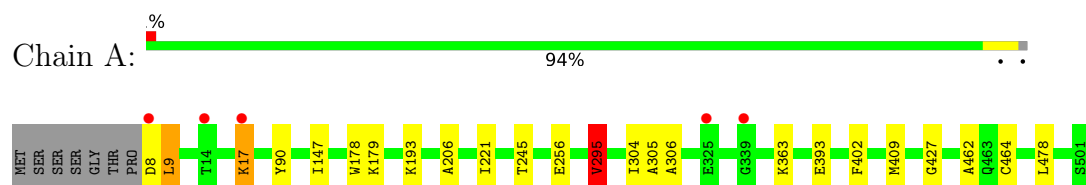
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	287	Total 287	O 287	0	0
5	H	284	Total 284	O 284	0	0

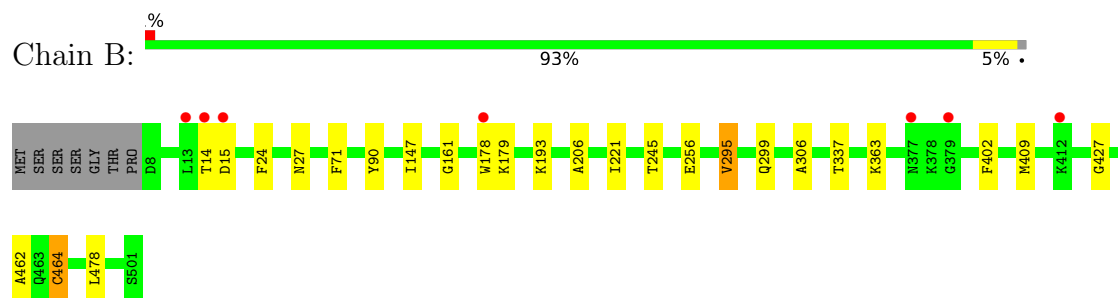
3 Residue-property plots [i](#)

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

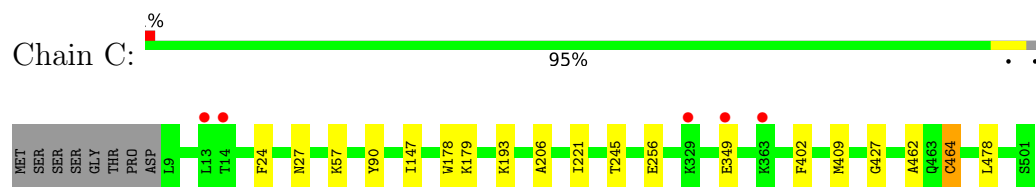
- Molecule 1: Retinal dehydrogenase 1



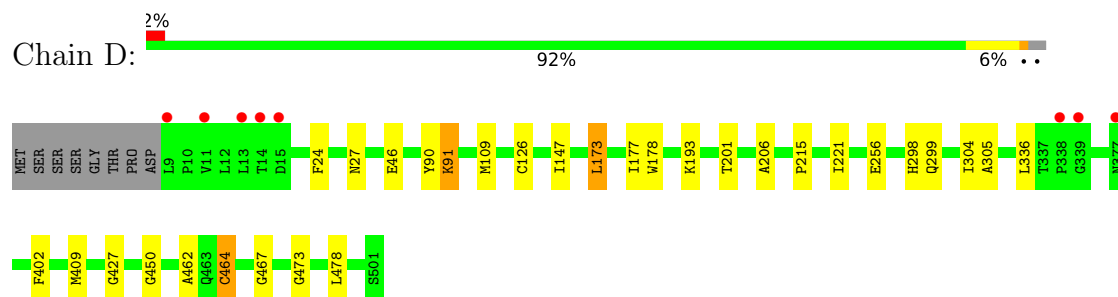
- Molecule 1: Retinal dehydrogenase 1



- Molecule 1: Retinal dehydrogenase 1



- Molecule 1: Retinal dehydrogenase 1



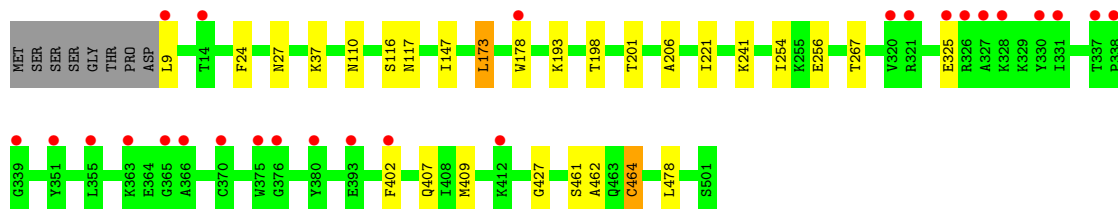
- Molecule 1: Retinal dehydrogenase 1

Chain E:  94% . . .



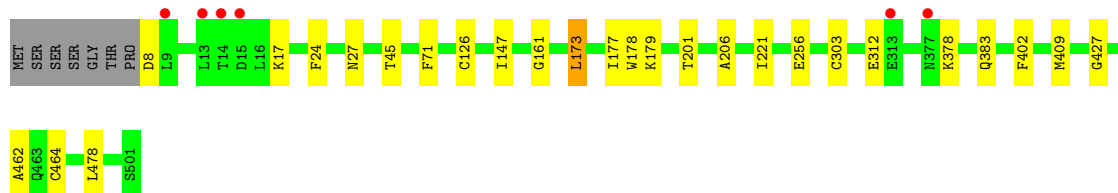
• Molecule 1: Retinal dehydrogenase 1

Chain F:  93% 5% .



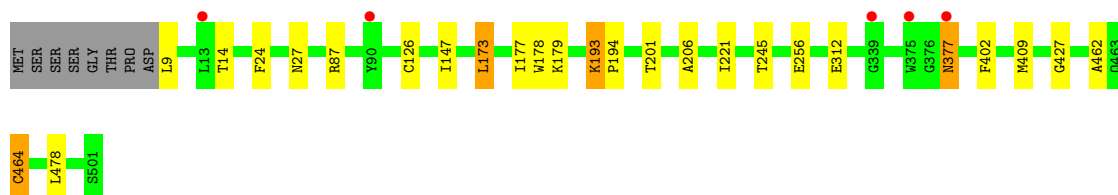
• Molecule 1: Retinal dehydrogenase 1

Chain G:  93% 5% .



• Molecule 1: Retinal dehydrogenase 1

Chain H:  93% . . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.98Å 98.29Å 127.32Å 80.55° 86.23° 64.36°	Depositor
Resolution (Å)	50.00 – 2.05 50.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.05) 90.6 (50.00-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.204 0.183 , 0.212	Depositor DCC
R_{free} test set	11177 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33056	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6ZW, CL, YB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	1/3917 (0.0%)	0.83	4/5301 (0.1%)
1	B	0.77	0/3917	0.82	1/5301 (0.0%)
1	C	0.79	1/3909 (0.0%)	0.84	4/5290 (0.1%)
1	D	0.81	3/3915 (0.1%)	0.86	3/5298 (0.1%)
1	E	0.76	1/3915 (0.0%)	0.85	4/5298 (0.1%)
1	F	0.75	3/3909 (0.1%)	0.86	5/5290 (0.1%)
1	G	0.77	0/3910	0.84	0/5291
1	H	0.77	1/3902 (0.0%)	0.83	4/5280 (0.1%)
All	All	0.77	10/31294 (0.0%)	0.84	25/42349 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	GLU	CD-OE2	8.57	1.41	1.25
1	C	349	GLU	CD-OE2	8.10	1.40	1.25
1	F	325	GLU	CA-CB	7.13	1.64	1.53
1	F	325	GLU	CD-OE2	5.99	1.36	1.25
1	D	46	GLU	CG-CD	5.77	1.66	1.52
1	E	359	GLU	CG-CD	5.71	1.66	1.52
1	A	9	LEU	C-O	-5.69	1.17	1.23
1	H	9	LEU	N-CA	5.66	1.56	1.46
1	F	325	GLU	CG-CD	5.61	1.66	1.52
1	D	215	PRO	CA-C	5.41	1.54	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	325	GLU	CA-CB-CG	9.30	132.71	114.10
1	E	359	GLU	OE1-CD-OE2	-7.34	105.29	122.90
1	D	91	LYS	CB-CG-CD	7.22	127.90	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	254	ILE	CB-CG1-CD1	6.74	127.95	113.80
1	E	359	GLU	CA-CB-CG	6.67	127.44	114.10
1	F	325	GLU	CG-CD-OE2	6.13	132.50	118.40
1	H	9	LEU	CA-C-N	-5.90	113.89	119.85
1	H	9	LEU	C-N-CA	-5.90	113.89	119.85
1	C	349	GLU	CG-CD-OE2	5.90	131.96	118.40
1	A	9	LEU	CA-C-N	-5.85	113.94	119.85
1	A	9	LEU	C-N-CA	-5.85	113.94	119.85
1	F	464	CYS	CB-CA-C	-5.77	100.85	108.76
1	F	254	ILE	CA-CB-CG1	-5.55	100.97	110.40
1	C	349	GLU	CB-CG-CD	5.48	121.92	112.60
1	E	193	LYS	CG-CD-CE	5.42	123.78	111.30
1	H	464	CYS	CB-CA-C	-5.42	101.33	108.76
1	A	363	LYS	CG-CD-CE	5.35	123.61	111.30
1	D	464	CYS	CB-CA-C	-5.33	101.46	108.76
1	E	359	GLU	CG-CD-OE1	5.27	130.52	118.40
1	B	464	CYS	CB-CA-C	-5.26	101.56	108.76
1	H	377	ASN	N-CA-C	5.23	118.88	112.03
1	D	473	GLY	N-CA-C	5.19	118.16	110.63
1	C	349	GLU	CG-CD-OE1	-5.17	106.50	118.40
1	A	295	VAL	CB-CA-C	-5.12	105.49	111.94
1	C	464	CYS	CB-CA-C	-5.06	101.83	108.76

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	3828	0	3827	13	0
1	B	3828	0	3827	13	0
1	C	3820	0	3823	10	0
1	D	3823	0	3828	18	0
1	E	3823	0	3829	15	0
1	F	3820	0	3824	15	0
1	G	3822	0	3824	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3814	0	3820	16	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
2	E	17	0	0	0	0
2	F	17	0	0	0	0
2	G	17	0	0	0	0
2	H	17	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	303	0	0	0	0
5	B	287	0	0	2	0
5	C	312	0	0	1	0
5	D	325	0	0	2	0
5	E	292	0	0	1	0
5	F	236	0	0	2	0
5	G	287	0	0	4	0
5	H	284	0	0	3	0
All	All	33056	0	30602	105	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 (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ALA:HA	1:B:478:LEU:HD23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ASN:ND2	5:F:701:HOH:O	2.23	0.70
1:E:126[B]:CYS:SG	1:E:177:ILE:HG13	2.33	0.68
1:D:126[B]:CYS:SG	1:D:177:ILE:HG13	2.35	0.67
1:G:45:THR:O	1:G:378:LYS:HE2	1.95	0.67
1:H:312:GLU:HG3	5:H:929:HOH:O	1.95	0.66
1:D:109:MET:HG2	1:D:336:LEU:HD11	1.79	0.64
1:A:8:ASP:OD1	1:A:9:LEU:HG	1.98	0.64
1:D:109:MET:CG	1:D:336:LEU:HD11	2.28	0.64
1:F:9:LEU:HD11	1:F:116:SER:HB3	1.79	0.64
1:H:126[B]:CYS:SG	1:H:177:ILE:HG13	2.40	0.62
1:F:462:ALA:HA	1:F:478:LEU:HD13	1.83	0.60
1:D:462:ALA:HA	1:D:478:LEU:HD13	1.83	0.60
1:E:147:ILE:HG13	1:F:461:SER:OG	2.02	0.59
1:G:126[B]:CYS:SG	1:G:177:ILE:HG13	2.42	0.58
1:F:241:LYS:NZ	1:F:267:THR:OG1	2.37	0.58
1:H:462:ALA:HA	1:H:478:LEU:HD13	1.86	0.57
1:G:462:ALA:HA	1:G:478:LEU:HD13	1.86	0.57
1:C:462:ALA:HA	1:C:478:LEU:HD13	1.86	0.57
1:E:126[B]:CYS:SG	1:E:177:ILE:CG1	2.93	0.56
1:A:90[B]:TYR:CE1	1:C:90[B]:TYR:CZ	2.92	0.56
1:B:90[B]:TYR:CZ	1:D:90[B]:TYR:CE1	2.93	0.56
1:E:462:ALA:HA	1:E:478:LEU:HD13	1.88	0.55
1:A:462:ALA:HA	1:A:478:LEU:HD13	1.88	0.54
1:F:9:LEU:HD11	1:F:116:SER:CB	2.38	0.54
1:B:178:TRP:CE3	1:B:478:LEU:HD13	2.43	0.53
1:H:178:TRP:CZ2	1:H:478:LEU:HD12	2.44	0.53
1:B:90[B]:TYR:CE1	1:D:90[B]:TYR:CZ	2.97	0.53
1:G:312:GLU:HG3	5:G:915:HOH:O	2.09	0.52
1:C:178:TRP:CZ2	1:C:478:LEU:HD12	2.44	0.52
1:A:393:GLU:N	1:A:393:GLU:OE1	2.44	0.51
1:A:90[B]:TYR:CZ	1:C:90[B]:TYR:CE1	2.98	0.51
1:D:178:TRP:CZ2	1:D:478:LEU:HD12	2.46	0.50
1:A:178:TRP:CZ2	1:A:478:LEU:HD12	2.46	0.50
1:C:256:GLU:HG3	1:D:256:GLU:HG3	1.93	0.50
1:F:178:TRP:CZ2	1:F:478:LEU:HD12	2.46	0.50
1:G:178:TRP:CZ2	1:G:478:LEU:HD12	2.47	0.49
1:G:179:LYS:HD3	5:G:778:HOH:O	2.12	0.49
1:E:178:TRP:CZ2	1:E:478:LEU:HD12	2.47	0.49
1:G:383:GLN:NE2	5:G:706:HOH:O	2.46	0.49
1:D:126[B]:CYS:SG	1:D:177:ILE:CG1	2.99	0.48
1:H:377:ASN:N	1:H:377:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:TRP:CE2	1:D:478:LEU:HD12	2.49	0.48
1:A:17:LYS:HE3	1:A:17:LYS:HA	1.95	0.48
1:E:193:LYS:HG2	1:E:222:VAL:O	2.14	0.48
1:A:295:VAL:HG23	1:A:306:ALA:O	2.14	0.47
1:H:178:TRP:CE2	1:H:478:LEU:HD12	2.49	0.47
1:A:206:ALA:HB2	1:A:221:ILE:HD12	1.96	0.47
1:D:298:HIS:HD2	5:D:738:HOH:O	1.96	0.47
1:H:87:ARG:HG2	5:H:827:HOH:O	2.13	0.47
1:E:178:TRP:CE2	1:E:478:LEU:HD12	2.50	0.47
1:A:256:GLU:HG3	1:B:256:GLU:HG3	1.96	0.46
1:B:337:THR:OG1	5:B:701:HOH:O	2.20	0.46
1:F:178:TRP:CE2	1:F:478:LEU:HD12	2.50	0.46
1:F:206:ALA:HB2	1:F:221:ILE:HD12	1.98	0.46
1:C:206:ALA:HB2	1:C:221:ILE:HD12	1.98	0.46
1:B:295:VAL:HG23	1:B:306:ALA:O	2.15	0.46
1:H:14:THR:HG22	5:H:957:HOH:O	2.15	0.46
1:B:299:GLN:HA	5:B:728:HOH:O	2.16	0.46
1:C:178:TRP:CE2	1:C:478:LEU:HD12	2.52	0.46
1:H:206:ALA:HB2	1:H:221:ILE:HD12	1.98	0.46
1:A:178:TRP:CE2	1:A:478:LEU:HD12	2.51	0.45
1:D:206:ALA:HB2	1:D:221:ILE:HD12	1.98	0.45
1:G:303[A]:CYS:SG	5:G:828:HOH:O	2.57	0.45
1:H:126[B]:CYS:SG	1:H:177:ILE:CG1	3.04	0.45
1:E:24:PHE:CZ	1:E:27:ASN:HA	2.52	0.45
1:E:299:GLN:HA	5:E:824:HOH:O	2.16	0.45
1:G:178:TRP:CE2	1:G:478:LEU:HD12	2.52	0.45
1:G:206:ALA:HB2	1:G:221:ILE:HD12	1.97	0.44
1:A:179:LYS:NZ	1:A:245:THR:OG1	2.49	0.44
1:F:37:LYS:HD2	5:F:708:HOH:O	2.16	0.44
1:F:407:GLN:N	1:F:407:GLN:OE1	2.50	0.44
1:C:24:PHE:CZ	1:C:27:ASN:HA	2.53	0.44
1:H:24:PHE:CZ	1:H:27:ASN:HA	2.53	0.44
1:D:24:PHE:CZ	1:D:27:ASN:HA	2.53	0.44
1:C:57:LYS:HE3	5:C:847:HOH:O	2.19	0.43
1:E:206:ALA:HB2	1:E:221:ILE:HD12	1.99	0.43
1:B:206:ALA:HB2	1:B:221:ILE:HD12	1.99	0.43
1:G:24:PHE:CZ	1:G:27:ASN:HA	2.54	0.43
1:D:299:GLN:HA	5:D:892:HOH:O	2.18	0.43
1:E:173:LEU:HD13	1:E:201:THR:HB	2.01	0.42
1:D:304:ILE:O	1:D:305:ALA:C	2.63	0.42
1:F:173:LEU:HD13	1:F:201:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:LYS:NZ	1:H:245:THR:OG1	2.49	0.42
1:H:173:LEU:HD13	1:H:201:THR:HB	2.01	0.42
1:B:24:PHE:CZ	1:B:27:ASN:HA	2.55	0.42
1:C:179:LYS:NZ	1:C:245:THR:OG1	2.49	0.42
1:E:147:ILE:HD13	1:E:147:ILE:HG21	1.76	0.42
1:E:179:LYS:NZ	1:E:245:THR:OG1	2.50	0.41
1:G:256:GLU:HG3	1:H:256:GLU:HG3	2.03	0.41
1:D:450:GLY:HA3	1:D:467:GLY:O	2.21	0.41
1:E:256:GLU:HG3	1:F:256:GLU:HG3	2.02	0.41
1:F:24:PHE:CZ	1:F:27:ASN:HA	2.56	0.41
1:B:71:PHE:CZ	1:B:161:GLY:HA2	2.56	0.41
1:B:179:LYS:NZ	1:B:245:THR:OG1	2.50	0.41
1:D:173:LEU:HD13	1:D:201:THR:HB	2.03	0.41
1:D:178:TRP:CE2	1:D:478:LEU:CD1	3.04	0.41
1:B:14:THR:HG22	1:B:15:ASP:N	2.36	0.41
1:H:178:TRP:CE2	1:H:478:LEU:CD1	3.03	0.41
1:G:173:LEU:HD13	1:G:201:THR:HB	2.03	0.40
1:G:71:PHE:CZ	1:G:161:GLY:HA2	2.57	0.40
1:A:304:ILE:O	1:A:305:ALA:C	2.64	0.40
1:H:193:LYS:HE3	1:H:194:PRO:O	2.21	0.40
1:E:178:TRP:CE2	1:E:478:LEU:CD1	3.05	0.40
1:F:110:ASN:HD21	1:F:198:THR:HA	1.87	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	494/501 (99%)	481 (97%)	12 (2%)	1 (0%)	43	37
1	B	494/501 (99%)	481 (97%)	12 (2%)	1 (0%)	43	37
1	C	493/501 (98%)	478 (97%)	14 (3%)	1 (0%)	43	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	494/501 (99%)	479 (97%)	14 (3%)	1 (0%)	43	37
1	E	494/501 (99%)	480 (97%)	13 (3%)	1 (0%)	43	37
1	F	493/501 (98%)	479 (97%)	13 (3%)	1 (0%)	43	37
1	G	494/501 (99%)	478 (97%)	15 (3%)	1 (0%)	43	37
1	H	493/501 (98%)	477 (97%)	15 (3%)	1 (0%)	43	37
All	All	3949/4008 (98%)	3833 (97%)	108 (3%)	8 (0%)	43	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	427	GLY
1	D	427	GLY
1	E	427	GLY
1	F	427	GLY
1	H	427	GLY
1	A	427	GLY
1	B	427	GLY
1	G	427	GLY

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	411/415 (99%)	404 (98%)	7 (2%)	53	53
1	B	411/415 (99%)	404 (98%)	7 (2%)	53	53
1	C	410/415 (99%)	405 (99%)	5 (1%)	63	65
1	D	411/415 (99%)	404 (98%)	7 (2%)	53	53
1	E	411/415 (99%)	406 (99%)	5 (1%)	63	65
1	F	410/415 (99%)	404 (98%)	6 (2%)	57	58
1	G	411/415 (99%)	404 (98%)	7 (2%)	53	53
1	H	410/415 (99%)	404 (98%)	6 (2%)	57	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3285/3320 (99%)	3235 (98%)	50 (2%)	57 58

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	147	ILE
1	A	193	LYS
1	A	295	VAL
1	A	402	PHE
1	A	409	MET
1	A	464	CYS
1	B	147	ILE
1	B	193	LYS
1	B	295	VAL
1	B	363	LYS
1	B	402	PHE
1	B	409	MET
1	B	464	CYS
1	C	147	ILE
1	C	193	LYS
1	C	402	PHE
1	C	409	MET
1	C	464	CYS
1	D	91	LYS
1	D	147	ILE
1	D	173	LEU
1	D	193	LYS
1	D	402	PHE
1	D	409	MET
1	D	464	CYS
1	E	147	ILE
1	E	173	LEU
1	E	402	PHE
1	E	409	MET
1	E	464	CYS
1	F	147	ILE
1	F	173	LEU
1	F	193	LYS
1	F	402	PHE
1	F	409	MET
1	F	464	CYS

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Mol	Chain	Res	Type
1	G	8	ASP
1	G	17	LYS
1	G	147	ILE
1	G	173	LEU
1	G	402	PHE
1	G	409	MET
1	G	464	CYS
1	H	147	ILE
1	H	173	LEU
1	H	193	LYS
1	H	402	PHE
1	H	409	MET
1	H	464	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	30	HIS
1	A	51	GLN
1	A	121	ASN
1	A	383	GLN
1	A	406	GLN
1	B	26	ASN
1	B	30	HIS
1	B	121	ASN
1	B	141	GLN
1	B	299	GLN
1	B	383	GLN
1	B	406	GLN
1	C	26	ASN
1	C	27	ASN
1	C	51	GLN
1	C	121	ASN
1	D	26	ASN
1	D	51	GLN
1	D	121	ASN
1	D	298	HIS
1	D	299	GLN
1	D	383	GLN
1	D	406	GLN
1	E	26	ASN

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Mol	Chain	Res	Type
1	E	30	HIS
1	E	121	ASN
1	E	383	GLN
1	E	406	GLN
1	F	26	ASN
1	F	121	ASN
1	F	141	GLN
1	F	383	GLN
1	F	406	GLN
1	G	26	ASN
1	G	121	ASN
1	G	383	GLN
1	G	406	GLN
1	H	26	ASN
1	H	121	ASN
1	H	406	GLN

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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	6ZW	G	601	-	18,18,18	1.64	4 (22%)	25,25,25	1.69	7 (28%)
2	6ZW	D	601	-	18,18,18	1.64	6 (33%)	25,25,25	1.88	7 (28%)
2	6ZW	A	601	-	18,18,18	1.57	4 (22%)	25,25,25	1.43	3 (12%)
2	6ZW	E	601	-	18,18,18	1.69	4 (22%)	25,25,25	1.55	6 (24%)
2	6ZW	C	601	-	18,18,18	1.46	3 (16%)	25,25,25	1.52	4 (16%)
2	6ZW	F	601	-	18,18,18	1.54	3 (16%)	25,25,25	1.70	6 (24%)
2	6ZW	H	601	-	18,18,18	1.78	3 (16%)	25,25,25	1.38	4 (16%)
2	6ZW	B	601	-	18,18,18	1.70	3 (16%)	25,25,25	1.95	9 (36%)

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	6ZW	G	601	-	-	3/8/8/8	0/2/2/2
2	6ZW	D	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	A	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	E	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	C	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	F	601	-	-	4/8/8/8	0/2/2/2
2	6ZW	H	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	B	601	-	-	4/8/8/8	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6ZW	C3-C2	4.76	1.49	1.40
2	H	601	6ZW	C9-C10	4.58	1.41	1.35
2	F	601	6ZW	C3-C2	4.20	1.48	1.40
2	H	601	6ZW	C3-C2	3.94	1.47	1.40
2	E	601	6ZW	C9-C10	3.90	1.40	1.35
2	E	601	6ZW	C3-C2	3.62	1.47	1.40
2	G	601	6ZW	C3-C2	3.59	1.47	1.40
2	C	601	6ZW	C3-C2	3.59	1.47	1.40
2	A	601	6ZW	C9-C10	3.40	1.39	1.35
2	A	601	6ZW	C3-C2	3.27	1.46	1.40
2	E	601	6ZW	C3-C10	3.12	1.50	1.45
2	B	601	6ZW	C9-C10	3.12	1.39	1.35
2	G	601	6ZW	C9-C10	2.99	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	6ZW	C3-C10	2.98	1.49	1.45
2	D	601	6ZW	C9-C8	-2.91	1.38	1.44
2	G	601	6ZW	C9-C8	-2.80	1.38	1.44
2	F	601	6ZW	C9-C10	2.79	1.38	1.35
2	F	601	6ZW	C9-C8	-2.71	1.38	1.44
2	D	601	6ZW	C9-C10	2.67	1.38	1.35
2	G	601	6ZW	C3-C10	2.54	1.49	1.45
2	D	601	6ZW	C3-C2	2.48	1.45	1.40
2	A	601	6ZW	C9-C8	-2.41	1.39	1.44
2	A	601	6ZW	C3-C10	2.35	1.48	1.45
2	C	601	6ZW	C9-C10	2.34	1.38	1.35
2	H	601	6ZW	C3-C10	2.23	1.48	1.45
2	C	601	6ZW	C9-C8	-2.23	1.39	1.44
2	D	601	6ZW	C6-N11	2.19	1.44	1.38
2	B	601	6ZW	C3-C10	2.09	1.48	1.45
2	D	601	6ZW	O7-C2	-2.03	1.35	1.38
2	E	601	6ZW	C9-C8	-2.03	1.40	1.44

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	6ZW	O7-C8-C9	5.08	123.35	117.16
2	F	601	6ZW	O7-C8-C9	4.74	122.93	117.16
2	C	601	6ZW	O7-C8-C9	4.69	122.87	117.16
2	G	601	6ZW	O7-C8-C9	4.27	122.35	117.16
2	A	601	6ZW	O7-C8-C9	4.26	122.34	117.16
2	H	601	6ZW	O7-C8-C9	4.21	122.28	117.16
2	E	601	6ZW	O7-C8-C9	4.05	122.09	117.16
2	D	601	6ZW	O7-C2-C3	-3.97	117.96	121.57
2	D	601	6ZW	C8-C9-C10	-3.65	119.97	123.06
2	B	601	6ZW	O7-C2-C1	3.56	120.87	115.83
2	E	601	6ZW	C8-C9-C10	-3.39	120.18	123.06
2	F	601	6ZW	O17-C8-C9	-3.38	119.11	125.92
2	D	601	6ZW	O7-C2-C1	3.38	120.62	115.83
2	D	601	6ZW	O7-C8-C9	3.37	121.26	117.16
2	B	601	6ZW	O7-C2-C3	-3.03	118.82	121.57
2	G	601	6ZW	O7-C2-C1	3.01	120.09	115.83
2	G	601	6ZW	O17-C8-C9	-3.00	119.90	125.92
2	D	601	6ZW	C16-C10-C3	2.95	123.28	119.94
2	E	601	6ZW	O7-C2-C1	2.90	119.94	115.83
2	B	601	6ZW	O17-C8-C9	-2.80	120.30	125.92
2	B	601	6ZW	C5-C6-N11	-2.74	117.58	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	6ZW	C16-C10-C9	-2.73	117.72	120.98
2	A	601	6ZW	O17-C8-C9	-2.64	120.60	125.92
2	C	601	6ZW	O7-C2-C1	2.62	119.54	115.83
2	F	601	6ZW	O7-C2-C1	2.58	119.48	115.83
2	B	601	6ZW	C4-C5-C6	2.57	123.55	120.30
2	G	601	6ZW	O7-C2-C3	-2.55	119.25	121.57
2	B	601	6ZW	C8-C9-C10	-2.50	120.94	123.06
2	F	601	6ZW	C16-C10-C3	2.41	122.67	119.94
2	E	601	6ZW	O7-C2-C3	-2.41	119.38	121.57
2	G	601	6ZW	C16-C10-C3	2.38	122.63	119.94
2	E	601	6ZW	C4-C5-C6	2.33	123.25	120.30
2	F	601	6ZW	C8-C9-C10	-2.30	121.10	123.06
2	H	601	6ZW	C3-C10-C9	-2.28	116.46	118.65
2	G	601	6ZW	C4-C5-C6	2.25	123.15	120.30
2	C	601	6ZW	C8-C9-C10	-2.22	121.18	123.06
2	C	601	6ZW	O7-C2-C3	-2.19	119.58	121.57
2	F	601	6ZW	O7-C2-C3	-2.12	119.64	121.57
2	E	601	6ZW	O17-C8-C9	-2.12	121.66	125.92
2	H	601	6ZW	C4-C5-C6	2.11	122.97	120.30
2	H	601	6ZW	O7-C2-C1	2.11	118.82	115.83
2	B	601	6ZW	C1-C6-N11	2.06	123.55	121.33
2	A	601	6ZW	O7-C2-C1	2.05	118.74	115.83
2	D	601	6ZW	C2-O7-C8	2.03	124.20	121.67
2	B	601	6ZW	C3-C10-C9	-2.03	116.69	118.65
2	G	601	6ZW	C12-N11-C6	2.03	124.39	121.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	601	6ZW	C13-C12-N11-C6
2	B	601	6ZW	C5-C6-N11-C12
2	B	601	6ZW	C1-C6-N11-C14
2	G	601	6ZW	C13-C12-N11-C14
2	B	601	6ZW	C5-C6-N11-C14
2	B	601	6ZW	C1-C6-N11-C12
2	F	601	6ZW	C5-C6-N11-C12
2	F	601	6ZW	C1-C6-N11-C12
2	F	601	6ZW	C5-C6-N11-C14
2	F	601	6ZW	C1-C6-N11-C14
2	G	601	6ZW	C5-C6-N11-C14

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	494/501 (98%)	-0.16	5 (1%) 79 81	7, 17, 33, 51	2 (0%)
1	B	494/501 (98%)	-0.14	7 (1%) 73 75	9, 18, 34, 60	2 (0%)
1	C	493/501 (98%)	-0.27	5 (1%) 79 81	7, 15, 31, 52	2 (0%)
1	D	493/501 (98%)	-0.23	8 (1%) 70 72	7, 15, 30, 62	3 (0%)
1	E	493/501 (98%)	-0.16	2 (0%) 88 90	7, 18, 31, 48	3 (0%)
1	F	493/501 (98%)	0.21	26 (5%) 32 32	9, 21, 46, 63	2 (0%)
1	G	494/501 (98%)	-0.20	6 (1%) 76 78	9, 16, 31, 63	2 (0%)
1	H	493/501 (98%)	-0.14	5 (1%) 79 81	10, 18, 31, 44	2 (0%)
All	All	3947/4008 (98%)	-0.14	64 (1%) 70 72	7, 17, 35, 63	18 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	375	TRP	4.9
1	D	13	LEU	4.7
1	F	327	ALA	4.5
1	D	338	PRO	3.9
1	F	380	TYR	3.6
1	C	14	THR	3.4
1	G	9	LEU	3.4
1	G	14	THR	3.3
1	D	377	ASN	3.2
1	B	13	LEU	3.2
1	B	14	THR	3.2
1	F	326	ARG	3.1
1	D	339	GLY	3.0
1	H	377	ASN	3.0
1	F	321	ARG	3.0
1	F	328	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	325	GLU	2.9
1	D	11	VAL	2.9
1	F	365	GLY	2.8
1	A	8	ASP	2.8
1	H	13	LEU	2.8
1	F	366	ALA	2.7
1	D	9	LEU	2.7
1	A	14	THR	2.7
1	D	14	THR	2.7
1	C	349	GLU	2.6
1	G	13	LEU	2.6
1	D	15	ASP	2.6
1	B	379	GLY	2.6
1	F	338	PRO	2.6
1	B	412	LYS	2.6
1	F	9	LEU	2.6
1	H	90	TYR	2.6
1	C	329	LYS	2.4
1	F	337	THR	2.4
1	G	313	GLU	2.4
1	B	15	ASP	2.4
1	E	363	LYS	2.4
1	F	14	THR	2.4
1	H	339	GLY	2.3
1	F	402	PHE	2.3
1	F	320	VAL	2.3
1	A	339	GLY	2.3
1	F	412	LYS	2.3
1	F	330	TYR	2.3
1	B	377	ASN	2.2
1	C	13	LEU	2.2
1	B	178	TRP	2.2
1	C	363	LYS	2.2
1	A	325	GLU	2.1
1	F	393	GLU	2.1
1	F	355	LEU	2.1
1	G	377	ASN	2.1
1	F	178	TRP	2.1
1	E	349	GLU	2.1
1	F	339	GLY	2.1
1	F	376	GLY	2.1
1	F	375	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	15	ASP	2.0
1	A	17	LYS	2.0
1	F	351	TYR	2.0
1	F	331	ILE	2.0
1	F	370	CYS	2.0
1	F	363	LYS	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(Å ²)	Q<0.9
2	6ZW	E	601	17/17	0.85	0.14	26,32,40,45	0
2	6ZW	C	601	17/17	0.89	0.12	20,23,29,31	0
2	6ZW	B	601	17/17	0.89	0.13	23,26,43,44	0
2	6ZW	F	601	17/17	0.89	0.11	25,27,36,36	0
2	6ZW	H	601	17/17	0.91	0.12	24,30,43,44	0
2	6ZW	D	601	17/17	0.92	0.10	17,19,34,37	0
2	6ZW	G	601	17/17	0.92	0.10	21,23,33,34	0
2	6ZW	A	601	17/17	0.92	0.11	22,26,36,37	0
3	YB	E	603	1/1	0.98	0.07	56,56,56,56	0
3	YB	F	602	1/1	0.98	0.11	49,49,49,49	0
3	YB	D	602	1/1	0.99	0.06	35,35,35,35	0
3	YB	E	602	1/1	0.99	0.05	32,32,32,32	0
3	YB	A	602	1/1	0.99	0.06	29,29,29,29	0
3	YB	B	602	1/1	0.99	0.04	27,27,27,27	0
3	YB	G	602	1/1	0.99	0.05	31,31,31,31	0
3	YB	H	602	1/1	0.99	0.04	25,25,25,25	0
4	CL	A	603	1/1	0.99	0.02	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	603	1/1	0.99	0.03	18,18,18,18	0
4	CL	C	602	1/1	0.99	0.04	17,17,17,17	0
4	CL	D	603	1/1	0.99	0.03	16,16,16,16	0
4	CL	E	604	1/1	0.99	0.02	17,17,17,17	0
4	CL	F	603	1/1	0.99	0.03	19,19,19,19	0
4	CL	G	603	1/1	0.99	0.03	16,16,16,16	0
4	CL	H	603	1/1	0.99	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.