



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:13 pm GMT

PDB ID : 2ZME  
Title : Integrated structural and functional model of the human ESCRT-II complex  
Authors : Im, Y.J.; Hurley, J.H.  
Deposited on : 2008-04-17  
Resolution : 2.90 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

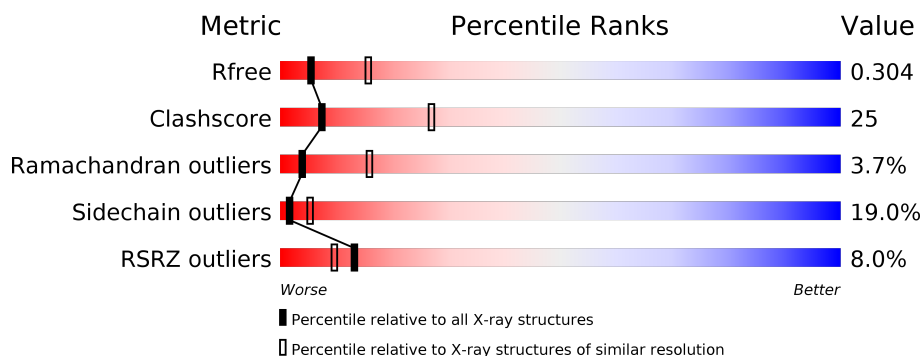
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	258	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>47%</span> <span>31%</span> <span>6%</span> <span>16%</span> </div> </div>
2	B	238	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>8%</span> <span>45%</span> <span>32%</span> <span>12%</span> <span>10%</span> </div> </div>
3	C	102	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>45%</span> <span>37%</span> <span>15%</span> <span>.</span> </div> </div>
3	D	102	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>28%</span> <span>40%</span> <span>41%</span> <span>12%</span> <span>5%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5127 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 Vacuolar-sorting protein SNF8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1718	1103	290	318	7			

- Molecule 2 is a protein called Vacuolar protein-sorting-associated protein 36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1678	1058	281	324	15			

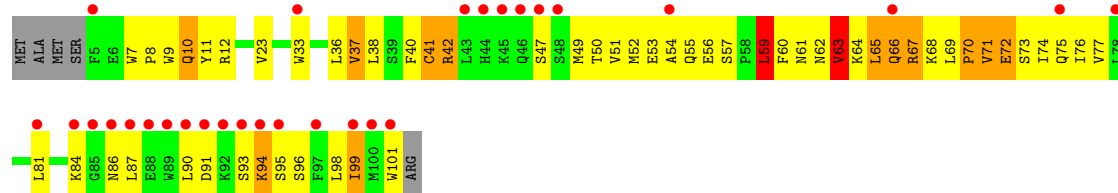
- Molecule 3 is a protein called Vacuolar protein-sorting-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	0	0
			838	546	144	143	5			
3	D	97	Total	C	N	O	S	0	0	0
			821	537	139	140	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	21	Total	O	0	0
			21	21		
4	C	12	Total	O	0	0
			12	12		
4	D	8	Total	O	0	0
			8	8		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.48Å 81.48Å 226.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.74 – 2.90 40.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.74-2.90) 99.6 (40.74-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.313 0.212 , 0.304	Depositor DCC
$R_{free}$ test set	990 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 90.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.052 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

### 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	0.88	1/1752 (0.1%)	0.90	1/2365 (0.0%)
2	B	0.73	2/1696 (0.1%)	0.82	2/2273 (0.1%)
3	C	0.85	0/862	0.82	1/1165 (0.1%)
3	D	0.60	0/845	0.72	1/1143 (0.1%)
All	All	0.78	3/5155 (0.1%)	0.83	5/6946 (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
1	A	0	1
3	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	271	CYS	CB-SG	-9.30	1.66	1.82
1	A	123	GLU	CG-CD	8.32	1.64	1.51
2	B	268	GLU	CG-CD	5.09	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	59	LEU	CA-CB-CG	6.30	129.80	115.30
1	A	118	LEU	CA-CB-CG	5.75	128.52	115.30
3	C	98	LEU	CA-CB-CG	5.37	127.64	115.30
2	B	271	CYS	CA-CB-SG	-5.26	104.54	114.00
2	B	372	VAL	CB-CA-C	-5.22	101.48	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	THR	Peptide
3	C	90	LEU	Peptide

## 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	1718	0	1730	63	0
2	B	1678	0	1735	118	0
3	C	838	0	846	48	0
3	D	821	0	828	47	0
4	A	31	0	0	1	0
4	B	21	0	0	5	0
4	C	12	0	0	4	0
4	D	8	0	0	2	0
All	All	5127	0	5139	252	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 25.

All (252) 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:265:SER:HB3	2:B:268:GLU:HG3	1.23	1.12
3:D:71:VAL:HA	4:D:103:HOH:O	1.49	1.09
4:A:261:HOH:O	3:C:67:ARG:HD2	1.52	1.08
1:A:194:THR:HG22	1:A:197:GLU:H	1.26	1.00
2:B:274:ASN:HD21	2:B:282:LEU:H	1.11	0.96
2:B:265:SER:HB3	2:B:268:GLU:CG	1.94	0.95
3:C:10:GLN:HE21	3:C:10:GLN:H	1.17	0.91
2:B:239:THR:HG22	2:B:242:HIS:H	1.40	0.86
3:C:22:ASN:HD22	3:C:25:THR:H	1.24	0.84
1:A:43:PHE:CZ	2:B:188:ALA:HB2	2.15	0.81
3:C:63:VAL:O	3:C:64:LYS:HB2	1.80	0.81
1:A:178:MET:O	1:A:182:VAL:HG23	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:SER:CB	2:B:268:GLU:HG3	2.07	0.79
3:C:62:ASN:ND2	4:C:107:HOH:O	2.17	0.78
2:B:384:THR:O	2:B:385:GLN:HB2	1.85	0.76
3:C:22:ASN:ND2	3:C:25:THR:H	1.84	0.74
3:C:52:MET:HA	3:C:52:MET:CE	2.17	0.74
3:D:62:ASN:OD1	3:D:65:LEU:HB3	1.85	0.74
2:B:217:PHE:O	2:B:220:TYR:HB3	1.87	0.73
2:B:248:GLN:HG3	4:B:64:HOH:O	1.88	0.73
2:B:226:ILE:O	2:B:228:ASN:CG	2.26	0.73
3:D:65:LEU:O	3:D:66:GLN:HB2	1.87	0.73
2:B:224:MET:HB3	2:B:226:ILE:HD12	1.71	0.73
2:B:224:MET:HE2	2:B:224:MET:HA	1.70	0.72
2:B:226:ILE:HG22	2:B:228:ASN:HD21	1.56	0.70
3:D:63:VAL:O	3:D:65:LEU:N	2.25	0.70
2:B:232:ARG:N	2:B:232:ARG:HE	1.90	0.70
3:C:52:MET:HE2	3:C:52:MET:HA	1.74	0.69
1:A:242:ASP:O	1:A:243:LEU:HB3	1.92	0.69
2:B:271:CYS:O	2:B:275:ARG:HB2	1.92	0.69
2:B:373:GLU:O	3:C:23:VAL:HG12	1.94	0.68
3:D:63:VAL:C	3:D:65:LEU:H	1.96	0.68
2:B:319:LYS:O	2:B:322:GLU:HG3	1.94	0.67
2:B:226:ILE:O	2:B:228:ASN:N	2.28	0.67
2:B:303:LEU:HG	2:B:304:ARG:N	2.10	0.66
2:B:274:ASN:ND2	2:B:282:LEU:H	1.90	0.66
2:B:233:GLU:C	2:B:235:TYR:H	2.00	0.66
2:B:274:ASN:HD21	2:B:282:LEU:N	1.88	0.65
3:C:71:VAL:HA	3:C:74:ILE:HG23	1.77	0.65
3:D:40:PHE:C	3:D:42:ARG:H	1.98	0.65
3:C:72:GLU:O	3:C:75:GLN:HB2	1.97	0.64
2:B:226:ILE:O	2:B:228:ASN:ND2	2.31	0.64
2:B:240:GLN:H	2:B:240:GLN:CD	2.00	0.63
1:A:104:ILE:HD13	1:A:148:ILE:HD13	1.80	0.63
3:C:60:PHE:CD2	3:C:69:LEU:HD12	2.34	0.63
1:A:72:CYS:HB3	1:A:77:VAL:HG23	1.80	0.62
1:A:75:ILE:CG2	2:B:192:VAL:HG21	2.29	0.61
1:A:154:LEU:HD13	2:B:267:THR:HB	1.82	0.61
2:B:359:LEU:O	2:B:362:LYS:HB2	1.99	0.61
1:A:40:LEU:HD13	2:B:220:TYR:HE1	1.65	0.61
1:A:172:VAL:O	1:A:172:VAL:HG23	2.01	0.60
1:A:40:LEU:HD13	2:B:220:TYR:CE1	2.36	0.60
2:B:373:GLU:CD	3:D:67:ARG:HH22	2.03	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:O	3:C:15:PRO:HB3	2.02	0.60
1:A:132:ARG:NH1	1:A:137:GLN:HB3	2.17	0.60
2:B:229:PRO:HA	2:B:232:ARG:NE	2.17	0.59
3:C:40:PHE:CG	3:C:59:LEU:HD13	2.38	0.59
2:B:231:THR:N	2:B:232:ARG:HH21	2.01	0.59
3:C:11:TYR:O	4:C:107:HOH:O	2.17	0.58
3:D:90:LEU:HB3	3:D:96:SER:HB2	1.85	0.58
2:B:172:LYS:O	2:B:176:GLU:HB2	2.03	0.58
2:B:228:ASN:C	2:B:230:VAL:H	2.07	0.58
3:D:38:LEU:O	3:D:101:TRP:HZ3	1.87	0.58
3:D:69:LEU:CD2	3:D:73:SER:HB2	2.33	0.58
3:D:51:VAL:CG2	3:D:95:SER:HA	2.34	0.58
2:B:191:MET:HG2	2:B:224:MET:SD	2.44	0.58
2:B:244:GLN:HB3	4:B:64:HOH:O	2.03	0.58
2:B:224:MET:CE	2:B:224:MET:HA	2.34	0.58
2:B:211:GLU:HG2	2:B:212:ASP:H	1.68	0.58
2:B:243:MET:HG3	2:B:297:LEU:HD11	1.86	0.58
3:D:33:TRP:O	3:D:37:VAL:HG12	2.04	0.58
1:A:186:LEU:HD21	1:A:202:LEU:HD21	1.86	0.57
2:B:319:LYS:HB2	2:B:322:GLU:HG2	1.85	0.57
3:D:7:TRP:HZ3	3:D:36:LEU:HD11	1.69	0.57
2:B:263:ILE:HD11	2:B:312:VAL:HG11	1.87	0.57
2:B:319:LYS:O	2:B:322:GLU:CG	2.53	0.57
1:A:95:ASP:OD1	2:B:280:GLU:N	2.38	0.56
3:C:8:PRO:HB2	3:C:10:GLN:NE2	2.21	0.56
3:C:61:ASN:ND2	3:C:68:LYS:HB3	2.21	0.56
3:D:8:PRO:O	3:D:11:TYR:N	2.36	0.56
3:D:33:TRP:CZ2	3:D:69:LEU:HD12	2.40	0.56
3:C:37:VAL:HB	3:C:59:LEU:HD21	1.88	0.56
3:C:33:TRP:O	3:C:37:VAL:HG12	2.06	0.55
2:B:254:GLN:O	2:B:258:GLU:HG3	2.07	0.55
2:B:384:THR:O	2:B:385:GLN:CB	2.55	0.55
3:C:20:GLN:HB3	4:C:106:HOH:O	2.07	0.55
2:B:369:ASP:HB3	2:B:376:ARG:HB2	1.89	0.55
3:D:67:ARG:NH1	4:D:110:HOH:O	2.38	0.55
2:B:239:THR:HG22	2:B:242:HIS:N	2.18	0.54
3:D:87:LEU:HA	3:D:98:LEU:O	2.07	0.54
2:B:302:ARG:HH21	2:B:304:ARG:HG3	1.71	0.54
1:A:77:VAL:HA	2:B:225:GLY:O	2.08	0.54
2:B:231:THR:H	2:B:232:ARG:HH21	1.54	0.54
3:C:22:ASN:HD22	3:C:25:THR:N	2.01	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:HG	2:B:304:ARG:H	1.71	0.54
3:D:69:LEU:HD23	3:D:73:SER:HB2	1.89	0.54
3:D:63:VAL:C	3:D:65:LEU:N	2.60	0.53
3:D:38:LEU:HD12	3:D:99:ILE:HD11	1.90	0.53
1:A:157:GLY:HA2	1:A:173:PRO:HG3	1.90	0.53
2:B:199:ALA:O	2:B:202:ILE:HG13	2.09	0.53
2:B:216:ARG:HH11	2:B:216:ARG:HB3	1.72	0.53
3:C:89:TRP:CE2	3:C:94:LYS:HG2	2.44	0.53
3:D:40:PHE:C	3:D:42:ARG:N	2.62	0.53
1:A:53:LYS:HG3	1:A:54:HIS:CE1	2.44	0.53
2:B:229:PRO:HA	2:B:232:ARG:CZ	2.39	0.52
1:A:104:ILE:HD13	1:A:148:ILE:CD1	2.39	0.52
1:A:75:ILE:HG22	2:B:192:VAL:HG21	1.92	0.52
1:A:104:ILE:HG21	1:A:148:ILE:CD1	2.40	0.52
1:A:114:ARG:HG2	3:C:9:TRP:CE2	2.45	0.51
3:C:23:VAL:O	3:C:27:GLN:HG3	2.11	0.51
1:A:38:LYS:O	1:A:41:ASP:OD1	2.28	0.51
1:A:213:LEU:HD23	1:A:234:TYR:CZ	2.46	0.51
2:B:334:LYS:HE3	2:B:345:LEU:HD11	1.92	0.50
2:B:233:GLU:O	2:B:236:GLY:O	2.29	0.50
2:B:320:GLU:OE1	2:B:356:ARG:HD3	2.11	0.50
2:B:294:LEU:HG	2:B:301:LEU:O	2.11	0.50
2:B:229:PRO:C	2:B:231:THR:H	2.15	0.50
3:D:74:ILE:O	3:D:77:VAL:HG12	2.11	0.50
1:A:62:PRO:O	1:A:66:VAL:HG23	2.12	0.50
2:B:212:ASP:HA	2:B:215:ILE:HD12	1.94	0.49
3:C:69:LEU:HD22	3:C:73:SER:HB3	1.95	0.49
2:B:264:MET:CE	2:B:268:GLU:HB2	2.42	0.49
2:B:320:GLU:OE1	2:B:356:ARG:CD	2.60	0.49
3:D:71:VAL:HG13	3:D:72:GLU:H	1.75	0.49
1:A:66:VAL:HG13	1:A:146:ARG:HH12	1.78	0.49
2:B:294:LEU:HD21	2:B:301:LEU:HD12	1.94	0.49
3:D:50:THR:HA	3:D:96:SER:HA	1.94	0.49
2:B:231:THR:OG1	2:B:232:ARG:NH2	2.47	0.48
2:B:264:MET:HE3	2:B:268:GLU:HB2	1.95	0.48
2:B:245:LEU:HD11	2:B:282:LEU:HD21	1.95	0.48
2:B:284:PRO:O	2:B:288:VAL:HG23	2.14	0.48
3:D:51:VAL:HG23	3:D:95:SER:HA	1.94	0.48
2:B:245:LEU:O	2:B:245:LEU:HD12	2.14	0.48
3:C:55:GLN:NE2	3:C:71:VAL:HB	2.28	0.48
3:D:61:ASN:HD22	3:D:62:ASN:N	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:O	1:A:240:PHE:HB3	2.13	0.48
3:D:7:TRP:HE3	3:D:8:PRO:HD2	1.78	0.48
1:A:158:PHE:HA	1:A:170:GLN:O	2.14	0.48
3:D:41:CYS:SG	3:D:99:ILE:HG21	2.54	0.48
1:A:235:TRP:CD1	3:C:15:PRO:HG3	2.48	0.48
2:B:362:LYS:HZ2	2:B:362:LYS:HB3	1.78	0.48
3:C:71:VAL:O	3:C:74:ILE:HG23	2.14	0.48
3:C:10:GLN:HB3	3:C:16:PHE:CD1	2.49	0.47
3:C:99:ILE:O	3:C:99:ILE:HD13	2.14	0.47
3:C:63:VAL:O	3:C:64:LYS:CB	2.52	0.47
2:B:360:ALA:HB3	2:B:366:LEU:HD12	1.96	0.47
1:A:112:LYS:HD3	1:A:172:VAL:CG1	2.44	0.47
1:A:207:GLU:HA	1:A:207:GLU:OE1	2.14	0.47
2:B:285:GLU:O	2:B:286:ASP:C	2.52	0.47
1:A:214:GLU:HG3	2:B:372:VAL:HG13	1.97	0.47
2:B:268:GLU:HA	4:B:19:HOH:O	2.13	0.47
3:C:62:ASN:OD1	3:C:65:LEU:HB2	2.15	0.47
3:C:72:GLU:H	3:C:72:GLU:CD	2.17	0.47
2:B:232:ARG:H	2:B:232:ARG:HE	1.60	0.47
3:D:33:TRP:HB3	3:D:77:VAL:HG21	1.96	0.47
3:C:7:TRP:HZ3	3:C:36:LEU:HD21	1.80	0.47
3:D:72:GLU:O	3:D:76:ILE:HG12	2.15	0.47
3:D:93:SER:O	3:D:94:LYS:HB2	2.15	0.47
3:C:69:LEU:CD2	3:C:73:SER:HB3	2.45	0.47
1:A:132:ARG:HH12	1:A:137:GLN:HB3	1.80	0.46
2:B:272:LEU:HD23	2:B:272:LEU:HA	1.66	0.46
2:B:194:LEU:HA	2:B:197:SER:OG	2.16	0.46
3:C:65:LEU:HD23	3:C:65:LEU:HA	1.60	0.46
1:A:58:ILE:O	1:A:59:ARG:HG3	2.14	0.46
2:B:369:ASP:OD2	3:D:67:ARG:NH1	2.48	0.46
1:A:43:PHE:HZ	2:B:188:ALA:HB2	1.76	0.46
1:A:188:GLU:HA	1:A:239:LEU:HD13	1.97	0.46
2:B:295:GLU:C	2:B:297:LEU:H	2.19	0.46
3:C:50:THR:HG23	3:C:53:GLU:H	1.80	0.46
1:A:192:TYR:C	1:A:192:TYR:CD2	2.90	0.46
2:B:358:LEU:O	2:B:362:LYS:HG3	2.16	0.46
1:A:85:GLY:O	1:A:89:GLU:HG2	2.16	0.45
3:D:7:TRP:CZ3	3:D:36:LEU:HD11	2.50	0.45
3:D:47:SER:O	3:D:98:LEU:HA	2.17	0.45
1:A:242:ASP:O	1:A:243:LEU:CB	2.62	0.45
1:A:137:GLN:OE1	1:A:137:GLN:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:ASN:O	2:B:232:ARG:NH2	2.49	0.45
3:D:10:GLN:HE21	3:D:10:GLN:HB2	1.61	0.45
2:B:233:GLU:C	2:B:235:TYR:N	2.69	0.45
1:A:84:LYS:HG3	2:B:241:TYR:CE1	2.52	0.45
2:B:373:GLU:CD	3:D:67:ARG:NH2	2.69	0.45
3:C:52:MET:CE	3:C:52:MET:CA	2.92	0.45
2:B:305:VAL:HG13	2:B:311:MET:HG2	1.97	0.45
3:D:59:LEU:HD13	3:D:60:PHE:N	2.32	0.45
2:B:373:GLU:OE2	3:D:67:ARG:NH2	2.50	0.44
1:A:69:GLN:HE22	1:A:146:ARG:HG2	1.82	0.44
3:D:8:PRO:O	3:D:10:GLN:N	2.51	0.44
2:B:321:GLU:N	2:B:321:GLU:OE2	2.46	0.44
1:A:39:GLN:HA	1:A:42:MET:HG3	1.98	0.44
2:B:275:ARG:HD3	2:B:275:ARG:HA	1.74	0.44
1:A:194:THR:HG22	1:A:197:GLU:N	2.11	0.44
1:A:86:PHE:CZ	2:B:223:SER:HB3	2.53	0.44
1:A:121:LEU:HD21	1:A:141:GLN:HB3	2.00	0.44
1:A:77:VAL:HG12	2:B:226:ILE:HG13	1.99	0.44
2:B:228:ASN:O	2:B:232:ARG:CZ	2.66	0.44
2:B:237:SER:HB3	4:B:26:HOH:O	2.17	0.44
2:B:274:ASN:HA	2:B:274:ASN:HD22	1.61	0.44
3:C:16:PHE:CE2	3:C:33:TRP:CE2	3.06	0.43
2:B:337:LEU:HD22	2:B:341:GLU:HB3	2.00	0.43
1:A:166:THR:HG23	1:A:167:TYR:N	2.33	0.43
1:A:84:LYS:HG3	2:B:241:TYR:CZ	2.53	0.43
2:B:263:ILE:CD1	2:B:312:VAL:HG11	2.48	0.43
1:A:61:ASN:CG	1:A:64:PHE:HB2	2.39	0.43
2:B:266:LEU:HA	2:B:266:LEU:HD23	1.56	0.43
3:D:81:LEU:HD12	3:D:84:LYS:HD3	2.01	0.43
3:D:53:GLU:C	3:D:55:GLN:H	2.22	0.43
2:B:226:ILE:O	2:B:227:ALA:C	2.57	0.43
2:B:233:GLU:O	2:B:235:TYR:N	2.48	0.43
1:A:61:ASN:OD1	1:A:61:ASN:C	2.57	0.43
2:B:229:PRO:C	2:B:231:THR:N	2.72	0.43
3:C:74:ILE:HD13	3:C:74:ILE:HG21	1.84	0.43
2:B:256:PRO:HA	2:B:259:GLU:OE2	2.19	0.42
3:C:12:ARG:CG	4:C:103:HOH:O	2.67	0.42
3:D:61:ASN:C	3:D:61:ASN:ND2	2.73	0.42
1:A:126:GLN:HE22	1:A:243:LEU:HD22	1.85	0.42
2:B:253:LEU:C	2:B:256:PRO:HD2	2.39	0.42
2:B:237:SER:OG	2:B:238:GLY:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:VAL:HG23	2:B:256:PRO:HD3	2.01	0.42
2:B:277:ARG:HG3	2:B:277:ARG:H	1.56	0.42
2:B:226:ILE:HG22	2:B:228:ASN:ND2	2.29	0.42
3:C:89:TRP:CD2	3:C:94:LYS:HG2	2.54	0.42
2:B:351:LEU:HD12	2:B:351:LEU:HA	1.78	0.42
2:B:196:LYS:O	2:B:199:ALA:HB3	2.20	0.41
3:C:71:VAL:HA	3:C:74:ILE:CG2	2.46	0.41
3:C:74:ILE:HA	3:C:77:VAL:HG13	2.02	0.41
3:D:40:PHE:O	3:D:42:ARG:N	2.52	0.41
1:A:72:CYS:SG	1:A:79:PRO:HG3	2.61	0.41
1:A:172:VAL:O	1:A:172:VAL:CG2	2.65	0.41
3:D:70:PRO:O	3:D:74:ILE:HG13	2.21	0.41
2:B:173:ASN:O	2:B:174:ILE:C	2.58	0.41
1:A:43:PHE:CE2	2:B:188:ALA:HB2	2.55	0.41
3:C:40:PHE:HZ	3:C:58:PRO:HG2	1.85	0.41
3:C:62:ASN:CG	3:C:65:LEU:HB2	2.40	0.41
1:A:219:GLU:HA	1:A:219:GLU:OE2	2.20	0.41
2:B:216:ARG:HB3	2:B:216:ARG:NH1	2.35	0.41
3:C:78:LEU:HA	3:C:78:LEU:HD12	1.87	0.41
1:A:144:LEU:O	1:A:148:ILE:HG12	2.21	0.41
1:A:237:PRO:O	1:A:239:LEU:O	2.39	0.41
2:B:256:PRO:O	2:B:260:ARG:HD2	2.21	0.41
3:D:72:GLU:O	3:D:75:GLN:HB2	2.21	0.41
3:D:84:LYS:HE3	3:D:86:ASN:ND2	2.36	0.41
2:B:188:ALA:O	2:B:191:MET:N	2.54	0.41
2:B:218:LYS:O	2:B:221:LEU:N	2.54	0.40
2:B:297:LEU:HB2	2:B:299:LEU:HD12	2.02	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD12	1.97	0.40
1:A:86:PHE:O	1:A:90:MET:HB2	2.21	0.40
2:B:228:ASN:C	2:B:230:VAL:N	2.73	0.40
1:A:202:LEU:HD13	1:A:202:LEU:HA	1.74	0.40
2:B:240:GLN:HB3	4:B:54:HOH:O	2.22	0.40
1:A:177:ASN:HB2	1:A:180:HIS:CD2	2.56	0.40
1:A:225:ASP:OD1	3:C:67:ARG:NH1	2.54	0.40
3:D:54:ALA:O	3:D:57:SER:HB3	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	215/258 (83%)	184 (86%)	22 (10%)	9 (4%)	3	12
2	B	213/238 (90%)	175 (82%)	32 (15%)	6 (3%)	6	22
3	C	97/102 (95%)	90 (93%)	6 (6%)	1 (1%)	18	51
3	D	95/102 (93%)	77 (81%)	11 (12%)	7 (7%)	1	3
All	All	620/700 (89%)	526 (85%)	71 (12%)	23 (4%)	4	16

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	243	LEU
1	A	245	SER
2	B	227	ALA
2	B	385	GLN
3	D	63	VAL
3	D	64	LYS
3	D	66	GLN
3	D	94	LYS
1	A	176	LEU
1	A	229	PRO
2	B	237	SER
3	C	64	LYS
3	D	9	TRP
1	A	58	ILE
1	A	137	GLN
1	A	249	THR
1	A	244	TYR
2	B	234	THR
2	B	174	ILE
2	B	230	VAL
3	D	71	VAL
3	D	70	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	182/211 (86%)	151 (83%)	31 (17%)	2	7
2	B	188/207 (91%)	153 (81%)	35 (19%)	2	5
3	C	95/97 (98%)	72 (76%)	23 (24%)	1	2
3	D	93/97 (96%)	76 (82%)	17 (18%)	2	6
All	All	558/612 (91%)	452 (81%)	106 (19%)	2	5

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	47	LEU
1	A	49	GLU
1	A	52	SER
1	A	56	GLN
1	A	59	ARG
1	A	60	LYS
1	A	71	MET
1	A	74	THR
1	A	89	GLU
1	A	93	VAL
1	A	107	VAL
1	A	112	LYS
1	A	118	LEU
1	A	122	GLU
1	A	130	LYS
1	A	145	ILE
1	A	168	LEU
1	A	176	LEU
1	A	178	MET
1	A	185	GLN
1	A	186	LEU
1	A	188	GLU
1	A	194	THR

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Mol	Chain	Res	Type
1	A	201	SER
1	A	202	LEU
1	A	205	GLU
1	A	206	THR
1	A	211	GLN
1	A	241	THR
1	A	246	GLN
2	B	174	ILE
2	B	181	LEU
2	B	182	SER
2	B	184	LEU
2	B	200	ASN
2	B	202	ILE
2	B	204	ASP
2	B	212	ASP
2	B	216	ARG
2	B	218	LYS
2	B	228	ASN
2	B	232	ARG
2	B	239	THR
2	B	240	GLN
2	B	245	LEU
2	B	248	GLN
2	B	255	VAL
2	B	259	GLU
2	B	266	LEU
2	B	267	THR
2	B	271	CYS
2	B	272	LEU
2	B	275	ARG
2	B	277	ARG
2	B	279	MET
2	B	285	GLU
2	B	301	LEU
2	B	304	ARG
2	B	316	GLN
2	B	330	THR
2	B	345	LEU
2	B	356	ARG
2	B	362	LYS
2	B	372	VAL
2	B	384	THR

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Mol	Chain	Res	Type
3	C	10	GLN
3	C	12	ARG
3	C	28	LYS
3	C	37	VAL
3	C	43	LEU
3	C	45	LYS
3	C	52	MET
3	C	61	ASN
3	C	63	VAL
3	C	65	LEU
3	C	66	GLN
3	C	69	LEU
3	C	73	SER
3	C	74	ILE
3	C	76	ILE
3	C	77	VAL
3	C	78	LEU
3	C	83	LYS
3	C	95	SER
3	C	98	LEU
3	C	99	ILE
3	C	100	MET
3	C	102	ARG
3	D	10	GLN
3	D	12	ARG
3	D	23	VAL
3	D	37	VAL
3	D	41	CYS
3	D	42	ARG
3	D	49	MET
3	D	52	MET
3	D	56	GLU
3	D	59	LEU
3	D	63	VAL
3	D	65	LEU
3	D	67	ARG
3	D	68	LYS
3	D	72	GLU
3	D	91	ASP
3	D	99	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	126	GLN
1	A	177	ASN
1	A	190	ASN
1	A	211	GLN
1	A	246	GLN
2	B	228	ASN
2	B	242	HIS
2	B	274	ASN
2	B	289	ASN
2	B	318	HIS
3	C	10	GLN
3	C	22	ASN
3	C	27	GLN
3	C	44	HIS
3	C	55	GLN
3	C	61	ASN
3	C	66	GLN
3	D	10	GLN
3	D	46	GLN
3	D	61	ASN
3	D	66	GLN
3	D	86	ASN

### 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](#)

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 ⓘ

### 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	217/258 (84%)	0.02	2 (0%) 84 83	57, 71, 107, 116	0
2	B	215/238 (90%)	0.47	18 (8%) 12 8	69, 94, 116, 120	0
3	C	99/102 (97%)	0.00	1 (1%) 82 81	57, 80, 103, 118	0
3	D	97/102 (95%)	1.29	29 (29%) 1 0	87, 114, 143, 146	0
All	All	628/700 (89%)	0.37	50 (7%) 13 10	57, 90, 124, 146	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	207	GLY	8.4
3	D	99	ILE	6.6
3	D	89	TRP	6.3
2	B	208	ASP	6.0
3	D	93	SER	5.3
2	B	206	GLN	4.8
3	D	100	MET	4.8
3	D	78	LEU	4.7
3	D	45	LYS	4.5
3	D	90	LEU	4.4
3	D	92	LYS	4.3
3	D	86	ASN	4.2
2	B	210	THR	3.9
3	D	101	TRP	3.9
3	D	94	LYS	3.8
2	B	231	THR	3.6
3	D	84	LYS	3.5
2	B	209	ILE	3.5
2	B	205	LYS	3.4
2	B	230	VAL	3.3
3	C	102	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	95	SER	3.1
2	B	172	LYS	3.0
3	D	43	LEU	2.9
3	D	85	GLY	2.9
3	D	44	HIS	2.9
3	D	97	PHE	2.9
2	B	234	THR	2.8
1	A	135	PHE	2.8
3	D	48	SER	2.8
3	D	88	GLU	2.7
3	D	75	GLN	2.7
2	B	235	TYR	2.7
3	D	54	ALA	2.6
3	D	87	LEU	2.5
2	B	365	HIS	2.5
3	D	47	SER	2.5
2	B	229	PRO	2.4
2	B	227	ALA	2.4
2	B	233	GLU	2.4
3	D	81	LEU	2.4
3	D	46	GLN	2.4
3	D	91	ASP	2.3
3	D	33	TRP	2.2
1	A	36	MET	2.2
2	B	345	LEU	2.2
3	D	66	GLN	2.1
2	B	178	PHE	2.1
2	B	220	TYR	2.0
3	D	5	PHE	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 [i](#)

There are no such residues in this entry.