W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 01:56 am BST

PDB ID	:	4Q9U
Title	:	Crystal structure of the Rab5, Rabex-5delta and Rabaptin-5C21 complex
Authors	:	Zhang, Z.; Zhang, T.; Ding, J.
Deposited on	:	2014-05-01
Resolution	:	4.62 Å(reported)

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

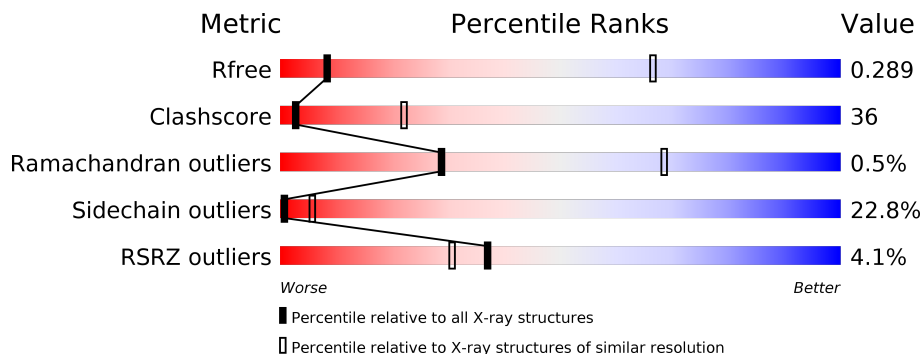|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.62 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		0.289
Clashscore		36
Ramachandran outliers		0.5%
Sidechain outliers		22.8%
RSRZ outliers		4.1%

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	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1114 (5.54-3.70)

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 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	317	28% 53% 15% •
1	E	317	2% / 35% 44% 14% 7%
2	B	171	8% / 35% 47% 7% 11%
2	F	171	18% / 38% 29% • 30%
3	C	92	26% 43% 20% • 10%
3	D	92	29% 41% 10% • 18%

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Mol	Chain	Length	Quality of chain
3	G	92	 32% 47% 13% 9%
3	H	92	24% 49% 16% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9679 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 Rab5 GDP/GTP exchange factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total 2492	C 1573	N 426	O 474	S 19	0	0	0
1	E	296	Total 2441	C 1541	N 419	O 462	S 19	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	EXPRESSION TAG	UNP Q9UJ41
A	125	GLY	-	EXPRESSION TAG	UNP Q9UJ41
A	126	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	127	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	128	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	129	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	130	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	131	HIS	-	EXPRESSION TAG	UNP Q9UJ41
A	?	-	LYS	DELETION	UNP Q9UJ41
A	?	-	GLN	DELETION	UNP Q9UJ41
A	?	-	GLU	DELETION	UNP Q9UJ41
A	?	-	ALA	DELETION	UNP Q9UJ41
A	?	-	GLU	DELETION	UNP Q9UJ41
A	?	-	SER	DELETION	UNP Q9UJ41
A	?	-	TRP	DELETION	UNP Q9UJ41
A	?	-	SER	DELETION	UNP Q9UJ41
A	?	-	PRO	DELETION	UNP Q9UJ41
A	?	-	ASP	DELETION	UNP Q9UJ41
A	?	-	ALA	DELETION	UNP Q9UJ41
A	?	-	CYS	DELETION	UNP Q9UJ41
A	?	-	LEU	DELETION	UNP Q9UJ41
A	?	-	GLY	DELETION	UNP Q9UJ41
A	?	-	VAL	DELETION	UNP Q9UJ41
E	124	MET	-	EXPRESSION TAG	UNP Q9UJ41
E	125	GLY	-	EXPRESSION TAG	UNP Q9UJ41

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Chain	Residue	Modelled	Actual	Comment	Reference
E	126	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	127	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	128	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	129	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	130	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	131	HIS	-	EXPRESSION TAG	UNP Q9UJ41
E	?	-	LYS	DELETION	UNP Q9UJ41
E	?	-	GLN	DELETION	UNP Q9UJ41
E	?	-	GLU	DELETION	UNP Q9UJ41
E	?	-	ALA	DELETION	UNP Q9UJ41
E	?	-	GLU	DELETION	UNP Q9UJ41
E	?	-	SER	DELETION	UNP Q9UJ41
E	?	-	TRP	DELETION	UNP Q9UJ41
E	?	-	SER	DELETION	UNP Q9UJ41
E	?	-	PRO	DELETION	UNP Q9UJ41
E	?	-	ASP	DELETION	UNP Q9UJ41
E	?	-	ALA	DELETION	UNP Q9UJ41
E	?	-	CYS	DELETION	UNP Q9UJ41
E	?	-	LEU	DELETION	UNP Q9UJ41
E	?	-	GLY	DELETION	UNP Q9UJ41
E	?	-	VAL	DELETION	UNP Q9UJ41

- Molecule 2 is a protein called Ras-related protein Rab-5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total 1194	C 759	N 201	O 229	S 5	0	0	0
2	F	120	Total 948	C 607	N 160	O 177	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	SER	-	EXPRESSION TAG	UNP P20339
F	14	SER	-	EXPRESSION TAG	UNP P20339

- Molecule 3 is a protein called Rab GTPase-binding effector protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total 667	C 406	N 119	O 138	S 4	0	0	0

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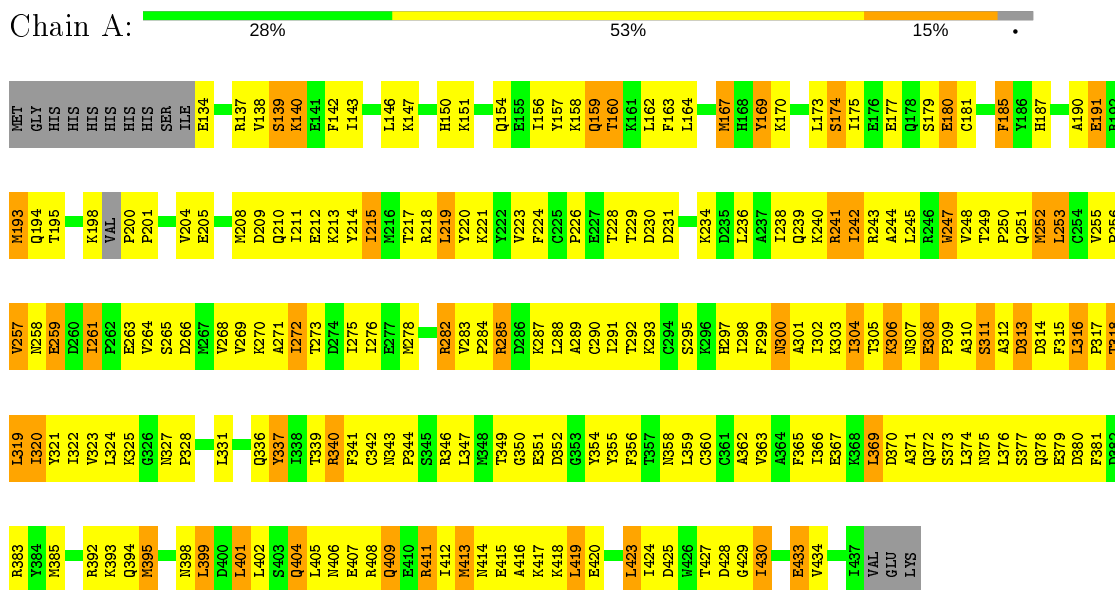| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	75	Total	C	N	O	S	0	0	0
			601	369	106	122	4			
3	G	84	Total	C	N	O	S	0	0	0
			678	412	123	139	4			
3	H	82	Total	C	N	O	S	0	0	0
			658	401	118	135	4			

There are 4 discrepancies between the modelled and reference sequences:

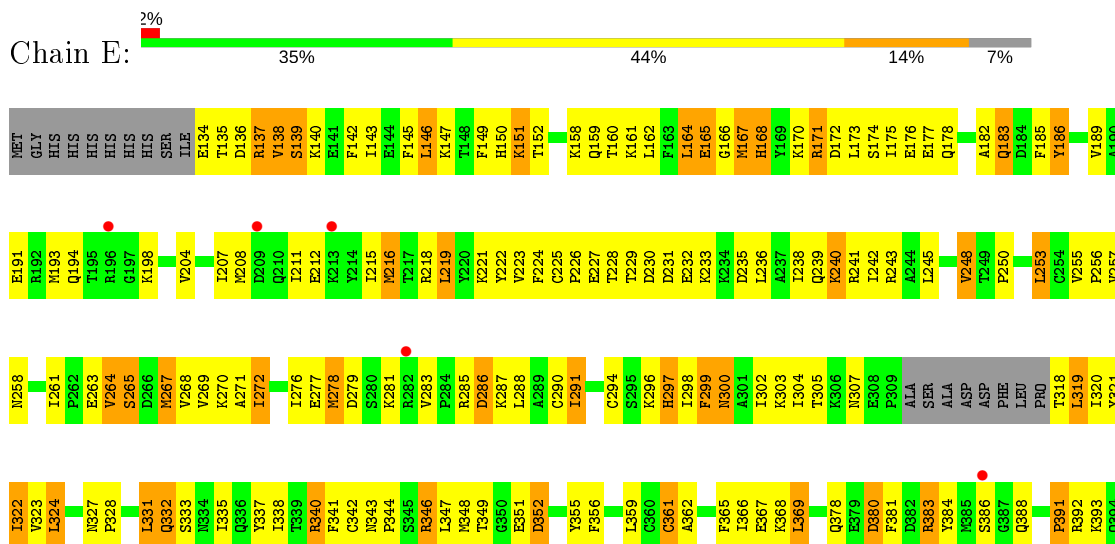| Chain	Residue	Modelled	Actual	Comment	Reference
C	551	MET	-	EXPRESSION TAG	UNP Q15276
D	551	MET	-	EXPRESSION TAG	UNP Q15276
G	551	MET	-	EXPRESSION TAG	UNP Q15276
H	551	MET	-	EXPRESSION TAG	UNP Q15276

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 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.
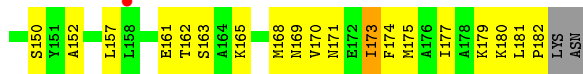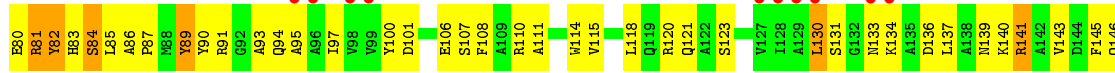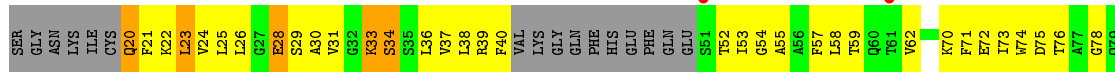
- Molecule 1: Rab5 GDP/GTP exchange factor
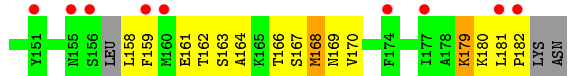

- Molecule 1: Rab5 GDP/GTP exchange factor

M395 Y396 K397 N398 L399 D400 L401 L402 S403 Q404 L405 N406 E407 R408 Q409 E410 R411 I412 M413 N414 E415 L419 E420 L423 W426 I430 A431 R432 Q435 D436 I437 VAL GLU LYS

- Molecule 2: Ras-related protein Rab-5A

Chain B:

8%

35%   47%   7%   11%

SER GLY ASN LYS ILE CYS Q20 F21 K22 L23 V24 L25 L26 G27 E28 S29 A30 V31 G32 K33 S34 L36 V37 L38 R39 F40 VAL LYS GLY GLN PHE HIS GLU PHE GLN GLU S51 T52 I53 G54 A55 A56 F57 L58 T59 Q60 T61 V62 K70 F71 E72 I73 W74 D75 T76 A77 G78 Q79

E80 R81 Y82 H83 S84 L85 A86 P87 M88 Y89 Y90 R91 G92 A93 Q94 A95 A96 I97 V98 V99 Y100 D101 E106 S107 F108 A109 R110 A111 W114 V115 L118 Q119 R120 Q121 A122 S123 V127 I128 A129 L130 S131 G132 N133 K134 A135 D136 L137 A138 N139 K140 R141 A142 V143 D144 F145 Q146

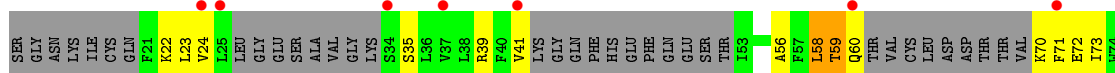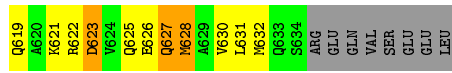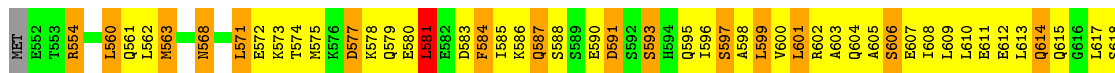S150 Y151 A152 L157 L158 E161 T162 S163 A164 K165 M168 N169 V170 N171 E172 I173 F174 M175 A176 I177 A178 K179 K180 L181 P182 LYS ASN

- Molecule 2: Ras-related protein Rab-5A

Chain F:

18%

38%   29%   ·   30%

SER GLY ASN LYS ILE CYS GLN F21 K22 L23 V24 L25 LEU GLY GLU SER ALA VAL GLY LYS S34 S35 L36 V37 L38 R39 F40 V41 LYS GLY GLN PHE HIS GLU PHE GLN GLU SER THR I53 A56 F57 L58 T59 Q60 THR VAL CYS LEU ASP ASP THR VAL K70 F71 E72 I73 W74

D75 T76 Y82 H83 S84 L85 A86 P87 M88 TYR TYR ARG GLY A93 Q94 A95 A96 I97 V98 V99 Y100 D101 ILE THR N104 E105 E106 S107 F108 A109 R110 A111 W114 V115 Q119 S123 I126 V127 I128 A129 L130 S131 G132 N133 LYS ALA ASP LEU ALA ASN LYS R141 A142 Q146

Y151 N155 S156 LEU L158 F159 M160 E161 T162 S163 A164 K165 T166 S167 M168 N169 V170 F174 I177 A178 K179 K180 L181 P182 LYS ASN

- Molecule 3: Rab GTPase-binding effector protein 1

Chain C:

26%   43%   20%   ·   10%

MET E552 T553 R554 L560 Q561 L562 M563 N568 L571 E572 K573 T574 M575 K576 S578 Q579 E580 L581 E582 D583 F584 I585 K586 Q587 S588 S589 E5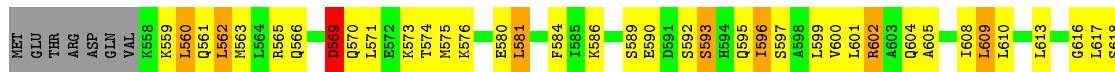90 D591 S592 S593 H594 Q595 I596 S597 A598 L599 V600 L601 R602 A603 Q604 A605 S606 E607 I608 L609 L610 E611 E612 L613 Q614 Q615 G616 L617 S618

Q619 A620 K621 R622 D623 V624 Q625 E626 Q627 M628 A629 V630 L631 M632 Q633 S634 ARG GLU GLN VAL SER GLU GLU LEU

- Molecule 3: Rab GTPase-binding effector protein 1

Chain D:

29%   41%   10%   ·   18%

MET GLU THR ARG ASP GLN VAL K558 K559 L560 Q561 L562 L564 R565 M563 Q566 D569 Q570 L571 E572 K573 T574 M575 K576 E580 L581 F584 I585 K586 S589 E590 D591 S592 S593 H594 Q595 I596 S597 A598 L599 V600 L601 R602 A603 Q604 A605 I608 L609 L610 L613 G616 L617 S618

Q619 A620 K621 R622 D623 V624 Q625 E626 Q627 M628 A629 V630 L631 M632 GLN SER ARG GLU GLN VAL SER GLU GLU LEU

• Molecule 3: Rab GTPase-binding effector protein 1

Chain G:

%

| 32% | 47% | 13% | 9% |

MET E552 T553 R554 D555 Q556 L560 Q561 L562 Q566 A567 N568 D569 Q570 L571 E572 K573 T574 M575 K576 D577 K578 Q579 E580 L581 E582 D583 F584 I585 K586 Q587 S588 S589 E590 D591 S592 S593 H594 Q595 I596 S597 A598 L599 V600 L601 R602 A603 Q604 A605 S606 E607 I608 L609 L610 E611 E612 L613 Q614

Q615 G616 L617 S618 Q619 A620 K621 R622 D623 V624 Q627 M628 A629 V630 L631 M632 Q633 S634 R635 GLU GLN VAL SER GLU GLU LEU

• Molecule 3: Rab GTPase-binding effector protein 1

Chain H:

| 24% | 49% | 16% | 11% |

MET GLU T553 R554 D555 K558 K559 L560 Q561 L562 M563 L564 R565 Q566 A567 N568 D569 Q570 L571 E572 K573 T574 M575 K576 D577 K578 Q579 E580 L581 F584 I585 K586 Q587 S588 S589 E590 D591 S592 S593 H594 Q595 I596 S597 A598 L599 V600 L601 R602 A603 Q604 A605 S606 E607 I608 L609 L610 E611 E612

L613 Q614 Q615 A620 K621 R622 D623 V624 Q625 E626 Q627 V630 L631 M632 Q633 S634 ARG GLU GLN VAL SER GLU GLU LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.82Å 174.82Å 149.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.78 – 4.62 48.49 – 4.62	Depositor EDS
% Data completeness (in resolution range)	95.9 (40.78-4.62) 95.9 (48.49-4.62)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.98 (at 4.64Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.251 , 0.343 0.258 , 0.289	Depositor DCC
R_{free} test set	621 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å²)	172.7	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 208.8	EDS
L-test for twinning[2]	$<|L|> = 0.50, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9679	wwPDB-VP
Average B, all atoms (Å²)	187.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% 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 (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	A	0.71	0/2535	0.92	2/3410 (0.1%)
1	E	0.60	0/2482	0.84	2/3338 (0.1%)
2	B	0.52	0/1213	0.71	0/1639
2	F	0.48	1/959 (0.1%)	0.60	0/1285
3	C	0.84	0/668	1.04	1/890 (0.1%)
3	D	0.82	0/602	1.09	1/801 (0.1%)
3	G	0.84	0/679	1.00	0/904
3	H	0.74	0/659	0.99	0/878
All	All	0.67	1/9797 (0.0%)	0.88	6/13145 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	86	ALA	CA-CB	5.09	1.63	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	581	LEU	CB-CG-CD1	-5.56	101.54	111.00
1	E	399	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	399	LEU	CB-CG-CD2	5.17	119.78	111.00
1	E	253	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	308	GLU	N-CA-C	-5.14	97.11	111.00

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	A	2492	0	2502	226	0
1	E	2441	0	2460	185	0
2	B	1194	0	1192	81	0
2	F	948	0	937	36	0
3	C	667	0	678	61	0
3	D	601	0	618	50	0
3	G	678	0	691	60	0
3	H	658	0	672	70	0
All	All	9679	0	9750	692	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 36.

The worst 5 of 692 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)
1:A:395:MET:HG3	1:A:399:LEU:HD23	1.45	0.99
1:A:250:PRO:HA	1:A:253:LEU:HG	1.49	0.92
1:A:238:ILE:HD13	1:A:331:LEU:HD23	1.53	0.89
1:E:258:ASN:H	1:E:305:THR:HG21	1.41	0.85
1:E:216:MET:HA	1:E:219:LEU:HD22	1.57	0.85

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	299/317 (94%)	279 (93%)	20 (7%)	0	100	100
1	E	292/317 (92%)	272 (93%)	18 (6%)	2 (1%)	22	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	149/171 (87%)	129 (87%)	17 (11%)	3 (2%)	7	40
2	F	104/171 (61%)	100 (96%)	3 (3%)	1 (1%)	15	54
3	C	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
3	D	73/92 (79%)	73 (100%)	0	0	100	100
3	G	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
3	H	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
All	All	1160/1344 (86%)	1088 (94%)	66 (6%)	6 (0%)	29	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	VAL
2	B	30	ALA
2	B	34	SER
1	E	391	PRO
2	F	168	MET

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	281/294 (96%)	217 (77%)	64 (23%)	1	6
1	E	276/294 (94%)	217 (79%)	59 (21%)	1	6
2	B	127/143 (89%)	106 (84%)	21 (16%)	2	14
2	F	100/143 (70%)	87 (87%)	13 (13%)	4	20
3	C	76/85 (89%)	49 (64%)	27 (36%)	0	1
3	D	68/85 (80%)	48 (71%)	20 (29%)	0	2
3	G	77/85 (91%)	54 (70%)	23 (30%)	0	2
3	H	75/85 (88%)	56 (75%)	19 (25%)	0	4
All	All	1080/1214 (89%)	834 (77%)	246 (23%)	1	6

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	628	MET
1	E	151	LYS
3	H	560	LEU
3	D	569	ASP
3	D	609	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	133	ASN
3	H	627	GLN
1	E	388	GLN
1	A	409	GLN
1	E	300	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 (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	303/317 (95%)	-0.37	0	100	100	45, 133, 270, 349	0
1	E	296/317 (93%)	-0.16	5 (1%)	70	61	39, 209, 344, 447	0
2	B	153/171 (89%)	0.29	13 (8%)	10	10	112, 238, 333, 441	0
2	F	120/171 (70%)	1.24	30 (25%)	0	1	137, 300, 407, 493	0
3	C	83/92 (90%)	-0.24	0	100	100	36, 120, 264, 425	0
3	D	75/92 (81%)	-0.43	0	100	100	71, 130, 262, 343	0
3	G	84/92 (91%)	-0.45	1 (1%)	79	70	54, 108, 252, 324	0
3	H	82/92 (89%)	-0.32	0	100	100	37, 116, 263, 327	0
All	All	1196/1344 (88%)	-0.07	49 (4%)	37	31	36, 178, 336, 493	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	130	LEU	6.1
2	B	128	ILE	4.9
2	F	98	VAL	4.8
2	F	76	THR	4.8
2	F	128	ILE	4.1

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.