



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:55 PM GMT

PDB ID : 4GM8  
Title : Crystal structure of human WD repeat domain 5 with compound MM-102  
Authors : Karatas, H.; Townsend, E.C.; Chen, Y.; Bernard, D.; Cao, F.; Liu, L.; Lei, M.; Dou, Y.; Wang, S.  
Deposited on : 2012-08-15  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

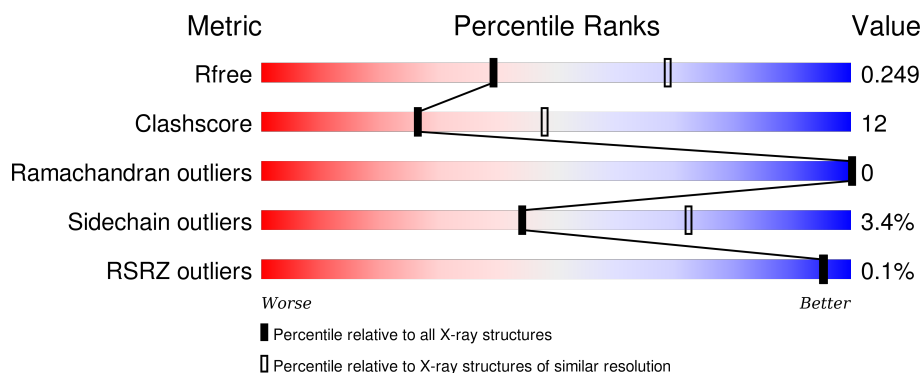
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	313	 70% 26% . .
1	B	313	 72% 23% . .
1	C	313	 72% 24% . .
1	D	313	 73% 22% .
2	E	5	 80% 20%

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Mol	Chain	Length	Quality of chain	
2	F	5	<div><div></div></div>	80% 20%
2	G	5	<div><div></div></div>	80% 20%
2	H	5	<div><div></div></div>	80% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0XL	G	2	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9805 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 WD repeat-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2333	1491	389	443	10			
1	B	300	Total	C	N	O	S	0	0	0
			2320	1481	387	442	10			
1	C	302	Total	C	N	O	S	0	0	0
			2336	1492	390	444	10			
1	D	300	Total	C	N	O	S	0	0	0
			2320	1484	387	439	10			

- Molecule 2 is a protein called MM-102.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	5	Total	C	F	N	O	0	0	0
			48	35	2	7	4			
2	F	5	Total	C	F	N	O	0	0	0
			48	35	2	7	4			
2	G	5	Total	C	F	N	O	0	0	0
			48	35	2	7	4			
2	H	5	Total	C	F	N	O	0	0	0
			48	35	2	7	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	79	Total	O	0	0
			79	79		
3	C	75	Total	O	0	0
			75	75		
3	D	75	Total	O	0	0
			75	75		

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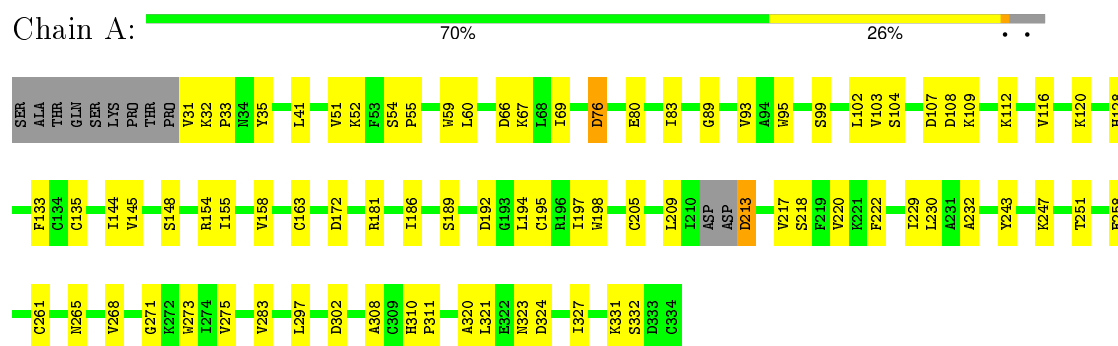
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total 2	O 2	0	0
3	F	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0

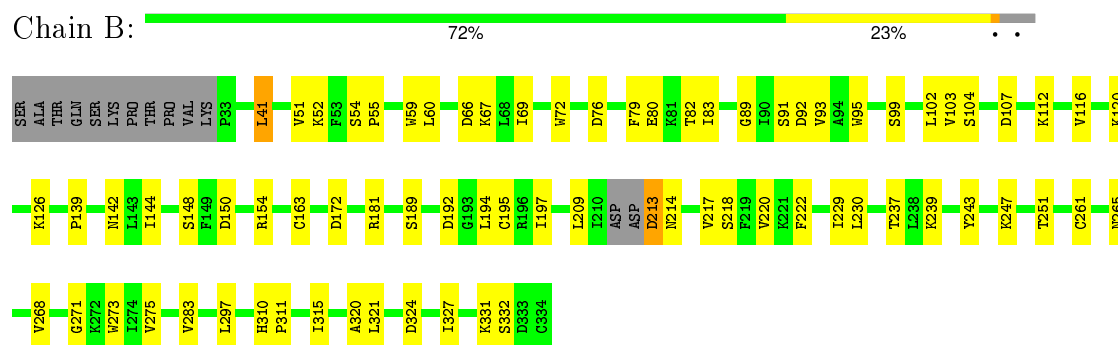
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

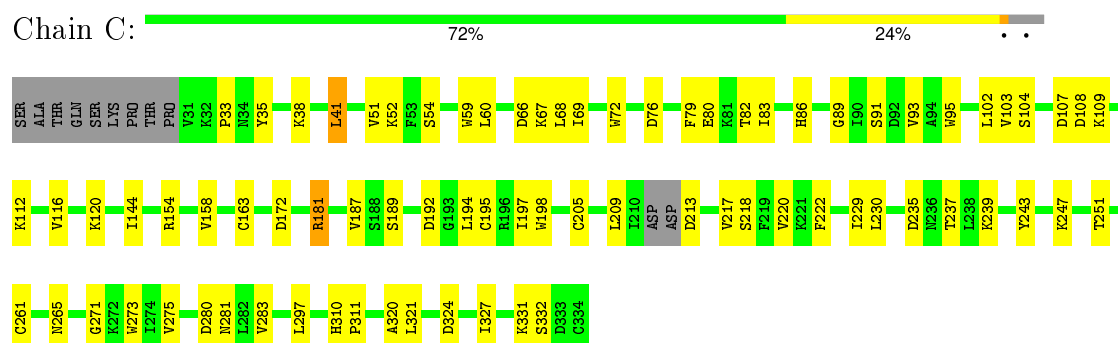
- Molecule 1: WD repeat-containing protein 5



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L297	K120	SER
H310	I144	ALA
P311	R154	THR
I315	V158	GLN
A320	K159	SER
L321	G163	LYS
D324	D172	PRO
I327	R181	THR
K331	S189	PRO
D333	D192	V31
C334	G193	Y35
	L194	K38
	C195	L41
	R196	V51
	I197	K52
	L209	F53
	T210	S54
	ASP	P55
	ASP	W59
	ASN	L60
	P215	D66
P216	P216	K67
V217	S218	L68
F219	V220	I69
	L229	D76
	L230	F79
A231	A232	E80
	Y243	K81
	K247	T82
	T251	I83
	C261	L88
N265	G271	G89
	K272	V93
	W273	A94
	L274	W95
V275	V283	S99
		L102
		V103
		S104
		D107
		D108
		K109
		K112
		V116

Chain E:  80% 20%

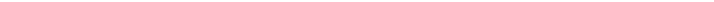
X1	X2	X3	X4	X5
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Chain F:  80% 20%

X1	X2	X3	X4	X5
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Chain G:  80% 20%

X1	X2	R3	X4	X5
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Chain H:  80% 20%

X1	X2	X3	X4	X5
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.86 Å 106.48 Å 120.72 Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	48.86 – 2.60 48.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.5 (48.86-2.60) 83.2 (48.86-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.193 , 0.249 0.192 , 0.249	Depositor DCC
$R_{free}$ test set	1764 reflections (5.78%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	1.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 21.0	EDS
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 35616 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.82 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.1512e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 0XL, 0XN, AC5, ALQ

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	0.43	0/2388	0.58	0/3239
1	B	0.43	0/2375	0.57	0/3221
1	C	0.43	0/2391	0.57	0/3243
1	D	0.43	0/2375	0.58	0/3220
2	E	2.79	1/10 (10.0%)	15.94	2/11 (18.2%)
2	F	3.01	1/10 (10.0%)	16.24	4/11 (36.4%)
2	G	2.92	1/10 (10.0%)	15.47	4/11 (36.4%)
2	H	2.77	1/10 (10.0%)	16.12	4/11 (36.4%)
All	All	0.47	4/9569 (0.0%)	1.09	14/12967 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	1
2	G	0	1
2	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	ARG	C-O	6.12	1.34	1.23
2	G	3	ARG	C-O	6.10	1.34	1.23
2	H	3	ARG	C-O	5.71	1.34	1.23
2	E	3	ARG	C-O	5.63	1.34	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	ARG	NE-CZ-NH2	47.73	144.17	120.30
2	F	3	ARG	NE-CZ-NH2	46.96	143.78	120.30
2	H	3	ARG	NE-CZ-NH2	46.85	143.72	120.30
2	G	3	ARG	NE-CZ-NH2	44.06	142.33	120.30
2	G	3	ARG	NH1-CZ-NH2	-24.67	92.27	119.40
2	F	3	ARG	NH1-CZ-NH2	-24.07	92.92	119.40
2	H	3	ARG	NH1-CZ-NH2	-24.00	93.00	119.40
2	E	3	ARG	NH1-CZ-NH2	-21.27	96.00	119.40
2	F	3	ARG	NE-CZ-NH1	-8.26	116.17	120.30
2	H	3	ARG	NE-CZ-NH1	-6.78	116.91	120.30
2	G	3	ARG	NE-CZ-NH1	-6.15	117.22	120.30
2	F	3	ARG	CA-C-O	-6.07	107.36	120.10
2	G	3	ARG	CA-C-O	-5.87	107.78	120.10
2	H	3	ARG	CA-C-O	-5.62	108.31	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	3	ARG	Sidechain
2	F	3	ARG	Sidechain
2	G	3	ARG	Sidechain
2	H	3	ARG	Sidechain

## 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	2333	0	2315	56	0
1	B	2320	0	2298	50	0
1	C	2336	0	2319	55	0
1	D	2320	0	2310	47	0
2	E	48	0	47	11	0
2	F	48	0	47	11	0
2	G	48	0	47	13	0
2	H	48	0	47	10	0
3	A	69	0	0	7	0
3	B	79	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	75	0	0	4	0
3	D	75	0	0	4	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	1	0
All	All	9805	0	9430	231	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 12.

All (231) 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)
2:H:3:ARG:O	3:H:101:HOH:O	1.81	0.96
1:A:194:LEU:HD12	3:A:434:HOH:O	1.74	0.88
2:E:2:0XL:H8	2:E:5:0XN:H34	1.56	0.88
1:A:258:GLU:OE1	3:A:467:HOH:O	1.93	0.85
1:A:89:GLY:HA3	2:E:1:ALQ:HB3	1.57	0.85
2:F:2:0XL:H8	2:F:5:0XN:H33	1.63	0.80
1:A:213:ASP:HB3	3:A:456:HOH:O	1.82	0.79
1:C:107:ASP:OD2	2:G:1:ALQ:HB2	1.82	0.78
2:E:2:0XL:OAG	2:E:5:0XN:H35	1.84	0.78
1:D:209:LEU:CD1	1:D:229:ILE:HD11	2.15	0.77
1:C:209:LEU:CD1	1:C:229:ILE:HD11	2.16	0.76
1:A:209:LEU:HD12	1:A:229:ILE:HD11	1.69	0.74
1:B:209:LEU:CD1	1:B:229:ILE:HD11	2.18	0.73
1:B:213:ASP:HB3	3:B:441:HOH:O	1.87	0.73
1:D:209:LEU:HD12	1:D:229:ILE:HD11	1.70	0.73
1:C:209:LEU:HD12	1:C:229:ILE:HD11	1.69	0.73
1:A:209:LEU:CD1	1:A:229:ILE:HD11	2.18	0.72
2:E:2:0XL:H8	2:E:5:0XN:CBQ	2.20	0.71
1:B:209:LEU:HD12	1:B:229:ILE:HD11	1.72	0.71
1:C:66:ASP:OD2	3:C:473:HOH:O	2.08	0.70
2:G:1:ALQ:O	2:G:4:AC5:HB22	1.93	0.69
1:C:68:LEU:HD12	3:C:473:HOH:O	1.92	0.68
1:D:215:PRO:N	3:D:435:HOH:O	2.27	0.68
2:E:1:ALQ:O	2:E:4:AC5:HB22	1.94	0.67
1:A:69:ILE:HB	1:A:83:ILE:HB	1.77	0.67
1:B:126:LYS:O	3:B:460:HOH:O	2.13	0.66
1:B:142:ASN:HB2	3:B:418:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ILE:HB	1:C:83:ILE:HB	1.79	0.64
1:B:69:ILE:HB	1:B:83:ILE:HB	1.81	0.63
1:D:107:ASP:OD2	2:H:1:ALQ:HB2	1.98	0.63
1:D:69:ILE:HB	1:D:83:ILE:HB	1.81	0.61
1:C:235:ASP:O	3:C:418:HOH:O	2.16	0.61
2:G:2:0XL:OAG	2:G:5:0XN:H35	2.01	0.60
1:C:181:ARG:NH2	1:D:59:TRP:CH2	2.70	0.59
2:G:2:0XL:H8	2:G:5:0XN:H34	1.83	0.59
1:D:218:SER:HB2	1:D:261:CYS:HA	1.84	0.59
1:D:192:ASP:OD1	1:D:194:LEU:HD12	2.03	0.59
1:C:89:GLY:HA3	2:G:1:ALQ:HB3	1.84	0.58
1:D:209:LEU:HD11	1:D:229:ILE:HD11	1.85	0.58
2:G:2:0XL:H8	2:G:5:0XN:CBQ	2.33	0.58
1:B:107:ASP:OD2	2:F:1:ALQ:HB2	2.04	0.57
1:C:67:LYS:O	3:C:412:HOH:O	2.18	0.57
1:B:218:SER:HB2	1:B:261:CYS:HA	1.85	0.57
1:C:218:SER:HB2	1:C:261:CYS:HA	1.85	0.57
1:A:268:VAL:O	3:A:444:HOH:O	2.18	0.57
2:H:1:ALQ:O	2:H:4:AC5:N	2.37	0.57
1:B:192:ASP:OD1	1:B:194:LEU:HD12	2.05	0.57
1:B:195:CYS:SG	1:B:220:VAL:HG11	2.44	0.57
1:A:218:SER:HB2	1:A:261:CYS:HA	1.86	0.56
1:B:321:LEU:CD2	2:F:4:AC5:HG12	2.35	0.56
1:C:103:VAL:HG21	1:C:144:ILE:HD13	1.87	0.56
1:A:107:ASP:OD2	2:E:1:ALQ:HB2	2.06	0.56
1:C:209:LEU:HD11	1:C:229:ILE:HD11	1.89	0.55
2:E:2:0XL:CAZ	2:E:5:0XN:H34	2.32	0.55
2:F:2:0XL:OAG	2:F:5:0XN:H32	2.06	0.55
1:A:232:ALA:HB1	3:A:409:HOH:O	2.06	0.54
1:C:181:ARG:HH21	1:D:59:TRP:HH2	1.52	0.54
2:G:2:0XL:H8	2:G:5:0XN:CBR	2.38	0.54
1:B:209:LEU:HD11	1:B:229:ILE:HD11	1.89	0.54
1:B:321:LEU:HD22	2:F:4:AC5:HG12	1.90	0.54
1:C:192:ASP:OD1	1:C:194:LEU:HD12	2.08	0.53
1:D:66:ASP:O	1:D:67:LYS:HB2	2.08	0.53
1:C:321:LEU:HD22	2:G:4:AC5:HG12	1.90	0.53
1:B:103:VAL:HG21	1:B:144:ILE:HD13	1.89	0.53
2:H:2:0XL:H8	2:H:5:0XN:H34	1.91	0.53
1:A:331:LYS:HG3	1:A:332:SER:N	2.24	0.52
1:D:103:VAL:HG21	1:D:144:ILE:HD13	1.91	0.52
1:D:321:LEU:HD22	2:H:4:AC5:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG21	1:A:144:ILE:HD13	1.91	0.51
1:C:310:HIS:CG	1:C:311:PRO:HD2	2.46	0.51
1:D:159:LYS:HG2	3:D:438:HOH:O	2.10	0.51
1:D:79:PHE:HZ	1:D:82:THR:HG1	1.59	0.51
2:G:2:0XL:H8	2:G:5:0XN:H35	1.91	0.51
1:A:31:VAL:HG12	1:A:32:LYS:HG3	1.92	0.51
1:A:66:ASP:O	1:A:67:LYS:HB2	2.11	0.50
1:A:209:LEU:HD11	1:A:229:ILE:HD11	1.92	0.50
1:A:89:GLY:HA3	2:E:1:ALQ:CB	2.37	0.50
1:B:283:VAL:HB	1:B:297:LEU:HB2	1.94	0.49
1:A:52:LYS:HG3	1:A:93:VAL:O	2.12	0.49
1:C:331:LYS:HG3	1:C:332:SER:N	2.26	0.49
1:B:102:LEU:HG	1:B:116:VAL:CG2	2.43	0.49
1:D:310:HIS:CG	1:D:311:PRO:HD2	2.47	0.49
2:G:1:ALQ:O	2:G:4:AC5:N	2.45	0.49
1:B:95:TRP:CZ3	1:B:116:VAL:HG21	2.47	0.49
1:A:195:CYS:SG	1:A:220:VAL:HG11	2.52	0.49
1:D:195:CYS:SG	1:D:220:VAL:HG11	2.52	0.49
2:H:2:0XL:CAZ	2:H:5:0XN:H34	2.42	0.49
1:B:92:ASP:OD2	3:B:455:HOH:O	2.20	0.49
1:B:66:ASP:O	1:B:67:LYS:HB2	2.13	0.49
1:C:102:LEU:HG	1:C:116:VAL:CG2	2.42	0.49
1:D:189:SER:HB2	1:D:217:VAL:CG1	2.43	0.49
2:H:3:ARG:O	2:H:3:ARG:HG2	2.13	0.49
1:D:89:GLY:HA3	2:H:1:ALQ:HB3	1.94	0.49
1:A:310:HIS:CG	1:A:311:PRO:HD2	2.47	0.49
1:D:95:TRP:CZ3	1:D:116:VAL:HG21	2.48	0.49
1:B:189:SER:HB2	1:B:217:VAL:CG1	2.43	0.49
2:F:2:0XL:H8	2:F:5:0XN:CBO	2.40	0.48
1:A:189:SER:HB2	1:A:217:VAL:CG1	2.43	0.48
1:B:268:VAL:HG22	3:B:470:HOH:O	2.12	0.48
1:A:154:ARG:HG2	1:A:163:CYS:SG	2.52	0.48
1:C:321:LEU:CD2	2:G:4:AC5:HG12	2.44	0.48
1:D:154:ARG:HG2	1:D:163:CYS:SG	2.53	0.48
1:C:189:SER:HB2	1:C:217:VAL:CG1	2.44	0.48
1:C:52:LYS:HG3	1:C:93:VAL:O	2.13	0.48
2:F:2:0XL:CAZ	2:F:5:0XN:H33	2.39	0.48
1:D:321:LEU:CD2	2:H:4:AC5:HG12	2.44	0.48
1:C:154:ARG:HG2	1:C:163:CYS:SG	2.54	0.48
1:A:172:ASP:HB2	1:A:192:ASP:HB3	1.95	0.47
1:B:197:ILE:HG13	1:B:243:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LEU:HD21	1:D:327:ILE:HG21	1.94	0.47
1:D:197:ILE:HG13	1:D:243:TYR:CE1	2.50	0.47
2:E:2:0XL:H8	2:E:5:0XN:CBR	2.43	0.47
1:A:192:ASP:OD1	1:A:194:LEU:HD12	2.14	0.47
1:A:55:PRO:HD2	1:A:99:SER:OG	2.14	0.47
1:A:320:ALA:HB3	1:A:324:ASP:HB3	1.96	0.47
1:B:154:ARG:HG2	1:B:163:CYS:SG	2.55	0.47
1:C:320:ALA:HB3	1:C:324:ASP:HB3	1.96	0.47
1:C:172:ASP:HB2	1:C:192:ASP:HB3	1.96	0.47
1:B:310:HIS:CG	1:B:311:PRO:HD2	2.49	0.47
1:B:52:LYS:HG3	1:B:93:VAL:O	2.15	0.47
1:D:52:LYS:HG3	1:D:93:VAL:O	2.14	0.47
2:H:1:ALQ:O	2:H:4:AC5:HB22	2.16	0.46
1:C:102:LEU:HG	1:C:116:VAL:HG22	1.97	0.46
1:D:102:LEU:HG	1:D:116:VAL:CG2	2.44	0.46
1:B:331:LYS:HG3	1:B:332:SER:N	2.31	0.46
1:B:220:VAL:HA	1:B:230:LEU:O	2.15	0.46
1:D:220:VAL:HA	1:D:230:LEU:O	2.14	0.46
1:A:102:LEU:HG	1:A:116:VAL:CG2	2.45	0.46
1:A:95:TRP:CZ3	1:A:116:VAL:HG21	2.51	0.46
1:D:271:GLY:HA3	1:D:273:TRP:CZ2	2.50	0.46
1:A:197:ILE:HG13	1:A:243:TYR:CE1	2.51	0.46
1:A:60:LEU:HD21	1:A:327:ILE:HG21	1.98	0.46
1:C:66:ASP:O	1:C:67:LYS:HB2	2.15	0.46
1:C:283:VAL:HB	1:C:297:LEU:HB2	1.98	0.46
1:C:197:ILE:HG13	1:C:243:TYR:CE1	2.51	0.46
1:C:198:TRP:CZ3	1:C:205:CYS:HB2	2.50	0.46
1:B:60:LEU:HD21	1:B:327:ILE:HG21	1.98	0.46
1:A:33:PRO:HD3	1:A:273:TRP:CH2	2.51	0.46
1:A:220:VAL:HA	1:A:230:LEU:O	2.15	0.46
1:C:310:HIS:CD2	1:C:311:PRO:HD2	2.50	0.45
1:B:54:SER:HB3	1:B:95:TRP:CE2	2.51	0.45
1:C:95:TRP:CZ3	1:C:116:VAL:HG21	2.51	0.45
1:D:197:ILE:HG13	1:D:243:TYR:HE1	1.81	0.45
1:D:232:ALA:HB1	3:D:407:HOH:O	2.16	0.45
1:B:79:PHE:HZ	1:B:82:THR:HG1	1.63	0.45
1:B:148:SER:HB3	1:B:150:ASP:OD1	2.16	0.45
1:B:89:GLY:HA3	2:F:1:ALQ:HB3	1.99	0.45
2:F:1:ALQ:O	2:F:4:AC5:N	2.49	0.45
1:C:33:PRO:HD3	1:C:273:TRP:CH2	2.51	0.45
1:A:247:LYS:HB2	1:A:247:LYS:HE3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:ARG:HG2	2:F:3:ARG:O	2.17	0.45
1:B:197:ILE:HG13	1:B:243:TYR:HE1	1.81	0.45
1:D:247:LYS:HB2	1:D:247:LYS:HE3	1.73	0.45
1:B:91:SER:HG	2:F:3:ARG:N	2.14	0.45
1:D:283:VAL:HB	1:D:297:LEU:HB2	1.99	0.45
1:C:79:PHE:HZ	1:C:82:THR:HG1	1.64	0.45
1:C:222:PHE:CD1	1:C:229:ILE:HG22	2.52	0.45
1:C:38:LYS:HD3	1:C:38:LYS:HA	1.78	0.45
1:D:320:ALA:HB3	1:D:324:ASP:HB3	1.99	0.44
1:A:197:ILE:HG13	1:A:243:TYR:HE1	1.82	0.44
1:B:222:PHE:CD1	1:B:229:ILE:HG22	2.53	0.44
1:B:102:LEU:HG	1:B:116:VAL:HG22	1.98	0.44
1:D:331:LYS:HG3	1:D:332:SER:N	2.31	0.44
1:B:320:ALA:HB3	1:B:324:ASP:HB3	1.99	0.44
1:C:197:ILE:HG13	1:C:243:TYR:HE1	1.82	0.44
1:A:271:GLY:HA3	1:A:273:TRP:CZ2	2.52	0.44
1:D:310:HIS:HB2	1:D:315:ILE:HB	1.99	0.44
1:D:102:LEU:HG	1:D:116:VAL:HG22	2.00	0.44
1:A:108:ASP:O	1:A:109:LYS:HB2	2.17	0.44
1:C:108:ASP:O	1:C:109:LYS:HB2	2.17	0.44
1:A:54:SER:HB3	1:A:95:TRP:CE2	2.53	0.44
1:A:283:VAL:HB	1:A:297:LEU:HB2	2.00	0.44
1:D:265:ASN:HB2	1:D:275:VAL:HB	2.00	0.44
1:A:321:LEU:HD22	2:E:4:AC5:HG12	2.00	0.44
1:A:222:PHE:CD1	1:A:229:ILE:HG22	2.53	0.44
1:D:108:ASP:O	1:D:109:LYS:HB2	2.18	0.44
1:D:103:VAL:HA	1:D:112:LYS:O	2.18	0.43
1:C:280:ASP:O	1:C:281:ASN:HB2	2.19	0.43
1:C:60:LEU:HD21	1:C:327:ILE:HG21	1.99	0.43
1:D:54:SER:HB3	1:D:95:TRP:CE2	2.53	0.43
1:C:187:VAL:HG23	1:C:197:ILE:HD13	2.00	0.43
1:B:265:ASN:HB2	1:B:275:VAL:HB	2.00	0.43
1:B:69:ILE:HD11	1:B:104:SER:HB3	2.00	0.43
1:A:308:ALA:HB1	3:A:429:HOH:O	2.18	0.43
1:D:69:ILE:HD11	1:D:104:SER:HB3	2.00	0.43
1:C:35:TYR:CD1	1:C:332:SER:HB2	2.53	0.43
1:C:220:VAL:HA	1:C:230:LEU:O	2.18	0.43
1:D:55:PRO:HD2	1:D:99:SER:OG	2.19	0.43
1:B:214:ASN:N	3:B:441:HOH:O	2.06	0.43
1:C:271:GLY:HA3	1:C:273:TRP:CZ2	2.54	0.42
1:A:76:ASP:HB3	1:B:139:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HB3	1:B:72:TRP:CE3	2.54	0.42
1:C:237:THR:HG21	1:C:239:LYS:HE2	2.01	0.42
1:A:69:ILE:HD11	1:A:104:SER:HB3	2.01	0.42
1:D:144:ILE:HG13	1:D:158:VAL:HG22	2.01	0.42
1:C:91:SER:HG	2:G:3:ARG:N	2.17	0.42
1:B:172:ASP:HB2	1:B:192:ASP:HB3	2.01	0.42
1:C:144:ILE:HG13	1:C:158:VAL:HG22	2.01	0.42
1:B:103:VAL:HA	1:B:112:LYS:O	2.20	0.42
1:A:103:VAL:HA	1:A:112:LYS:O	2.20	0.42
1:A:102:LEU:HG	1:A:116:VAL:HG22	2.01	0.42
1:D:172:ASP:HB2	1:D:192:ASP:HB3	2.02	0.42
1:D:35:TYR:CD1	1:D:332:SER:HB2	2.54	0.42
1:B:247:LYS:HE3	1:B:247:LYS:HB2	1.75	0.42
1:A:155:ILE:HD11	1:A:186:ILE:CD1	2.49	0.42
1:C:54:SER:HB3	1:C:95:TRP:CE2	2.55	0.42
1:A:310:HIS:CD2	1:A:311:PRO:HD2	2.55	0.42
1:C:265:ASN:HB2	1:C:275:VAL:HB	2.02	0.42
1:B:55:PRO:HD2	1:B:99:SER:OG	2.20	0.42
1:A:128:HIS:CE1	1:A:148:SER:HB2	2.54	0.41
1:C:247:LYS:HB2	1:C:247:LYS:HE3	1.75	0.41
1:A:133:PHE:CZ	2:E:3:ARG:HG3	2.55	0.41
1:D:88:LEU:HB3	3:D:448:HOH:O	2.20	0.41
1:C:86:HIS:CE1	1:C:112:LYS:HG3	2.55	0.41
1:A:35:TYR:CD1	1:A:332:SER:HB2	2.55	0.41
1:B:41:LEU:HB3	1:B:72:TRP:CZ3	2.54	0.41
1:A:198:TRP:CZ3	1:A:205:CYS:HB2	2.55	0.41
1:A:265:ASN:HB2	1:A:275:VAL:HB	2.02	0.41
2:G:2:0XL:CAZ	2:G:5:0XN:H34	2.49	0.41
1:A:144:ILE:HG13	1:A:158:VAL:HG22	2.03	0.41
1:A:135:CYS:HA	1:A:145:VAL:O	2.21	0.41
1:C:41:LEU:HB3	1:C:72:TRP:CE3	2.56	0.41
1:C:69:ILE:HD11	1:C:104:SER:HB3	2.02	0.41
1:A:232:ALA:CB	3:A:409:HOH:O	2.67	0.41
1:C:195:CYS:SG	1:C:220:VAL:HG11	2.60	0.41
1:A:302:ASP:OD2	1:A:323:ASN:HB2	2.21	0.41
1:B:310:HIS:HB2	1:B:315:ILE:HB	2.02	0.40
1:D:38:LYS:HD3	1:D:38:LYS:HA	1.82	0.40
1:C:103:VAL:HA	1:C:112:LYS:O	2.21	0.40
1:B:237:THR:HG21	1:B:239:LYS:HE2	2.03	0.40
1:B:271:GLY:HA3	1:B:273:TRP:CZ2	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	298/313 (95%)	278 (93%)	20 (7%)	0	100	100
1	B	296/313 (95%)	276 (93%)	20 (7%)	0	100	100
1	C	298/313 (95%)	280 (94%)	18 (6%)	0	100	100
1	D	296/313 (95%)	276 (93%)	20 (7%)	0	100	100
All	All	1188/1252 (95%)	1110 (93%)	78 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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	262/274 (96%)	253 (97%)	9 (3%)	44	72
1	B	261/274 (95%)	252 (97%)	9 (3%)	44	72
1	C	263/274 (96%)	254 (97%)	9 (3%)	44	72
1	D	261/274 (95%)	252 (97%)	9 (3%)	44	72
2	E	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
2	G	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
All	All	1051/1100 (96%)	1015 (97%)	36 (3%)	44	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	51	VAL
1	A	59	TRP
1	A	76	ASP
1	A	80	GLU
1	A	120	LYS
1	A	181	ARG
1	A	213	ASP
1	A	251	THR
1	B	41	LEU
1	B	51	VAL
1	B	59	TRP
1	B	76	ASP
1	B	80	GLU
1	B	120	LYS
1	B	181	ARG
1	B	213	ASP
1	B	251	THR
1	C	41	LEU
1	C	51	VAL
1	C	59	TRP
1	C	76	ASP
1	C	80	GLU
1	C	120	LYS
1	C	181	ARG
1	C	213	ASP
1	C	251	THR
1	D	31	VAL
1	D	41	LEU
1	D	51	VAL
1	D	59	TRP
1	D	76	ASP
1	D	80	GLU
1	D	120	LYS
1	D	181	ARG
1	D	251	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	0XL	E	2	2	3,7,8	2.78	1 (33%)	2,9,11	4.40	1 (50%)
2	AC5	E	4	2	6,8,9	3.77	3 (50%)	9,11,13	2.42	1 (11%)
2	0XL	F	2	2	3,7,8	2.95	1 (33%)	2,9,11	4.69	1 (50%)
2	AC5	F	4	2	6,8,9	3.78	3 (50%)	9,11,13	2.29	1 (11%)
2	0XL	G	2	2	3,7,8	2.73	1 (33%)	2,9,11	4.18	1 (50%)
2	AC5	G	4	2	6,8,9	3.77	3 (50%)	9,11,13	2.12	2 (22%)
2	0XL	H	2	2	3,7,8	3.04	1 (33%)	2,9,11	4.78	1 (50%)
2	AC5	H	4	2	6,8,9	3.73	3 (50%)	9,11,13	2.29	1 (11%)

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	0XL	E	2	2	-	0/4/9/12	0/0/0/0
2	AC5	E	4	2	-	0/2/12/15	0/1/1/1
2	0XL	F	2	2	-	0/4/9/12	0/0/0/0
2	AC5	F	4	2	-	0/2/12/15	0/1/1/1
2	0XL	G	2	2	-	0/4/9/12	0/0/0/0
2	AC5	G	4	2	-	0/2/12/15	0/1/1/1
2	0XL	H	2	2	-	0/4/9/12	0/0/0/0
2	AC5	H	4	2	-	0/2/12/15	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	AC5	CB2-CA	-6.56	1.46	1.54
2	G	4	AC5	CB2-CA	-6.32	1.46	1.54
2	H	4	AC5	CB2-CA	-6.31	1.46	1.54
2	E	4	AC5	CB2-CA	-6.31	1.46	1.54
2	E	4	AC5	CB1-CA	-4.87	1.48	1.54
2	G	4	AC5	CB1-CA	-4.61	1.48	1.54
2	F	4	AC5	CB1-CA	-4.60	1.48	1.54
2	H	4	AC5	CB1-CA	-4.47	1.49	1.54
2	F	4	AC5	O-C	4.60	1.34	1.20
2	E	4	AC5	O-C	4.64	1.34	1.20
2	G	2	0XL	OAG-CAE	4.72	1.35	1.20
2	E	2	0XL	OAG-CAE	4.81	1.35	1.20
2	H	4	AC5	O-C	4.81	1.35	1.20
2	G	4	AC5	O-C	4.91	1.35	1.20
2	F	2	0XL	OAG-CAE	5.11	1.36	1.20
2	H	2	0XL	OAG-CAE	5.25	1.36	1.20

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	0XL	OAG-CAE-CAD	-6.75	109.63	125.16
2	E	4	AC5	O-C-CA	-6.68	109.79	125.16
2	F	2	0XL	OAG-CAE-CAD	-6.44	110.36	125.16
2	H	4	AC5	O-C-CA	-6.34	110.58	125.16
2	F	4	AC5	O-C-CA	-6.26	110.77	125.16
2	E	2	0XL	OAG-CAE-CAD	-6.21	110.88	125.16
2	G	2	0XL	OAG-CAE-CAD	-5.85	111.72	125.16
2	G	4	AC5	O-C-CA	-5.73	111.98	125.16
2	G	4	AC5	CB2-CA-CB1	2.15	107.57	103.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	0XL	5	0
2	E	4	AC5	2	0
2	F	2	0XL	4	0
2	F	4	AC5	3	0
2	G	2	0XL	6	0
2	G	4	AC5	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	0XL	2	0
2	H	4	AC5	4	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	302/313 (96%)	-0.49	0 100 100	14, 23, 45, 62	0
1	B	300/313 (95%)	-0.50	0 100 100	15, 24, 44, 61	0
1	C	302/313 (96%)	-0.49	0 100 100	15, 23, 45, 61	0
1	D	300/313 (95%)	-0.47	1 (0%) 94 93	15, 24, 44, 61	0
2	E	1/5 (20%)	-1.07	0 100 100	15, 15, 15, 15	0
2	F	1/5 (20%)	-1.19	0 100 100	16, 16, 16, 16	0
2	G	1/5 (20%)	-1.06	0 100 100	17, 17, 17, 17	0
2	H	1/5 (20%)	-0.90	0 100 100	15, 15, 15, 15	0
All	All	1208/1272 (94%)	-0.49	1 (0%) 95 95	14, 23, 45, 62	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	VAL	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AC5	F	4	8/9	0.95	0.13	-	15,21,30,31	0
2	0XL	H	2	8/9	0.97	0.17	-	15,19,23,32	0
2	AC5	G	4	8/9	0.97	0.12	-	13,15,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AC5	E	4	8/9	0.96	0.14	-	14,21,26,27	0
2	0XL	E	2	8/9	0.97	0.13	-	14,17,22,27	0
2	0XL	G	2	8/9	0.96	0.17	-	10,16,21,22	0
2	AC5	H	4	8/9	0.96	0.11	-	12,19,25,25	0
2	0XL	F	2	8/9	0.97	0.17	-	13,16,23,27	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.