



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:15 AM GMT

PDB ID : 2CAZ
Title : ESCRT-I CORE
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Deposited on : 2005-12-23
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

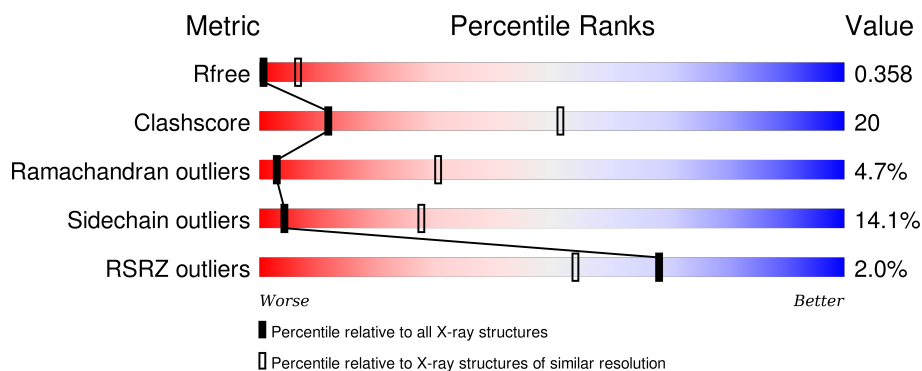
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



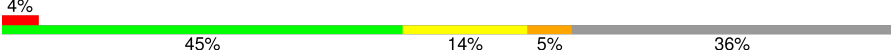
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 ≥ 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	82	<div> <div>49%</div> <div>17%</div> <div>5%</div> <div>28%</div> </div>
1	D	82	<div> <div>48%</div> <div>22%</div> <div>26%</div> </div>
2	B	155	<div> <div>30%</div> <div>29%</div> <div>5%</div> <div>35%</div> </div>
2	E	155	<div> <div>26%</div> <div>31%</div> <div>8%</div> <div>34%</div> </div>
3	C	85	<div> <div>5%</div> <div>47%</div> <div>22%</div> <div>6%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	85	 <p>A horizontal bar chart showing the quality of chain F. The bar is divided into five segments: a small red segment at the beginning labeled '4%', followed by a green segment labeled '45%', a yellow segment labeled '14%', an orange segment labeled '5%', and a grey segment at the end labeled '36%'.</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3602 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 SUPPRESSOR PROTEIN STP22 OF TEMPERATURE-SENSITIVE ALPHA-FACTOR RECEPTOR AND ARGININE PERMEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	59	Total	C	N	O	S	0	0	1
			484	306	91	85	2			
1	D	61	Total	C	N	O	S	0	0	1
			499	317	93	87	2			

- Molecule 2 is a protein called VACUOLAR PROTEIN SORTING-ASSOCIATED PROTEIN VPS28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	1
			813	515	131	166	1			
2	E	102	Total	C	N	O	S	0	0	1
			820	520	132	167	1			

- Molecule 3 is a protein called PROTEIN SRN2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	65	Total	C	N	O	0	0	1
			536	331	93	112			
3	F	54	Total	C	N	O	0	0	1
			450	277	81	92			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	140	ASP	GLU	CONFLICT	UNP Q99176
C	143	GLU	LYS	CONFLICT	UNP Q99176

3 Residue-property plots [i](#)

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: SUPPRESSOR PROTEIN STP22 OF TEMPERATURE-SENSITIVE ALPHA-FACTOR RECEPTOR AND ARGININE PERMEASE

Chain A: 



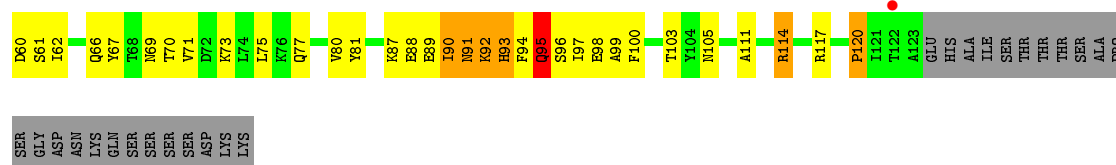
- Molecule 1: SUPPRESSOR PROTEIN STP22 OF TEMPERATURE-SENSITIVE ALPHA-FACTOR RECEPTOR AND ARGININE PERMEASE

Chain D: 




- Molecule 2: VACUOLAR PROTEIN SORTING-ASSOCIATED PROTEIN VPS28

Chain B: 



- Molecule 2: VACUOLAR PROTEIN SORTING-ASSOCIATED PROTEIN VPS28

Chain E: 



SER
ALA
PRO
SER
GLY
ASP
ASN
LYS
GLN
SER
SER
SER
SER
ASP
LYS
LYS

● Molecule 3: PROTEIN SRN2



MET
TYR
VAL
ALA
SER
TRP
GLN
ASP
TYR
HIS
S139
S142
E143
K144
Y146
G146
D147
I148
A149
K152
E155
E169
R173
S174
I175
D176
S177
D180
Q183
F184
I185
K186
L189
D190
I191
R192
T193
Q194
L197
R198
R199
E200
K201
L202
A203
THR
TRP
ASP
LYS
GLN
GLY

ASN
LEU
LYS
TYR

● Molecule 3: PROTEIN SRN2



MET
TYR
VAL
ALA
SER
TRP
GLN
ASP
TYR
HIS
SER
ASP
PHE
SER
GLU
LYS
TYR
GLY
ASP
ILE
ALA
L150
K151
K152
E155
Q156
I175
D176
S177
D180
I185
K186
L189
D190
I191
R192
T193
Q194
R198
R199
E200
K201
L202
A203
THR
TRP
ASP
LYS
GLN
GLY
ASN
LEU
LYS
TYR

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	167.91Å 167.91Å 50.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	145.86 – 3.60 43.11 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (145.86-3.60) 99.9 (43.11-3.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.328 , 0.357 0.328 , 0.358	Depositor DCC
R_{free} test set	465 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	134.8	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.3	EDS
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 9652 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3602	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.29	5/492 (1.0%)	0.81	3/666 (0.5%)
1	D	0.84	2/508 (0.4%)	0.81	2/689 (0.3%)
2	B	0.55	0/825	0.63	0/1117
2	E	0.56	0/832	0.66	0/1128
3	C	0.83	1/541 (0.2%)	0.57	0/723
3	F	0.45	0/453	0.60	0/605
All	All	0.77	8/3651 (0.2%)	0.68	5/4928 (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
2	E	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	ARG	CZ-NH2	20.61	1.59	1.33
3	C	142	SER	CB-OG	16.11	1.63	1.42
1	D	368	ARG	CZ-NH2	12.78	1.49	1.33
1	A	326	ASN	CG-ND2	11.83	1.62	1.32
1	A	368	ARG	NE-CZ	7.28	1.42	1.33
1	A	382	SER	C-N	-5.50	1.23	1.34
1	A	326	ASN	CG-OD1	5.32	1.35	1.24
1	D	368	ARG	NE-CZ	5.05	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ARG	NE-CZ-NH2	-12.34	114.13	120.30
1	A	326	ASN	OD1-CG-ND2	10.52	146.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	326	ASN	CB-CG-ND2	-6.26	101.68	116.70
1	D	368	ARG	NH1-CZ-NH2	5.73	125.70	119.40
1	A	368	ARG	CD-NE-CZ	5.04	130.66	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	24	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	484	0	491	27	0
1	D	499	0	509	27	0
2	B	813	0	809	43	0
2	E	820	0	817	55	0
3	C	536	0	529	13	0
3	F	450	0	455	10	0
All	All	3602	0	3610	146	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 20.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
2:B:40:LEU:HA	2:B:43:ILE:HD12	1.42	1.02
2:E:40:LEU:HA	2:E:43:ILE:HD12	1.49	0.95
1:D:368:ARG:HH11	1:D:368:ARG:HG3	1.32	0.92
2:B:54:GLU:OE1	2:B:114:ARG:HD2	1.75	0.85
2:E:42:GLU:HG2	2:E:81:TYR:CZ	2.12	0.84
2:B:42:GLU:HG2	2:B:81:TYR:CZ	2.13	0.84
1:A:376:HIS:CD2	2:B:24:LEU:HD22	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:HIS:NE2	2:E:24:LEU:HA	1.97	0.78
1:A:356:LEU:HD22	2:B:66:GLN:HG3	1.67	0.75
1:D:374:ARG:HG2	2:E:104:TYR:HD1	1.52	0.74
1:A:343:GLU:HB3	1:A:347:ARG:HH21	1.53	0.72
2:E:101:CYS:HA	2:E:106:ILE:HD11	1.69	0.72
2:B:96:SER:O	2:B:99:ALA:HB3	1.90	0.72
1:D:374:ARG:HG2	2:E:104:TYR:CD1	2.24	0.71
2:E:30:THR:HB	2:E:33:ASP:H	1.58	0.69
2:E:32:LYS:O	2:E:36:VAL:HG23	1.93	0.68
2:E:51:ASP:OD1	2:E:110:ASN:HB3	1.92	0.68
2:E:93:HIS:HB3	2:E:94:PHE:CE1	2.28	0.68
2:B:54:GLU:OE2	2:B:114:ARG:HB2	1.94	0.67
3:F:152:LYS:HA	3:F:155:GLU:HB2	1.75	0.67
1:A:356:LEU:HD12	1:A:356:LEU:H	1.58	0.67
2:E:112:ILE:O	2:E:116:GLU:HG2	1.95	0.67
3:F:185:ILE:HG22	3:F:186:LYS:N	2.10	0.67
1:A:356:LEU:HD13	2:B:66:GLN:NE2	2.09	0.67
2:B:93:HIS:HB3	2:B:94:PHE:CE1	2.31	0.66
1:D:356:LEU:HD22	2:E:66:GLN:HG3	1.77	0.65
3:C:185:ILE:HG22	3:C:186:LYS:N	2.11	0.65
1:D:343:GLU:HB3	1:D:347:ARG:HH21	1.62	0.64
1:D:328:LEU:O	1:D:332:VAL:HG23	1.98	0.64
1:A:368:ARG:HG3	1:A:368:ARG:HH11	1.61	0.64
2:B:91:ASN:O	2:B:95:GLN:HG3	1.97	0.63
2:B:32:LYS:O	2:B:36:VAL:HG23	1.98	0.63
2:B:30:THR:HB	2:B:33:ASP:H	1.64	0.62
1:D:382:SER:HB3	1:D:383:PRO:HD3	1.84	0.60
2:B:89:GLU:HA	2:B:92:LYS:HB3	1.84	0.58
1:D:368:ARG:NH1	1:D:368:ARG:HG3	2.10	0.58
1:D:355:PRO:HD3	3:F:175:ILE:HG22	1.85	0.58
2:B:51:ASP:HB2	2:B:111:ALA:HB2	1.85	0.58
1:D:371:PHE:HB2	2:E:44:TYR:CD2	2.39	0.58
1:D:356:LEU:HD13	2:E:66:GLN:NE2	2.19	0.58
1:A:378:GLN:HA	1:A:381:THR:HG22	1.85	0.57
2:E:89:GLU:HA	2:E:92:LYS:HB3	1.86	0.56
1:A:364:ARG:HG2	2:B:45:SER:OG	2.05	0.56
2:E:91:ASN:O	2:E:95:GLN:HG3	2.06	0.56
1:A:368:ARG:NH1	2:B:42:GLU:OE2	2.39	0.56
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.70	0.56
1:A:371:PHE:HB2	2:B:44:TYR:CD2	2.41	0.55
2:E:108:ALA:O	2:E:110:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:ASN:H	2:E:91:ASN:HD22	1.55	0.54
1:A:328:LEU:O	1:A:332:VAL:HG23	2.08	0.54
2:E:42:GLU:HG2	2:E:81:TYR:OH	2.08	0.54
1:A:376:HIS:HD2	2:B:24:LEU:HD22	1.69	0.53
1:D:364:ARG:HH11	1:D:364:ARG:HG2	1.74	0.53
2:E:54:GLU:OE1	2:E:114:ARG:HD2	2.09	0.52
3:F:194:GLN:HG3	3:F:198:ARG:NH1	2.24	0.52
1:A:327:GLN:HE22	2:B:23:PRO:N	2.07	0.52
2:B:73:LYS:HG2	2:B:77:GLN:HE21	1.75	0.52
3:C:191:ILE:HG22	3:C:192:ARG:N	2.25	0.51
2:E:91:ASN:N	2:E:91:ASN:HD22	2.09	0.50
1:D:368:ARG:NH1	2:E:42:GLU:OE2	2.44	0.50
2:E:77:GLN:O	2:E:80:VAL:HB	2.12	0.50
1:D:356:LEU:HD23	2:E:62:ILE:HG13	1.93	0.50
2:B:91:ASN:H	2:B:91:ASN:HD22	1.58	0.50
2:B:42:GLU:HG2	2:B:81:TYR:OH	2.13	0.49
1:D:356:LEU:HD12	1:D:356:LEU:H	1.77	0.49
3:C:200:GLU:O	3:C:201:LYS:C	2.51	0.49
1:D:350:HIS:HA	2:E:61:SER:HB3	1.94	0.49
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.27	0.49
1:A:350:HIS:HA	2:B:61:SER:HB3	1.93	0.49
2:E:22:VAL:N	2:E:23:PRO:CD	2.76	0.48
2:B:91:ASN:N	2:B:91:ASN:HD22	2.10	0.48
3:C:198:ARG:O	3:C:199:ARG:C	2.51	0.48
2:B:97:ILE:O	2:B:98:GLU:C	2.49	0.48
1:A:351:ARG:NH2	3:C:169:GLU:OE1	2.47	0.48
2:B:30:THR:HG22	2:B:32:LYS:H	1.79	0.48
2:E:73:LYS:HG2	2:E:77:GLN:HE21	1.78	0.48
1:A:376:HIS:NE2	2:B:24:LEU:HA	2.27	0.48
1:A:343:GLU:HB3	1:A:347:ARG:NH2	2.22	0.47
2:E:101:CYS:HA	2:E:106:ILE:CD1	2.41	0.47
1:D:356:LEU:HD13	2:E:66:GLN:HE21	1.79	0.47
2:B:67:TYR:CE2	2:B:71:VAL:HG21	2.50	0.47
1:D:356:LEU:CD2	2:E:62:ILE:HG13	2.45	0.47
2:E:59:LYS:C	2:E:61:SER:H	2.18	0.47
2:E:60:ASP:O	2:E:61:SER:C	2.53	0.47
1:A:356:LEU:HD13	2:B:66:GLN:HE21	1.80	0.47
2:E:117:ARG:O	2:E:119:ILE:N	2.48	0.47
3:C:174:SER:O	3:C:176:ASP:N	2.48	0.47
3:C:152:LYS:HD2	3:C:152:LYS:HA	1.73	0.47
3:F:191:ILE:HG22	3:F:192:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:HIS:O	2:B:53:VAL:C	2.53	0.46
3:F:185:ILE:O	3:F:186:LYS:C	2.53	0.46
3:C:194:GLN:HG3	3:C:198:ARG:NH1	2.30	0.46
1:A:370:GLN:O	1:A:371:PHE:C	2.55	0.45
2:E:39:THR:HG22	2:E:43:ILE:HD11	1.98	0.45
1:A:356:LEU:HD23	2:B:62:ILE:HG13	1.97	0.45
2:B:77:GLN:O	2:B:80:VAL:HB	2.16	0.45
2:E:98:GLU:HA	2:E:98:GLU:OE2	2.17	0.45
2:E:33:ASP:O	2:E:36:VAL:N	2.49	0.45
2:B:71:VAL:HG11	2:B:120:PRO:HB3	1.98	0.45
2:E:87:LYS:O	2:E:90:ILE:HB	2.17	0.44
1:A:364:ARG:HH12	2:B:46:ILE:HG13	1.82	0.44
2:E:90:ILE:O	2:E:91:ASN:C	2.55	0.44
3:F:185:ILE:CG2	3:F:186:LYS:N	2.79	0.44
2:E:24:LEU:O	2:E:25:PHE:CG	2.71	0.44
2:B:60:ASP:O	2:B:61:SER:C	2.56	0.43
1:D:370:GLN:O	1:D:371:PHE:C	2.56	0.43
3:C:185:ILE:O	3:C:186:LYS:C	2.56	0.43
2:E:118:GLY:O	2:E:119:ILE:HG23	2.18	0.43
2:E:101:CYS:O	2:E:106:ILE:HG13	2.19	0.43
3:C:177:SER:OG	3:C:180:ASP:HB2	2.18	0.43
2:B:87:LYS:O	2:B:90:ILE:HB	2.19	0.43
2:E:50:LEU:O	2:E:51:ASP:C	2.57	0.43
1:D:364:ARG:HG2	2:E:45:SER:OG	2.18	0.43
2:E:67:TYR:CE2	2:E:71:VAL:HG21	2.53	0.43
2:B:26:ASP:C	2:B:28:SER:H	2.21	0.43
1:D:353:THR:O	3:F:175:ILE:HG23	2.19	0.42
1:A:368:ARG:CG	1:A:368:ARG:HH11	2.31	0.42
1:D:382:SER:CB	1:D:383:PRO:HD3	2.49	0.42
3:F:198:ARG:O	3:F:199:ARG:C	2.58	0.42
3:F:177:SER:OG	3:F:180:ASP:HB2	2.20	0.42
3:C:175:ILE:H	3:C:175:ILE:HG13	1.49	0.42
1:D:367:ALA:O	1:D:368:ARG:C	2.58	0.42
2:B:59:LYS:C	2:B:61:SER:H	2.23	0.42
1:A:356:LEU:CD2	2:B:62:ILE:HG13	2.50	0.41
2:E:106:ILE:O	2:E:107:THR:C	2.59	0.41
2:E:59:LYS:O	2:E:61:SER:N	2.51	0.41
1:A:364:ARG:HG2	1:A:364:ARG:NH1	2.35	0.41
2:B:117:ARG:HB2	2:B:117:ARG:NH1	2.36	0.41
2:B:90:ILE:HG22	2:B:91:ASN:N	2.36	0.41
2:E:90:ILE:HG22	2:E:91:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:GLY:C	1:D:354:ILE:H	2.22	0.41
2:E:52:HIS:O	2:E:53:VAL:C	2.59	0.41
2:B:87:LYS:HE2	2:B:87:LYS:C	2.42	0.41
2:B:50:LEU:O	2:B:51:ASP:C	2.60	0.41
2:E:22:VAL:N	2:E:23:PRO:HD2	2.36	0.41
3:C:146:GLY:O	3:C:149:ALA:HB3	2.21	0.41
2:E:51:ASP:HB2	2:E:111:ALA:HB2	2.03	0.41
2:E:121:ILE:HD13	2:E:121:ILE:HA	1.88	0.41
2:E:93:HIS:C	2:E:94:PHE:CG	2.94	0.40
1:D:343:GLU:O	1:D:346:SER:HB3	2.20	0.40
3:C:173:ARG:C	3:C:175:ILE:H	2.24	0.40
2:E:30:THR:C	2:E:32:LYS:H	2.25	0.40
2:E:93:HIS:C	2:E:94:PHE:CD1	2.95	0.40
1:D:371:PHE:C	1:D:371:PHE:CD2	2.94	0.40
2:E:87:LYS:HE2	2:E:87:LYS:C	2.41	0.40
1:A:371:PHE:C	1:A:371:PHE:CD2	2.95	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	57/82 (70%)	50 (88%)	7 (12%)	0	100	100
1	D	59/82 (72%)	50 (85%)	9 (15%)	0	100	100
2	B	99/155 (64%)	69 (70%)	23 (23%)	7 (7%)	1	19
2	E	100/155 (64%)	65 (65%)	28 (28%)	7 (7%)	1	20
3	C	63/85 (74%)	44 (70%)	15 (24%)	4 (6%)	2	23
3	F	52/85 (61%)	37 (71%)	13 (25%)	2 (4%)	4	37
All	All	430/644 (67%)	315 (73%)	95 (22%)	20 (5%)	3	30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	ILE
2	B	92	LYS
3	C	175	ILE
2	E	92	LYS
2	E	95	GLN
2	E	109	SER
2	E	118	GLY
2	B	24	LEU
2	B	95	GLN
2	E	90	ILE
3	F	177	SER
2	B	120	PRO
2	E	25	PHE
2	B	27	ASN
3	F	201	LYS
2	B	100	PHE
3	C	143	GLU
3	C	177	SER
2	E	117	ARG
3	C	185	ILE

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	53/74 (72%)	46 (87%)	7 (13%)	5	30
1	D	55/74 (74%)	49 (89%)	6 (11%)	8	39
2	B	95/145 (66%)	81 (85%)	14 (15%)	4	25
2	E	96/145 (66%)	79 (82%)	17 (18%)	2	16
3	C	61/79 (77%)	53 (87%)	8 (13%)	5	30
3	F	52/79 (66%)	46 (88%)	6 (12%)	7	36
All	All	412/596 (69%)	354 (86%)	58 (14%)	4	28

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	LEU
1	A	329	TYR
1	A	351	ARG
1	A	356	LEU
1	A	368	ARG
1	A	369	GLN
1	A	370	GLN
2	B	24	LEU
2	B	33	ASP
2	B	35	GLU
2	B	42	GLU
2	B	69	ASN
2	B	70	THR
2	B	75	LEU
2	B	88	GLU
2	B	91	ASN
2	B	93	HIS
2	B	95	GLN
2	B	103	THR
2	B	105	ASN
2	B	114	ARG
3	C	155	GLU
3	C	169	GLU
3	C	175	ILE
3	C	176	ASP
3	C	183	GLN
3	C	189	LEU
3	C	194	GLN
3	C	202	LEU
1	D	351	ARG
1	D	353	THR
1	D	356	LEU
1	D	368	ARG
1	D	369	GLN
1	D	370	GLN
2	E	26	ASP
2	E	30	THR
2	E	33	ASP
2	E	35	GLU
2	E	69	ASN
2	E	70	THR
2	E	75	LEU

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Mol	Chain	Res	Type
2	E	88	GLU
2	E	91	ASN
2	E	93	HIS
2	E	95	GLN
2	E	112	ILE
2	E	113	THR
2	E	117	ARG
2	E	119	ILE
2	E	121	ILE
2	E	122	THR
3	F	155	GLU
3	F	175	ILE
3	F	176	ASP
3	F	189	LEU
3	F	194	GLN
3	F	202	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	77	GLN
2	B	83	ASN
2	B	91	ASN
2	B	93	HIS
2	B	95	GLN
2	B	105	ASN
1	D	334	GLN
2	E	27	ASN
2	E	77	GLN
2	E	83	ASN
2	E	91	ASN
2	E	93	HIS
2	E	95	GLN

5.3.3 RNA ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	59/82 (71%)	-0.04	0	100 100	73, 73, 73, 73	0
1	D	61/82 (74%)	0.06	0	100 100	73, 73, 73, 73	0
2	B	101/155 (65%)	-0.11	1 (0%)	84 73	73, 73, 73, 73	0
2	E	102/155 (65%)	-0.13	1 (0%)	84 73	73, 73, 73, 73	0
3	C	65/85 (76%)	0.33	4 (6%)	24 16	73, 73, 73, 73	0
3	F	54/85 (63%)	0.28	3 (5%)	28 19	73, 73, 73, 73	0
All	All	442/644 (68%)	0.03	9 (2%)	68 54	73, 73, 73, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	139	SER	6.5
3	C	147	ASP	3.4
3	F	156	GLN	2.9
3	F	200	GLU	2.6
3	C	197	LEU	2.4
3	C	145	TYR	2.2
3	F	155	GLU	2.2
2	B	122	THR	2.2
2	E	93	HIS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.