Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 06:58 pm BST

PDB ID	:	6GMA
Title	:	Crystal structure of the FIP200 C-terminal region
Authors	:	Witt, M.; Bock, T.; Daumke, O.
Deposited on	:	2018-05-24
Resolution	:	3.20 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 3.20 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.
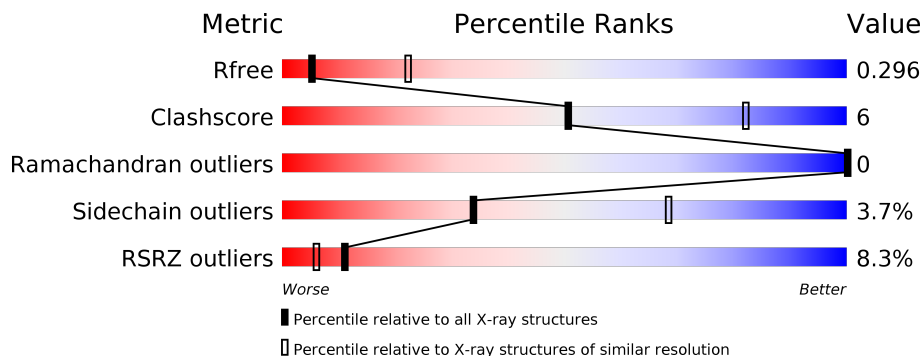
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	140	71% 19% · 9%
1	B	140	76% 13% · 9%
1	C	140	76% 16% · 7%
1	D	140	76% 16% · 6%
1	E	140	76% 12% 12%
1	F	140	79% 7% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5952 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 RB1-inducible coiled-coil protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1044	670	187	182	5			
1	B	127	Total	C	N	O	S	0	0	0
			1033	662	185	181	5			
1	C	130	Total	C	N	O	S	0	0	0
			1054	675	187	187	5			
1	D	131	Total	C	N	O	S	0	0	0
			1047	671	184	187	5			
1	E	123	Total	C	N	O	S	0	0	0
			940	604	164	168	4			
1	F	120	Total	C	N	O	S	0	0	0
			834	519	151	159	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1455	GLY	-	expression tag	UNP Q8TDY2
A	1456	ALA	-	expression tag	UNP Q8TDY2
A	1457	ALA	-	expression tag	UNP Q8TDY2
B	1455	GLY	-	expression tag	UNP Q8TDY2
B	1456	ALA	-	expression tag	UNP Q8TDY2
B	1457	ALA	-	expression tag	UNP Q8TDY2
C	1455	GLY	-	expression tag	UNP Q8TDY2
C	1456	ALA	-	expression tag	UNP Q8TDY2
C	1457	ALA	-	expression tag	UNP Q8TDY2
D	1455	GLY	-	expression tag	UNP Q8TDY2
D	1456	ALA	-	expression tag	UNP Q8TDY2
D	1457	ALA	-	expression tag	UNP Q8TDY2
E	1455	GLY	-	expression tag	UNP Q8TDY2
E	1456	ALA	-	expression tag	UNP Q8TDY2
E	1457	ALA	-	expression tag	UNP Q8TDY2
F	1455	GLY	-	expression tag	UNP Q8TDY2
F	1456	ALA	-	expression tag	UNP Q8TDY2

Continued on next page...

Continued from previous page...

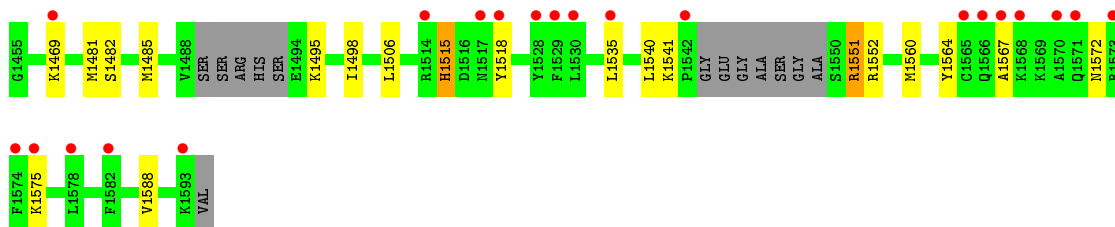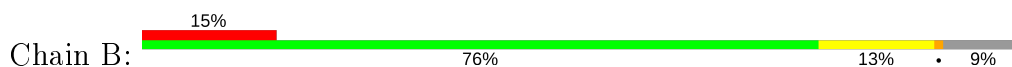| Chain	Residue	Modelled	Actual	Comment	Reference
F	1457	ALA	-	expression tag	UNP Q8TDY2

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.
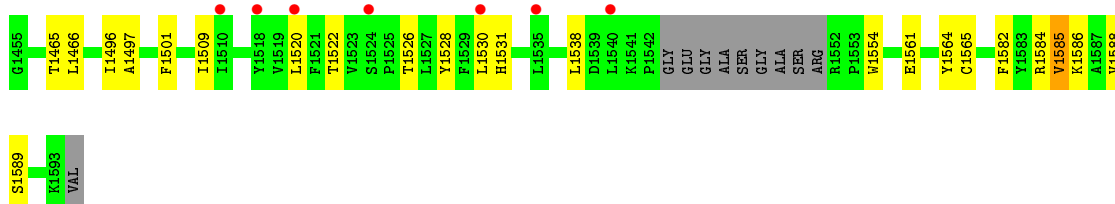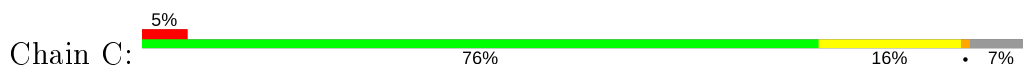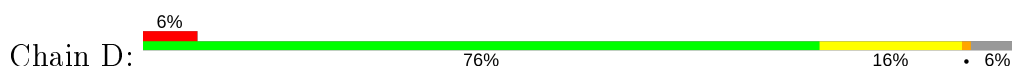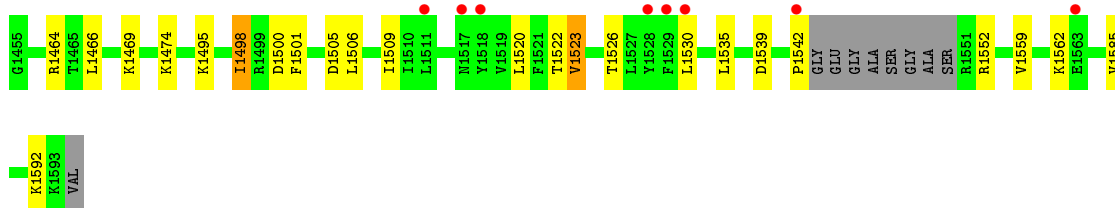
- Molecule 1: RB1-inducible coiled-coil protein 1
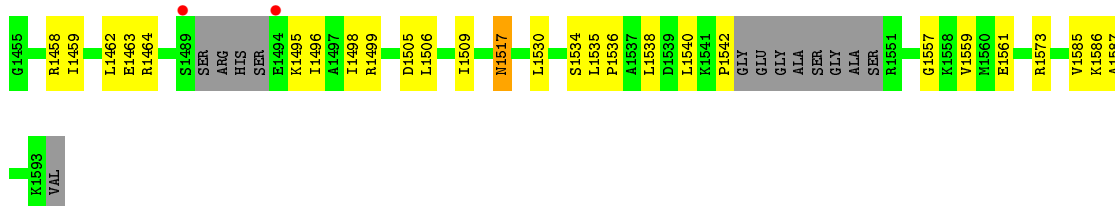
- Molecule 1: RB1-inducible coiled-coil protein 1

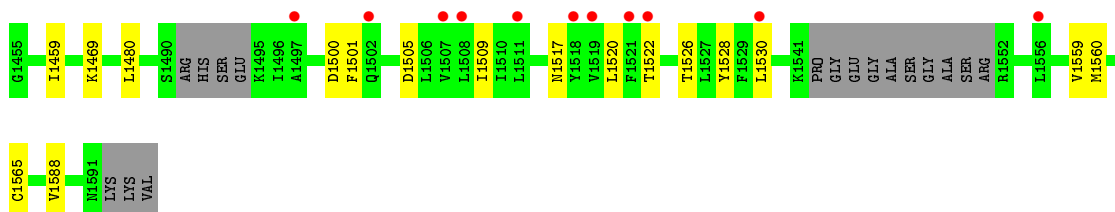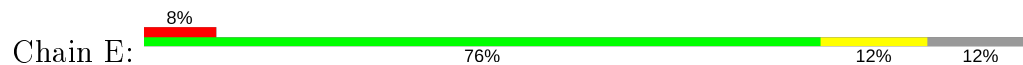- Molecule 1: RB1-inducible coiled-coil protein 1

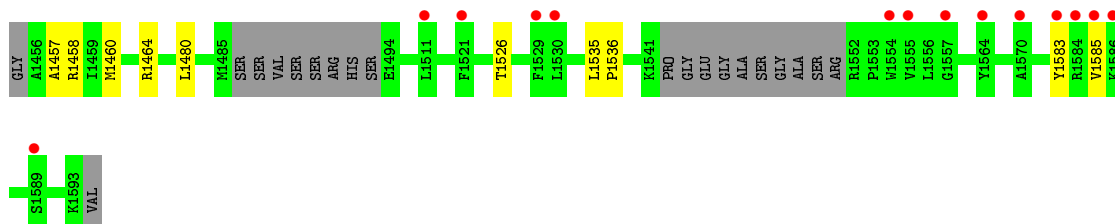- Molecule 1: RB1-inducible coiled-coil protein 1

• Molecule 1: RB1-inducible coiled-coil protein 1

Chain E:

• Molecule 1: RB1-inducible coiled-coil protein 1

Chain F:
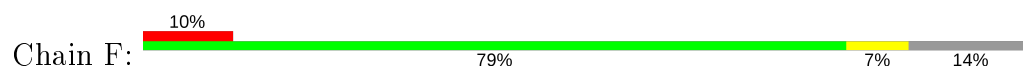
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.05Å 187.17Å 55.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.76 – 3.20 44.69 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.1 (37.76-3.20) 97.2 (44.69-3.17)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.267 , 0.295 0.267 , 0.296	Depositor DCC
R_{free} test set	1647 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	135.9	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 101.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5952	wwPDB-VP
Average B, all atoms (Å^2)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[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	0.30	0/1061	0.55	0/1422
1	B	0.29	0/1050	0.55	0/1410
1	C	0.28	0/1073	0.52	0/1442
1	D	0.28	0/1065	0.52	0/1433
1	E	0.27	0/956	0.51	0/1293
1	F	0.27	0/845	0.49	0/1151
All	All	0.28	0/6050	0.52	0/8151

There are no bond length outliers.

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	A	1044	0	1088	15	0
1	B	1033	0	1056	13	0
1	C	1054	0	1083	17	0
1	D	1047	0	1069	17	0
1	E	940	0	903	9	0
1	F	834	0	697	6	0
All	All	5952	0	5896	67	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 6.

All (67) 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:1517:ASN:OD1	1:A:1573:ARG:NH1	2.26	0.68
1:D:1539:ASP:OD1	1:D:1552:ARG:NH1	2.26	0.68
1:B:1541:LYS:HE3	1:B:1551:ARG:HG2	1.78	0.64
1:C:1509:ILE:HG21	1:C:1530:LEU:HD22	1.80	0.63
1:D:1509:ILE:HG21	1:D:1530:LEU:HD22	1.83	0.61
1:C:1497:ALA:HB2	1:D:1495:LYS:HE2	1.84	0.60
1:D:1592:LYS:H	1:E:1565:CYS:HA	1.68	0.58
1:A:1509:ILE:HG21	1:A:1530:LEU:HD22	1.85	0.58
1:A:1535:LEU:HD23	1:A:1542:PRO:HB3	1.86	0.57
1:C:1538:LEU:HG	1:C:1589:SER:HB3	1.88	0.56
1:B:1482:SER:HA	1:B:1485:MET:HE2	1.88	0.56
1:C:1554:TRP:HH2	1:D:1523:VAL:HG23	1.72	0.54
1:E:1520:LEU:O	1:E:1522:THR:HG23	2.07	0.54
1:C:1538:LEU:HD11	1:C:1588:VAL:HA	1.89	0.53
1:B:1560:MET:HG3	1:B:1588:VAL:HG23	1.91	0.52
1:B:1535:LEU:HD23	1:B:1540:LEU:HD22	1.91	0.52
1:C:1554:TRP:CH2	1:D:1523:VAL:HG23	2.45	0.52
1:B:1518:TYR:CE1	1:B:1540:LEU:HD21	2.46	0.50
1:B:1481:MET:O	1:B:1485:MET:HG3	2.12	0.49
1:B:1515:HIS:ND1	1:B:1515:HIS:N	2.60	0.49
1:C:1465:THR:HG22	1:D:1466:LEU:HD11	1.95	0.49
1:E:1509:ILE:HG22	1:E:1520:LEU:HD12	1.95	0.48
1:A:1535:LEU:HB3	1:A:1536:PRO:HD3	1.95	0.48
1:F:1535:LEU:HB3	1:F:1536:PRO:HD3	1.94	0.48
1:D:1535:LEU:HD13	1:D:1542:PRO:HG2	1.96	0.48
1:F:1464:ARG:HH21	1:F:1464:ARG:HG3	1.79	0.48
1:D:1464:ARG:HG2	1:D:1464:ARG:HH11	1.79	0.47
1:B:1551:ARG:HA	1:B:1551:ARG:HD3	1.62	0.47
1:A:1506:LEU:HD12	1:A:1557:GLY:O	2.15	0.47
1:A:1505:ASP:O	1:A:1559:VAL:HG22	2.15	0.47
1:D:1523:VAL:HG13	1:D:1523:VAL:O	2.15	0.47
1:A:1496:ILE:HG12	1:A:1506:LEU:HG	1.96	0.46
1:C:1520:LEU:HD22	1:C:1585:VAL:HG21	1.96	0.46
1:D:1505:ASP:O	1:D:1559:VAL:HG12	2.15	0.46
1:A:1534:SER:OG	1:A:1587:ALA:O	2.33	0.46
1:D:1559:VAL:HG23	1:D:1585:VAL:HG13	1.98	0.46
1:B:1515:HIS:HA	1:B:1575:LYS:HB2	1.98	0.46
1:C:1565:CYS:HB2	1:C:1582:PHE:CE1	2.51	0.45
1:F:1457:ALA:HA	1:F:1460:MET:HE2	1.98	0.45
1:F:1526:THR:HG21	1:F:1583:TYR:HD1	1.80	0.45

<div align="center">Continued on next page...</div>

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1509:ILE:HG21	1:E:1530:LEU:HD13	1.97	0.45
1:C:1531:HIS:CD2	1:C:1584:ARG:HD3	2.51	0.45
1:A:1495:LYS:HB3	1:B:1495:LYS:HB3	1.98	0.45
1:E:1560:MET:HG3	1:E:1588:VAL:HG23	1.97	0.45
1:D:1501:PHE:O	1:D:1562:LYS:NZ	2.32	0.45
1:E:1480:LEU:HD21	1:F:1480:LEU:HA	1.99	0.45
1:A:1496:ILE:HG13	1:B:1498:ILE:HG13	1.99	0.45
1:C:1520:LEU:O	1:C:1522:THR:HG23	2.17	0.44
1:A:1538:LEU:HD12	1:A:1540:LEU:HG	2.01	0.43
1:C:1466:LEU:HD23	1:C:1466:LEU:HA	1.89	0.43
1:C:1561:GLU:HG2	1:C:1586:LYS:HB3	2.01	0.43
1:E:1505:ASP:O	1:E:1559:VAL:HG12	2.19	0.42
1:C:1501:PHE:HE2	1:C:1520:LEU:HB3	1.83	0.42
1:D:1520:LEU:O	1:D:1522:THR:HG23	2.19	0.42
1:A:1458:ARG:O	1:A:1462:LEU:HD13	2.19	0.42
1:A:1459:ILE:O	1:A:1463:GLU:HG3	2.18	0.42
1:E:1501:PHE:HD2	1:E:1528:TYR:CE2	2.38	0.42
1:A:1573:ARG:HE	1:A:1573:ARG:HB2	1.74	0.42
1:C:1496:ILE:HG12	1:D:1498:ILE:HD11	2.01	0.41
1:D:1474:LYS:HB2	1:D:1474:LYS:HE3	1.80	0.41
1:E:1459:ILE:HD13	1:F:1458:ARG:HD3	2.02	0.41
1:A:1561:GLU:HB3	1:A:1586:LYS:HE3	2.03	0.41
1:C:1501:PHE:CE2	1:C:1520:LEU:HD23	2.55	0.41
1:B:1469:LYS:HA	1:B:1469:LYS:HD3	1.87	0.40
1:D:1469:LYS:HA	1:D:1469:LYS:HD3	1.83	0.40
1:C:1522:THR:HG21	1:C:1528:TYR:CD1	2.57	0.40
1:B:1567:ALA:HB1	1:B:1572:ASN:HD22	1.87	0.40

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	121/140 (86%)	115 (95%)	6 (5%)	0	100	100
1	B	121/140 (86%)	116 (96%)	5 (4%)	0	100	100
1	C	126/140 (90%)	121 (96%)	5 (4%)	0	100	100
1	D	127/140 (91%)	120 (94%)	7 (6%)	0	100	100
1	E	117/140 (84%)	110 (94%)	7 (6%)	0	100	100
1	F	114/140 (81%)	109 (96%)	5 (4%)	0	100	100
All	All	726/840 (86%)	691 (95%)	35 (5%)	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	A	115/124 (93%)	110 (96%)	5 (4%)	29	64
1	B	111/124 (90%)	106 (96%)	5 (4%)	27	63
1	C	116/124 (94%)	113 (97%)	3 (3%)	46	76
1	D	114/124 (92%)	109 (96%)	5 (4%)	28	64
1	E	93/124 (75%)	89 (96%)	4 (4%)	29	64
1	F	68/124 (55%)	67 (98%)	1 (2%)	65	85
All	All	617/744 (83%)	594 (96%)	23 (4%)	34	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1464	ARG
1	A	1498	ILE
1	A	1499	ARG
1	A	1517	ASN
1	A	1585	VAL
1	B	1506	LEU
1	B	1515	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1551	ARG
1	B	1552	ARG
1	B	1564	TYR
1	C	1526	THR
1	C	1564	TYR
1	C	1585	VAL
1	D	1498	ILE
1	D	1500	ASP
1	D	1506	LEU
1	D	1523	VAL
1	D	1526	THR
1	E	1469	LYS
1	E	1500	ASP
1	E	1517	ASN
1	E	1526	THR
1	F	1585	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1502	GLN
1	C	1517	ASN
1	C	1531	HIS
1	E	1531	HIS
1	F	1478	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 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(Å²)	Q<0.9
1	A	127/140 (90%)	0.22	2 (1%)	72	59	80, 121, 180, 230	0
1	B	127/140 (90%)	0.79	21 (16%)	1	1	115, 169, 224, 237	0
1	C	130/140 (92%)	0.30	7 (5%)	25	14	100, 148, 186, 217	0
1	D	131/140 (93%)	0.28	8 (6%)	21	12	94, 151, 187, 234	0
1	E	123/140 (87%)	0.40	11 (8%)	9	5	101, 178, 205, 215	0
1	F	120/140 (85%)	0.36	14 (11%)	4	2	90, 197, 231, 245	0
All	All	758/840 (90%)	0.39	63 (8%)	11	6	80, 157, 217, 245	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1530	LEU	8.3
1	F	1529	PHE	6.6
1	B	1568	LYS	5.7
1	F	1555	VAL	5.7
1	B	1530	LEU	5.3
1	B	1574	PHE	5.2
1	B	1582	PHE	4.9
1	B	1573	ARG	4.9
1	B	1529	PHE	4.6
1	E	1521	PHE	4.5
1	B	1566	GLN	4.2
1	B	1578	LEU	4.2
1	D	1542	PRO	4.1
1	F	1557	GLY	4.1
1	B	1567	ALA	4.0
1	F	1584	ARG	3.8
1	A	1489	SER	3.8
1	D	1529	PHE	3.6
1	F	1585	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1518	TYR	3.5
1	C	1530	LEU	3.4
1	D	1563	GLU	3.4
1	E	1530	LEU	3.3
1	F	1570	ALA	3.3
1	B	1565	CYS	3.2
1	E	1511	LEU	3.1
1	B	1575	LYS	3.0
1	F	1554	TRP	3.0
1	D	1511	LEU	3.0
1	F	1583	TYR	3.0
1	B	1514	ARG	2.9
1	D	1518	TYR	2.8
1	F	1530	LEU	2.8
1	F	1521	PHE	2.7
1	B	1570	ALA	2.7
1	B	1542	PRO	2.6
1	E	1502	GLN	2.6
1	B	1518	TYR	2.5
1	B	1571	GLN	2.5
1	B	1593	LYS	2.5
1	C	1520	LEU	2.4
1	D	1517	ASN	2.4
1	C	1535	LEU	2.4
1	F	1511	LEU	2.3
1	D	1528	TYR	2.3
1	E	1497	ALA	2.3
1	B	1535	LEU	2.3
1	E	1556	LEU	2.3
1	C	1540	LEU	2.2
1	B	1517	ASN	2.2
1	B	1528	TYR	2.2
1	E	1519	VAL	2.2
1	F	1586	LYS	2.2
1	E	1522	THR	2.2
1	C	1518	TYR	2.2
1	F	1589	SER	2.2
1	F	1564	TYR	2.1
1	E	1508	LEU	2.1
1	C	1510	ILE	2.1
1	A	1494	GLU	2.1
1	E	1507	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1469	LYS	2.1
1	C	1524	SER	2.1

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.