Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 09:06 PM EDT

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)

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

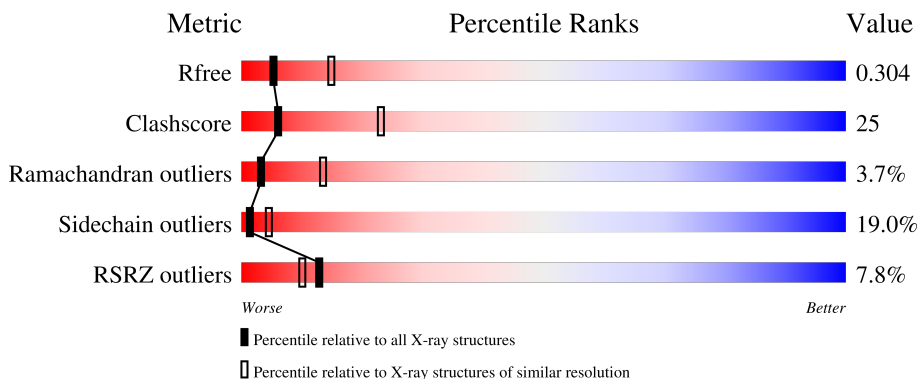|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.304
Clashscore		25
Ramachandran outliers		3.7%
Sidechain outliers		19.0%
RSRZ outliers		7.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% — 47% / 31% / 6% / 16%
2	B	238	7% — 45% / 32% / 12% · 10%
3	C	102	% — 45% / 37% / 15% ·
3	D	102	28% — 40% / 41% / 12% · 5%

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.

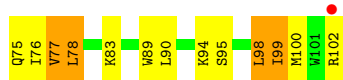| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1718	1103	290	318	7			

- 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.

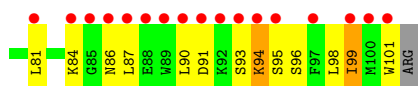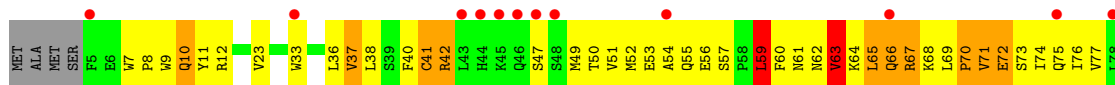| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	0	0
			838	546	144	143	5			
3	D	97	Total	C	N	O	S	0	0	0
			821	537	139	140	5			

- 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		

3 Residue-property plots ⓘ

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

- Molecule 1: Vacuolar-sorting protein SNF8

- Molecule 2: Vacuolar protein-sorting-associated protein 36

- Molecule 3: Vacuolar protein-sorting-associated protein 25

MET ALA MET S4 W7 P8 W9 Q10 Y11 R12 P15 F16 Q20 P21 N22 V23 D24 T25 R26 Q27 K28 W33 L36 V37 F40 L43 H44 K45 T50 V51 M52 E53 A54 Q55 P58 L59 F60 N61 N62 V63 K64 L65 Q66 R67 K68 L69 P70 V71 E72 S73 I74

Q75 I76 V77 L78 K83 W89 L90 K94 S95 L98 I99 M100 W101 R102

• Molecule 3: Vacuolar protein-sorting-associated protein 25

Chain D:

28%

40%   41%   12%   5%

MET ALA MET SER F5 E6 W7 P8 W9 Q10 Y11 R12 V23 W33 L36 V37 L38 S39 F40 C41 R42 L43 H44 K45 Q46 S47 S48 M49 T50 V51 M52 E53 A54 Q55 E56 S57 P58 L59 F60 N61 N62 V63 K64 L65 Q66 R67 K68 L69 P70 V71 E72 S73 I74 Q75 I76 V77 L78

L81 K84 G85 N86 L87 E88 W89 L90 D91 K92 S93 K94 S95 S96 F97 L98 I99 M100 W101 ARG

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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 (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	94.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 90.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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^2)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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:H	3:C:10:GLN:HE21	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:HA	3:C:52:MET:HE2	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:CD	2:B:240:GLN:H	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:51:VAL:CG2	3:D:95:SER:HA	2.34	0.58
3:D:69:LEU:CD2	3:D:73:SER:HB2	2.33	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:HA	2:B:224:MET:CE	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:245:LEU:HD11	2:B:282:LEU:HD21	1.95	0.48
2:B:264:MET:HE3	2:B:268:GLU:HB2	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:HB3	2:B:362:LYS:HZ2	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:OE1	1:A:207:GLU:HA	2.14	0.47
1:A:214:GLU:HG3	2:B:372:VAL:HG13	1.97	0.47
2:B:285:GLU:O	2:B:286:ASP:C	2.52	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:HE	2:B:232:ARG:H	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:HA	1:A:137:GLN:OE1	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
1:A:84:LYS:HG3	2:B:241:TYR:CE1	2.52	0.45
2:B:233:GLU:C	2:B:235:TYR:N	2.69	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:OE2	2:B:321:GLU:N	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:86:PHE:CZ	2:B:223:SER:HB3	2.53	0.44
1:A:194:THR:HG22	1:A:197:GLU:N	2.11	0.44
1:A:77:VAL:HG12	2:B:226:ILE:HG13	1.99	0.44
1:A:121:LEU:HD21	1:A:141:GLN:HB3	2.00	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:HD22	2:B:274:ASN:HA	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:84:LYS:HG3	2:B:241:TYR:CZ	2.53	0.43
1:A:166:THR:HG23	1:A:167:TYR:N	2.33	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:HD23	2:B:266:LEU:HA	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:C	1:A:61:ASN:OD1	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:H	2:B:277:ARG:HG3	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
1:A:43:PHE:CE2	2:B:188:ALA:HB2	2.55	0.41
2:B:173:ASN:O	2:B:174:ILE:C	2.58	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:OE2	1:A:219:GLU:HA	2.20	0.41
2:B:216:ARG:HB3	2:B:216:ARG:NH1	2.35	0.41
3:C:78:LEU:HD12	3:C:78:LEU:HA	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:86:PHE:O	1:A:90:MET:HB2	2.21	0.40
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.97	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	10
2	B	213/238 (90%)	175 (82%)	32 (15%)	6 (3%)	5	19
3	C	97/102 (95%)	90 (93%)	6 (6%)	1 (1%)	15	45
3	D	95/102 (93%)	77 (81%)	11 (12%)	7 (7%)	1	2
All	All	620/700 (89%)	526 (85%)	71 (12%)	23 (4%)	3	13

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 (i)

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	6
2	B	188/207 (91%)	153 (81%)	35 (19%)	1	5
3	C	95/97 (98%)	72 (76%)	23 (24%)	0	2
3	D	93/97 (96%)	76 (82%)	17 (18%)	1	5
All	All	558/612 (91%)	452 (81%)	106 (19%)	1	4

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

Sometimes 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 ⓘ

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 monosaccharides 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, 95th 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(Å²)	Q<0.9
1	A	217/258 (84%)	0.01	2 (0%)	84	84	57, 71, 107, 116	0
2	B	215/238 (90%)	0.47	17 (7%)	12	10	69, 94, 116, 120	0
3	C	99/102 (97%)	-0.00	1 (1%)	82	82	57, 80, 103, 118	0
3	D	97/102 (95%)	1.29	29 (29%)	0	0	87, 114, 143, 146	0
All	All	628/700 (89%)	0.37	49 (7%)	13	10	57, 90, 124, 146	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	207	GLY	8.6
3	D	99	ILE	6.7
3	D	89	TRP	6.4
2	B	208	ASP	6.0
3	D	93	SER	5.3
3	D	78	LEU	4.7
3	D	100	MET	4.7
2	B	206	GLN	4.7
3	D	45	LYS	4.4
3	D	90	LEU	4.4
3	D	92	LYS	4.3
3	D	86	ASN	4.2
2	B	210	THR	4.1
3	D	101	TRP	3.8
3	D	94	LYS	3.8
2	B	231	THR	3.6
2	B	209	ILE	3.6
3	D	84	LYS	3.5
2	B	205	LYS	3.4
2	B	230	VAL	3.2
3	C	102	ARG	3.2

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