



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:08 AM EDT

PDB ID : 9EC1 / pdb\_00009ec1  
Title : The Structure of Human Dystrophin Spectrin Repeat 24  
Authors : Streeter, O.; Shi, K.; Bui, H.N.; Ervasti, J.M.; Evans III, R.L.; Muretta, J.M.  
Deposited on : 2024-11-13  
Resolution : 2.14 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](mailto: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>.

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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

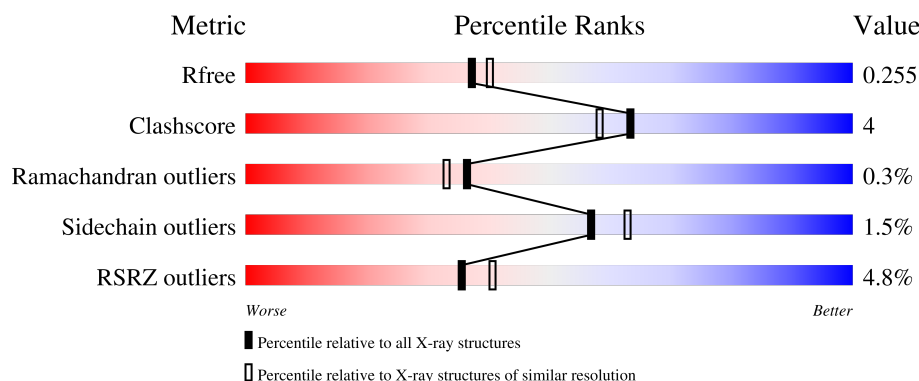
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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  $\geq 3$ , 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	117	<div> <div>3%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
1	B	117	<div> <div>%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	C	117	<div> <div>%</div> <div>91%</div> <div>9%</div> <div>.</div> </div>
1	D	117	<div> <div>3%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	E	117	<div> <div>5%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	117	<div><div></div><div>4%</div><div>90%</div><div>8%</div><div>••</div></div>
1	G	117	<div><div></div><div>4%</div><div>84%</div><div>15%</div><div>•</div></div>
1	H	117	<div><div></div><div>17%</div><div>81%</div><div>16%</div><div>•</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7630 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 Dystrophin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	0	0	0
			940	586	170	184			
1	B	117	Total	C	N	O	0	0	0
			940	586	170	184			
1	C	117	Total	C	N	O	0	0	0
			940	586	170	184			
1	D	116	Total	C	N	O	0	0	0
			934	583	169	182			
1	E	117	Total	C	N	O	0	0	0
			940	586	170	184			
1	F	115	Total	C	N	O	0	0	0
			929	581	168	180			
1	G	116	Total	C	N	O	0	0	0
			934	583	169	182			
1	H	114	Total	C	N	O	0	0	0
			898	560	164	174			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P11532
A	2	THR	-	expression tag	UNP P11532
A	3	GLY	-	expression tag	UNP P11532
A	8	GLN	ARG	variant	UNP P11532
B	1	SER	-	expression tag	UNP P11532
B	2	THR	-	expression tag	UNP P11532
B	3	GLY	-	expression tag	UNP P11532
B	8	GLN	ARG	variant	UNP P11532
C	1	SER	-	expression tag	UNP P11532
C	2	THR	-	expression tag	UNP P11532
C	3	GLY	-	expression tag	UNP P11532
C	8	GLN	ARG	variant	UNP P11532
D	1	SER	-	expression tag	UNP P11532

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	THR	-	expression tag	UNP P11532
D	3	GLY	-	expression tag	UNP P11532
D	8	GLN	ARG	variant	UNP P11532
E	1	SER	-	expression tag	UNP P11532
E	2	THR	-	expression tag	UNP P11532
E	3	GLY	-	expression tag	UNP P11532
E	8	GLN	ARG	variant	UNP P11532
F	1	SER	-	expression tag	UNP P11532
F	2	THR	-	expression tag	UNP P11532
F	3	GLY	-	expression tag	UNP P11532
F	8	GLN	ARG	variant	UNP P11532
G	1	SER	-	expression tag	UNP P11532
G	2	THR	-	expression tag	UNP P11532
G	3	GLY	-	expression tag	UNP P11532
G	8	GLN	ARG	variant	UNP P11532
H	1	SER	-	expression tag	UNP P11532
H	2	THR	-	expression tag	UNP P11532
H	3	GLY	-	expression tag	UNP P11532
H	8	GLN	ARG	variant	UNP P11532

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	3	Total	Cl	0	0
			3	3		
3	D	2	Total	Cl	0	0
			2	2		
3	F	1	Total	Cl	0	0
			1	1		
3	G	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		

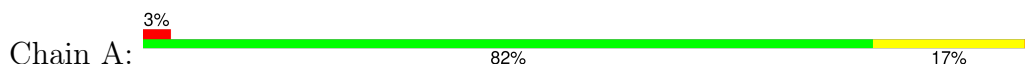
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	19	Total 19	O 19	0	0
4	C	11	Total 11	O 11	0	0
4	D	9	Total 9	O 9	0	0
4	E	8	Total 8	O 8	0	0
4	F	12	Total 12	O 12	0	0
4	G	15	Total 15	O 15	0	0
4	H	10	Total 10	O 10	0	0

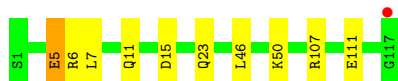
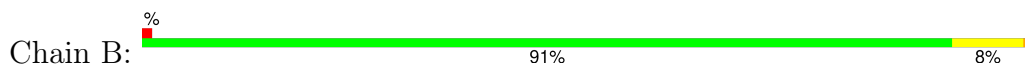
### 3 Residue-property plots [i](#)

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.

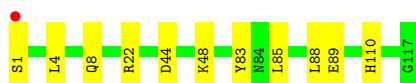
- Molecule 1: Dystrophin



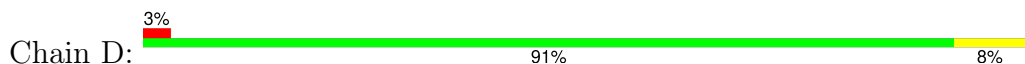
- Molecule 1: Dystrophin



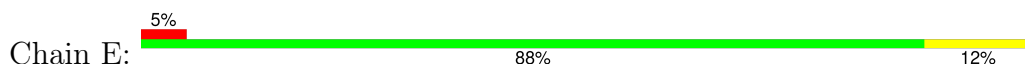
- Molecule 1: Dystrophin



- Molecule 1: Dystrophin

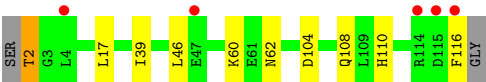
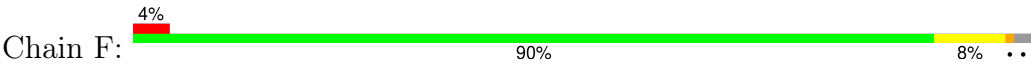


- Molecule 1: Dystrophin

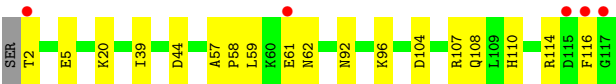
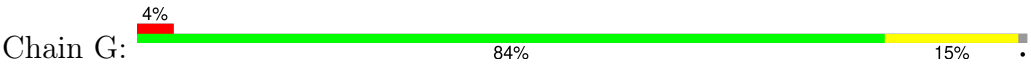


- Molecule 1: Dystrophin

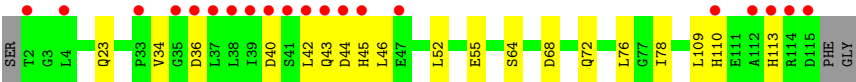
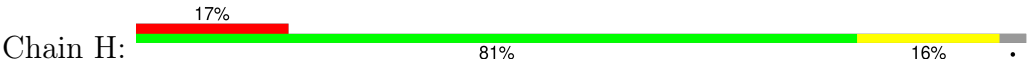




● Molecule 1: Dystrophin



● Molecule 1: Dystrophin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.00Å 106.00Å 614.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.48 – 2.14 34.48 – 2.14	Depositor EDS
% Data completeness (in resolution range)	62.5 (34.48-2.14) 62.6 (34.48-2.14)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.217 , 0.255 0.215 , 0.255	Depositor DCC
$R_{free}$ test set	3593 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/952	0.40	0/1287
1	B	0.23	0/952	0.41	0/1287
1	C	0.23	0/952	0.36	0/1287
1	D	0.23	0/946	0.37	0/1279
1	E	0.23	0/952	0.38	0/1287
1	F	0.22	0/941	0.37	0/1274
1	G	0.23	0/946	0.40	0/1279
1	H	0.22	0/909	0.36	0/1232
All	All	0.23	0/7550	0.38	0/10212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	940	0	952	12	0
1	B	940	0	952	6	0
1	C	940	0	952	6	0
1	D	934	0	944	6	0
1	E	940	0	952	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	929	0	941	6	0
1	G	934	0	944	12	0
1	H	898	0	894	8	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	20	0	0	0	0
3	A	2	0	0	0	0
3	B	3	0	0	1	0
3	D	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	16	0	0	0	0
4	B	19	0	0	0	0
4	C	11	0	0	0	0
4	D	9	0	0	0	0
4	E	8	0	0	0	0
4	F	12	0	0	0	0
4	G	15	0	0	1	0
4	H	10	0	0	0	0
All	All	7630	0	7531	60	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 4.

All (60) 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:E:23:GLN:NE2	1:H:23:GLN:OE1	2.18	0.70
1:A:44:ASP:OD2	1:A:48:LYS:NZ	2.25	0.69
1:B:15:ASP:OD1	1:C:83:TYR:OH	2.12	0.66
1:E:2:THR:HA	1:E:5:GLU:OE2	1.95	0.66
1:E:99:GLN:O	1:E:103:GLU:HG2	1.97	0.65
1:F:104:ASP:O	1:F:108:GLN:HG3	1.95	0.65
1:G:58:PRO:O	1:G:61:GLU:HG3	1.96	0.64
1:D:111:GLU:HG2	1:D:114:ARG:HH22	1.63	0.64
1:E:16:GLU:HG3	1:E:20:LYS:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:ARG:NH1	4:G:301:HOH:O	2.32	0.58
1:A:104:ASP:OD1	1:A:107:ARG:NH2	2.36	0.58
1:B:107:ARG:O	1:B:111:GLU:HG3	2.03	0.58
1:A:23:GLN:NE2	1:D:23:GLN:OE1	2.34	0.55
1:B:46:LEU:O	1:B:50:LYS:HG3	2.07	0.55
1:C:85:LEU:O	1:C:89:GLU:HG3	2.08	0.54
1:H:72:GLN:O	1:H:76:LEU:HG	2.08	0.53
1:A:6:ARG:HH11	1:A:72:GLN:NE2	2.05	0.53
1:E:46:LEU:HD21	1:E:110:HIS:CD2	2.43	0.53
1:G:92:ASN:O	1:G:96:LYS:HD2	2.07	0.52
1:F:46:LEU:HD21	1:F:110:HIS:CE1	2.44	0.52
1:F:39:ILE:HD12	1:F:116:PHE:HB2	1.92	0.51
1:D:111:GLU:HG2	1:D:114:ARG:NH2	2.26	0.51
1:H:68:ASP:O	1:H:72:GLN:HG3	2.10	0.51
1:A:1:SER:O	1:A:6:ARG:NH2	2.39	0.50
1:C:44:ASP:OD1	1:C:48:LYS:HE2	2.11	0.50
1:E:39:ILE:HD11	1:E:117:GLY:HA3	1.94	0.49
1:C:110:HIS:NE2	2:C:201:SO4:O3	2.35	0.47
1:A:84:ASN:O	1:A:88:LEU:HD23	2.14	0.47
1:G:59:LEU:O	1:G:62:ASN:HB2	2.14	0.47
1:A:18:ASP:O	1:A:22:ARG:HG3	2.14	0.47
3:B:203:CL:CL	1:C:22:ARG:NH1	2.85	0.47
1:E:43:GLN:OE1	1:E:113:HIS:NE2	2.48	0.46
1:G:104:ASP:O	1:G:108:GLN:HG2	2.15	0.46
1:H:46:LEU:HD12	1:H:109:LEU:HB3	1.97	0.46
1:F:17:LEU:HD13	1:F:62:ASN:HB3	1.98	0.45
1:B:7:LEU:O	1:B:11:GLN:HG3	2.15	0.45
1:H:76:LEU:HB2	1:H:78:ILE:HD12	1.99	0.45
1:A:49:VAL:HG21	1:A:105:ARG:HG2	1.99	0.44
1:G:44:ASP:OD2	1:G:44:ASP:N	2.51	0.44
1:H:44:ASP:C	1:H:45:HIS:HD1	2.26	0.44
1:C:4:LEU:O	1:C:8:GLN:HG3	2.18	0.44
1:A:32:GLN:O	1:A:105:ARG:NH1	2.36	0.43
1:D:71:ARG:HD3	1:D:71:ARG:HA	1.69	0.43
1:D:2:THR:HB	1:D:6:ARG:HH21	1.84	0.43
1:F:2:THR:O	1:F:2:THR:OG1	2.36	0.43
1:D:59:LEU:O	1:D:62:ASN:HB2	2.19	0.43
1:H:52:LEU:HA	1:H:55:GLU:OE1	2.19	0.42
1:G:104:ASP:OD2	1:G:107:ARG:NH2	2.52	0.42
1:G:39:ILE:HB	1:G:116:PHE:CZ	2.54	0.42
1:A:68:ASP:OD1	1:A:71:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD11	1:A:116:PHE:CZ	2.54	0.42
1:E:39:ILE:HD11	1:E:117:GLY:CA	2.49	0.42
1:F:60:LYS:HA	1:F:60:LYS:HD2	1.73	0.41
1:G:2:THR:HB	1:G:5:GLU:HB3	2.02	0.41
1:G:39:ILE:HB	1:G:116:PHE:CE1	2.55	0.41
1:B:23:GLN:NE2	1:G:20:LYS:HD3	2.35	0.41
1:B:5:GLU:OE1	1:B:6:ARG:NH1	2.53	0.41
1:G:57:ALA:N	1:G:58:PRO:HD2	2.36	0.40
1:A:56:ILE:O	1:A:59:LEU:HB2	2.22	0.40
1:H:113:HIS:ND1	1:H:113:HIS:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
1	B	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	C	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
1	D	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
1	E	115/117 (98%)	115 (100%)	0	0	100	100
1	F	113/117 (97%)	113 (100%)	0	0	100	100
1	G	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
1	H	112/117 (96%)	103 (92%)	6 (5%)	3 (3%)	4	1
All	All	913/936 (98%)	897 (98%)	13 (1%)	3 (0%)	36	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	43	GLN
1	H	36	ASP
1	H	42	LEU

### 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	104/104 (100%)	103 (99%)	1 (1%)	68	74
1	B	104/104 (100%)	103 (99%)	1 (1%)	68	74
1	C	104/104 (100%)	102 (98%)	2 (2%)	50	55
1	D	103/104 (99%)	102 (99%)	1 (1%)	68	74
1	E	104/104 (100%)	103 (99%)	1 (1%)	68	74
1	F	103/104 (99%)	102 (99%)	1 (1%)	68	74
1	G	103/104 (99%)	102 (99%)	1 (1%)	68	74
1	H	96/104 (92%)	92 (96%)	4 (4%)	26	23
All	All	821/832 (99%)	809 (98%)	12 (2%)	57	63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	B	5	GLU
1	C	1	SER
1	C	88	LEU
1	D	66	VAL
1	E	64	SER
1	F	2	THR
1	G	110	HIS
1	H	34	VAL
1	H	40	ASP
1	H	64	SER
1	H	110	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	67	ASN
1	A	72	GLN
1	A	92	ASN
1	B	67	ASN
1	B	92	ASN
1	C	32	GLN
1	C	43	GLN
1	C	62	ASN
1	C	67	ASN
1	C	84	ASN
1	C	92	ASN
1	D	45	HIS
1	D	65	HIS
1	D	67	ASN
1	D	84	ASN
1	D	92	ASN
1	D	99	GLN
1	D	108	GLN
1	E	45	HIS
1	E	72	GLN
1	E	79	GLN
1	E	84	ASN
1	E	110	HIS
1	F	45	HIS
1	F	65	HIS
1	F	79	GLN
1	G	23	GLN
1	G	67	ASN
1	G	72	GLN
1	G	92	ASN
1	H	65	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	SO4	E	201	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	A	202	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	F	202	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	B	202	-	4,4,4	0.32	0	6,6,6	0.20	0
2	SO4	G	201	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	A	201	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	C	201	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	B	201	-	4,4,4	0.25	0	6,6,6	0.24	0
2	SO4	G	203	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	G	204	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	D	201	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	F	201	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	G	202	-	4,4,4	0.25	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	117/117 (100%)	0.08	4 (3%)	48	52	25, 37, 60, 86	0
1	B	117/117 (100%)	-0.23	1 (0%)	81	84	21, 32, 53, 59	0
1	C	117/117 (100%)	-0.05	1 (0%)	81	84	24, 37, 59, 71	0
1	D	116/117 (99%)	0.09	3 (2%)	57	61	25, 36, 65, 87	0
1	E	117/117 (100%)	0.19	6 (5%)	33	38	25, 39, 66, 95	0
1	F	115/117 (98%)	0.08	5 (4%)	40	45	23, 36, 67, 98	0
1	G	116/117 (99%)	0.13	5 (4%)	40	45	24, 36, 62, 86	0
1	H	114/117 (97%)	0.71	20 (17%)	4	5	24, 43, 99, 113	0
All	All	929/936 (99%)	0.12	45 (4%)	35	41	21, 37, 72, 113	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	44	ASP	5.8
1	G	116	PHE	5.8
1	H	42	LEU	5.6
1	D	116	PHE	4.9
1	E	1	SER	4.8
1	H	41	SER	4.8
1	H	39	ILE	4.2
1	H	43	GLN	3.9
1	H	113	HIS	3.8
1	D	2	THR	3.7
1	H	112	ALA	3.6
1	B	117	GLY	3.6
1	H	35	GLY	3.6
1	F	115	ASP	3.6
1	A	117	GLY	3.4
1	H	38	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	2	THR	3.3
1	A	5	GLU	3.2
1	G	115	ASP	3.1
1	E	4	LEU	3.0
1	H	4	LEU	3.0
1	G	2	THR	3.0
1	F	116	PHE	3.0
1	H	40	ASP	2.9
1	G	117	GLY	2.8
1	A	2	THR	2.8
1	E	117	GLY	2.7
1	G	61	GLU	2.5
1	H	37	LEU	2.5
1	H	33	PRO	2.5
1	E	114	ARG	2.5
1	H	110	HIS	2.5
1	H	114	ARG	2.5
1	H	47	GLU	2.4
1	E	2	THR	2.4
1	H	45	HIS	2.4
1	H	36	ASP	2.3
1	A	1	SER	2.3
1	F	114	ARG	2.2
1	H	115	ASP	2.2
1	F	47	GLU	2.2
1	D	115	ASP	2.2
1	C	1	SER	2.1
1	E	116	PHE	2.1
1	F	4	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	202	5/5	0.65	0.19	65,69,89,131	0
2	SO4	A	202	5/5	0.75	0.13	56,76,86,118	0
2	SO4	G	204	5/5	0.75	0.13	64,75,90,109	0
2	SO4	G	202	5/5	0.76	0.20	61,69,76,113	0
2	SO4	G	203	5/5	0.77	0.11	76,76,79,100	0
2	SO4	D	201	5/5	0.79	0.10	68,83,127,129	0
2	SO4	F	202	5/5	0.81	0.17	58,58,100,126	0
2	SO4	F	201	5/5	0.81	0.10	59,92,116,126	0
2	SO4	G	201	5/5	0.86	0.11	64,75,101,105	0
3	CL	G	205	1/1	0.86	0.20	77,77,77,77	0
3	CL	B	204	1/1	0.87	0.25	71,71,71,71	0
2	SO4	E	201	5/5	0.89	0.07	61,65,92,95	0
3	CL	F	203	1/1	0.90	0.14	70,70,70,70	0
3	CL	B	203	1/1	0.91	0.11	72,72,72,72	0
2	SO4	C	201	5/5	0.93	0.09	48,60,90,93	0
3	CL	D	202	1/1	0.93	0.12	61,61,61,61	0
3	CL	D	203	1/1	0.93	0.09	56,56,56,56	0
3	CL	A	203	1/1	0.93	0.12	68,68,68,68	0
2	SO4	B	201	5/5	0.93	0.08	58,59,67,73	0
2	SO4	A	201	5/5	0.94	0.08	47,60,73,85	0
3	CL	B	205	1/1	0.95	0.10	54,54,54,54	0
3	CL	H	201	1/1	0.96	0.08	63,63,63,63	0
3	CL	A	204	1/1	0.97	0.07	55,55,55,55	0

## 6.5 Other polymers

There are no such residues in this entry.