



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:14 pm BST

PDB ID : 3FM8  
Title : Crystal structure of full length centaurin alpha-1 bound with the FHA domain of KIF13B (CAPRI target)  
Authors : Shen, L.; Tong, Y.; Tempel, W.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-12-19  
Resolution : 2.30 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.

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

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

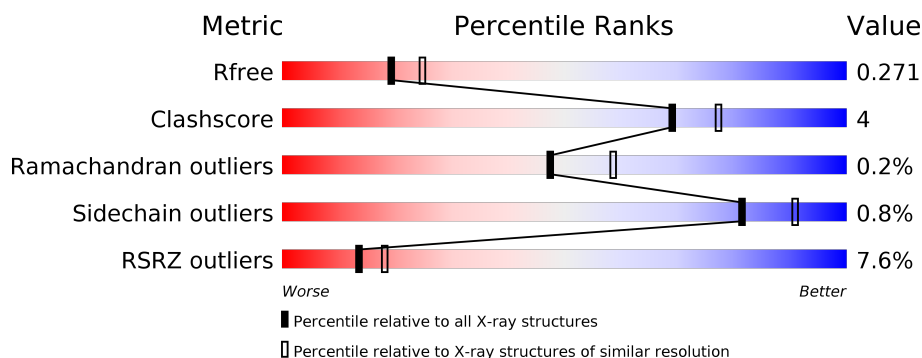
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	124	<div> <div>6%</div> <div>65%</div> <div>14%</div> <div>21%</div> </div>
1	B	124	<div> <div>11%</div> <div>68%</div> <div>9%</div> <div>23%</div> </div>
2	C	392	<div> <div>6%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
2	D	392	<div> <div>6%</div> <div>82%</div> <div>8%</div> <div>10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	6	-	-	-	X
3	UNX	A	7	-	-	-	X
3	UNX	A	8	-	-	-	X
3	UNX	B	20	-	-	-	X
3	UNX	C	376	-	-	-	X
3	UNX	C	377	-	-	-	X
3	UNX	C	378	-	-	-	X
3	UNX	C	379	-	-	-	X
3	UNX	C	380	-	-	-	X
3	UNX	C	381	-	-	-	X
3	UNX	D	377	-	-	-	X
3	UNX	D	378	-	-	-	X
3	UNX	D	379	-	-	-	X
3	UNX	D	380	-	-	-	X
3	UNX	D	381	-	-	-	X
3	UNX	D	382	-	-	-	X
3	UNX	D	383	-	-	-	X
3	UNX	D	384	-	-	-	X
3	UNX	D	385	-	-	-	X
3	UNX	D	386	-	-	-	X
3	UNX	D	387	-	-	-	X
3	UNX	D	388	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7335 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 Kinesin-like protein KIF13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			760	484	131	140	5			
1	B	95	Total	C	N	O	S	0	0	0
			724	466	124	129	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	MET	-	EXPRESSION TAG	UNP Q9NQT8
A	423	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	424	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	425	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	426	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	427	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	428	HIS	-	EXPRESSION TAG	UNP Q9NQT8
A	429	SER	-	EXPRESSION TAG	UNP Q9NQT8
A	430	SER	-	EXPRESSION TAG	UNP Q9NQT8
A	431	GLY	-	EXPRESSION TAG	UNP Q9NQT8
A	432	ARG	-	EXPRESSION TAG	UNP Q9NQT8
A	433	GLU	-	EXPRESSION TAG	UNP Q9NQT8
A	434	ASN	-	EXPRESSION TAG	UNP Q9NQT8
A	435	LEU	-	EXPRESSION TAG	UNP Q9NQT8
A	436	TYR	-	EXPRESSION TAG	UNP Q9NQT8
A	437	PHE	-	EXPRESSION TAG	UNP Q9NQT8
A	438	GLN	-	EXPRESSION TAG	UNP Q9NQT8
A	439	GLY	-	EXPRESSION TAG	UNP Q9NQT8
B	422	MET	-	EXPRESSION TAG	UNP Q9NQT8
B	423	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	424	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	425	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	426	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	427	HIS	-	EXPRESSION TAG	UNP Q9NQT8
B	428	HIS	-	EXPRESSION TAG	UNP Q9NQT8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	SER	-	EXPRESSION TAG	UNP Q9NQT8
B	430	SER	-	EXPRESSION TAG	UNP Q9NQT8
B	431	GLY	-	EXPRESSION TAG	UNP Q9NQT8
B	432	ARG	-	EXPRESSION TAG	UNP Q9NQT8
B	433	GLU	-	EXPRESSION TAG	UNP Q9NQT8
B	434	ASN	-	EXPRESSION TAG	UNP Q9NQT8
B	435	LEU	-	EXPRESSION TAG	UNP Q9NQT8
B	436	TYR	-	EXPRESSION TAG	UNP Q9NQT8
B	437	PHE	-	EXPRESSION TAG	UNP Q9NQT8
B	438	GLN	-	EXPRESSION TAG	UNP Q9NQT8
B	439	GLY	-	EXPRESSION TAG	UNP Q9NQT8

- Molecule 2 is a protein called Centaurin-alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	364	Total	C	N	O	S	0	0	0
			2903	1865	515	510	13			
2	D	353	Total	C	N	O	S	0	1	0
			2775	1791	475	497	12			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	EXPRESSION TAG	UNP O75689
C	-16	HIS	-	EXPRESSION TAG	UNP O75689
C	-15	HIS	-	EXPRESSION TAG	UNP O75689
C	-14	HIS	-	EXPRESSION TAG	UNP O75689
C	-13	HIS	-	EXPRESSION TAG	UNP O75689
C	-12	HIS	-	EXPRESSION TAG	UNP O75689
C	-11	HIS	-	EXPRESSION TAG	UNP O75689
C	-10	SER	-	EXPRESSION TAG	UNP O75689
C	-9	SER	-	EXPRESSION TAG	UNP O75689
C	-8	GLY	-	EXPRESSION TAG	UNP O75689
C	-7	ARG	-	EXPRESSION TAG	UNP O75689
C	-6	GLU	-	EXPRESSION TAG	UNP O75689
C	-5	ASN	-	EXPRESSION TAG	UNP O75689
C	-4	LEU	-	EXPRESSION TAG	UNP O75689
C	-3	TYR	-	EXPRESSION TAG	UNP O75689
C	-2	PHE	-	EXPRESSION TAG	UNP O75689
C	-1	GLN	-	EXPRESSION TAG	UNP O75689
C	0	GLY	-	EXPRESSION TAG	UNP O75689
C	241	SER	GLY	SEE REMARK 999	UNP O75689

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	MET	-	EXPRESSION TAG	UNP O75689
D	-16	HIS	-	EXPRESSION TAG	UNP O75689
D	-15	HIS	-	EXPRESSION TAG	UNP O75689
D	-14	HIS	-	EXPRESSION TAG	UNP O75689
D	-13	HIS	-	EXPRESSION TAG	UNP O75689
D	-12	HIS	-	EXPRESSION TAG	UNP O75689
D	-11	HIS	-	EXPRESSION TAG	UNP O75689
D	-10	SER	-	EXPRESSION TAG	UNP O75689
D	-9	SER	-	EXPRESSION TAG	UNP O75689
D	-8	GLY	-	EXPRESSION TAG	UNP O75689
D	-7	ARG	-	EXPRESSION TAG	UNP O75689
D	-6	GLU	-	EXPRESSION TAG	UNP O75689
D	-5	ASN	-	EXPRESSION TAG	UNP O75689
D	-4	LEU	-	EXPRESSION TAG	UNP O75689
D	-3	TYR	-	EXPRESSION TAG	UNP O75689
D	-2	PHE	-	EXPRESSION TAG	UNP O75689
D	-1	GLN	-	EXPRESSION TAG	UNP O75689
D	0	GLY	-	EXPRESSION TAG	UNP O75689
D	241	SER	GLY	SEE REMARK 999	UNP O75689

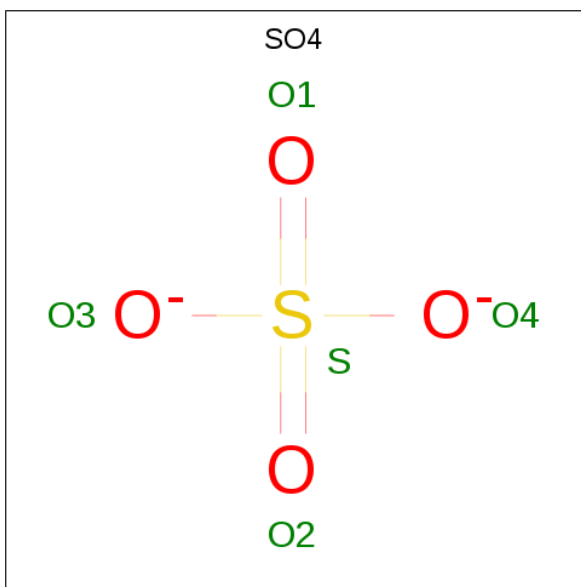
- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total X 1 1	0	0
3	A	3	Total X 3 3	0	0
3	D	12	Total X 12 12	0	0
3	C	6	Total X 6 6	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

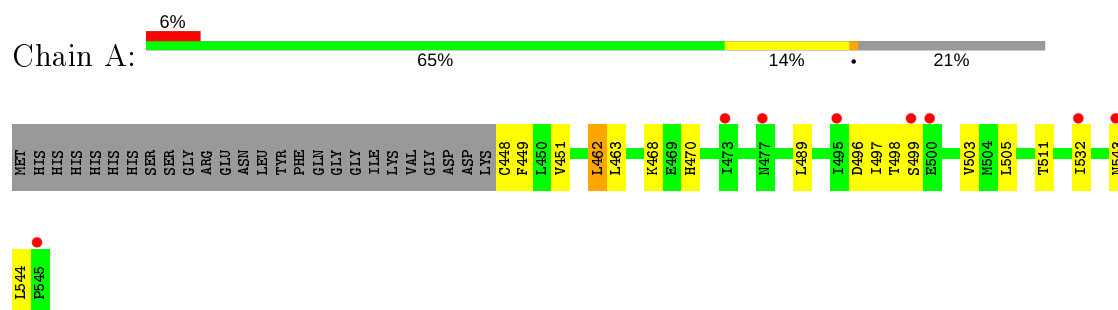
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	8	Total	O	0	0
			8	8		
6	C	71	Total	O	0	0
			71	71		
6	D	50	Total	O	0	0
			50	50		

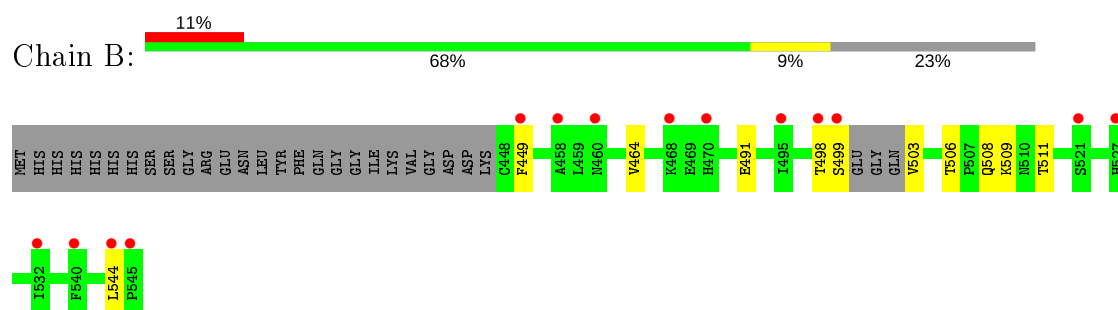
### 3 Residue-property plots [i](#)

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

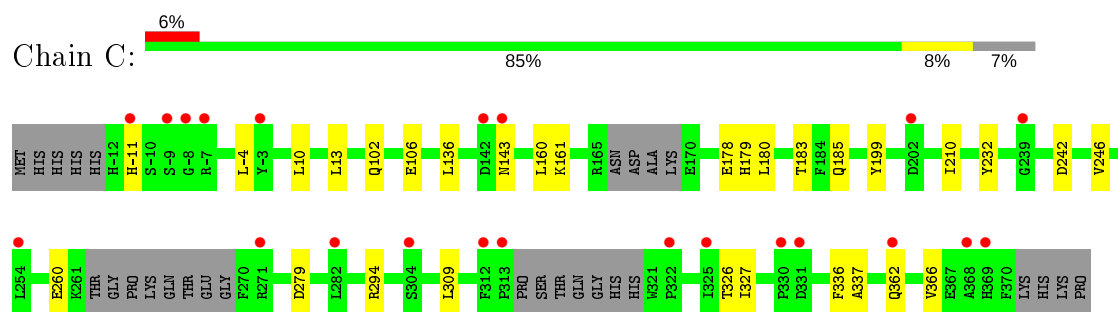
- Molecule 1: Kinesin-like protein KIF13B



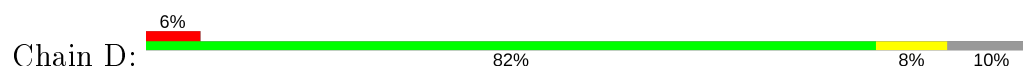
- Molecule 1: Kinesin-like protein KIF13B



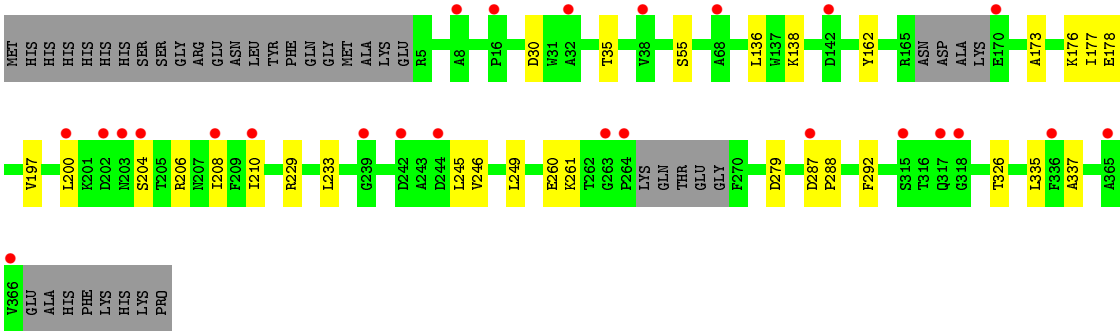
- Molecule 2: Centaurin-alpha-1



- Molecule 2: Centaurin-alpha-1







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.63 Å 115.63 Å 189.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.30 19.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.86-2.30) 99.7 (19.83-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.30 Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.231 , 0.272 0.233 , 0.271	Depositor DCC
$R_{free}$ test set	2023 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: UNX, ZN, 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	0.63	0/777	0.74	0/1058
1	B	0.57	0/740	0.69	0/1009
2	C	0.71	0/2987	0.72	0/4042
2	D	0.64	0/2860	0.67	0/3882
All	All	0.66	0/7364	0.70	0/9991

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	760	0	747	10	0
1	B	724	0	705	8	0
2	C	2903	0	2728	14	0
2	D	2775	0	2591	19	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	6	0	0	0	0
3	D	12	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	1	0
6	A	5	0	0	0	0
6	B	8	0	0	0	0
6	C	71	0	0	0	0
6	D	50	0	0	0	0
All	All	7335	0	6771	51	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 (51) 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:503:VAL:HG21	1:B:544:LEU:HD21	1.58	0.86
2:D:138:LYS:HE2	2:D:208[A]:ILE:HD12	1.72	0.72
2:C:178:GLU:HG3	2:C:232:TYR:CZ	2.26	0.69
2:C:260:GLU:HB2	2:C:337:ALA:HB3	1.77	0.66
2:D:197:VAL:O	2:D:208[B]:ILE:HG23	1.95	0.66
1:A:489:LEU:HD12	1:A:511:THR:HG22	1.78	0.64
2:C:136:LEU:HD13	2:C:210:ILE:HD12	1.81	0.62
2:D:197:VAL:HB	2:D:208[B]:ILE:HG23	1.81	0.61
2:D:200:LEU:HD12	2:D:204:SER:C	2.22	0.60
1:B:449:PHE:CD1	1:B:464:VAL:HG13	2.37	0.60
1:B:503:VAL:CG2	1:B:544:LEU:HD21	2.32	0.59
1:A:503:VAL:HG21	1:A:544:LEU:HD21	1.84	0.59
2:D:233:LEU:HB3	2:D:245:LEU:HD22	1.85	0.58
2:D:197:VAL:O	2:D:208[B]:ILE:CG2	2.52	0.57
2:D:206:ARG:NH1	2:D:292:PHE:CG	2.72	0.57
2:C:183:THR:HG23	2:C:185:GLN:HG2	1.87	0.56
2:D:200:LEU:HD12	2:D:204:SER:O	2.06	0.55
2:D:162:TYR:CE2	2:D:173:ALA:HB3	2.42	0.54
1:A:468:LYS:O	1:A:497:ILE:HD12	2.11	0.50
1:A:470:HIS:ND1	1:A:496:ASP:OD1	2.33	0.50
1:A:462:LEU:C	1:A:462:LEU:HD23	2.33	0.48
2:C:102:GLN:NE2	2:C:106:GLU:OE1	2.46	0.48
1:A:449:PHE:CZ	1:A:543:ASN:ND2	2.81	0.48
1:B:498:THR:CG2	1:B:499:SER:N	2.77	0.47
1:A:498:THR:HG22	1:A:499:SER:N	2.29	0.47
2:D:260:GLU:HB2	2:D:337:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:THR:OG1	2:D:55:SER:HA	2.15	0.47
1:A:451:VAL:HG13	1:A:463:LEU:HD11	1.96	0.46
2:C:178:GLU:CG	2:C:232:TYR:CZ	2.96	0.46
2:C:242:ASP:O	2:C:246:VAL:HG23	2.16	0.46
1:B:498:THR:HG22	1:B:499:SER:N	2.30	0.46
1:A:503:VAL:HG21	1:A:544:LEU:CD2	2.45	0.46
2:D:136:LEU:HD13	2:D:210:ILE:HD12	1.97	0.46
2:D:200:LEU:HA	2:D:200:LEU:HD12	1.84	0.45
2:D:261:LYS:NZ	5:D:376:SO4:O4	2.50	0.45
2:C:179:HIS:HB2	2:C:199:TYR:CE1	2.52	0.44
2:D:326:THR:HG23	2:D:335:LEU:HD23	1.99	0.44
2:C:327:ILE:HD12	2:C:336:PHE:HE1	1.83	0.44
2:D:176:LYS:HB3	2:D:178:GLU:OE2	2.18	0.43
2:D:177:ILE:HD11	2:D:229:ARG:HG2	1.99	0.43
2:C:160:LEU:HB3	2:C:180:LEU:HD11	2.01	0.43
2:C:-11:HIS:HA	2:C:-4:LEU:O	2.19	0.43
2:D:287:ASP:CG	2:D:288:PRO:HD2	2.39	0.42
1:B:506:THR:HG23	1:B:506:THR:O	2.20	0.42
1:B:509:LYS:O	1:B:511:THR:HG23	2.19	0.42
1:B:491:GLU:O	1:B:508:GLN:HG3	2.20	0.42
2:C:309:LEU:HB2	2:C:326:THR:HB	2.02	0.42
1:A:505:LEU:CD1	1:A:532:ILE:HD13	2.51	0.41
2:D:246:VAL:HA	2:D:249:LEU:HG	2.03	0.40
2:C:10:LEU:HD12	2:C:13:LEU:HD12	2.03	0.40
2:C:362:GLN:O	2:C:366:VAL:HG23	2.21	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	96/124 (77%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	91/124 (73%)	89 (98%)	2 (2%)	0	100	100
2	C	356/392 (91%)	351 (99%)	4 (1%)	1 (0%)	41	50
2	D	348/392 (89%)	340 (98%)	7 (2%)	1 (0%)	41	50
All	All	891/1032 (86%)	873 (98%)	16 (2%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	279	ASP
2	D	279	ASP

### 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	86/110 (78%)	84 (98%)	2 (2%)	50	67
1	B	79/110 (72%)	79 (100%)	0	100	100
2	C	283/334 (85%)	280 (99%)	3 (1%)	73	86
2	D	269/334 (80%)	268 (100%)	1 (0%)	91	96
All	All	717/888 (81%)	711 (99%)	6 (1%)	81	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	448	CYS
1	A	462	LEU
2	C	143	ASN
2	C	161	LYS
2	C	294	ARG
2	D	30	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	352	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 22 are unknown and 2 are monoatomic - leaving 3 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	$\# Z  > 2$
5	SO4	D	376	-	4,4,4	0.22	0	6,6,6	0.25	0
5	SO4	D	375	-	4,4,4	0.22	0	6,6,6	0.31	0
5	SO4	C	375	-	4,4,4	0.25	0	6,6,6	0.36	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
5	D	376	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	98/124 (79%)	0.53	8 (8%) 11 15	28, 44, 62, 82	0
1	B	95/124 (76%)	0.66	14 (14%) 2 3	31, 52, 73, 84	0
2	C	364/392 (92%)	0.24	22 (6%) 21 28	19, 39, 67, 84	0
2	D	353/392 (90%)	0.30	25 (7%) 16 21	24, 42, 77, 129	0
All	All	910/1032 (88%)	0.34	69 (7%) 13 18	19, 42, 72, 129	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	PRO	6.4
2	C	142	ASP	6.3
2	C	312	PHE	5.5
2	C	313	PRO	5.5
2	D	202	ASP	4.4
2	D	239	GLY	4.4
1	A	499	SER	4.4
2	D	318	GLY	4.4
2	C	-11	HIS	4.2
1	A	500	GLU	4.2
2	C	331	ASP	4.1
1	A	545	PRO	4.0
2	D	8	ALA	3.8
1	B	460	ASN	3.8
1	A	495	ILE	3.7
2	D	336	PHE	3.7
2	D	365	ALA	3.7
1	B	521	SER	3.7
2	C	-8	GLY	3.6
1	A	532	ILE	3.6
2	D	264	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	210	ILE	3.3
2	D	242	ASP	3.1
2	D	208[A]	ILE	3.1
1	A	543	ASN	3.1
2	C	-9	SER	3.1
2	D	315	SER	3.1
2	C	-7	ARG	3.1
2	C	202	ASP	3.0
2	D	366	VAL	3.0
1	B	499	SER	3.0
2	D	38	VAL	3.0
2	C	282	LEU	2.9
2	C	322	PRO	2.9
2	C	271	ARG	2.9
2	D	68	ALA	2.8
1	B	540	PHE	2.7
2	D	203	ASN	2.7
2	D	16	PRO	2.7
2	C	239	GLY	2.7
2	D	142	ASP	2.6
2	C	362	GLN	2.6
1	B	458	ALA	2.6
2	C	368	ALA	2.6
2	D	263	GLY	2.6
2	D	200	LEU	2.5
2	D	244	ASP	2.5
1	B	449	PHE	2.5
1	A	477	ASN	2.4
2	C	304	SER	2.4
2	C	254	LEU	2.4
2	D	317	GLN	2.4
2	D	170	GLU	2.4
1	B	495	ILE	2.3
2	C	330	PRO	2.3
1	B	498	THR	2.3
1	A	473	ILE	2.3
2	C	369	HIS	2.3
2	C	-3	TYR	2.3
2	C	325	ILE	2.2
1	B	532	ILE	2.2
1	B	468	LYS	2.2
2	D	32	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	470	HIS	2.1
2	D	287	ASP	2.1
2	C	143	ASN	2.1
1	B	527	HIS	2.1
2	D	204	SER	2.0
1	B	544	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	UNX	D	383	1/1	-0.85	2.50	2,2,2,2	1
3	UNX	D	384	1/1	-0.55	2.30	2,2,2,2	1
3	UNX	D	380	1/1	-0.51	1.71	2,2,2,2	1
3	UNX	D	377	1/1	-0.43	1.97	2,2,2,2	1
3	UNX	A	7	1/1	-0.40	1.43	2,2,2,2	1
3	UNX	D	386	1/1	-0.28	1.60	2,2,2,2	1
3	UNX	D	378	1/1	-0.06	2.42	2,2,2,2	1
3	UNX	A	6	1/1	-0.01	2.34	2,2,2,2	1
3	UNX	C	378	1/1	0.01	1.86	2,2,2,2	1
3	UNX	C	379	1/1	0.19	1.19	2,2,2,2	1
3	UNX	A	8	1/1	0.21	1.50	2,2,2,2	1
3	UNX	B	20	1/1	0.37	2.36	2,2,2,2	1
3	UNX	D	385	1/1	0.38	1.49	2,2,2,2	1
3	UNX	C	381	1/1	0.40	1.73	2,2,2,2	1
3	UNX	D	382	1/1	0.42	3.21	2,2,2,2	1
3	UNX	D	379	1/1	0.49	3.05	2,2,2,2	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UNX	C	380	1/1	0.55	2.33	2,2,2,2	1
3	UNX	D	387	1/1	0.57	3.93	2,2,2,2	1
3	UNX	C	376	1/1	0.57	2.58	2,2,2,2	1
3	UNX	C	377	1/1	0.65	2.56	2,2,2,2	1
3	UNX	D	381	1/1	0.68	1.93	2,2,2,2	1
3	UNX	D	388	1/1	0.73	2.70	2,2,2,2	1
5	SO4	D	376	5/5	0.98	0.10	41,49,55,64	0
4	ZN	D	401	1/1	0.98	0.09	44,44,44,44	0
5	SO4	D	375	5/5	0.98	0.09	45,47,49,51	0
4	ZN	C	401	1/1	0.99	0.11	25,25,25,25	0
5	SO4	C	375	5/5	0.99	0.15	34,37,47,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.