Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:06 PM GMT

PDB ID	:	4NQS
Title	:	Knob-into-hole IgG Fc
Authors	:	Eigenbrot, C.; Ultsch, M.
Deposited on	:	2013-11-25
Resolution	:	2.64 Å(reported)

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

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

The reported resolution of this entry is 2.64 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		0.277
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		3.9%
RSRZ outliers		9.8%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
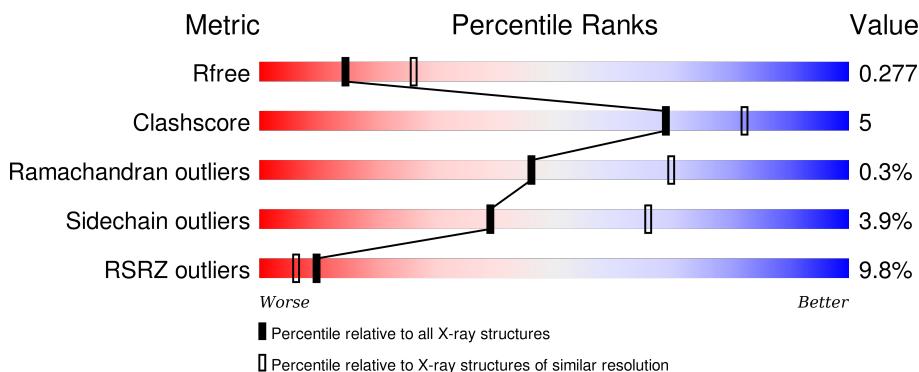
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	213	13% / 82% 15% ••
1	G	213	22% / 82% 15% •
2	B	213	3% / 78% 19% •
2	H	213	5% / 83% 14% ••
3	D	34	94% 6%
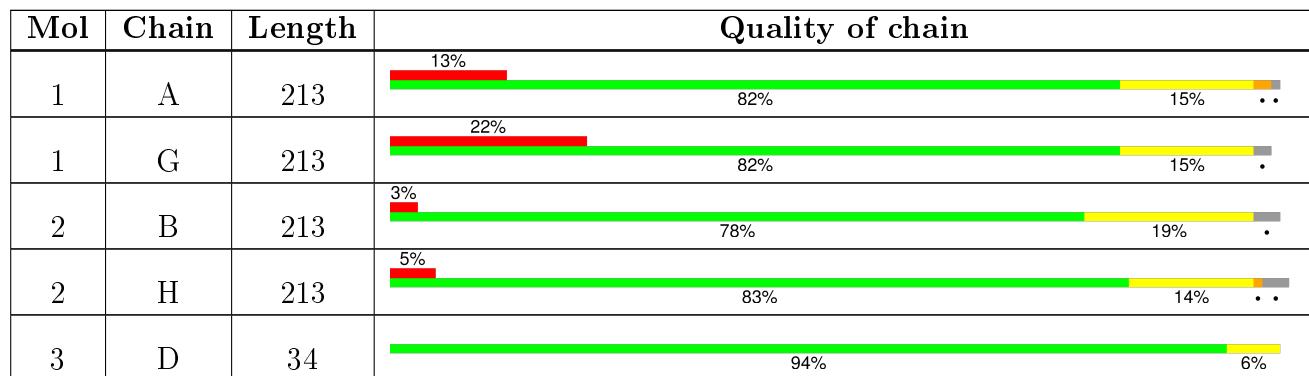
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Mol	Chain	Length	Quality of chain
3	E	34	3% 94% 6%
3	I	34	100%
3	J	34	6% 97%
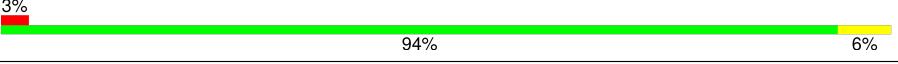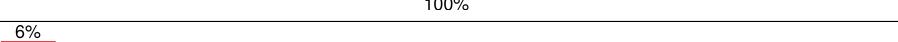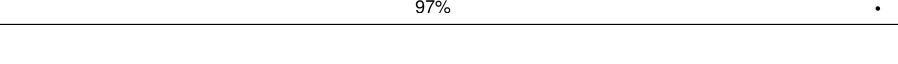
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7832 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 Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total 1668	C 1059	N 282	O 320	S 7	0	0	0
1	G	208	Total 1656	C 1051	N 280	O 318	S 7	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	GLU	ASP	SEE REMARK 999	UNP P01857
A	358	MET	LEU	SEE REMARK 999	UNP P01857
A	366	SER	THR	ENGINEERED MUTATION	UNP P01857
A	368	ALA	LEU	ENGINEERED MUTATION	UNP P01857
A	407	VAL	TYR	ENGINEERED MUTATION	UNP P01857
G	356	GLU	ASP	SEE REMARK 999	UNP P01857
G	358	MET	LEU	SEE REMARK 999	UNP P01857
G	366	SER	THR	ENGINEERED MUTATION	UNP P01857
G	368	ALA	LEU	ENGINEERED MUTATION	UNP P01857
G	407	VAL	TYR	ENGINEERED MUTATION	UNP P01857

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total 1666	C 1063	N 280	O 316	S 7	0	0	0
2	H	207	Total 1666	C 1063	N 280	O 316	S 7	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	356	GLU	ASP	SEE REMARK 999	UNP P01857
B	358	MET	LEU	SEE REMARK 999	UNP P01857

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Chain	Residue	Modelled	Actual	Comment	Reference
B	366	TRP	THR	ENGINEERED MUTATION	UNP P01857
H	356	GLU	ASP	SEE REMARK 999	UNP P01857
H	358	MET	LEU	SEE REMARK 999	UNP P01857
H	366	TRP	THR	ENGINEERED MUTATION	UNP P01857

- Molecule 3 is a protein called miniZ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	34	Total 291	C 176	N 57	O 55	S 3	0	0	0
3	E	34	Total 291	C 176	N 57	O 55	S 3	0	0	0
3	I	34	Total 291	C 176	N 57	O 55	S 3	0	0	0
3	J	34	Total 291	C 176	N 57	O 55	S 3	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	3	Total 3	O 3	0	0
4	D	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0
4	H	4	Total 4	O 4	0	0
4	I	1	Total 1	O 1	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 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: Ig gamma-1 chain C region
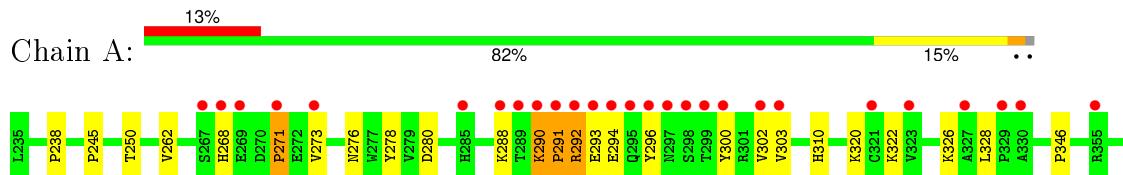
- Molecule 1: Ig gamma-1 chain C region
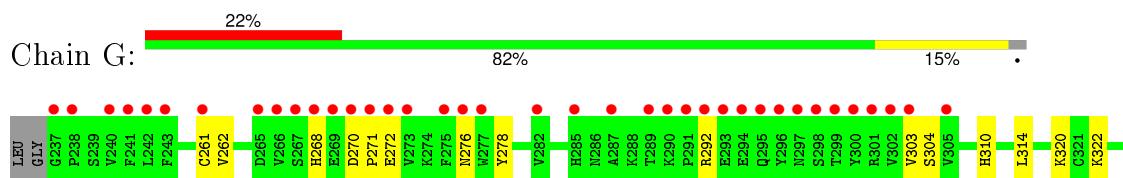
- Molecule 2: Ig gamma-1 chain C region

- Molecule 2: Ig gamma-1 chain C region

D399 Y407 H429 E430 A431 L443 SER PRO GLY LYS

• Molecule 3: miniZ

Chain D:

94%   6%

F6 L23 Q27 C39
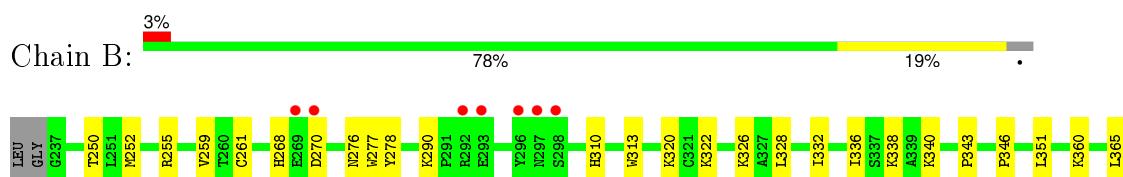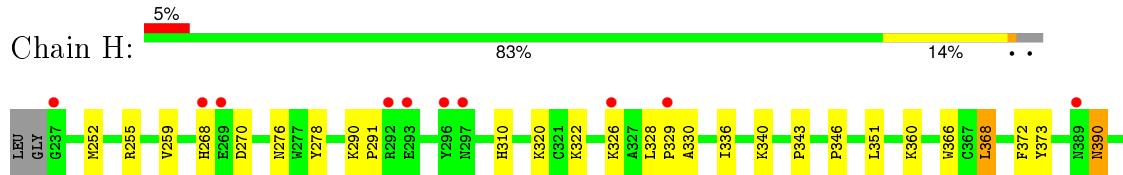
• Molecule 3: miniZ

Chain E:

3%

94%   6%

F6 Q9 C10 C39
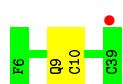
• Molecule 3: miniZ

Chain I:

100%

There are no outlier residues recorded for this chain.

• Molecule 3: miniZ

Chain J:

6%

97%   .

F6 D38 C39

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.24Å 66.08Å 102.90Å 90.00° 95.18° 90.00°	Depositor
Resolution (Å)	46.50 – 2.64 44.86 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.50-2.64) 97.1 (44.86-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.24 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.229 , 0.266 0.238 , 0.277	Depositor DCC
R_{free} test set	961 reflections (3.26%)	DCC
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<\lvert L \rvert> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 30472 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7832	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.19% 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 $<\lvert L \rvert>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (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	0.40	0/1713	0.62	0/2332
1	G	0.39	0/1701	0.58	0/2316
2	B	0.39	0/1714	0.60	0/2335
2	H	0.37	0/1714	0.62	0/2335
3	D	0.38	0/295	0.59	0/393
3	E	0.38	0/295	0.61	0/393
3	I	0.37	0/295	0.55	0/393
3	J	0.39	0/295	0.58	0/393
All	All	0.39	0/8022	0.60	0/10890

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	1668	0	1637	25	0
1	G	1656	0	1623	16	0
2	B	1666	0	1629	16	0
2	H	1666	0	1629	17	0
3	D	291	0	272	1	0
3	E	291	0	272	0	0
3	I	291	0	272	0	0
3	J	291	0	272	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	4	0	0	0	0
4	I	1	0	0	0	0
All	All	7832	0	7606	71	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 5.

All (71) 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)
2:B:346:PRO:HB3	2:B:372:PHE:HB3	1.62	0.82
2:H:252:MET:HB2	2:H:255:ARG:HG3	1.75	0.68
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.77	0.66
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.80	0.63
2:H:346:PRO:HB3	2:H:372:PHE:HB3	1.81	0.61
1:G:346:PRO:HB3	1:G:372:PHE:HB3	1.83	0.61
1:A:291:PRO:HB2	1:A:292:ARG:HD3	1.86	0.57
1:G:367:CYS:HB2	1:G:381:TRP:CZ2	2.40	0.56
2:H:276:ASN:HB2	2:H:322:LYS:HB3	1.88	0.56
1:G:271:PRO:HB2	1:G:292:ARG:HD2	1.90	0.54
2:B:310:HIS:CD2	2:B:310:HIS:H	2.24	0.54
2:B:365:LEU:HD12	2:B:410:LEU:HD23	1.90	0.53
2:H:343:PRO:HA	2:H:373:TYR:O	2.09	0.52
2:B:328:LEU:HD21	2:B:332:ILE:HG13	1.91	0.52
2:H:252:MET:HB2	2:H:255:ARG:CG	2.39	0.52
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.92	0.52
2:H:368:LEU:HG	2:H:407:TYR:CE1	2.45	0.51
2:B:416:ARG:HG2	2:B:423:PHE:HZ	1.74	0.51
1:A:290:LYS:NZ	1:A:303:VAL:HB	2.26	0.51
1:A:296:TYR:HB2	2:H:330:ALA:HB3	1.93	0.50
1:G:339:ALA:HB3	1:G:374:PRO:HB3	1.94	0.50
2:B:261:CYS:HB2	2:B:277:TRP:CZ2	2.48	0.49
2:B:351:LEU:HB2	2:B:366:TRP:HB2	1.93	0.49
1:A:291:PRO:O	1:A:302:VAL:HA	2.13	0.49
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.47	0.49
2:H:310:HIS:H	2:H:310:HIS:CD2	2.31	0.49
1:G:276:ASN:HB2	1:G:322:LYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:CD2	1:A:431:ALA:H	2.31	0.48
1:A:374:PRO:O	1:A:429:HIS:HE1	1.95	0.48
1:A:292:ARG:HB3	1:A:300:TYR:CD1	2.49	0.48
2:H:429:HIS:CD2	2:H:431:ALA:H	2.31	0.48
2:H:259:VAL:HG13	2:H:336:ILE:HD11	1.96	0.48
2:B:252:MET:HB2	2:B:255:ARG:HG3	1.96	0.48
2:B:278:TYR:HB2	2:B:320:LYS:HB3	1.95	0.47
2:B:259:VAL:HG13	2:B:336:ILE:HD11	1.95	0.47
2:B:276:ASN:HB2	2:B:322:LYS:HB3	1.96	0.47
2:H:290:LYS:HG2	2:H:291:PRO:HD2	1.96	0.47
1:G:310:HIS:H	1:G:310:HIS:CD2	2.34	0.46
1:G:314:LEU:HD22	1:G:430:GLU:HG3	1.96	0.46
2:B:379:VAL:HG21	2:B:406:LEU:HD11	1.97	0.46
2:B:343:PRO:HA	2:B:373:TYR:O	2.15	0.46
2:H:429:HIS:HD2	2:H:431:ALA:H	1.64	0.46
2:H:368:LEU:HG	2:H:407:TYR:CZ	2.51	0.46
1:A:238:PRO:HG2	1:A:328:LEU:HD13	1.98	0.46
1:A:262:VAL:HG22	1:A:303:VAL:HG13	1.98	0.45
1:A:290:LYS:HB2	1:A:303:VAL:O	2.16	0.45
1:G:262:VAL:HG22	1:G:303:VAL:HG13	1.97	0.45
1:G:379:VAL:HG22	1:G:427:VAL:HG22	1.98	0.45
1:A:294:GLU:HB3	2:H:329:PRO:HB3	1.99	0.45
1:A:245:PRO:HB2	1:A:250:THR:HG23	1.99	0.45
1:A:310:HIS:CD2	1:A:310:HIS:H	2.34	0.45
1:A:273:VAL:HB	1:A:302:VAL:HG11	1.98	0.44
1:G:278:TYR:HB2	1:G:320:LYS:HB3	1.98	0.44
1:G:429:HIS:CD2	1:G:431:ALA:H	2.35	0.44
1:A:291:PRO:HA	1:A:302:VAL:HG13	1.99	0.43
1:A:430:GLU:HA	1:A:435:HIS:CD2	2.54	0.43
1:G:261:CYS:HB3	1:G:304:SER:HB3	2.01	0.43
1:G:368:ALA:HB1	2:H:366:TRP:CZ2	2.53	0.43
2:H:351:LEU:HB2	2:H:366:TRP:HB2	2.01	0.43
1:A:290:LYS:HD3	1:A:303:VAL:C	2.39	0.42
3:D:23:LEU:HD22	3:D:27:GLN:HB3	2.01	0.42
1:G:272:GLU:HB3	1:G:326:LYS:HE2	2.01	0.42
2:H:278:TYR:HB2	2:H:320:LYS:HB3	2.01	0.42
1:G:346:PRO:CB	1:G:372:PHE:HB3	2.48	0.42
1:A:271:PRO:HB2	1:A:292:ARG:HD2	2.01	0.42
1:G:328:LEU:HD21	1:G:332:ILE:HG13	2.02	0.41
1:A:397:VAL:HG21	2:B:394:THR:HG22	2.01	0.41
2:B:250:THR:HG21	2:B:313:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:O	1:A:293:GLU:HG3	2.20	0.41
2:B:426:SER:HB2	2:B:436:TYR:CE2	2.56	0.41
1:A:268:HIS:HA	1:A:300:TYR:HE2	1.86	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	208/213 (98%)	196 (94%)	10 (5%)	2 (1%)	19	37
1	G	206/213 (97%)	199 (97%)	7 (3%)	0	100	100
2	B	205/213 (96%)	198 (97%)	7 (3%)	0	100	100
2	H	205/213 (96%)	198 (97%)	6 (3%)	1 (0%)	34	57
3	D	32/34 (94%)	32 (100%)	0	0	100	100
3	E	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
3	I	32/34 (94%)	32 (100%)	0	0	100	100
3	J	32/34 (94%)	32 (100%)	0	0	100	100
All	All	952/988 (96%)	918 (96%)	31 (3%)	3 (0%)	46	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	PRO
2	H	390	ASN
1	A	271	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	194/196 (99%)	188 (97%)	6 (3%)	47	74
1	G	193/196 (98%)	187 (97%)	6 (3%)	47	74
2	B	193/197 (98%)	182 (94%)	11 (6%)	25	47
2	H	193/197 (98%)	184 (95%)	9 (5%)	32	57
3	D	32/32 (100%)	32 (100%)	0	100	100
3	E	32/32 (100%)	30 (94%)	2 (6%)	22	42
3	I	32/32 (100%)	32 (100%)	0	100	100
3	J	32/32 (100%)	31 (97%)	1 (3%)	47	74
All	All	901/914 (99%)	866 (96%)	35 (4%)	39	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	ASP
1	A	288	LYS
1	A	290	LYS
1	A	292	ARG
1	A	326	LYS
1	A	442	SER
2	B	268	HIS
2	B	270	ASP
2	B	290	LYS
2	B	326	LYS
2	B	338	LYS
2	B	340	LYS
2	B	360	LYS
2	B	390	ASN
2	B	399	ASP
2	B	415	SER
2	B	440	SER
3	E	9	GLN
3	E	10	CYS

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Mol	Chain	Res	Type
1	G	268	HIS
1	G	270	ASP
1	G	326	LYS
1	G	382	GLU
1	G	407	VAL
1	G	442	SER
2	H	268	HIS
2	H	270	ASP
2	H	326	LYS
2	H	328	LEU
2	H	340	LYS
2	H	360	LYS
2	H	368	LEU
2	H	390	ASN
2	H	399	ASP
3	J	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	HIS
1	A	390	ASN
1	A	429	HIS
1	A	434	ASN
2	B	268	HIS
2	B	310	HIS
2	B	390	ASN
2	B	429	HIS
2	B	434	ASN
3	E	9	GLN
1	G	310	HIS
1	G	429	HIS
1	G	434	ASN
2	H	268	HIS
2	H	310	HIS
2	H	390	ASN
2	H	429	HIS
2	H	434	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(Å²)	Q<0.9
1	A	210/213 (98%)	0.83	28 (13%)	4	2	20, 50, 126, 172	0
1	G	208/213 (97%)	1.05	47 (22%)	1	0	20, 59, 133, 149	0
2	B	207/213 (97%)	0.02	7 (3%)	49	42	19, 34, 85, 117	0
2	H	207/213 (97%)	-0.00	10 (4%)	34	28	19, 35, 82, 107	0
3	D	34/34 (100%)	-0.05	0	100	100	26, 34, 57, 61	0
3	E	34/34 (100%)	-0.03	1 (2%)	55	49	19, 41, 58, 64	0
3	I	34/34 (100%)	-0.15	0	100	100	25, 35, 60, 69	0
3	J	34/34 (100%)	0.19	2 (5%)	26	20	22, 42, 64, 68	0
All	All	968/988 (97%)	0.41	95 (9%)	10	6	19, 41, 112, 172	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	GLN	14.7
1	A	296	TYR	14.0
1	A	291	PRO	13.1
1	A	292	ARG	12.2
1	G	297	ASN	11.1
1	A	294	GLU	9.4
1	A	290	LYS	8.9
1	A	300	TYR	8.7
1	G	296	TYR	8.1
1	A	297	ASN	7.6
1	A	298	SER	7.6
1	G	269	GLU	7.5
1	A	289	THR	7.3
1	G	267	SER	6.8
1	A	299	THR	6.8
1	G	299	THR	6.8

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Mol	Chain	Res	Type	RSRZ
1	G	268	HIS	6.1
1	G	292	ARG	5.9
1	G	275	PHE	5.7
2	B	298	SER	5.4
1	G	298	SER	5.4
1	G	294	GLU	5.2
1	G	329	PRO	5.2
1	A	268	HIS	5.2
2	H	297	ASN	5.1
1	G	273	VAL	5.0
1	G	300	TYR	5.0
1	A	302	VAL	4.8
1	G	271	PRO	4.8
1	G	277	TRP	4.6
1	G	291	PRO	4.5
2	B	292	ARG	4.5
2	B	297	ASN	4.4
3	J	38	ASP	4.3
3	J	39	CYS	4.2
1	A	293	GLU	4.1
1	G	293	GLU	4.1
1	G	266	VAL	4.0
1	G	285	HIS	4.0
1	G	243	PHE	3.9
1	G	295	GLN	3.9
1	G	305	VAL	3.9
1	A	269	GLU	3.7
2	H	296	TYR	3.7
1	G	330	ALA	3.6
1	A	330	ALA	3.6
1	G	261	CYS	3.6
1	G	241	PHE	3.5
1	G	287	ALA	3.5
1	G	237	GLY	3.3
2	B	293	GLU	3.3
1	G	328	LEU	3.3
1	G	270	ASP	3.2
1	A	303	VAL	3.2
1	A	267	SER	3.2
2	B	269	GLU	3.1
1	G	240	VAL	3.1
1	G	327	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	332	ILE	3.0
1	A	285	HIS	3.0
1	A	359	THR	3.0
1	G	238	PRO	2.9
1	G	242	LEU	2.9
1	G	355	ARG	2.9
1	G	276	ASN	2.9
1	A	273	VAL	2.9
1	G	289	THR	2.9
1	A	321	CYS	2.8
2	H	329	PRO	2.8
1	G	331	PRO	2.7
1	A	355	ARG	2.7
1	G	265	ASP	2.7
2	H	389	ASN	2.7
1	G	302	VAL	2.6
1	G	303	VAL	2.6
1	A	271	PRO	2.5
2	H	237	GLY	2.5
2	H	269	GLU	2.5
2	B	270	ASP	2.5
2	B	296	TYR	2.5
1	G	290	LYS	2.4
2	H	326	LYS	2.3
1	G	301	ARG	2.3
3	E	39	CYS	2.3
1	G	361	ASN	2.2
1	A	288	LYS	2.2
1	A	323	VAL	2.1
1	G	282	VAL	2.1
2	H	293	GLU	2.1
2	H	268	HIS	2.1
1	G	326	LYS	2.1
2	H	292	ARG	2.0
1	G	272	GLU	2.0
1	A	329	PRO	2.0
1	A	327	ALA	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 (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.