



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3F1I / pdb_00003f1i
Title : Human ESCRT-0 Core Complex
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Deposited on : 2008-10-28
Resolution : 2.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

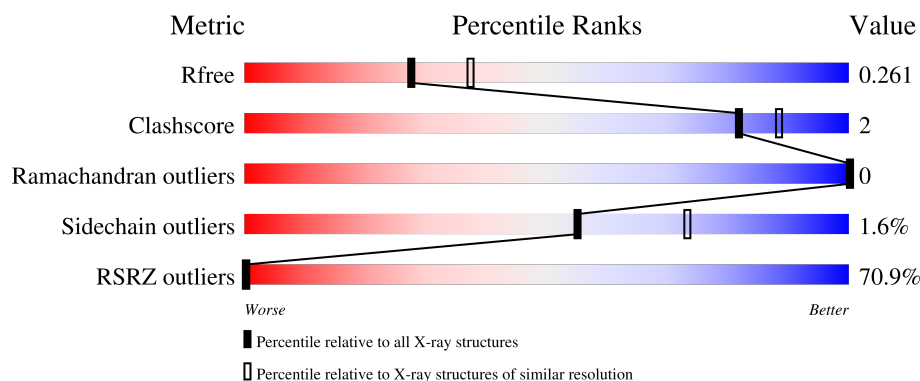
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	H	98	72% 92% 7% .
2	C	77	31% 29% . 69%
2	S	77	60% 92% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1642 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 Hepatocyte growth factor-regulated tyrosine kinase substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	98	Total	C	N	O	S	0	0	0
			798	490	156	149	3			

- Molecule 2 is a protein called Signal transducing adapter molecule 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	77	Total	C	N	O	S	0	0	0
			621	386	98	130	7			
2	C	24	Total	C	N	O	S	0	0	0
			195	119	33	42	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	20	Total	O	0	0
			20	20		
3	S	7	Total	O	0	0
			7	7		
3	C	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	78.06Å 78.06Å 152.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 2.30 44.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.77-2.30) 99.2 (44.77-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.239 , 0.253 0.242 , 0.261	Depositor DCC
R_{free} test set	1019 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1642	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	H	0.95	1/807 (0.1%)	1.02	0/1080
2	C	0.76	0/196	0.88	0/261
2	S	0.84	0/629	0.98	0/847
All	All	0.89	1/1632 (0.1%)	0.99	0/2188

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	493	GLU	CD-OE1	5.25	1.35	1.25

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	H	798	0	801	3	1
2	C	195	0	190	1	0
2	S	621	0	606	4	0
3	C	1	0	0	0	0
3	H	20	0	0	1	0
3	S	7	0	0	0	0
All	All	1642	0	1597	8	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 2.

All (8) 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:S:371:TYR:OH	2:S:375:MET:HE3	1.97	0.64
1:H:420:VAL:HG12	1:H:424:LYS:HE3	1.89	0.54
2:S:371:TYR:CZ	2:S:375:MET:HE3	2.46	0.48
2:S:371:TYR:CE1	2:S:375:MET:HE2	2.50	0.47
1:H:432:SER:OG	1:H:434:THR:HG22	2.15	0.46
1:H:471:GLN:NE2	3:H:7:HOH:O	2.49	0.44
2:S:331:HIS:O	2:S:335:MET:HG3	2.18	0.43
2:C:338:GLN:O	2:C:341:PRO:HD2	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:ASP:OD2	1:H:479:ASP:OD2[6_555]	1.80	0.40

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	H	96/98 (98%)	96 (100%)	0	0	100	100
2	C	22/77 (29%)	21 (96%)	1 (4%)	0	100	100
2	S	75/77 (97%)	75 (100%)	0	0	100	100
All	All	193/252 (77%)	192 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	H	85/85 (100%)	84 (99%)	1 (1%)	63	79
2	C	23/74 (31%)	23 (100%)	0	100	100
2	S	74/74 (100%)	72 (97%)	2 (3%)	39	58
All	All	182/233 (78%)	179 (98%)	3 (2%)	55	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	471	GLN
2	S	312	GLN
2	S	326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	447	ASN
1	H	476	GLN
2	C	338	GLN

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 oligosaccharides 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(Å ²)	Q<0.9
1	H	98/98 (100%)	2.56	71 (72%)  	55, 59, 68, 72	0
2	C	24/77 (31%)	3.98	24 (100%)  	74, 81, 94, 95	0
2	S	77/77 (100%)	2.29	46 (59%)  	56, 59, 64, 65	0
All	All	199/252 (78%)	2.63	141 (70%)  	55, 60, 83, 95	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	360	LEU	6.5
2	C	357	LEU	5.4
1	H	429	ARG	5.3
1	H	433	ILE	5.2
2	C	339	MET	5.0
2	C	338	GLN	5.0
1	H	478	ARG	4.9
2	C	342	LEU	4.8
1	H	474	LEU	4.8
1	H	434	THR	4.7
1	H	497	ARG	4.7
2	C	340	GLY	4.6
2	S	326	LEU	4.5
2	C	352	ARG	4.4
2	C	353	LYS	4.4
2	C	355	SER	4.3
1	H	501	GLU	4.3
1	H	498	ALA	4.2
1	H	444	GLN	4.1
2	S	325	ASP	4.1
2	C	349	ASP	4.1
1	H	404	SER	4.1
2	C	356	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
2	S	330	LEU	4.0
2	S	320	SER	4.0
2	C	354	HIS	3.9
2	C	347	LEU	3.9
2	S	312	GLN	3.8
1	H	464	ARG	3.8
1	H	427	HIS	3.8
2	S	328	GLU	3.8
2	C	359	GLU	3.8
2	C	345	GLU	3.7
1	H	443	PHE	3.7
1	H	431	ARG	3.7
2	S	376	ASN	3.6
2	C	361	ASN	3.6
1	H	405	HIS	3.6
2	S	337	HIS	3.6
2	S	329	LEU	3.6
1	H	477	ILE	3.5
1	H	471	GLN	3.5
2	S	327	PRO	3.5
2	C	350	ILE	3.5
2	S	377	GLU	3.5
1	H	448	GLY	3.4
1	H	406	GLU	3.4
2	C	351	ASP	3.4
1	H	416	VAL	3.3
2	S	332	LEU	3.3
2	C	343	ILE	3.3
2	S	336	CYS	3.2
2	S	317	THR	3.2
2	S	364	VAL	3.2
2	S	357	LEU	3.1
2	C	358	SER	3.1
2	C	346	LYS	3.1
1	H	419	PHE	3.1
1	H	473	LYS	3.1
2	C	341	PRO	3.1
1	H	432	SER	3.0
2	S	301	PHE	3.0
1	H	500	GLU	3.0
2	S	324	PRO	3.0
1	H	468	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	410	LYS	3.0
1	H	465	LEU	2.9
1	H	467	TYR	2.9
1	H	470	LEU	2.9
2	S	353	LYS	2.9
1	H	439	VAL	2.9
1	H	496	ARG	2.8
1	H	440	LEU	2.8
1	H	475	ALA	2.8
2	S	303	ASP	2.8
1	H	454	LEU	2.8
1	H	423	MET	2.8
1	H	407	GLN	2.8
1	H	412	LEU	2.8
2	S	311	LEU	2.8
2	S	333	GLU	2.7
1	H	409	LEU	2.7
2	S	338	GLN	2.7
1	H	437	SER	2.7
2	S	319	PRO	2.7
1	H	426	ASN	2.7
2	S	347	LEU	2.7
2	C	344	ASP	2.6
2	S	359	GLU	2.6
1	H	420	VAL	2.6
1	H	425	SER	2.6
1	H	442	LEU	2.6
1	H	495	LEU	2.6
2	S	363	LYS	2.6
1	H	481	ARG	2.6
1	H	458	ASN	2.5
1	H	428	MET	2.5
2	S	351	ASP	2.5
2	S	352	ARG	2.5
1	H	453	LEU	2.5
2	S	342	LEU	2.5
2	S	334	ALA	2.5
1	H	451	PRO	2.5
1	H	441	SER	2.5
1	H	445	SER	2.5
1	H	435	ASN	2.5
1	H	446	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	463	ARG	2.4
2	S	302	ILE	2.4
1	H	430	GLY	2.4
2	S	369	SER	2.4
2	S	313	MET	2.4
1	H	489	GLU	2.4
2	S	360	LEU	2.3
1	H	490	GLU	2.3
2	S	367	ALA	2.3
2	S	371	TYR	2.3
1	H	415	ALA	2.3
2	S	309	GLN	2.3
2	S	343	ILE	2.3
1	H	414	ASN	2.2
2	S	321	ASP	2.2
2	S	358	SER	2.2
2	S	314	LEU	2.2
1	H	462	GLU	2.2
2	S	354	HIS	2.2
1	H	485	SER	2.2
1	H	460	LEU	2.1
2	S	322	ASP	2.1
1	H	455	GLU	2.1
2	S	373	LYS	2.1
2	S	331	HIS	2.1
1	H	466	TYR	2.1
2	C	348	GLU	2.1
1	H	422	ARG	2.1
1	H	456	LEU	2.1
1	H	472	ASP	2.1
1	H	494	LYS	2.1
1	H	447	ASN	2.0
1	H	483	ALA	2.0
1	H	476	GLN	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.