WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 11:13 am BST

PDB ID	:	2X6G
Title	:	X-ray Structure of Macrophage Inflammatory Protein-1 alpha (D27A)
Authors	:	Guo, Q.; Ren, M.; Tang, W.
Deposited on	:	2010-02-17
Resolution	:	2.18 Å(reported)

The following versions of software and data (see references (1)) 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 (i)

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

The reported resolution of this entry is 2.18 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.

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
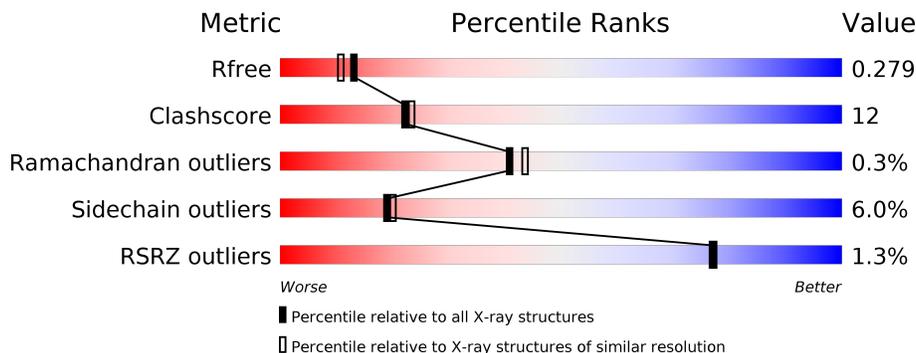
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	70	73% 20% • 6%
1	B	70	70% 23% 7%
1	C	70	77% 14% • 7%
1	D	70	83% 9% • 7%
1	E	70	70% 20% • 6%
1	F	70	76% 17% • 6%

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Mol	Chain	Length	Quality of chain
1	G	70	64% 24% 10%
1	H	70	74% 13% 7%
1	I	70	% 83% 13%
1	J	70	74% 17% 7%
1	K	70	6% 59% 26% 13%
1	L	70	4% 61% 24% 11%
1	M	70	64% 21% 11%
1	N	70	% 69% 24% 7%
1	O	70	63% 27% 7%
1	P	70	61% 27% 9%
1	Q	70	9% 66% 24% 10%
1	R	70	63% 23% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9591 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 C-C MOTIF CHEMOKINE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			518	326	85	103	4			
1	B	65	Total	C	N	O	S	0	0	0
			512	323	84	101	4			
1	C	65	Total	C	N	O	S	0	0	0
			513	323	84	102	4			
1	D	65	Total	C	N	O	S	0	0	0
			513	323	84	102	4			
1	E	66	Total	C	N	O	S	0	0	0
			517	326	85	102	4			
1	F	66	Total	C	N	O	S	0	0	0
			518	326	85	103	4			
1	G	63	Total	C	N	O	S	0	0	0
			502	317	82	99	4			
1	H	65	Total	C	N	O	S	0	0	0
			512	323	84	101	4			
1	I	67	Total	C	N	O	S	0	0	0
			523	329	86	104	4			
1	J	65	Total	C	N	O	S	0	0	0
			513	323	84	102	4			
1	K	61	Total	C	N	O	S	0	0	0
			485	306	80	95	4			
1	L	62	Total	C	N	O	S	0	0	0
			493	312	81	96	4			
1	M	62	Total	C	N	O	S	0	0	0
			494	313	81	96	4			
1	N	65	Total	C	N	O	S	0	0	0
			513	323	84	102	4			
1	O	65	Total	C	N	O	S	0	0	0
			512	323	84	101	4			
1	P	64	Total	C	N	O	S	0	0	0
			508	320	83	101	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	63	Total 494	C 313	N 79	O 98	S 4	0	0	0
1	R	63	Total 502	C 317	N 82	O 99	S 4	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	ASP	SEE REMARK 999	UNP P10147
B	27	ALA	ASP	SEE REMARK 999	UNP P10147
C	27	ALA	ASP	SEE REMARK 999	UNP P10147
D	27	ALA	ASP	SEE REMARK 999	UNP P10147
E	27	ALA	ASP	SEE REMARK 999	UNP P10147
F	27	ALA	ASP	SEE REMARK 999	UNP P10147
G	27	ALA	ASP	SEE REMARK 999	UNP P10147
H	27	ALA	ASP	SEE REMARK 999	UNP P10147
I	27	ALA	ASP	SEE REMARK 999	UNP P10147
J	27	ALA	ASP	SEE REMARK 999	UNP P10147
K	27	ALA	ASP	SEE REMARK 999	UNP P10147
L	27	ALA	ASP	SEE REMARK 999	UNP P10147
M	27	ALA	ASP	SEE REMARK 999	UNP P10147
N	27	ALA	ASP	SEE REMARK 999	UNP P10147
O	27	ALA	ASP	SEE REMARK 999	UNP P10147
P	27	ALA	ASP	SEE REMARK 999	UNP P10147
Q	27	ALA	ASP	SEE REMARK 999	UNP P10147
R	27	ALA	ASP	SEE REMARK 999	UNP P10147

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total 44	O 44	0	0
2	B	30	Total 30	O 30	0	0
2	C	34	Total 34	O 34	0	0
2	D	34	Total 34	O 34	0	0
2	E	44	Total 44	O 44	0	0
2	F	28	Total 28	O 28	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	28	Total 28	O 28	0	0
2	H	26	Total 26	O 26	0	0
2	I	37	Total 37	O 37	0	0
2	J	18	Total 18	O 18	0	0
2	K	9	Total 9	O 9	0	0
2	L	10	Total 10	O 10	0	0
2	M	16	Total 16	O 16	0	0
2	N	19	Total 19	O 19	0	0
2	O	25	Total 25	O 25	0	0
2	P	20	Total 20	O 20	0	0
2	Q	11	Total 11	O 11	0	0
2	R	16	Total 16	O 16	0	0

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: C-C MOTIF CHEMOKINE 3

Chain A:

- Molecule 1: C-C MOTIF CHEMOKINE 3

Chain B:

- Molecule 1: C-C MOTIF CHEMOKINE 3

Chain C:

- Molecule 1: C-C MOTIF CHEMOKINE 3

Chain D:

- Molecule 1: C-C MOTIF CHEMOKINE 3

Chain E:

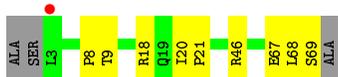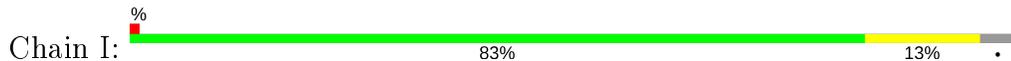- Molecule 1: C-C MOTIF CHEMOKINE 3

Chain F:

ALA SER LEU ALA A5 D6 T7 P8 T9 F13 P21 F24 Y28 R48 D53 P54 S55 E56 V59 Q60 K61 Y62 V63 A70

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain G:

| 64% | 24% | • 10% |

ALA SER LEU ALA A5 D6 T7 P8 R18 N23 F24 I25 A26 P38 G39 V40 I41 K45 R46 C51 ALA D53 P54 K61 Y62 V63 S64 D65 L66 E67 L68 SER ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain H:

| 74% | 13% | • • 7% |

ALA SER LEU A4 P8 T9 Q22 Y28 F42 R46 E57 W58 V59 Q60 K61 Y62 V63 E67 L68 SER ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain I:

%

| 83% | 13% | • |

ALA SER L3 P8 T9 R18 Q19 I20 P21 R46 E67 L68 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain J:

| 74% | 17% | • 7% |

ALA SER LEU ALA A5 T9 R18 Q22 N23 F24 I41 R46 S47 D53 E57 W58 V59 Q60 K61 Y62 L66 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain K:

6%

| 59% | 26% | • 13% |

ALA SER LEU ALA ALA D6 T7 P8 T9 F13 Q19 I20 P21 Q22 N23 F24 I25 Y28 F29 S36 K45 R48 A52 D53 P54 W58 V59 Q60 K61 Y62 V63 L66 GLU LEU SER ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain L:

4%

| 61% | 24% | • 11% |

ALA SER LEU ALA ALA ASP THR P8 T9 I20 N23 F24 F29 E30 S33 Q34 P38 M58 I41 T44 K45 R46 S47 D53 P54 S55 E56 E57 W58 V59 Q60 K61 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain M:

| 64% | 21% | • 11% |

ALA SER LEU ALA ASP **T7** I20 P21 Q22 N23 F24 F29 E30 T31 S32 S33 Q34 V50 D53 E56 E57 W58 K61 L66 E67 L68 SER ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain N:

| 69% | 24% | 7% |

ALA SER LEU ALA A5 S14 Y15 R18 Q19 I20 F24 F29 E30 T31 S32 I41 F42 L43 S47 R48 Q49 V50 W58 K61 L66 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain O:

| 63% | 27% | 7% |

ALA SER LEU ALA A5 D6 T7 P8 T9 F13 R18 P21 F24 S36 K45 R46 S47 R48 D53 P54 S55 E56 E57 W58 V59 Q60 V63 L68 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain P:

| 61% | 27% | 9% |

ALA SER LEU ALA D6 T9 R18 Q22 I25 E30 V40 I41 F42 L43 T44 K45 R46 S47 R48 D53 P54 S55 E56 E57 Q60 K61 Y62 E67 L68 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain Q:

| 9% | 66% | 24% | 10% |

ALA SER LEU A4 T9 Y15 THR SER ARG Q19 I20 P21 Q22 N23 F24 Y28 F29 E30 C35 P38 I41 F42 L43 R46 S47 R48 Q49 V50 C51 A52 D53 E56 E57 K61 Y62 V63 S69 ALA

• Molecule 1: C-C MOTIF CHEMOKINE 3

Chain R:

| 63% | 23% | 10% |

ALA SER LEU ALA ALA D6 T7 P8 T9 F13 R18 Q19 I20 P21 Q22 I25 S32 L43 S47 R48 D53 P54 S55 E56 K61 Y62 L66 E67 L68 SER ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.21Å 113.53Å 173.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.18 49.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.7 (49.01-2.18) 95.7 (49.01-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	6.08 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.210 , 0.286 0.206 , 0.279	Depositor DCC
R_{free} test set	3120 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.5	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	0.94	EDS
Total number of atoms	9591	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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	0.51	0/530	0.65	0/720
1	B	0.44	0/524	0.58	0/712
1	C	0.48	0/525	0.63	0/713
1	D	0.42	0/525	0.57	0/713
1	E	0.42	0/529	0.61	0/719
1	F	0.46	0/530	0.57	0/720
1	G	0.47	0/513	0.63	0/695
1	H	0.41	0/524	0.61	0/712
1	I	0.46	0/535	0.61	0/727
1	J	0.40	0/525	0.55	0/713
1	K	0.35	0/497	0.47	0/675
1	L	0.38	0/505	0.53	0/684
1	M	0.36	0/506	0.55	0/687
1	N	0.38	0/525	0.55	0/713
1	O	0.42	0/524	0.55	0/712
1	P	0.41	0/520	0.58	0/706
1	Q	0.37	0/505	0.48	0/685
1	R	0.36	0/514	0.51	0/698
All	All	0.42	0/9356	0.57	0/12704

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
1	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	67	GLU	Peptide

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	518	0	491	14	0
1	B	512	0	483	7	0
1	C	513	0	486	9	0
1	D	513	0	486	6	0
1	E	517	0	488	19	0
1	F	518	0	491	12	0
1	G	502	0	475	13	0
1	H	512	0	486	11	0
1	I	523	0	493	9	0
1	J	513	0	486	12	0
1	K	485	0	459	24	0
1	L	493	0	471	16	0
1	M	494	0	472	15	0
1	N	513	0	486	17	0
1	O	512	0	483	17	0
1	P	508	0	481	21	0
1	Q	494	0	465	16	0
1	R	502	0	476	20	0
2	A	44	0	0	0	0
2	B	30	0	0	0	0
2	C	34	0	0	0	0
2	D	34	0	0	2	0
2	E	44	0	0	0	0
2	F	28	0	0	1	0
2	G	28	0	0	3	0
2	H	26	0	0	0	0
2	I	37	0	0	1	0
2	J	18	0	0	0	0
2	K	9	0	0	1	0
2	L	10	0	0	0	0
2	M	16	0	0	1	0
2	N	19	0	0	0	0
2	O	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	20	0	0	1	0
2	Q	11	0	0	1	0
2	R	16	0	0	3	0
All	All	9591	0	8658	208	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 12.

The worst 5 of 208 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:J:18:ARG:HG3	1:J:18:ARG:HH21	1.17	1.02
1:P:30:GLU:HG3	1:R:18:ARG:CZ	1.92	0.98
1:H:67:GLU:HB2	1:J:24:PHE:HE2	1.28	0.96
1:R:53:ASP:HB3	1:R:56:GLU:HG3	1.49	0.94
1:H:67:GLU:HB2	1:J:24:PHE:CE2	2.06	0.90

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	64/70 (91%)	64 (100%)	0	0	100	100
1	B	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
1	C	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
1	D	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
1	E	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
1	F	64/70 (91%)	64 (100%)	0	0	100	100
1	G	59/70 (84%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	63/70 (90%)	63 (100%)	0	0	100	100
1	I	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
1	J	63/70 (90%)	63 (100%)	0	0	100	100
1	K	59/70 (84%)	51 (86%)	7 (12%)	1 (2%)	9	5
1	L	60/70 (86%)	59 (98%)	1 (2%)	0	100	100
1	M	60/70 (86%)	60 (100%)	0	0	100	100
1	N	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
1	O	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
1	P	62/70 (89%)	59 (95%)	3 (5%)	0	100	100
1	Q	59/70 (84%)	56 (95%)	2 (3%)	1 (2%)	9	5
1	R	61/70 (87%)	56 (92%)	4 (7%)	1 (2%)	9	6
All	All	1118/1260 (89%)	1087 (97%)	28 (2%)	3 (0%)	41	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	35	CYS
1	R	32	SER
1	K	21	PRO

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	59/61 (97%)	55 (93%)	4 (7%)	16	15
1	B	58/61 (95%)	54 (93%)	4 (7%)	15	15
1	C	59/61 (97%)	56 (95%)	3 (5%)	24	26
1	D	59/61 (97%)	58 (98%)	1 (2%)	60	72
1	E	58/61 (95%)	53 (91%)	5 (9%)	10	9
1	F	59/61 (97%)	56 (95%)	3 (5%)	24	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	58/61 (95%)	55 (95%)	3 (5%)	23	26
1	H	58/61 (95%)	52 (90%)	6 (10%)	7	6
1	I	59/61 (97%)	57 (97%)	2 (3%)	37	44
1	J	59/61 (97%)	55 (93%)	4 (7%)	16	15
1	K	56/61 (92%)	53 (95%)	3 (5%)	22	24
1	L	57/61 (93%)	53 (93%)	4 (7%)	15	14
1	M	57/61 (93%)	53 (93%)	4 (7%)	15	14
1	N	59/61 (97%)	58 (98%)	1 (2%)	60	72
1	O	58/61 (95%)	51 (88%)	7 (12%)	5	3
1	P	59/61 (97%)	56 (95%)	3 (5%)	24	26
1	Q	56/61 (92%)	54 (96%)	2 (4%)	35	42
1	R	58/61 (95%)	54 (93%)	4 (7%)	15	15
All	All	1046/1098 (95%)	983 (94%)	63 (6%)	19	20

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	68	LEU
1	K	9	THR
1	Q	48	ARG
1	I	9	THR
1	J	9	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	34	GLN
1	L	34	GLN
1	Q	60	GLN
1	J	22	GLN
1	K	22	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(Å^2)	Q<0.9
1	A	66/70 (94%)	-0.29	0	100	100	23, 30, 37, 45	0
1	B	65/70 (92%)	-0.27	0	100	100	26, 34, 44, 49	0
1	C	65/70 (92%)	-0.36	0	100	100	25, 34, 42, 48	0
1	D	65/70 (92%)	-0.35	0	100	100	24, 34, 43, 50	0
1	E	66/70 (94%)	-0.27	0	100	100	28, 34, 45, 49	0
1	F	66/70 (94%)	-0.27	0	100	100	25, 33, 40, 43	0
1	G	63/70 (90%)	-0.32	0	100	100	27, 35, 42, 45	0
1	H	65/70 (92%)	-0.22	0	100	100	27, 33, 47, 53	0
1	I	67/70 (95%)	-0.31	1 (1%)	73	74	24, 31, 46, 60	0
1	J	65/70 (92%)	-0.17	0	100	100	27, 38, 48, 53	0
1	K	61/70 (87%)	0.39	4 (6%)	18	19	44, 56, 64, 72	0
1	L	62/70 (88%)	0.13	3 (4%)	30	32	36, 47, 57, 61	0
1	M	62/70 (88%)	-0.26	0	100	100	32, 42, 54, 57	0
1	N	65/70 (92%)	-0.20	1 (1%)	73	74	30, 38, 48, 53	0
1	O	65/70 (92%)	-0.41	0	100	100	29, 34, 45, 55	0
1	P	64/70 (91%)	-0.21	0	100	100	28, 39, 49, 58	0
1	Q	63/70 (90%)	0.30	6 (9%)	8	8	36, 53, 65, 72	0
1	R	63/70 (90%)	0.13	0	100	100	38, 46, 60, 69	0
All	All	1158/1260 (91%)	-0.17	15 (1%)	77	77	23, 37, 57, 72	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	52	ALA	4.7
1	K	29	PHE	4.0
1	Q	46	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	Q	43	LEU	2.9
1	Q	24	PHE	2.6

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.