



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:08 AM GMT

PDB ID : 3HCU  
Title : Crystal structure of TRAF6 in complex with Ubc13 in the C2 space group  
Authors : Yin, Q.; Lin, S.-C.; Lamothe, B.; Lu, M.; Lo, Y.-C.; Hura, G.; Zheng, L.; Rich, R.L.; Campos, A.D.; Myszkka, D.G.; Lenardo, M.J.; Darnay, B.G.; Wu, H.  
Deposited on : 2009-05-06  
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.

---

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

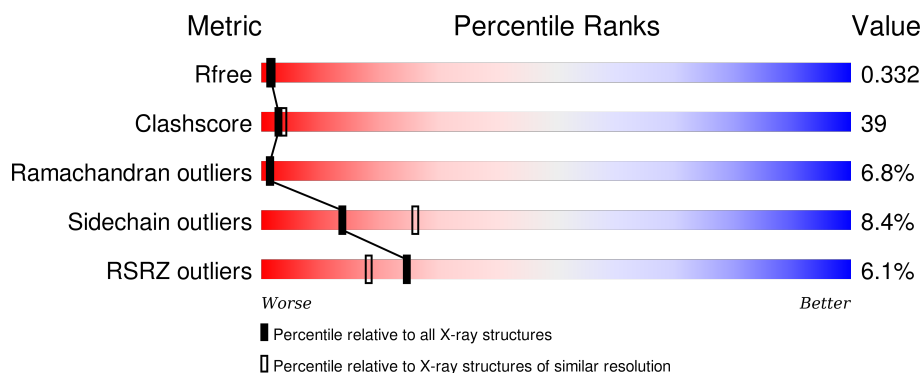
# 1 Overall quality at a glance

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	118	 7% 42% 42% 7% 10%
1	C	118	 7% 34% 43% 11% 12%
2	B	155	 6% 46% 41% 10% 10%
2	D	155	 9% 45% 39% 13% 10%

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
3	ZN	A	302	-	-	-	X
3	ZN	C	305	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4098 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 TNF receptor-associated factor 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	0	0
			847	533	148	154	12			
1	C	104	Total	C	N	O	S	0	0	0
			834	524	146	152	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	LEU	-	EXPRESSION TAG	UNP Q9Y4K3
A	161	GLU	-	EXPRESSION TAG	UNP Q9Y4K3
A	162	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
A	163	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
A	164	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
A	165	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
A	166	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
A	167	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
C	160	LEU	-	EXPRESSION TAG	UNP Q9Y4K3
C	161	GLU	-	EXPRESSION TAG	UNP Q9Y4K3
C	162	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
C	163	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
C	164	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
C	165	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
C	166	HIS	-	EXPRESSION TAG	UNP Q9Y4K3
C	167	HIS	-	EXPRESSION TAG	UNP Q9Y4K3

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1195	767	206	218	4			
2	D	149	Total	C	N	O	S	0	0	0
			1183	760	204	215	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP P61088
B	-1	SER	-	EXPRESSION TAG	UNP P61088
B	0	HIS	-	EXPRESSION TAG	UNP P61088
D	-2	GLY	-	EXPRESSION TAG	UNP P61088
D	-1	SER	-	EXPRESSION TAG	UNP P61088
D	0	HIS	-	EXPRESSION TAG	UNP P61088

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Zn 3 3	0	0
3	C	3	Total Zn 3 3	0	0

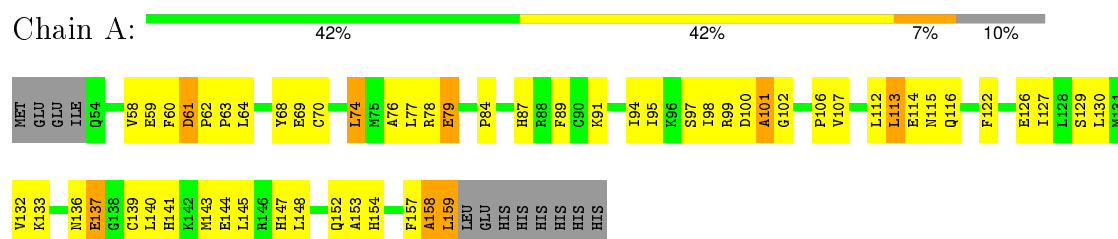
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	10	Total O 10 10	0	0
4	C	5	Total O 5 5	0	0
4	D	5	Total O 5 5	0	0

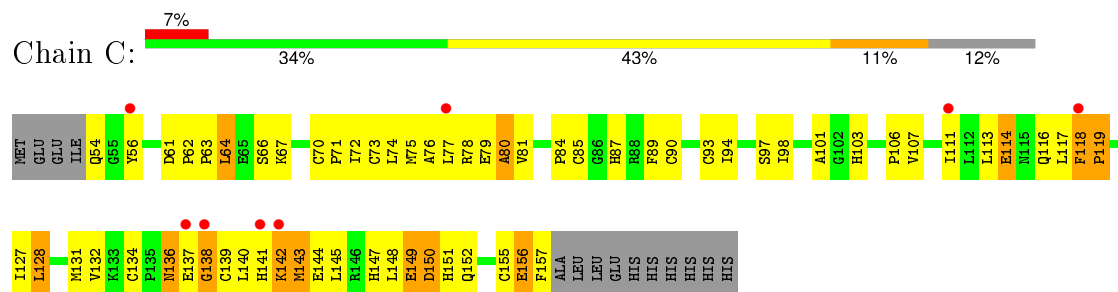
### 3 Residue-property plots

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.

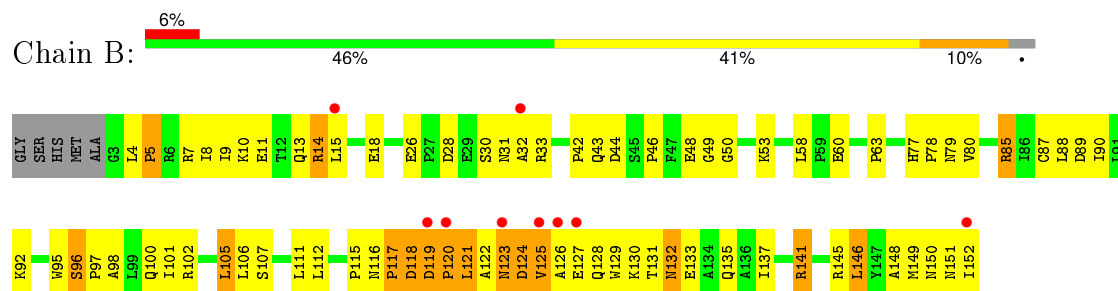
#### • Molecule 1: TNF receptor-associated factor 6



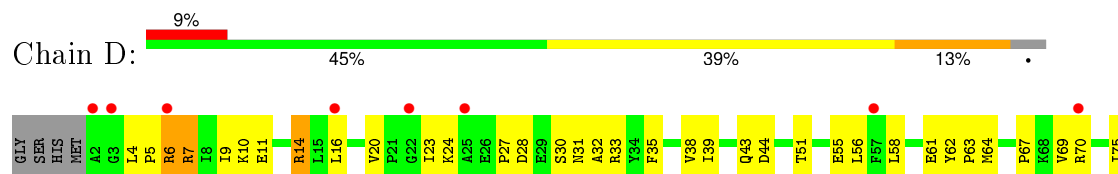
#### • Molecule 1: TNF receptor-associated factor 6

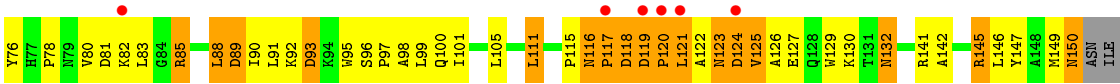


#### • Molecule 2: Ubiquitin-conjugating enzyme E2 N



#### • Molecule 2: Ubiquitin-conjugating enzyme E2 N





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.49Å 41.39Å 123.75Å 90.00° 116.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 40.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-2.60) 94.3 (40.35-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.09 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.256 , 0.333 0.255 , 0.332	Depositor DCC
$R_{free}$ test set	1733 reflections (9.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18484 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0.48	0/866	0.72	0/1167
1	C	0.35	0/853	0.68	0/1149
2	B	0.44	0/1225	0.64	0/1667
2	D	0.41	0/1213	0.63	0/1652
All	All	0.42	0/4157	0.66	0/5635

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	847	0	821	59	0
1	C	834	0	809	66	1
2	B	1195	0	1208	85	0
2	D	1183	0	1196	118	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
4	A	13	0	0	1	0
4	B	10	0	0	0	0
4	C	5	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	1	0
All	All	4098	0	4034	318	1

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 39.

All (318) 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:B:121:LEU:HD22	2:B:126:ALA:HB1	1.29	1.13
2:D:88:LEU:HD22	2:D:90:ILE:HG22	1.38	1.02
1:C:56:TYR:HB2	1:C:76:ALA:HB3	1.43	1.00
2:B:145:ARG:HA	2:B:149:MET:HG3	1.47	0.96
2:D:23:ILE:HG21	2:D:105:LEU:HD12	1.49	0.91
1:A:159:LEU:HD13	1:A:159:LEU:H	1.35	0.91
1:C:81:VAL:HG12	1:C:119:PRO:HB3	1.53	0.89
2:B:137:ILE:O	2:B:141:ARG:HG3	1.73	0.89
2:B:5:PRO:HG2	2:B:8:ILE:HD12	1.55	0.89
2:D:14:ARG:HB2	2:D:14:ARG:HH11	1.39	0.86
2:D:90:ILE:HG23	2:D:91:LEU:HD12	1.60	0.84
2:D:85:ARG:H	2:D:85:ARG:HD2	1.44	0.81
2:D:7:ARG:HG3	2:D:7:ARG:HH11	1.45	0.80
2:D:117:PRO:HA	2:D:121:LEU:HD11	1.64	0.79
2:B:132:ASN:HD22	2:B:132:ASN:N	1.79	0.78
1:C:63:PRO:O	1:C:64:LEU:HB3	1.81	0.78
2:D:145:ARG:HA	2:D:149:MET:SD	2.25	0.77
2:D:132:ASN:HD22	2:D:132:ASN:N	1.83	0.77
2:D:78:PRO:O	2:D:121:LEU:HD22	1.83	0.76
2:D:6:ARG:H	2:D:6:ARG:HD2	1.51	0.76
1:C:90:CYS:HB2	1:C:93:CYS:SG	2.26	0.75
1:A:97:SER:O	1:A:101:ALA:HB3	1.85	0.75
1:A:106:PRO:HB2	2:B:98:ALA:HB2	1.69	0.75
2:D:83:LEU:HB2	2:D:85:ARG:NE	2.01	0.75
2:D:14:ARG:HB2	2:D:14:ARG:NH1	2.02	0.74
2:D:81:ASP:HB2	2:D:85:ARG:CD	2.17	0.74
1:C:131:MET:HG3	1:C:142:LYS:HB3	1.66	0.74
2:D:6:ARG:HD2	2:D:6:ARG:N	2.02	0.74
1:C:148:LEU:HG	1:C:149:GLU:H	1.52	0.74
1:A:136:ASN:HD21	1:A:152:GLN:HE22	1.36	0.73
2:D:4:LEU:HD12	2:D:5:PRO:HD2	1.69	0.73
2:D:56:LEU:HG	2:D:69:VAL:HG22	1.71	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PRO:HG2	1:C:116:GLN:NE2	2.05	0.71
1:C:81:VAL:HG21	1:C:117:LEU:HD13	1.71	0.71
2:D:81:ASP:HB2	2:D:85:ARG:HD3	1.72	0.71
2:D:90:ILE:HG13	2:D:99:LEU:HD13	1.73	0.70
1:C:148:LEU:O	1:C:150:ASP:N	2.24	0.70
1:C:149:GLU:O	1:C:152:GLN:HB3	1.92	0.70
2:B:53:LYS:HD2	2:B:152:ILE:OXT	1.92	0.70
2:B:4:LEU:HD22	2:B:32:ALA:HB3	1.75	0.69
1:C:113:LEU:O	1:C:116:GLN:HB2	1.93	0.69
2:D:124:ASP:OD1	2:D:125:VAL:HG23	1.92	0.69
1:C:89:PHE:CZ	1:C:106:PRO:HG2	2.27	0.69
2:D:43:GLN:HB3	4:D:403:HOH:O	1.93	0.69
1:A:158:ALA:HB1	1:A:159:LEU:HD13	1.74	0.68
2:D:43:GLN:O	2:D:44:ASP:HB2	1.92	0.68
2:D:75:ILE:HG23	2:D:80:VAL:HG21	1.75	0.66
2:D:146:LEU:HD23	2:D:146:LEU:O	1.96	0.66
2:D:117:PRO:HA	2:D:121:LEU:CD1	2.25	0.65
1:A:74:LEU:HD22	2:B:7:ARG:HD3	1.78	0.65
2:B:119:ASP:H	2:B:120:PRO:C	1.99	0.65
2:D:78:PRO:HB2	2:D:121:LEU:CD1	2.27	0.65
2:D:145:ARG:NH1	2:D:145:ARG:HB3	2.12	0.64
1:A:113:LEU:CD2	1:A:115:ASN:H	2.11	0.64
1:C:80:ALA:O	1:C:119:PRO:HB2	1.98	0.64
1:C:63:PRO:O	1:C:64:LEU:CB	2.46	0.63
2:B:132:ASN:ND2	2:B:132:ASN:N	2.46	0.63
2:B:10:LYS:HG2	2:B:14:ARG:NH1	2.13	0.63
1:A:132:VAL:HG22	1:A:133:LYS:N	2.14	0.63
2:D:83:LEU:HB2	2:D:85:ARG:CD	2.29	0.62
2:B:117:PRO:O	2:B:121:LEU:HD23	1.99	0.62
2:D:119:ASP:H	2:D:120:PRO:C	2.01	0.62
1:C:118:PHE:HB3	1:C:119:PRO:HA	1.82	0.62
2:B:4:LEU:HD12	2:B:5:PRO:HD2	1.82	0.62
2:D:78:PRO:HB2	2:D:121:LEU:HD11	1.81	0.62
2:D:123:ASN:O	2:D:126:ALA:HB3	1.99	0.62
1:A:153:ALA:O	1:A:154:HIS:HD2	1.83	0.62
2:B:152:ILE:HD11	2:D:118:ASP:OD2	2.00	0.61
2:D:62:TYR:CE1	2:D:67:PRO:HG3	2.35	0.61
2:B:78:PRO:HD3	2:B:129:TRP:CE3	2.35	0.61
1:A:159:LEU:H	1:A:159:LEU:CD1	2.12	0.61
1:C:78:ARG:O	1:C:79:GLU:HB2	2.00	0.60
1:C:142:LYS:N	1:C:142:LYS:HD2	2.16	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:LEU:HD12	2:B:116:ASN:HD22	1.66	0.60
1:C:139:CYS:SG	1:C:151:HIS:NE2	2.74	0.60
1:A:113:LEU:HD22	1:A:115:ASN:H	1.66	0.59
1:A:60:PHE:O	1:A:63:PRO:HA	2.02	0.59
2:D:90:ILE:HG13	2:D:99:LEU:CD1	2.31	0.59
1:A:122:PHE:O	1:A:126:GLU:HG2	2.02	0.59
2:D:7:ARG:HG3	2:D:7:ARG:NH1	2.18	0.59
2:D:24:LYS:HE3	2:D:38:VAL:HB	1.85	0.59
1:C:142:LYS:HD2	1:C:142:LYS:H	1.68	0.58
2:D:11:GLU:OE1	2:D:100:GLN:HB3	2.02	0.58
2:B:77:HIS:CE1	2:B:79:ASN:HB2	2.38	0.58
1:A:112:LEU:O	1:A:113:LEU:HB3	2.02	0.58
1:C:77:LEU:HB2	1:C:127:ILE:CD1	2.34	0.58
2:D:61:GLU:HG2	2:D:64:MET:HB2	1.86	0.58
2:D:145:ARG:CB	2:D:145:ARG:HH11	2.16	0.58
2:D:75:ILE:CG2	2:D:80:VAL:HG21	2.33	0.58
1:C:142:LYS:O	1:C:143:MET:HB3	2.04	0.58
2:D:95:TRP:CE3	2:D:99:LEU:HD12	2.40	0.57
1:A:113:LEU:HD22	1:A:115:ASN:OD1	2.03	0.57
2:B:33:ARG:HD2	2:B:58:LEU:O	2.05	0.57
2:D:141:ARG:HB3	2:D:141:ARG:NH1	2.19	0.57
1:A:91:LYS:O	1:A:95:ILE:HG12	2.05	0.57
2:D:78:PRO:HD3	2:D:129:TRP:CE3	2.40	0.57
2:D:101:ILE:HG22	2:D:105:LEU:HD23	1.87	0.56
1:C:139:CYS:O	1:C:141:HIS:N	2.38	0.56
1:C:139:CYS:SG	1:C:151:HIS:CE1	2.98	0.56
1:C:136:ASN:O	1:C:138:GLY:N	2.38	0.56
1:A:84:PRO:HG2	1:A:116:GLN:NE2	2.19	0.56
2:B:117:PRO:O	2:B:130:LYS:NZ	2.39	0.56
1:C:70:CYS:SG	1:C:93:CYS:SG	3.04	0.56
2:D:6:ARG:H	2:D:6:ARG:CD	2.18	0.56
1:A:84:PRO:HD3	1:A:116:GLN:O	2.04	0.56
2:D:90:ILE:HG23	2:D:91:LEU:CD1	2.33	0.56
2:D:90:ILE:CG1	2:D:99:LEU:HD13	2.35	0.56
2:D:90:ILE:O	2:D:95:TRP:HE3	1.88	0.56
1:A:74:LEU:HD22	2:B:7:ARG:CD	2.35	0.56
2:B:131:THR:OG1	2:B:132:ASN:N	2.38	0.56
1:C:156:GLU:N	1:C:156:GLU:CD	2.59	0.56
2:B:127:GLU:HA	2:B:130:LYS:HE2	1.88	0.56
1:C:118:PHE:HB3	1:C:119:PRO:CA	2.35	0.56
2:D:5:PRO:O	2:D:9:ILE:HG13	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:O	1:A:158:ALA:HB2	2.05	0.55
2:D:92:LYS:NZ	2:D:120:PRO:HD2	2.21	0.55
1:C:149:GLU:HA	1:C:152:GLN:HB3	1.86	0.55
1:A:129:SER:HA	1:A:144:GLU:HG2	1.88	0.55
2:D:10:LYS:HB2	2:D:10:LYS:NZ	2.21	0.55
2:B:146:LEU:HD11	2:D:111:LEU:HD13	1.88	0.55
2:B:123:ASN:O	2:B:126:ALA:HB3	2.07	0.55
2:D:58:LEU:HD11	2:D:101:ILE:HD11	1.87	0.55
1:C:56:TYR:CE2	1:C:78:ARG:HD3	2.43	0.54
2:D:145:ARG:HB3	2:D:145:ARG:HH11	1.71	0.54
2:B:89:ASP:CG	2:B:90:ILE:H	2.11	0.54
1:A:113:LEU:HD23	1:A:114:GLU:N	2.22	0.54
1:C:62:PRO:HB3	1:C:63:PRO:HD2	1.87	0.54
1:C:138:GLY:HA2	1:C:157:PHE:CD1	2.43	0.54
1:C:144:GLU:O	1:C:147:HIS:N	2.41	0.54
2:B:125:VAL:HA	2:B:128:GLN:HG2	1.90	0.53
2:D:132:ASN:N	2:D:132:ASN:ND2	2.56	0.53
2:B:43:GLN:O	2:B:44:ASP:HB2	2.08	0.53
2:D:83:LEU:HD22	2:D:83:LEU:N	2.24	0.53
2:D:62:TYR:HE1	2:D:67:PRO:HG3	1.73	0.53
1:A:136:ASN:HD21	1:A:152:GLN:NE2	2.06	0.53
2:D:149:MET:C	2:D:150:ASN:HD22	2.12	0.53
1:C:156:GLU:HG2	1:C:157:PHE:CE1	2.43	0.53
2:B:88:LEU:HD21	2:B:107:SER:OG	2.08	0.53
1:A:61:ASP:HA	1:A:62:PRO:C	2.29	0.53
1:A:69:GLU:OE2	2:B:14:ARG:NH2	2.39	0.52
1:A:95:ILE:CG2	1:A:99:ARG:HE	2.22	0.52
2:D:150:ASN:HD22	2:D:150:ASN:N	2.06	0.52
2:B:43:GLN:HA	2:B:48:GLU:HG3	1.91	0.52
1:C:97:SER:O	1:C:101:ALA:HB3	2.09	0.52
2:B:4:LEU:CD2	2:B:32:ALA:HB3	2.38	0.52
2:D:76:TYR:CE1	2:D:125:VAL:HG22	2.45	0.52
2:B:4:LEU:HD11	2:B:33:ARG:NE	2.24	0.52
2:D:119:ASP:H	2:D:120:PRO:CA	2.23	0.52
1:C:81:VAL:HA	1:C:119:PRO:HA	1.91	0.51
1:A:132:VAL:CG2	1:A:133:LYS:N	2.73	0.51
2:B:28:ASP:HB3	2:B:31:ASN:O	2.10	0.51
1:C:74:LEU:HD22	1:C:74:LEU:N	2.25	0.51
2:B:43:GLN:NE2	2:B:48:GLU:CD	2.63	0.51
1:C:71:PRO:HB2	1:C:89:PHE:CE2	2.45	0.51
2:D:61:GLU:O	2:D:64:MET:HB2	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:CYS:SG	1:C:90:CYS:SG	3.08	0.51
2:B:89:ASP:CG	2:B:90:ILE:N	2.64	0.51
2:D:142:ALA:O	2:D:145:ARG:HG2	2.11	0.51
2:D:117:PRO:O	2:D:118:ASP:HB3	2.11	0.51
2:B:146:LEU:CD1	2:D:111:LEU:HD13	2.41	0.51
2:D:117:PRO:HB2	2:D:130:LYS:HE3	1.93	0.51
2:B:119:ASP:N	2:B:120:PRO:O	2.36	0.51
1:C:77:LEU:HB2	1:C:127:ILE:HD11	1.93	0.51
2:B:49:GLY:O	2:B:149:MET:SD	2.69	0.50
2:D:63:PRO:O	2:D:97:PRO:HA	2.11	0.50
2:B:117:PRO:C	2:B:121:LEU:HD23	2.31	0.50
2:B:9:ILE:O	2:B:13:GLN:HG3	2.12	0.50
1:C:143:MET:SD	1:C:148:LEU:HD12	2.52	0.50
2:D:7:ARG:HE	2:D:63:PRO:HB3	1.76	0.50
1:A:139:CYS:SG	1:A:141:HIS:HB2	2.52	0.49
2:D:7:ARG:HE	2:D:63:PRO:CB	2.25	0.49
1:A:112:LEU:O	1:A:113:LEU:CB	2.60	0.49
1:C:61:ASP:N	1:C:62:PRO:O	2.45	0.49
2:D:28:ASP:C	2:D:30:SER:H	2.16	0.49
1:A:136:ASN:ND2	1:A:152:GLN:HE22	2.06	0.49
1:C:155:CYS:SG	1:C:156:GLU:N	2.86	0.49
1:C:142:LYS:O	1:C:143:MET:CB	2.61	0.49
2:B:119:ASP:H	2:B:120:PRO:CA	2.26	0.49
2:B:141:ARG:HH11	2:B:141:ARG:HB3	1.78	0.48
2:D:7:ARG:CG	2:D:7:ARG:HH11	2.21	0.48
1:A:87:HIS:CD2	1:A:107:VAL:HG11	2.48	0.48
2:D:120:PRO:O	2:D:121:LEU:HD23	2.13	0.48
1:C:113:LEU:O	1:C:114:GLU:C	2.50	0.48
2:D:124:ASP:OD1	2:D:125:VAL:N	2.46	0.48
2:B:117:PRO:O	2:B:118:ASP:CB	2.62	0.48
1:A:153:ALA:C	1:A:154:HIS:CD2	2.87	0.48
1:A:98:ILE:HA	1:A:102:GLY:O	2.13	0.48
2:B:133:GLU:O	2:B:137:ILE:HG13	2.13	0.48
2:D:4:LEU:HD22	2:D:32:ALA:HB3	1.96	0.48
2:B:78:PRO:HB3	2:B:126:ALA:HA	1.96	0.48
2:B:87:CYS:SG	2:B:92:LYS:NZ	2.87	0.48
2:D:88:LEU:HD22	2:D:90:ILE:CG2	2.27	0.48
1:C:72:ILE:HB	1:C:93:CYS:HB3	1.95	0.48
1:A:60:PHE:CE2	1:A:76:ALA:HB2	2.49	0.48
1:C:128:LEU:HD23	1:C:145:LEU:HG	1.96	0.48
1:C:81:VAL:HG12	1:C:119:PRO:CB	2.35	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ARG:HE	2:D:63:PRO:HG3	1.78	0.47
2:B:127:GLU:HA	2:B:130:LYS:HG3	1.95	0.47
1:A:58:VAL:HG21	1:A:132:VAL:HG21	1.97	0.47
1:C:94:ILE:O	1:C:98:ILE:HG13	2.13	0.47
2:B:42:PRO:HG2	2:B:112:LEU:HB2	1.95	0.47
2:D:90:ILE:CD1	2:D:99:LEU:HD13	2.44	0.47
1:C:151:HIS:CE1	4:C:402:HOH:O	2.67	0.47
1:A:70:CYS:O	1:A:74:LEU:HD12	2.14	0.47
1:A:68:TYR:OH	1:A:126:GLU:HG3	2.14	0.47
2:B:63:PRO:O	2:B:97:PRO:HA	2.14	0.47
1:C:149:GLU:CA	1:C:152:GLN:HB3	2.45	0.47
2:B:90:ILE:O	2:B:95:TRP:HB2	2.15	0.47
1:C:73:CYS:C	1:C:75:MET:N	2.69	0.46
1:C:89:PHE:HZ	1:C:107:VAL:HG23	1.79	0.46
2:D:4:LEU:HD22	2:D:32:ALA:CB	2.45	0.46
1:C:71:PRO:HB2	1:C:89:PHE:HE2	1.80	0.46
2:D:85:ARG:HH11	2:D:85:ARG:HG3	1.80	0.46
1:A:89:PHE:CE1	1:A:94:ILE:HD13	2.51	0.46
2:B:15:LEU:HD23	2:B:102:ARG:HH21	1.81	0.46
2:B:15:LEU:HD23	2:B:102:ARG:NH2	2.31	0.46
2:B:115:PRO:C	2:B:117:PRO:HD3	2.36	0.46
1:A:136:ASN:O	1:A:137:GLU:O	2.34	0.46
1:A:79:GLU:HB3	1:A:91:LYS:HB3	1.98	0.46
2:B:102:ARG:HG2	2:B:106:LEU:HD12	1.98	0.46
2:D:88:LEU:HD23	2:D:89:ASP:N	2.30	0.46
1:C:87:HIS:CD2	1:C:107:VAL:HB	2.51	0.46
1:A:74:LEU:N	1:A:74:LEU:CD1	2.79	0.46
2:B:43:GLN:HE22	2:B:48:GLU:CD	2.18	0.46
2:B:101:ILE:HG22	2:B:105:LEU:HD22	1.98	0.45
2:D:80:VAL:HA	2:D:85:ARG:O	2.16	0.45
2:B:77:HIS:HE1	2:B:79:ASN:HB2	1.79	0.45
1:C:103:HIS:O	1:C:111:ILE:HG23	2.16	0.45
2:D:78:PRO:HB2	2:D:121:LEU:HD13	1.99	0.45
2:B:131:THR:C	2:B:132:ASN:HD22	2.18	0.45
2:B:131:THR:OG1	2:B:132:ASN:ND2	2.49	0.45
1:A:84:PRO:HG2	1:A:116:GLN:HE21	1.81	0.45
2:B:124:ASP:OD2	2:B:125:VAL:N	2.49	0.45
2:B:33:ARG:HH12	2:B:60:GLU:HG3	1.82	0.45
2:D:119:ASP:N	2:D:120:PRO:O	2.39	0.45
1:A:107:VAL:HG12	1:A:107:VAL:O	2.15	0.45
2:D:56:LEU:HG	2:D:69:VAL:CG2	2.44	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:ASP:C	2:B:30:SER:H	2.18	0.45
2:D:146:LEU:HD22	2:D:147:TYR:CE1	2.52	0.45
1:C:78:ARG:O	1:C:79:GLU:CB	2.64	0.44
2:B:80:VAL:HA	2:B:85:ARG:O	2.16	0.44
2:D:23:ILE:CG2	2:D:105:LEU:HD12	2.34	0.44
2:D:115:PRO:O	2:D:117:PRO:HD3	2.17	0.44
2:B:92:LYS:NZ	2:B:120:PRO:HD2	2.33	0.44
2:B:11:GLU:OE1	2:B:100:GLN:HB3	2.18	0.44
2:D:118:ASP:N	2:D:121:LEU:HG	2.33	0.44
2:D:127:GLU:O	2:D:130:LYS:HB2	2.18	0.44
2:B:46:PRO:HG3	2:B:137:ILE:HG23	1.99	0.44
2:D:7:ARG:HE	2:D:63:PRO:CG	2.31	0.44
2:B:5:PRO:O	2:B:9:ILE:HG12	2.18	0.44
2:D:123:ASN:OD1	2:D:124:ASP:N	2.50	0.44
1:C:73:CYS:O	1:C:75:MET:N	2.51	0.43
1:A:157:PHE:CD1	1:A:157:PHE:N	2.86	0.43
1:A:64:LEU:HD11	1:A:68:TYR:HB2	2.00	0.43
1:A:94:ILE:HD12	1:A:94:ILE:HA	1.89	0.43
2:D:96:SER:C	2:D:98:ALA:H	2.21	0.43
2:D:121:LEU:HB3	2:D:126:ALA:HB2	2.01	0.43
2:D:69:VAL:HG12	2:D:70:ARG:N	2.33	0.43
1:A:59:GLU:OE1	1:A:133:LYS:HE2	2.17	0.43
2:D:122:ALA:O	2:D:123:ASN:C	2.56	0.43
2:D:20:VAL:HG11	2:D:23:ILE:HD12	1.99	0.43
2:B:122:ALA:O	2:B:123:ASN:C	2.56	0.43
1:A:106:PRO:HB2	2:B:98:ALA:CB	2.44	0.43
1:A:59:GLU:O	1:A:132:VAL:HG23	2.19	0.43
1:A:127:ILE:HA	1:A:130:LEU:CD1	2.49	0.43
2:B:126:ALA:O	2:B:130:LYS:HG3	2.18	0.43
2:B:150:ASN:ND2	2:B:152:ILE:HG13	2.34	0.43
2:D:146:LEU:HD23	2:D:146:LEU:C	2.39	0.43
2:D:119:ASP:N	2:D:120:PRO:CA	2.81	0.42
1:C:74:LEU:HD11	2:D:100:GLN:OE1	2.19	0.42
2:D:7:ARG:CG	2:D:7:ARG:NH1	2.79	0.42
1:A:78:ARG:NH1	4:A:403:HOH:O	2.47	0.42
1:C:56:TYR:O	1:C:75:MET:HG3	2.19	0.42
2:D:92:LYS:HB2	2:D:92:LYS:HE3	1.76	0.42
2:B:95:TRP:CG	2:B:96:SER:N	2.87	0.42
1:A:70:CYS:HB2	1:A:77:LEU:HD23	2.02	0.42
2:B:123:ASN:O	2:B:124:ASP:O	2.38	0.42
2:D:82:LYS:H	2:D:82:LYS:HD3	1.85	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:VAL:CG1	2:D:23:ILE:HD12	2.50	0.42
2:D:85:ARG:H	2:D:85:ARG:CD	2.18	0.42
2:D:146:LEU:HD22	2:D:147:TYR:CZ	2.55	0.42
2:B:50:GLY:HA2	2:B:148:ALA:O	2.20	0.42
2:D:33:ARG:NH1	2:D:58:LEU:O	2.53	0.42
1:C:142:LYS:H	1:C:142:LYS:CD	2.31	0.42
1:A:147:HIS:O	1:A:148:LEU:C	2.57	0.42
2:D:124:ASP:O	2:D:125:VAL:C	2.58	0.42
1:A:132:VAL:CG2	1:A:133:LYS:H	2.32	0.42
1:A:84:PRO:CG	1:A:116:GLN:HB3	2.50	0.42
2:D:123:ASN:O	2:D:124:ASP:O	2.38	0.42
1:A:145:LEU:O	1:A:145:LEU:HD12	2.20	0.42
2:D:81:ASP:CB	2:D:85:ARG:HD3	2.47	0.41
2:D:23:ILE:HG23	2:D:39:ILE:HG12	2.02	0.41
2:D:116:ASN:HA	2:D:116:ASN:HD22	1.67	0.41
2:B:124:ASP:C	2:B:124:ASP:OD2	2.57	0.41
2:B:124:ASP:O	2:B:125:VAL:C	2.59	0.41
1:A:89:PHE:CD1	1:A:94:ILE:HD13	2.55	0.41
1:C:54:GLN:N	2:D:6:ARG:NH1	2.69	0.41
1:A:139:CYS:SG	1:A:140:LEU:N	2.93	0.41
2:D:92:LYS:HG2	2:D:93:ASP:N	2.35	0.41
2:D:4:LEU:O	2:D:9:ILE:HD11	2.20	0.41
2:B:79:ASN:HB2	2:B:111:LEU:HD21	2.02	0.41
1:C:98:ILE:CD1	1:C:114:GLU:HA	2.50	0.41
2:B:4:LEU:CD1	2:B:5:PRO:HD2	2.48	0.41
2:B:96:SER:C	2:B:98:ALA:H	2.24	0.41
1:C:132:VAL:HG21	1:C:148:LEU:HD13	2.02	0.41
1:C:84:PRO:HG2	1:C:116:GLN:HE21	1.84	0.41
2:B:92:LYS:HZ2	2:B:120:PRO:HD2	1.86	0.41
2:B:10:LYS:O	2:B:14:ARG:HG2	2.21	0.41
2:D:111:LEU:HA	2:D:111:LEU:HD12	1.82	0.41
2:D:27:PRO:HG3	2:D:35:PHE:CE1	2.56	0.41
2:B:115:PRO:O	2:B:117:PRO:HD3	2.19	0.40
2:B:119:ASP:N	2:B:120:PRO:CA	2.84	0.40
1:A:153:ALA:O	1:A:154:HIS:CD2	2.70	0.40
1:C:149:GLU:C	1:C:152:GLN:HB3	2.40	0.40
1:C:151:HIS:CD2	1:C:151:HIS:O	2.74	0.40
2:D:90:ILE:O	2:D:90:ILE:HG12	2.21	0.40
2:D:92:LYS:NZ	2:D:120:PRO:CD	2.85	0.40
2:B:135:GLN:HE21	2:B:135:GLN:HB2	1.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LYS:NZ	1:C:67:LYS:NZ[2_555]	1.70	0.50

## 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	104/118 (88%)	92 (88%)	8 (8%)	4 (4%)	4	5
1	C	102/118 (86%)	75 (74%)	13 (13%)	14 (14%)	0	0
2	B	148/155 (96%)	126 (85%)	13 (9%)	9 (6%)	2	2
2	D	147/155 (95%)	125 (85%)	15 (10%)	7 (5%)	3	3
All	All	501/546 (92%)	418 (83%)	49 (10%)	34 (7%)	1	1

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	158	ALA
2	B	118	ASP
2	B	119	ASP
2	B	123	ASN
2	B	124	ASP
2	B	151	ASN
1	C	118	PHE
2	D	118	ASP
2	D	119	ASP
2	D	123	ASN
2	D	124	ASP
1	C	64	LEU
1	C	80	ALA
1	C	114	GLU
1	C	136	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	138	GLY
1	C	143	MET
1	C	149	GLU
2	D	125	VAL
1	A	101	ALA
1	C	137	GLU
1	C	140	LEU
1	C	142	LYS
2	B	117	PRO
2	B	125	VAL
1	C	66	SER
1	C	134	CYS
1	C	128	LEU
2	D	117	PRO
1	A	113	LEU
2	B	5	PRO
2	D	120	PRO
2	B	120	PRO

### 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	95/107 (89%)	89 (94%)	6 (6%)	22	44
1	C	94/107 (88%)	90 (96%)	4 (4%)	35	64
2	B	128/131 (98%)	118 (92%)	10 (8%)	16	30
2	D	126/131 (96%)	109 (86%)	17 (14%)	5	8
All	All	443/476 (93%)	406 (92%)	37 (8%)	14	26

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	74	LEU
1	A	79	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	100	ASP
1	A	143	MET
1	A	159	LEU
2	B	14	ARG
2	B	18	GLU
2	B	26	GLU
2	B	85	ARG
2	B	96	SER
2	B	105	LEU
2	B	121	LEU
2	B	132	ASN
2	B	141	ARG
2	B	146	LEU
1	C	85	CYS
1	C	119	PRO
1	C	150	ASP
1	C	156	GLU
2	D	6	ARG
2	D	7	ARG
2	D	14	ARG
2	D	16	LEU
2	D	31	ASN
2	D	51	THR
2	D	55	GLU
2	D	85	ARG
2	D	88	LEU
2	D	89	ASP
2	D	93	ASP
2	D	111	LEU
2	D	116	ASN
2	D	121	LEU
2	D	132	ASN
2	D	145	ARG
2	D	150	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	109	ASN
1	A	116	GLN
1	A	152	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	154	HIS
2	B	43	GLN
2	B	100	GLN
2	B	116	ASN
2	B	132	ASN
2	B	135	GLN
1	C	82	GLN
1	C	147	HIS
2	D	31	ASN
2	D	116	ASN
2	D	132	ASN
2	D	150	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

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, 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	106/118 (89%)	0.03	0 100 100	42, 63, 82, 89	0
1	C	104/118 (88%)	0.61	8 (7%) 16 11	64, 92, 126, 139	0
2	B	150/155 (96%)	0.43	9 (6%) 25 18	48, 73, 115, 130	0
2	D	149/155 (96%)	0.54	14 (9%) 11 6	54, 79, 110, 132	0
All	All	509/546 (93%)	0.41	31 (6%) 25 18	42, 77, 120, 139	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	126	ALA	6.2
2	D	124	ASP	5.5
1	C	141	HIS	5.1
1	C	138	GLY	4.9
2	D	121	LEU	4.8
1	C	137	GLU	3.9
2	B	120	PRO	3.7
2	D	2	ALA	3.7
2	D	117	PRO	3.5
1	C	118	PHE	3.5
1	C	56	TYR	3.5
1	C	142	LYS	3.4
2	B	119	ASP	3.3
2	B	152	ILE	3.2
2	D	16	LEU	2.9
2	D	70	ARG	2.7
2	D	120	PRO	2.7
2	B	15	LEU	2.6
2	D	57	PHE	2.4
2	D	82	LYS	2.4
2	B	32	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	127	GLU	2.3
2	B	125	VAL	2.2
2	D	3	GLY	2.2
2	B	123	ASN	2.2
2	D	6	ARG	2.1
2	D	119	ASP	2.1
1	C	111	ILE	2.0
2	D	25	ALA	2.0
2	D	22	GLY	2.0
1	C	77	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. 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( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	302	1/1	0.98	0.27	4.33	66,66,66,66	0
3	ZN	C	305	1/1	0.99	0.23	2.59	75,75,75,75	0
3	ZN	A	303	1/1	0.98	0.20	0.57	84,84,84,84	0
3	ZN	A	301	1/1	0.98	0.15	-0.74	48,48,48,48	0
3	ZN	C	306	1/1	0.97	0.15	-0.93	132,132,132,132	0
3	ZN	C	304	1/1	0.95	0.16	-1.31	84,84,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.