Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:14 PM GMT

PDB ID	:	4ZTD
Title	:	Crystal Structure of Human PCNA in complex with a TRAIP peptide
Authors	:	Montoya, G.; Mortuza, G.B.; Blanco, F.J.; Ibanez de Opakua, A.
Deposited on	:	2015-05-14
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

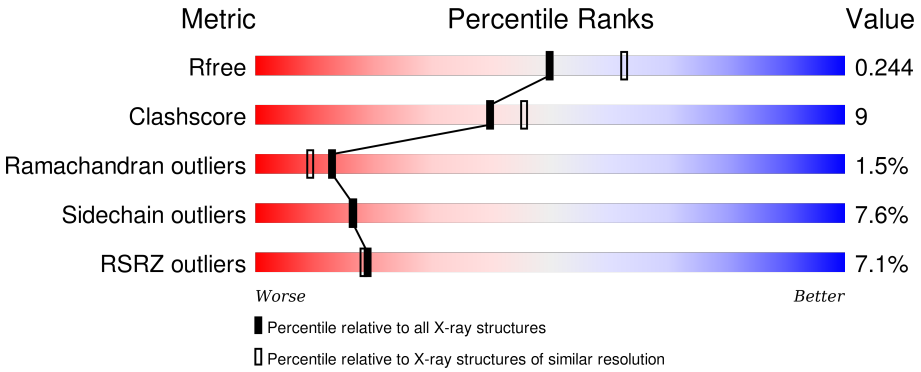
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	253	4% 77% 20%
1	B	253	8% 75% 22%
1	C	253	8% 75% 22%
2	D	12	8% 58% 42%
2	E	12	8% 75% 17% 8%

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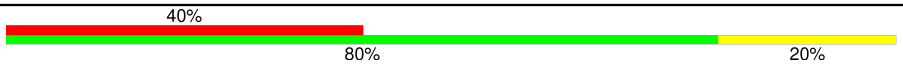
Mol	Chain	Length	Quality of chain
3	F	5	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6245 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1947	1222	320	390	15			
1	B	253	Total	C	N	O	S	0	0	0
			1947	1222	320	390	15			
1	C	252	Total	C	N	O	S	0	0	0
			1938	1216	318	389	15			

- Molecule 2 is a protein called ALA-PHE-GLN-ALA-LYS-LEU-ASP-THR-PHE-LEU-TRP-SER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	0	0	0
			101	69	15	17			
2	E	12	Total	C	N	O	0	0	0
			101	69	15	17			

- Molecule 3 is a protein called ALA-GLY-ALA-GLY-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			23	13	5	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	57	Total	O	0	0
			57	57		
4	C	50	Total	O	0	0
			50	50		
4	D	3	Total	O	0	0
			3	3		

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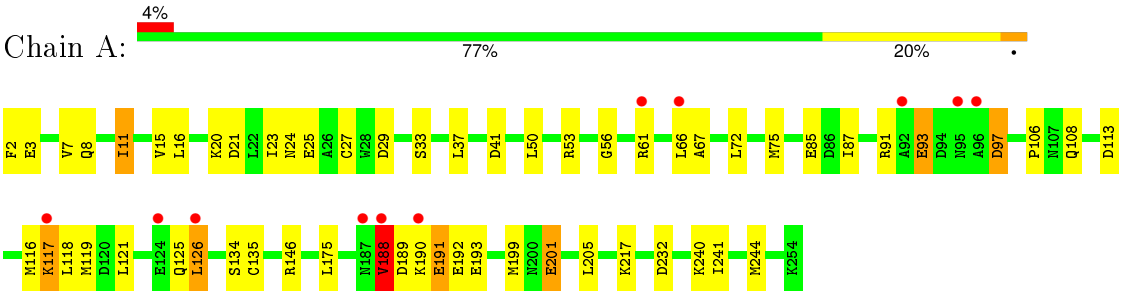
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	4	Total O 4 4	0	0

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.

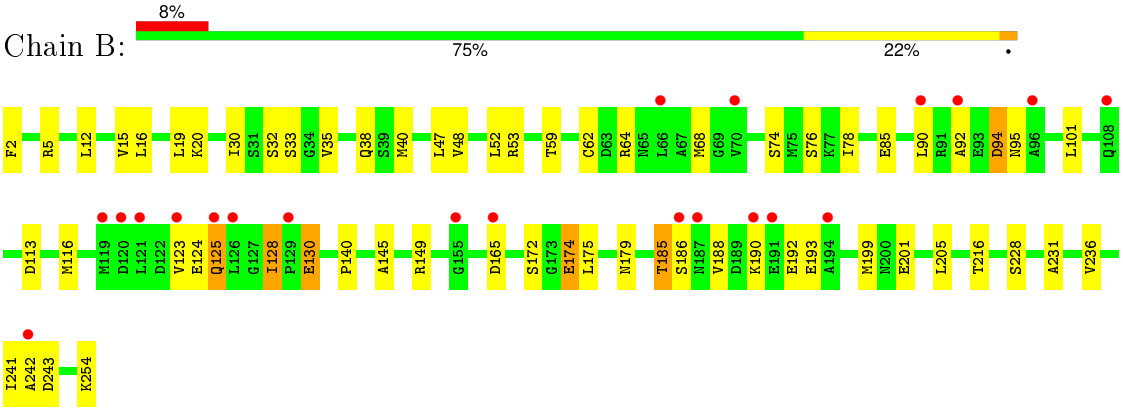
- Molecule 1: Proliferating cell nuclear antigen

Chain A:



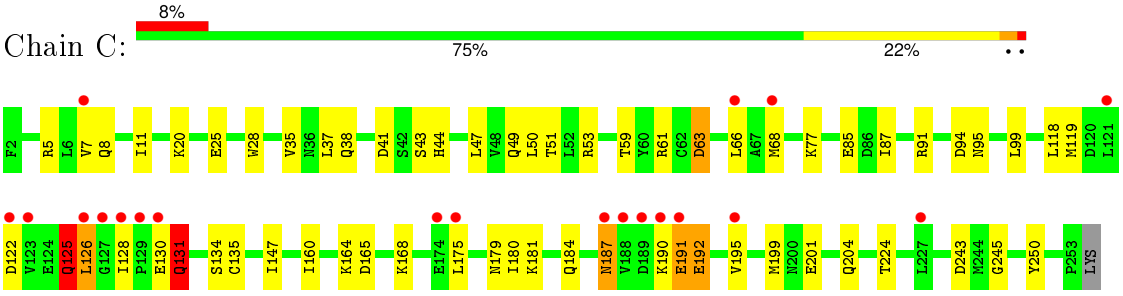
- Molecule 1: Proliferating cell nuclear antigen

Chain B:



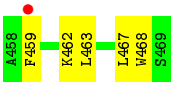
- Molecule 1: Proliferating cell nuclear antigen

Chain C:



- Molecule 2: ALA-PHE-GLN-ALA-LYS-LEU-ASP-THR-PHE-LEU-TRP-SER

Chain D:



• Molecule 2: ALA-PHE-GLN-ALA-LYS-LEU-ASP-THR-PHE-LEU-TRP-SER

Chain E:

• Molecule 3: ALA-GLY-ALA-GLY-ALA

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	84.36Å 84.36Å 210.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.75 – 2.20 42.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.75-2.20) 99.2 (42.75-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.203 , 0.234 0.214 , 0.244	Depositor DCC
R_{free} test set	2132 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 63.8	EDS
Estimated twinning fraction	0.110 for h,-h-k,-l 0.095 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.110 for h,-h-k,-l	Depositor
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	2 of 42654 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6245	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, 0.375 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	0.30	0/1973	0.50	0/2666
1	B	0.29	0/1973	0.53	0/2666
1	C	0.28	0/1964	0.50	0/2655
2	D	0.31	0/104	0.41	0/140
2	E	0.33	0/104	0.45	0/140
3	F	0.16	0/22	0.28	0/28
All	All	0.29	0/6140	0.50	0/8295

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

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	1947	0	1950	35	0
1	B	1947	0	1950	38	1
1	C	1938	0	1937	35	1
2	D	101	0	96	7	0
2	E	101	0	96	4	0
3	F	23	0	20	0	0
4	A	74	0	0	3	0
4	B	57	0	0	2	0
4	C	50	0	0	4	0
4	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	4	0	0	1	0
All	All	6245	0	6049	107	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 9.

All (107) 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:117:LYS:NZ	1:B:174:GLU:O	2.10	0.83
1:A:29:ASP:OD2	1:A:125:GLN:NE2	2.15	0.80
1:B:185:THR:HG23	1:B:188:VAL:HG23	1.67	0.76
1:A:97:ASP:HB3	1:A:118:LEU:HD12	1.69	0.73
1:B:38:GLN:NE2	1:B:125:GLN:OE1	2.23	0.71
1:C:134:SER:HB3	1:C:201:GLU:HG3	1.74	0.69
1:B:113:ASP:OD1	1:C:181:LYS:NZ	2.25	0.69
1:C:5:ARG:HB3	1:C:59:THR:HG22	1.75	0.69
1:C:77:LYS:NZ	4:C:306:HOH:O	2.26	0.68
1:C:130:GLU:O	1:C:131:GLN:HB2	1.92	0.68
1:C:25:GLU:HB3	1:C:119:MET:HE1	1.76	0.68
2:E:458:ALA:N	4:E:501:HOH:O	2.28	0.67
2:E:468:TRP:HA	2:E:468:TRP:CE3	2.28	0.67
1:B:185:THR:HG21	1:B:190:LYS:HB2	1.77	0.66
2:E:468:TRP:HA	2:E:468:TRP:HE3	1.61	0.66
1:B:5:ARG:HB3	1:B:59:THR:HB	1.79	0.65
1:B:2:PHE:HB3	1:B:92:ALA:HB3	1.80	0.63
1:A:2:PHE:N	1:A:3:GLU:HA	2.13	0.63
1:A:61:ARG:NH2	1:A:93:GLU:OE1	2.32	0.63
1:B:179:ASN:ND2	4:B:305:HOH:O	2.32	0.62
1:B:30:ILE:HG13	1:B:35:VAL:HG22	1.82	0.62
1:A:33:SER:O	1:A:53:ARG:NH1	2.33	0.61
1:A:126:LEU:HB3	2:E:467:LEU:HB3	1.83	0.60
1:C:41:ASP:OD2	1:C:43:SER:OG	2.13	0.58
1:C:190:LYS:C	1:C:192:GLU:H	2.07	0.57
1:A:191:GLU:HB3	1:A:193:GLU:OE1	2.05	0.57
1:B:130:GLU:N	1:B:130:GLU:OE1	2.37	0.57
1:B:254:LYS:HA	2:D:459:PHE:O	2.04	0.56
1:A:20:LYS:NZ	4:A:309:HOH:O	2.38	0.56
1:C:122:ASP:N	1:C:122:ASP:OD1	2.37	0.55
1:A:188:VAL:HG13	1:A:189:ASP:N	2.22	0.55
1:B:12:LEU:HD11	1:B:90:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:GLN:NE2	2:D:467:LEU:HD22	2.22	0.54
1:C:47:LEU:HB3	1:C:250:TYR:HB2	1.90	0.53
1:A:23:ILE:HG22	1:A:41:ASP:HA	1.91	0.53
1:A:188:VAL:HG13	1:A:189:ASP:H	1.73	0.53
1:A:56:GLY:HA3	1:A:244:MET:HB2	1.89	0.52
1:B:149:ARG:NH1	4:B:308:HOH:O	2.40	0.52
1:A:134:SER:HB3	1:A:201:GLU:HG2	1.91	0.52
1:C:5:ARG:HB3	1:C:59:THR:CG2	2.39	0.52
1:A:108:GLN:O	4:A:301:HOH:O	2.19	0.51
1:A:75:MET:HA	1:A:116:MET:HE1	1.91	0.51
1:C:38:GLN:NE2	1:C:126:LEU:HB3	2.25	0.51
1:B:128:ILE:HD12	1:B:128:ILE:H	1.75	0.51
1:A:23:ILE:HG13	1:A:72:LEU:HD12	1.92	0.51
1:B:205:LEU:HD21	1:B:231:ALA:HA	1.93	0.51
1:A:240:LYS:NZ	4:A:314:HOH:O	2.43	0.51
1:C:147:ILE:HG23	1:C:180:ILE:HD12	1.92	0.51
1:B:40:MET:SD	2:D:467:LEU:HD11	2.51	0.50
1:C:49:GLN:NE2	1:C:51:THR:OG1	2.33	0.49
1:C:191:GLU:O	1:C:192:GLU:HB2	2.13	0.49
1:B:140:PRO:HG3	1:B:193:GLU:HA	1.94	0.48
1:C:165:ASP:OD1	1:C:165:ASP:N	2.44	0.48
1:B:2:PHE:HD2	1:B:92:ALA:HB2	1.77	0.48
1:B:20:LYS:HD3	1:B:76:SER:OG	2.14	0.48
1:C:168:LYS:NZ	4:C:311:HOH:O	2.38	0.47
1:B:101:LEU:HD11	1:B:116:MET:HE2	1.95	0.47
1:B:94:ASP:OD1	1:B:95:ASN:N	2.47	0.47
1:C:184:GLN:HG3	1:C:195:VAL:O	2.14	0.47
1:A:27:CYS:SG	1:A:67:ALA:HB1	2.55	0.47
1:A:25:GLU:HB3	1:A:119:MET:HE1	1.97	0.46
1:A:21:ASP:OD2	1:A:217:LYS:NZ	2.44	0.46
1:C:160:ILE:O	1:C:204:GLN:HA	2.15	0.46
1:C:122:ASP:OD2	4:C:302:HOH:O	2.21	0.46
1:C:63:ASP:OD1	1:C:63:ASP:N	2.48	0.45
1:C:190:LYS:HG2	1:C:191:GLU:H	1.81	0.45
1:A:205:LEU:HD21	1:A:232:ASP:H	1.80	0.45
1:C:187:ASN:OD1	1:C:187:ASN:N	2.50	0.45
1:B:113:ASP:OD1	1:C:179:ASN:HB2	2.16	0.44
1:B:15:VAL:O	1:B:19:LEU:HG	2.17	0.44
2:D:463:LEU:O	2:D:467:LEU:HG	2.17	0.44
1:C:37:LEU:HB3	1:C:50:LEU:HB3	1.99	0.44
1:A:113:ASP:OD1	1:A:113:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.72	0.44
1:B:192:GLU:HG2	1:B:193:GLU:OE2	2.18	0.44
1:A:175:LEU:HD11	1:C:77:LYS:HE2	1.99	0.44
1:A:113:ASP:OD1	1:B:179:ASN:HB2	2.18	0.44
1:B:145:ALA:HA	1:B:216:THR:HG21	2.00	0.44
1:C:7:VAL:HA	1:C:87:ILE:HG23	2.00	0.44
1:B:165:ASP:OD1	1:B:165:ASP:N	2.50	0.44
1:B:52:LEU:HD21	1:B:241:ILE:HD12	2.00	0.43
1:B:40:MET:HE3	2:D:463:LEU:HB2	2.01	0.43
1:A:7:VAL:HA	1:A:87:ILE:HG23	1.99	0.43
1:C:125:GLN:HB3	1:C:126:LEU:H	1.36	0.43
1:A:8:GLN:HB2	1:A:11:ILE:HD12	2.01	0.43
1:A:135:CYS:SG	1:A:199:MET:HG3	2.59	0.42
1:B:68:MET:HB3	1:B:68:MET:HE2	1.93	0.42
1:B:38:GLN:HA	1:B:48:VAL:O	2.20	0.42
1:B:116:MET:HE2	1:B:116:MET:HB2	1.77	0.42
1:A:15:VAL:HG22	1:A:241:ILE:HD13	2.02	0.42
1:C:99:LEU:HB2	1:C:118:LEU:HD21	2.02	0.42
1:A:37:LEU:HB3	1:A:50:LEU:HB3	2.02	0.41
1:B:47:LEU:HB2	2:D:463:LEU:HD12	2.02	0.41
1:C:51:THR:O	1:C:245:GLY:HA3	2.20	0.41
1:B:78:ILE:HG21	1:B:101:LEU:HD13	2.02	0.41
1:A:116:MET:HE2	1:A:116:MET:HB2	1.84	0.41
1:B:228:SER:HB2	1:B:236:VAL:HB	2.02	0.41
1:B:30:ILE:HG22	1:B:62:CYS:SG	2.61	0.41
1:B:74:SER:HB3	1:C:175:LEU:HB2	2.02	0.41
1:C:135:CYS:SG	1:C:199:MET:HG3	2.60	0.41
1:C:91:ARG:NH2	4:C:323:HOH:O	2.53	0.41
1:A:2:PHE:N	1:A:3:GLU:CA	2.83	0.40
1:C:28:TRP:CE3	1:C:35:VAL:HG11	2.56	0.40
2:D:463:LEU:HA	2:D:463:LEU:HD23	1.84	0.40
1:A:21:ASP:HB2	1:A:217:LYS:HZ3	1.86	0.40
1:A:2:PHE:N	1:A:91:ARG:HA	2.36	0.40
1:C:66:LEU:HD23	1:C:68:MET:HG3	2.03	0.40

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:B:64:ARG:NH2	1:C:63:ASP:OD1[1_445]	2.16	0.04

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	251/253 (99%)	236 (94%)	12 (5%)	3 (1%)	16 12
1	B	251/253 (99%)	238 (95%)	10 (4%)	3 (1%)	16 12
1	C	250/253 (99%)	235 (94%)	10 (4%)	5 (2%)	9 5
2	D	10/12 (83%)	10 (100%)	0	0	100 100
2	E	10/12 (83%)	10 (100%)	0	0	100 100
3	F	3/5 (60%)	2 (67%)	0	1 (33%)	0 0
All	All	775/788 (98%)	731 (94%)	32 (4%)	12 (2%)	13 9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	LEU
1	C	131	GLN
1	A	188	VAL
1	B	94	ASP
1	C	125	GLN
1	B	242	ALA
1	C	94	ASP
1	C	192	GLU
3	F	463	ALA
1	B	125	GLN
1	A	11	ILE
1	A	106	PRO

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	221/221 (100%)	206 (93%)	15 (7%)	20 21
1	B	221/221 (100%)	204 (92%)	17 (8%)	16 16
1	C	220/221 (100%)	203 (92%)	17 (8%)	16 16
2	D	10/10 (100%)	8 (80%)	2 (20%)	1 1
2	E	10/10 (100%)	9 (90%)	1 (10%)	9 8
All	All	682/683 (100%)	630 (92%)	52 (8%)	16 16

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	24	ASN
1	A	66	LEU
1	A	85	GLU
1	A	93	GLU
1	A	97	ASP
1	A	117	LYS
1	A	121	LEU
1	A	126	LEU
1	A	146	ARG
1	A	188	VAL
1	A	190	LYS
1	A	191	GLU
1	A	192	GLU
1	A	201	GLU
1	B	16	LEU
1	B	32	SER
1	B	33	SER
1	B	53	ARG
1	B	85	GLU
1	B	123	VAL
1	B	124	GLU
1	B	128	ILE
1	B	130	GLU
1	B	172	SER
1	B	174	GLU
1	B	175	LEU
1	B	185	THR
1	B	186	SER

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Mol	Chain	Res	Type
1	B	199	MET
1	B	201	GLU
1	B	243	ASP
1	C	8	GLN
1	C	11	ILE
1	C	20	LYS
1	C	44	HIS
1	C	53	ARG
1	C	61	ARG
1	C	63	ASP
1	C	85	GLU
1	C	95	ASN
1	C	125	GLN
1	C	128	ILE
1	C	131	GLN
1	C	164	LYS
1	C	187	ASN
1	C	191	GLU
1	C	224	THR
1	C	243	ASP
2	D	462	LYS
2	D	468	TRP
2	E	468	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	125	GLN

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 carbohydrates 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, 95^{th} 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	253/253 (100%)	0.44	11 (4%)	39	38	26, 44, 87, 102	0
1	B	253/253 (100%)	0.67	21 (8%)	14	13	31, 55, 98, 117	0
1	C	252/253 (99%)	0.68	20 (7%)	15	15	31, 54, 99, 125	0
2	D	12/12 (100%)	0.90	1 (8%)	14	13	51, 59, 82, 84	0
2	E	12/12 (100%)	0.76	1 (8%)	14	13	35, 45, 80, 80	0
3	F	5/5 (100%)	1.60	2 (40%)	0	0	82, 86, 87, 89	0
All	All	787/788 (99%)	0.61	56 (7%)	19	18	26, 51, 97, 125	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	188	VAL	9.9
1	B	123	VAL	9.8
1	C	191	GLU	9.7
1	C	190	LYS	6.9
1	C	187	ASN	6.7
1	B	186	SER	5.6
1	B	187	ASN	5.5
1	C	127	GLY	5.5
1	A	188	VAL	5.4
1	C	123	VAL	4.8
1	B	191	GLU	4.6
1	B	126	LEU	4.5
1	A	190	LYS	4.3
2	E	468	TRP	4.3
1	B	129	PRO	3.8
1	C	122	ASP	3.6
1	C	128	ILE	3.5
1	C	129	PRO	3.5
1	B	194	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASN	3.3
1	B	121	LEU	3.2
1	B	70	VAL	3.2
1	C	175	LEU	3.1
1	B	190	LYS	3.1
1	A	187	ASN	3.1
1	C	7	VAL	3.0
1	B	96	ALA	3.0
3	F	465	ALA	3.0
1	B	242	ALA	2.9
1	A	96	ALA	2.8
1	B	120	ASP	2.8
1	B	66	LEU	2.8
1	C	126	LEU	2.8
1	B	119	MET	2.6
1	C	130	GLU	2.6
1	A	92	ALA	2.6
3	F	461	ALA	2.6
1	C	66	LEU	2.5
1	C	195	VAL	2.5
1	B	108	GLN	2.5
1	A	66	LEU	2.4
1	B	125	GLN	2.3
1	C	189	ASP	2.3
1	A	117	LYS	2.3
1	C	68	MET	2.3
1	B	92	ALA	2.3
1	A	126	LEU	2.3
1	C	174	GLU	2.2
1	C	227	LEU	2.2
1	B	90	LEU	2.2
1	C	121	LEU	2.1
1	A	61	ARG	2.1
1	A	124	GLU	2.1
2	D	459	PHE	2.1
1	B	155	GLY	2.0
1	B	165	ASP	2.0

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

There are no carbohydrates 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.