



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:41 PM GMT

PDB ID : 2GD5  
Title : Structural basis for budding by the ESCRTIII factor CHMP3  
Authors : Muziol, T.M.; Pineda-Molina, E.; Ravelli, R.B.; Zamborlini, A.; Usami, Y.;  
Gottlinger, H.; Weissenhorn, W.  
Deposited on : 2006-03-15  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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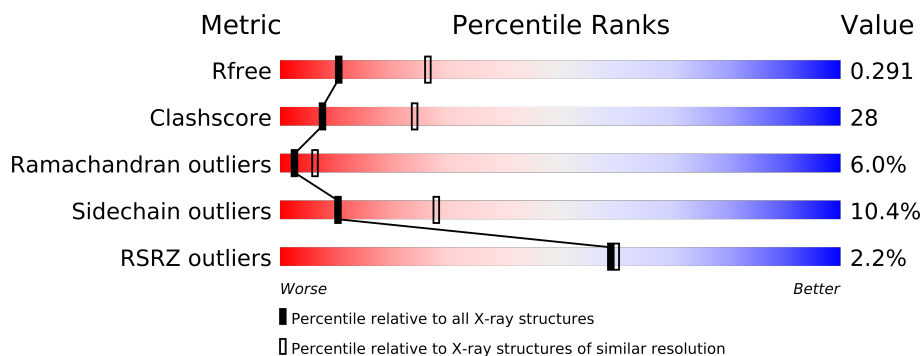
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	179	
1	B	179	
1	C	179	
1	D	179	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4746 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Charged multivesicular body protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	Se	0	0	0
			1134	710	207	205	1	11			
1	B	156	Total	C	N	O	S	Se	0	0	0
			1219	763	223	220	1	12			
1	C	142	Total	C	N	O	S	Se	0	0	0
			1123	703	204	204	1	11			
1	D	162	Total	C	N	O	S	Se	0	0	0
			1270	793	229	234	1	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
A	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
A	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
A	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
A	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
B	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
B	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
B	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
B	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
C	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
C	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
C	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
C	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
D	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
D	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
D	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
D	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7

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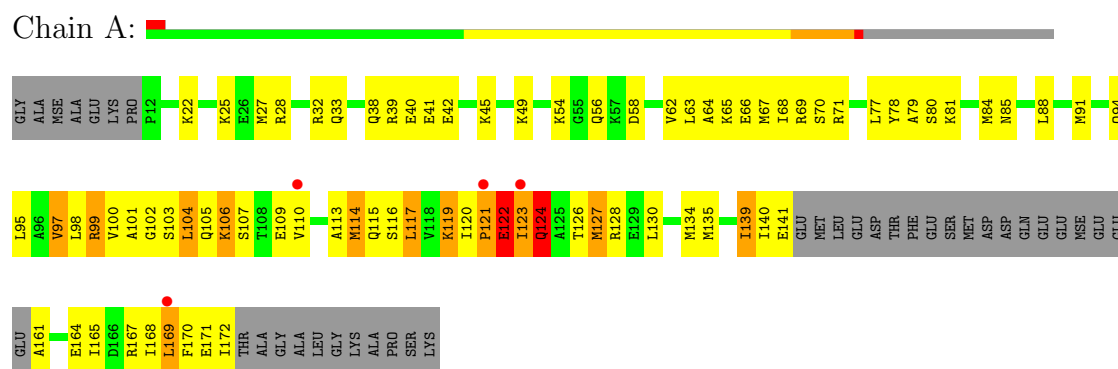
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Chain	Residue	Modelled	Actual	Comment	Reference
D	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7

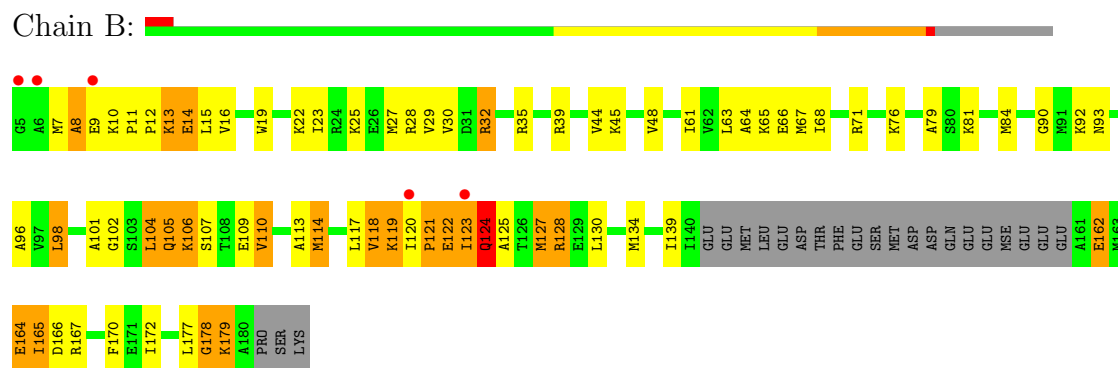
### 3 Residue-property plots

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.

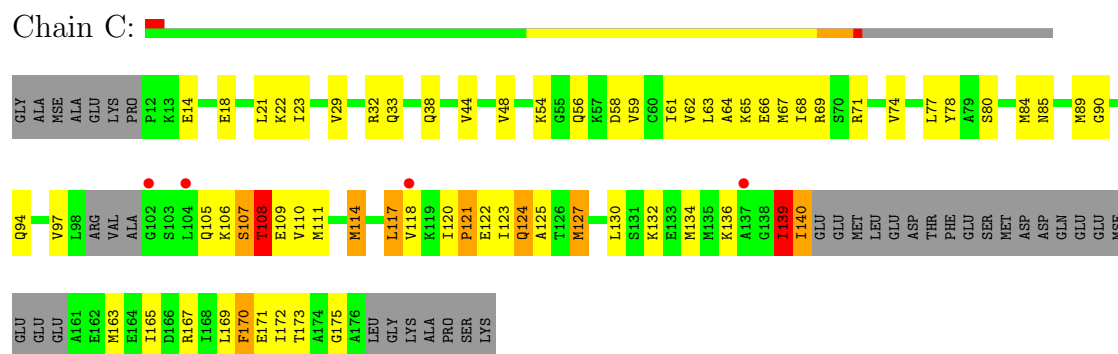
- Molecule 1: Charged multivesicular body protein 3



- Molecule 1: Charged multivesicular body protein 3

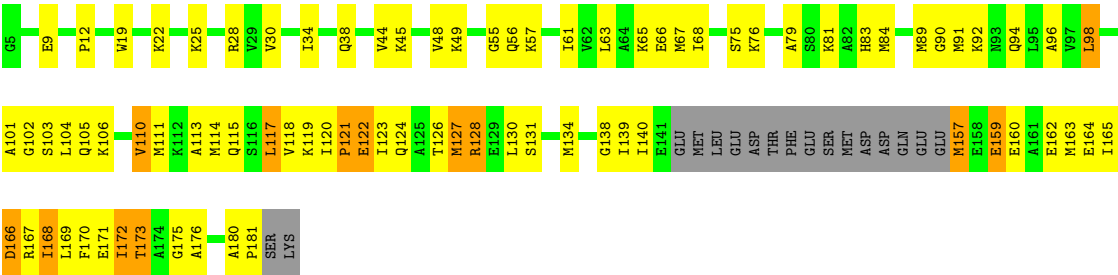


- Molecule 1: Charged multivesicular body protein 3



- Molecule 1: Charged multivesicular body protein 3

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	33.58Å 72.57Å 89.23Å 68.68° 83.61° 76.70°	Depositor
Resolution (Å)	20.00 – 2.80 33.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.80) 95.6 (33.09-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.259 , 0.301 0.252 , 0.291	Depositor DCC
$R_{free}$ test set	914 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 17886 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

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	0.72	0/1128	0.74	0/1476
1	B	0.72	0/1213	0.76	0/1589
1	C	0.71	0/1116	0.70	0/1459
1	D	0.73	0/1265	0.74	0/1659
All	All	0.72	0/4722	0.74	0/6183

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1134	0	1232	78	0
1	B	1219	0	1325	78	0
1	C	1123	0	1218	68	0
1	D	1270	0	1365	68	0
All	All	4746	0	5140	273	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

All (273) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:169:LEU:O	1:D:173:THR:HG22	1.37	1.20
1:C:33:GLN:HE22	1:C:122:GLU:HG2	1.16	1.09
1:C:33:GLN:NE2	1:C:122:GLU:HG2	1.74	1.00
1:D:160:GLU:HB3	1:D:163:MSE:HE2	1.40	1.00
1:C:71:ARG:NH2	1:D:101:ALA:HB2	1.77	0.99
1:C:71:ARG:HH22	1:D:101:ALA:HB2	1.25	0.96
1:C:172:ILE:HD12	1:C:173:THR:HG22	1.46	0.96
1:C:139:ILE:H	1:C:139:ILE:HD13	1.27	0.94
1:D:165:ILE:HD12	1:D:166:ASP:N	1.82	0.93
1:C:58:ASP:O	1:C:62:VAL:HG23	1.67	0.93
1:D:165:ILE:HD12	1:D:166:ASP:H	1.34	0.92
1:C:33:GLN:HE22	1:C:122:GLU:CG	1.84	0.89
1:A:120:ILE:HG13	1:A:121:PRO:HD2	1.54	0.88
1:A:101:ALA:HB2	1:B:71:ARG:HH22	1.39	0.87
1:A:116:SER:HA	1:A:119:LYS:HE2	1.56	0.85
1:D:124:GLN:O	1:D:128:ARG:HB2	1.77	0.84
1:A:38:GLN:HE22	1:B:96:ALA:HB1	1.43	0.83
1:A:164:GLU:HA	1:A:167:ARG:HB2	1.61	0.82
1:C:172:ILE:CD1	1:C:173:THR:HG22	2.09	0.82
1:A:45:LYS:HA	1:A:67:MSE:HE1	1.61	0.81
1:B:98:LEU:HD23	1:B:102:GLY:HA2	1.65	0.79
1:A:67:MSE:HE3	1:B:172:ILE:HD13	1.66	0.78
1:A:71:ARG:NH2	1:B:101:ALA:HB2	1.99	0.78
1:B:166:ASP:HB3	1:B:179:LYS:HA	1.63	0.77
1:C:139:ILE:H	1:C:139:ILE:CD1	1.98	0.76
1:B:125:ALA:HA	1:B:128:ARG:HH12	1.50	0.76
1:A:27:MSE:HG2	1:A:84:MSE:HE3	1.66	0.76
1:D:111:MSE:HG3	1:D:140:ILE:HG23	1.67	0.76
1:A:71:ARG:HH22	1:B:101:ALA:HB2	1.50	0.74
1:A:68:ILE:HG13	1:A:69:ARG:N	2.01	0.73
1:A:114:MSE:HE2	1:A:134:MSE:SE	2.39	0.73
1:D:169:LEU:C	1:D:173:THR:HG22	2.08	0.73
1:B:128:ARG:HB2	1:B:128:ARG:HH11	1.52	0.73
1:D:123:ILE:HD12	1:D:127:MSE:HE2	1.71	0.73
1:C:48:VAL:HG11	1:D:172:ILE:HD11	1.68	0.73
1:B:113:ALA:O	1:B:117:LEU:HB2	1.88	0.72
1:C:169:LEU:O	1:C:172:ILE:HG13	1.90	0.72
1:C:172:ILE:HD12	1:C:173:THR:CG2	2.20	0.72
1:B:162:GLU:OE1	1:B:165:ILE:HD12	1.90	0.72
1:B:125:ALA:HA	1:B:128:ARG:NH1	2.04	0.72
1:D:157:MSE:HG3	1:D:159:GLU:HB2	1.71	0.71
1:A:117:LEU:O	1:A:120:ILE:HG22	1.91	0.71
1:C:139:ILE:HD13	1:C:139:ILE:N	2.03	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:29:VAL:O	1:C:33:GLN:HG3	1.90	0.71
1:D:106:LYS:HG3	1:D:138:GLY:O	1.91	0.70
1:B:120:ILE:HG23	1:B:121:PRO:HD3	1.74	0.69
1:A:109:GLU:HA	1:A:109:GLU:OE2	1.90	0.69
1:C:111:MSE:SE	1:C:140:ILE:HB	2.43	0.69
1:B:76:LYS:HB2	1:B:76:LYS:NZ	2.08	0.69
1:C:170:PHE:O	1:C:172:ILE:N	2.26	0.68
1:B:25:LYS:HA	1:B:28:ARG:NH1	2.09	0.68
1:D:94:GLN:HE22	1:D:105:GLN:H	1.41	0.68
1:B:165:ILE:HD13	1:B:166:ASP:H	1.59	0.67
1:C:111:MSE:SE	1:C:140:ILE:HD13	2.45	0.67
1:C:63:LEU:O	1:C:66:GLU:HB3	1.95	0.67
1:B:119:LYS:C	1:B:119:LYS:HD3	2.16	0.66
1:A:94:GLN:NE2	1:A:94:GLN:HA	2.11	0.65
1:D:157:MSE:CG	1:D:159:GLU:HB2	2.26	0.65
1:A:45:LYS:CA	1:A:67:MSE:HE1	2.25	0.65
1:B:25:LYS:HA	1:B:28:ARG:HH11	1.62	0.65
1:A:161:ALA:O	1:A:165:ILE:HG23	1.97	0.65
1:B:118:VAL:HG12	1:B:127:MSE:HB3	1.79	0.64
1:C:107:SER:H	1:C:139:ILE:HG22	1.63	0.64
1:D:63:LEU:O	1:D:66:GLU:HB3	1.98	0.64
1:B:11:PRO:HB2	1:B:15:LEU:HD11	1.81	0.63
1:A:101:ALA:HB2	1:B:71:ARG:NH2	2.12	0.63
1:B:32:ARG:HH11	1:B:32:ARG:HG3	1.64	0.63
1:B:114:MSE:HE2	1:B:134:MSE:SE	2.49	0.62
1:C:22:LYS:HD2	1:C:130:LEU:HD21	1.81	0.62
1:B:128:ARG:NH1	1:B:128:ARG:HB2	2.15	0.62
1:A:22:LYS:HD2	1:A:130:LEU:HD21	1.82	0.62
1:D:122:GLU:CD	1:D:122:GLU:H	2.03	0.62
1:D:76:LYS:HB2	1:D:76:LYS:NZ	2.14	0.61
1:C:65:LYS:O	1:C:68:ILE:HG12	2.00	0.61
1:B:109:GLU:HA	1:B:109:GLU:OE2	2.01	0.61
1:B:11:PRO:HB2	1:B:15:LEU:CD1	2.31	0.60
1:D:114:MSE:HE2	1:D:134:MSE:SE	2.51	0.60
1:B:29:VAL:O	1:B:32:ARG:HB3	2.01	0.60
1:A:123:ILE:HD12	1:A:124:GLN:N	2.17	0.60
1:B:63:LEU:O	1:B:66:GLU:HB3	2.01	0.60
1:C:106:LYS:HA	1:C:139:ILE:HA	1.83	0.60
1:B:105:GLN:OE1	1:B:106:LYS:O	2.19	0.60
1:C:68:ILE:HG13	1:C:69:ARG:N	2.17	0.60
1:B:9:GLU:HG2	1:B:9:GLU:O	2.02	0.59
1:C:71:ARG:HH22	1:D:101:ALA:CB	2.09	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:94:GLN:HA	1:C:94:GLN:NE2	2.17	0.59
1:C:56:GLN:HB3	1:C:59:VAL:HG23	1.84	0.59
1:A:168:ILE:C	1:A:170:PHE:H	2.05	0.59
1:D:164:GLU:HG3	1:D:167:ARG:NH1	2.18	0.59
1:D:169:LEU:O	1:D:172:ILE:HG12	2.03	0.59
1:A:67:MSE:HE3	1:B:172:ILE:CD1	2.33	0.59
1:C:61:ILE:O	1:C:64:ALA:HB3	2.04	0.58
1:D:124:GLN:HG2	1:D:128:ARG:CZ	2.34	0.57
1:B:104:LEU:HD13	1:B:139:ILE:HD11	1.86	0.57
1:D:79:ALA:O	1:D:83:HIS:HD2	1.87	0.57
1:C:54:LYS:HD2	1:C:56:GLN:HE22	1.68	0.57
1:A:81:LYS:HA	1:A:84:MSE:CE	2.34	0.57
1:B:22:LYS:HD2	1:B:130:LEU:HD21	1.84	0.57
1:B:120:ILE:CG2	1:B:121:PRO:HD3	2.35	0.57
1:D:34:ILE:O	1:D:38:GLN:HG2	2.04	0.57
1:D:157:MSE:HE3	1:D:157:MSE:HA	1.87	0.57
1:A:58:ASP:O	1:A:62:VAL:HG23	2.04	0.56
1:C:74:VAL:O	1:C:77:LEU:HB2	2.06	0.56
1:A:167:ARG:O	1:A:170:PHE:HB2	2.06	0.56
1:B:30:VAL:HG21	1:B:84:MSE:HE1	1.88	0.56
1:C:173:THR:HG23	1:C:175:GLY:H	1.71	0.56
1:A:169:LEU:O	1:A:172:ILE:HG12	2.06	0.55
1:C:33:GLN:HE22	1:C:122:GLU:CD	2.09	0.55
1:B:123:ILE:O	1:B:125:ALA:N	2.33	0.55
1:A:120:ILE:HG13	1:A:121:PRO:CD	2.33	0.55
1:A:38:GLN:HE22	1:B:96:ALA:CB	2.17	0.55
1:D:44:VAL:O	1:D:48:VAL:HG23	2.06	0.54
1:A:122:GLU:O	1:A:124:GLN:HG3	2.08	0.54
1:A:68:ILE:HG13	1:A:69:ARG:H	1.73	0.54
1:C:134:MSE:HB3	1:C:139:ILE:HG12	1.90	0.54
1:A:65:LYS:O	1:A:68:ILE:HG12	2.08	0.54
1:B:93:ASN:O	1:B:96:ALA:HB3	2.08	0.54
1:D:25:LYS:HA	1:D:28:ARG:NH1	2.22	0.53
1:B:45:LYS:HA	1:B:67:MSE:HE1	1.90	0.53
1:B:7:MSE:O	1:B:8:ALA:O	2.26	0.53
1:B:170:PHE:HD2	1:B:178:GLY:HA2	1.73	0.53
1:C:54:LYS:HD2	1:C:56:GLN:NE2	2.24	0.53
1:A:63:LEU:O	1:A:64:ALA:C	2.44	0.53
1:C:71:ARG:NH2	1:D:101:ALA:CB	2.62	0.53
1:D:157:MSE:CE	1:D:157:MSE:HA	2.38	0.53
1:D:45:LYS:HE2	1:D:49:LYS:HE3	1.90	0.53
1:B:122:GLU:C	1:B:124:GLN:H	2.11	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:33:GLN:HE22	1:A:122:GLU:CD	2.12	0.53
1:C:106:LYS:O	1:C:106:LYS:HG3	2.09	0.53
1:A:105:GLN:O	1:A:107:SER:N	2.41	0.53
1:B:81:LYS:HA	1:B:84:MSE:HE3	1.90	0.53
1:A:140:ILE:HG22	1:A:141:GLU:N	2.24	0.53
1:D:115:GLN:HE21	1:D:119:LYS:HE2	1.74	0.53
1:D:118:VAL:HG12	1:D:127:MSE:HB3	1.91	0.52
1:A:45:LYS:HA	1:A:67:MSE:CE	2.38	0.52
1:B:121:PRO:O	1:B:122:GLU:HB2	2.10	0.52
1:B:76:LYS:HB2	1:B:76:LYS:HZ3	1.74	0.52
1:C:120:ILE:HD13	1:C:123:ILE:HD11	1.92	0.52
1:C:78:TYR:CZ	1:D:92:LYS:HG2	2.44	0.52
1:C:140:ILE:HD12	1:C:140:ILE:H	1.75	0.52
1:B:15:LEU:HB3	1:B:19:TRP:CZ2	2.45	0.52
1:B:12:PRO:O	1:B:14:GLU:N	2.33	0.52
1:B:119:LYS:HD2	1:B:124:GLN:HG2	1.93	0.51
1:A:104:LEU:HB3	1:A:139:ILE:HG22	1.93	0.51
1:A:54:LYS:HB2	1:A:56:GLN:HE21	1.75	0.51
1:B:123:ILE:C	1:B:125:ALA:H	2.13	0.51
1:C:170:PHE:C	1:C:172:ILE:H	2.13	0.51
1:D:79:ALA:O	1:D:83:HIS:CD2	2.64	0.51
1:C:80:SER:OG	1:C:120:ILE:HG12	2.11	0.51
1:B:61:ILE:O	1:B:64:ALA:HB3	2.10	0.51
1:D:84:MSE:HG3	1:D:117:LEU:HD21	1.92	0.51
1:C:23:ILE:HD11	1:C:114:MSE:HE1	1.93	0.51
1:D:127:MSE:O	1:D:131:SER:HB2	2.11	0.51
1:B:44:VAL:O	1:B:48:VAL:HG23	2.11	0.51
1:A:49:LYS:HE2	1:B:172:ILE:O	2.09	0.51
1:C:68:ILE:CG1	1:C:69:ARG:N	2.74	0.51
1:B:13:LYS:HE2	1:B:13:LYS:N	2.25	0.51
1:C:38:GLN:NE2	1:D:96:ALA:HB1	2.26	0.51
1:C:90:GLY:HA3	1:C:110:VAL:HG11	1.92	0.50
1:D:45:LYS:HA	1:D:67:MSE:HE1	1.92	0.50
1:B:23:ILE:O	1:B:27:MSE:HG3	2.12	0.50
1:D:103:SER:O	1:D:105:GLN:NE2	2.43	0.50
1:D:165:ILE:CD1	1:D:166:ASP:H	2.17	0.50
1:A:117:LEU:HG	1:A:127:MSE:HE3	1.93	0.49
1:D:157:MSE:HG3	1:D:159:GLU:H	1.77	0.49
1:A:67:MSE:O	1:A:70:SER:HB2	2.12	0.49
1:C:120:ILE:O	1:C:124:GLN:N	2.38	0.49
1:A:40:GLU:OE2	1:A:40:GLU:HA	2.13	0.49
1:C:90:GLY:HA3	1:C:110:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:GLU:O	1:A:168:ILE:HG13	2.13	0.49
1:B:121:PRO:O	1:B:122:GLU:CB	2.60	0.49
1:A:139:ILE:O	1:A:139:ILE:HG13	2.12	0.48
1:D:30:VAL:HG21	1:D:84:MSE:HE1	1.95	0.48
1:D:159:GLU:O	1:D:162:GLU:HG2	2.13	0.48
1:C:44:VAL:O	1:C:48:VAL:HG23	2.13	0.48
1:D:139:ILE:O	1:D:139:ILE:HG22	2.13	0.48
1:A:99:ARG:HA	1:A:99:ARG:CZ	2.44	0.48
1:D:173:THR:OG1	1:D:176:ALA:HB3	2.14	0.48
1:D:81:LYS:HA	1:D:84:MSE:HE3	1.96	0.48
1:D:98:LEU:HA	1:D:102:GLY:H	1.79	0.48
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.95	0.47
1:C:48:VAL:HG11	1:D:172:ILE:CD1	2.42	0.47
1:B:107:SER:HB3	1:B:110:VAL:HG22	1.96	0.47
1:B:13:LYS:HE2	1:B:13:LYS:CA	2.44	0.47
1:D:170:PHE:CE1	1:D:175:GLY:HA2	2.49	0.47
1:D:120:ILE:O	1:D:124:GLN:HB2	2.14	0.47
1:B:15:LEU:N	1:B:15:LEU:HD12	2.30	0.47
1:C:84:MSE:HG3	1:C:117:LEU:HD21	1.96	0.47
1:A:88:LEU:O	1:A:91:MSE:HB2	2.14	0.47
1:D:110:VAL:HG23	1:D:110:VAL:O	2.14	0.46
1:C:107:SER:O	1:C:109:GLU:N	2.49	0.46
1:B:128:ARG:HH11	1:B:128:ARG:CB	2.25	0.46
1:C:109:GLU:HA	1:C:109:GLU:OE2	2.16	0.46
1:C:117:LEU:O	1:C:120:ILE:HD12	2.16	0.46
1:A:140:ILE:CG2	1:A:141:GLU:N	2.79	0.46
1:B:30:VAL:CG2	1:B:84:MSE:HE1	2.46	0.46
1:B:170:PHE:CD2	1:B:178:GLY:HA2	2.51	0.45
1:D:65:LYS:O	1:D:68:ILE:HG12	2.17	0.45
1:A:25:LYS:HA	1:A:28:ARG:NH1	2.31	0.45
1:B:170:PHE:CD2	1:B:179:LYS:HG2	2.51	0.45
1:B:90:GLY:HA3	1:B:110:VAL:CG1	2.46	0.45
1:D:61:ILE:O	1:D:65:LYS:HG3	2.17	0.45
1:A:67:MSE:O	1:A:68:ILE:C	2.55	0.45
1:A:63:LEU:O	1:A:66:GLU:HB3	2.17	0.45
1:A:139:ILE:O	1:A:140:ILE:HD13	2.17	0.45
1:C:33:GLN:NE2	1:C:122:GLU:OE2	2.50	0.44
1:D:89:MSE:O	1:D:90:GLY:C	2.56	0.44
1:D:98:LEU:HG	1:D:102:GLY:HA2	1.98	0.44
1:D:55:GLY:O	1:D:57:LYS:N	2.49	0.44
1:A:168:ILE:C	1:A:170:PHE:N	2.71	0.44
1:A:78:TYR:OH	1:B:92:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:173:THR:HG23	1:C:175:GLY:N	2.32	0.44
1:A:81:LYS:HA	1:A:84:MSE:HE2	1.97	0.44
1:A:63:LEU:O	1:A:66:GLU:N	2.51	0.44
1:D:89:MSE:O	1:D:92:LYS:N	2.51	0.44
1:B:35:ARG:HG2	1:B:39:ARG:HH21	1.83	0.44
1:D:22:LYS:HD2	1:D:130:LEU:HD21	2.00	0.44
1:C:114:MSE:HE2	1:C:134:MSE:SE	2.68	0.43
1:A:97:VAL:HG12	1:A:103:SER:O	2.17	0.43
1:A:105:GLN:HE22	1:A:167:ARG:HH12	1.67	0.43
1:C:77:LEU:HA	1:C:77:LEU:HD23	1.86	0.43
1:A:121:PRO:HB2	1:A:122:GLU:H	1.60	0.43
1:A:22:LYS:CD	1:A:130:LEU:HD21	2.47	0.43
1:A:124:GLN:HE21	1:A:128:ARG:HH22	1.67	0.43
1:B:65:LYS:O	1:B:68:ILE:HG12	2.19	0.43
1:B:164:GLU:OE1	1:B:167:ARG:NH2	2.52	0.43
1:A:124:GLN:NE2	1:A:128:ARG:HH22	2.16	0.43
1:A:39:ARG:HA	1:A:42:GLU:OE1	2.19	0.43
1:D:114:MSE:CE	1:D:134:MSE:SE	3.16	0.43
1:C:77:LEU:O	1:C:80:SER:HB2	2.19	0.43
1:A:95:LEU:O	1:A:98:LEU:HB2	2.19	0.43
1:A:41:GLU:CD	1:A:70:SER:HB3	2.40	0.42
1:B:13:LYS:HG3	1:B:98:LEU:HD21	2.01	0.42
1:B:76:LYS:O	1:B:79:ALA:HB3	2.19	0.42
1:C:18:GLU:O	1:C:21:LEU:HB2	2.19	0.42
1:C:54:LYS:HB2	1:C:56:GLN:HE21	1.85	0.42
1:D:169:LEU:C	1:D:173:THR:CG2	2.85	0.42
1:A:94:GLN:CA	1:A:94:GLN:HE21	2.32	0.42
1:C:122:GLU:N	1:C:122:GLU:OE1	2.27	0.42
1:A:106:LYS:HE3	1:A:106:LYS:HB2	1.82	0.42
1:D:12:PRO:HB3	1:D:104:LEU:HG	2.02	0.42
1:A:117:LEU:C	1:A:119:LYS:H	2.23	0.42
1:B:81:LYS:HA	1:B:84:MSE:CE	2.50	0.42
1:A:99:ARG:HA	1:A:99:ARG:NH1	2.35	0.42
1:C:85:ASN:O	1:C:89:MSE:HG2	2.20	0.42
1:D:139:ILE:O	1:D:139:ILE:CG2	2.68	0.42
1:A:77:LEU:O	1:A:80:SER:HB2	2.19	0.41
1:D:120:ILE:HA	1:D:121:PRO:HD2	1.63	0.41
1:C:121:PRO:HA	1:C:124:GLN:OE1	2.20	0.41
1:A:135:MSE:HA	1:A:140:ILE:HB	2.02	0.41
1:A:113:ALA:C	1:A:115:GLN:H	2.24	0.41
1:A:65:LYS:HA	1:A:68:ILE:HG12	2.03	0.41
1:A:81:LYS:HA	1:A:84:MSE:HE3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:162:GLU:CD	1:B:162:GLU:C	2.80	0.41
1:D:113:ALA:O	1:D:117:LEU:HB2	2.21	0.41
1:B:110:VAL:HG23	1:B:110:VAL:O	2.19	0.41
1:A:78:TYR:O	1:A:79:ALA:C	2.56	0.41
1:D:19:TRP:HE3	1:D:91:MSE:SE	2.54	0.41
1:D:168:ILE:O	1:D:169:LEU:C	2.60	0.41
1:A:94:GLN:HE21	1:A:94:GLN:HA	1.80	0.41
1:C:132:LYS:HB2	1:C:132:LYS:HE3	1.84	0.41
1:C:106:LYS:O	1:C:108:THR:N	2.55	0.40
1:B:165:ILE:CD1	1:B:166:ASP:H	2.30	0.40
1:C:56:GLN:HB3	1:C:59:VAL:CG2	2.50	0.40
1:B:12:PRO:C	1:B:14:GLU:H	2.19	0.40
1:A:38:GLN:NE2	1:B:96:ALA:HB1	2.22	0.40
1:C:67:MSE:O	1:C:68:ILE:C	2.58	0.40
1:A:110:VAL:HG23	1:A:110:VAL:O	2.21	0.40
1:B:114:MSE:HE2	1:B:134:MSE:CE	2.51	0.40
1:B:14:GLU:C	1:B:16:VAL:N	2.72	0.40
1:C:172:ILE:HD12	1:C:173:THR:CB	2.52	0.40
1:B:177:LEU:O	1:B:178:GLY:O	2.40	0.40
1:A:54:LYS:HD2	1:A:56:GLN:NE2	2.36	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	138/179 (77%)	118 (86%)	12 (9%)	8 (6%)	3	7
1	B	152/179 (85%)	121 (80%)	20 (13%)	11 (7%)	2	4
1	C	136/179 (76%)	108 (79%)	16 (12%)	12 (9%)	1	2
1	D	158/179 (88%)	143 (90%)	11 (7%)	4 (2%)	9	28
All	All	584/716 (82%)	490 (84%)	59 (10%)	35 (6%)	2	6

All (35) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	121	PRO
1	A	122	GLU
1	B	8	ALA
1	B	122	GLU
1	B	124	GLN
1	C	107	SER
1	C	136	LYS
1	C	163	MSE
1	C	171	GLU
1	A	106	LYS
1	A	124	GLN
1	A	171	GLU
1	B	13	LYS
1	C	118	VAL
1	C	125	ALA
1	C	127	MSE
1	C	165	ILE
1	D	171	GLU
1	B	104	LEU
1	B	118	VAL
1	C	108	THR
1	D	56	GLN
1	A	169	LEU
1	A	100	VAL
1	B	123	ILE
1	B	178	GLY
1	C	121	PRO
1	C	139	ILE
1	B	106	LYS
1	A	102	GLY
1	B	110	VAL
1	B	121	PRO
1	D	172	ILE
1	C	97	VAL
1	D	121	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	126/142 (89%)	112 (89%)	14 (11%)	9	25
1	B	132/142 (93%)	118 (89%)	14 (11%)	10	27
1	C	124/142 (87%)	112 (90%)	12 (10%)	12	32
1	D	138/142 (97%)	124 (90%)	14 (10%)	11	30
All	All	520/568 (92%)	466 (90%)	54 (10%)	10	28

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	85	ASN
1	A	97	VAL
1	A	99	ARG
1	A	104	LEU
1	A	114	MSE
1	A	117	LEU
1	A	119	LYS
1	A	122	GLU
1	A	123	ILE
1	A	124	GLN
1	A	126	THR
1	A	127	MSE
1	A	139	ILE
1	B	10	LYS
1	B	14	GLU
1	B	32	ARG
1	B	98	LEU
1	B	105	GLN
1	B	114	MSE
1	B	119	LYS
1	B	124	GLN
1	B	127	MSE
1	B	128	ARG
1	B	162	GLU
1	B	164	GLU
1	B	165	ILE
1	B	179	LYS
1	C	14	GLU
1	C	32	ARG
1	C	105	GLN
1	C	108	THR
1	C	114	MSE

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Mol	Chain	Res	Type
1	C	117	LEU
1	C	124	GLN
1	C	127	MSE
1	C	139	ILE
1	C	140	ILE
1	C	167	ARG
1	C	170	PHE
1	D	9	GLU
1	D	75	SER
1	D	98	LEU
1	D	110	VAL
1	D	117	LEU
1	D	122	GLU
1	D	126	THR
1	D	127	MSE
1	D	128	ARG
1	D	157	MSE
1	D	159	GLU
1	D	166	ASP
1	D	168	ILE
1	D	173	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	38	GLN
1	A	56	GLN
1	A	94	GLN
1	A	105	GLN
1	A	124	GLN
1	B	38	GLN
1	B	94	GLN
1	C	33	GLN
1	C	38	GLN
1	C	94	GLN
1	D	17	ASN
1	D	83	HIS
1	D	94	GLN
1	D	115	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 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	142/179 (79%)	0.12	4 (2%) 50 52	23, 58, 91, 94	0
1	B	156/179 (87%)	0.19	5 (3%) 45 46	38, 58, 82, 90	0
1	C	142/179 (79%)	0.13	4 (2%) 50 52	34, 62, 92, 98	0
1	D	162/179 (90%)	-0.01	0 100 100	29, 55, 71, 82	0
All	All	602/716 (84%)	0.11	13 (2%) 59 60	23, 58, 88, 98	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	ALA	5.5
1	B	9	GLU	3.3
1	A	110	VAL	2.8
1	B	5	GLY	2.8
1	A	121	PRO	2.7
1	B	120	ILE	2.6
1	B	123	ILE	2.6
1	A	169	LEU	2.3
1	B	6	ALA	2.3
1	C	118	VAL	2.1
1	C	102	GLY	2.1
1	A	123	ILE	2.1
1	C	104	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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.