



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:28 PM UTC

PDB ID : 4NQS / pdb_00004nqs
Title : Knob-into-hole IgG Fc
Authors : Eigenbrot, C.; Ultsch, M.
Deposited on : 2013-11-25
Resolution : 2.64 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

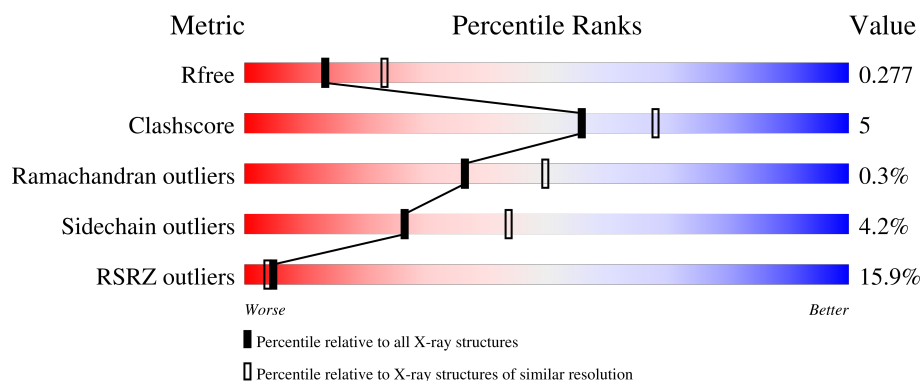
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



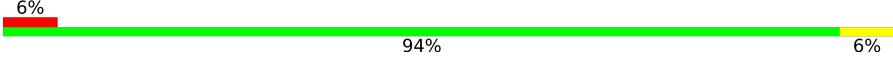
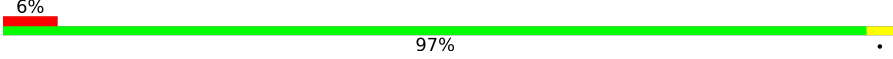
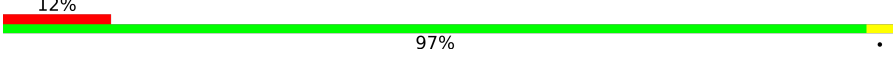
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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 of 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 $\leq 5\%$. 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	
1	G	213	
2	B	213	
2	H	213	
3	D	34	

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Mol	Chain	Length	Quality of chain
3	E	34	 6% 94% 6%
3	I	34	 6% 97% •
3	J	34	 12% 97% •

2 Entry composition

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	C	N	O	S	0	0	0
			1668	1059	282	320	7			
1	G	208	Total	C	N	O	S	0	0	0
			1656	1051	280	318	7			

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	C	N	O	S	0	0	0
			1666	1063	280	316	7			
2	H	207	Total	C	N	O	S	0	0	0
			1666	1063	280	316	7			

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

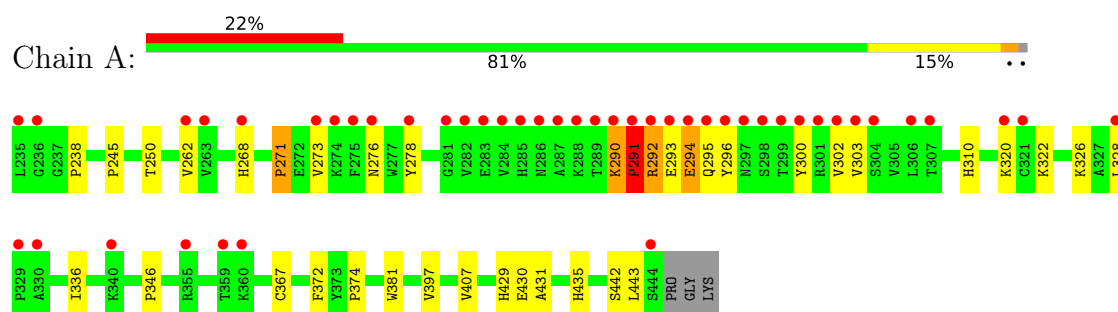
- Molecule 4 is water.

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

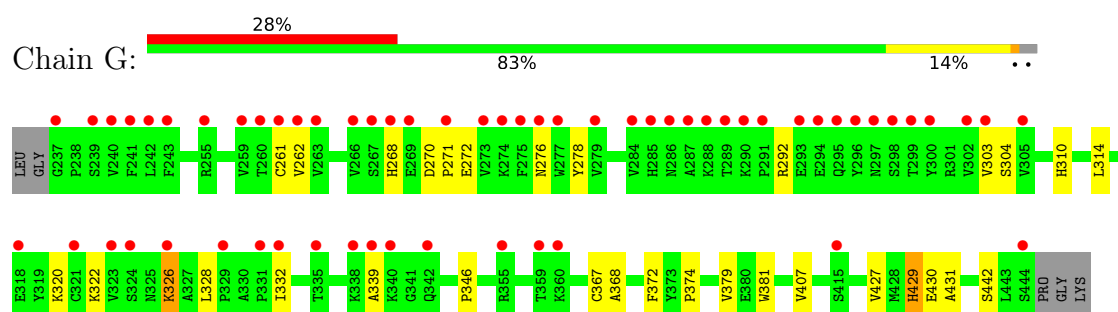
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

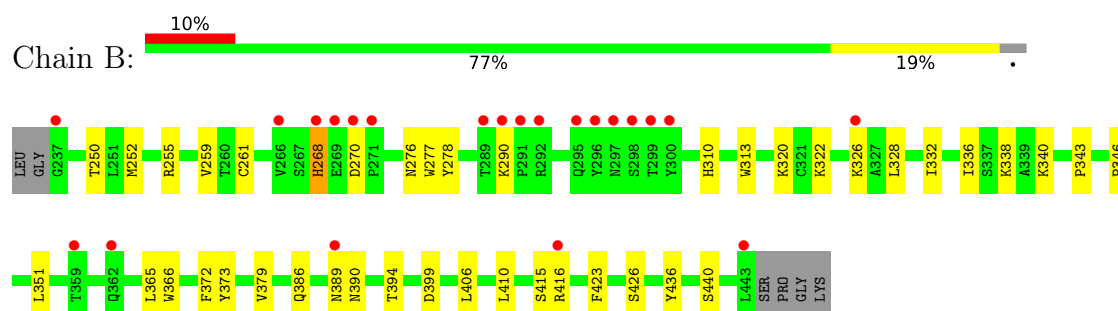
- Molecule 1: Ig gamma-1 chain C region



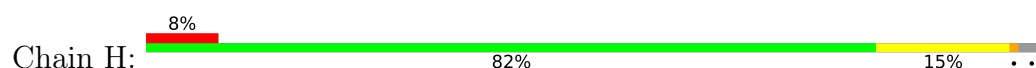
- Molecule 1: Ig gamma-1 chain C region

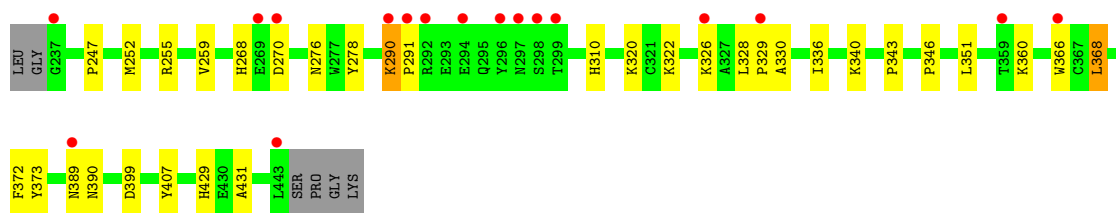


- Molecule 2: Ig gamma-1 chain C region



- Molecule 2: Ig gamma-1 chain C region

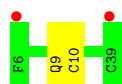




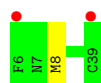
● Molecule 3: miniZ



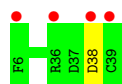
● Molecule 3: miniZ



● Molecule 3: miniZ



● Molecule 3: miniZ



4 Data and refinement statistics

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 46.50 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.50-2.64) 97.1 (46.50-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (3.15%)	wwPDB-VP
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 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.74	0/1713	1.16	2/2332 (0.1%)
1	G	0.71	0/1701	1.09	2/2316 (0.1%)
2	B	0.68	0/1714	1.08	2/2335 (0.1%)
2	H	0.66	0/1714	1.12	4/2335 (0.2%)
3	D	0.67	0/295	1.48	0/393
3	E	0.66	0/295	1.49	0/393
3	I	0.66	0/295	1.33	0/393
3	J	0.67	0/295	1.43	0/393
All	All	0.70	0/8022	1.16	10/10890 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	PRO	CA-C-N	5.80	129.10	120.87
1	A	291	PRO	C-N-CA	5.80	129.10	120.87
2	H	389	ASN	CA-C-N	5.51	132.07	121.54
2	H	389	ASN	C-N-CA	5.51	132.07	121.54
2	B	268	HIS	CA-C-N	5.43	127.82	120.65
2	B	268	HIS	C-N-CA	5.43	127.82	120.65
2	H	247	PRO	CA-C-N	5.37	127.74	120.38
2	H	247	PRO	C-N-CA	5.37	127.74	120.38
1	G	429	HIS	CA-C-N	5.28	127.66	120.54
1	G	429	HIS	C-N-CA	5.28	127.66	120.54

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	26	0
1	G	1656	0	1623	16	0
2	B	1666	0	1629	16	0
2	H	1666	0	1629	18	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
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	72	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 (72) 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:H	2:B:310:HIS:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:NZ	1:A:303:VAL:HB	2.26	0.51
2:B:416:ARG:HG2	2:B:423:PHE:HZ	1.74	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
1:G:276:ASN:HB2	1:G:322:LYS:HB3	1.95	0.49
2:H:310:HIS:H	2:H:310:HIS:CD2	2.31	0.49
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:B:252:MET:HB2	2:B:255:ARG:HG3	1.96	0.48
2:H:259:VAL:HG13	2:H:336:ILE:HD11	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
1:A:290:LYS:HD3	1:A:303:VAL:C	2.39	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
1:A:238:PRO:HG2	1:A:328:LEU:HD13	1.98	0.46
2:H:368:LEU:HG	2:H:407:TYR:CZ	2.51	0.46
1:A:262:VAL:HG22	1:A:303:VAL:HG13	1.98	0.45
1:A:295:GLN:C	2:H:329:PRO:HB2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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%)	12	18
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%)	24	36
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%)	36	50

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%)	186 (96%)	8 (4%)	27	44
1	G	193/196 (98%)	188 (97%)	5 (3%)	40	61
2	B	193/197 (98%)	181 (94%)	12 (6%)	16	28
2	H	193/197 (98%)	184 (95%)	9 (5%)	23	38
3	D	32/32 (100%)	32 (100%)	0	100	100
3	E	32/32 (100%)	30 (94%)	2 (6%)	16	27
3	I	32/32 (100%)	31 (97%)	1 (3%)	35	55
3	J	32/32 (100%)	31 (97%)	1 (3%)	35	55
All	All	901/914 (99%)	863 (96%)	38 (4%)	26	44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	LYS
1	A	292	ARG
1	A	294	GLU
1	A	326	LYS
1	A	336	ILE
1	A	407	VAL
1	A	442	SER
1	A	443	LEU
2	B	268	HIS
2	B	270	ASP
2	B	290	LYS

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Mol	Chain	Res	Type
2	B	326	LYS
2	B	338	LYS
2	B	340	LYS
2	B	386	GLN
2	B	389	ASN
2	B	390	ASN
2	B	399	ASP
2	B	415	SER
2	B	440	SER
3	E	9	GLN
3	E	10	CYS
1	G	268	HIS
1	G	270	ASP
1	G	326	LYS
1	G	407	VAL
1	G	442	SER
2	H	268	HIS
2	H	270	ASP
2	H	290	LYS
2	H	326	LYS
2	H	328	LEU
2	H	340	LYS
2	H	360	LYS
2	H	368	LEU
2	H	399	ASP
3	I	8	MET
3	J	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	310	HIS
1	A	386	GLN
1	A	390	ASN
1	A	429	HIS
1	A	434	ASN
2	B	268	HIS
2	B	276	ASN
2	B	310	HIS
2	B	389	ASN
2	B	390	ASN

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Mol	Chain	Res	Type
2	B	429	HIS
2	B	434	ASN
3	D	19	HIS
3	E	9	GLN
1	G	286	ASN
1	G	310	HIS
1	G	384	ASN
1	G	429	HIS
1	G	433	HIS
1	G	434	ASN
2	H	268	HIS
2	H	310	HIS
2	H	389	ASN
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 oligosaccharides 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 ⓘ

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, 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	210/213 (98%)	0.97	46 (21%) 2 1	20, 50, 126, 172	0
1	G	208/213 (97%)	1.18	60 (28%) 1 1	20, 59, 133, 149	0
2	B	207/213 (97%)	0.42	22 (10%) 11 9	19, 34, 85, 117	0
2	H	207/213 (97%)	0.41	17 (8%) 17 14	18, 35, 82, 107	0
3	D	34/34 (100%)	0.25	1 (2%) 53 48	26, 34, 57, 61	0
3	E	34/34 (100%)	0.47	2 (5%) 28 23	19, 41, 58, 64	0
3	I	34/34 (100%)	0.27	2 (5%) 28 23	25, 35, 60, 69	0
3	J	34/34 (100%)	0.73	4 (11%) 9 7	22, 42, 64, 68	0
All	All	968/988 (97%)	0.70	154 (15%) 5 4	18, 41, 112, 172	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	296	TYR	6.0
1	A	296	TYR	5.9
3	J	39	CYS	5.8
1	A	291	PRO	5.4
1	A	289	THR	5.4
1	G	275	PHE	5.3
1	A	290	LYS	4.6
2	B	296	TYR	4.5
1	A	285	HIS	4.5
2	H	296	TYR	4.3
1	A	295	GLN	4.1
2	B	298	SER	4.1
1	A	297	ASN	4.0
1	G	288	LYS	4.0
1	A	303	VAL	4.0
1	A	288	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	284	VAL	3.9
1	A	294	GLU	3.9
1	G	273	VAL	3.8
2	H	389	ASN	3.8
2	H	326	LYS	3.8
1	G	297	ASN	3.7
1	A	299	THR	3.6
1	A	302	VAL	3.6
1	G	305	VAL	3.6
1	G	299	THR	3.5
3	J	38	ASP	3.5
2	B	443	LEU	3.5
2	B	326	LYS	3.4
1	A	235	LEU	3.4
1	A	292	ARG	3.4
3	I	39	CYS	3.4
1	G	261	CYS	3.4
1	G	243	PHE	3.4
1	A	300	TYR	3.4
1	G	287	ALA	3.4
1	G	298	SER	3.3
1	G	291	PRO	3.3
1	G	237	GLY	3.3
1	A	275	PHE	3.3
1	G	323	VAL	3.3
1	G	241	PHE	3.2
1	G	262	VAL	3.2
2	H	443	LEU	3.2
1	G	277	TRP	3.2
1	G	284	VAL	3.2
1	A	298	SER	3.1
1	G	255	ARG	3.1
1	G	286	ASN	3.1
1	G	329	PRO	3.1
1	G	290	LYS	3.1
1	A	286	ASN	3.0
1	G	240	VAL	3.0
2	B	291	PRO	3.0
1	A	321	CYS	3.0
3	D	39	CYS	3.0
1	G	271	PRO	3.0
2	B	389	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	359	THR	2.9
1	G	324	SER	2.9
1	G	444	SER	2.9
1	G	285	HIS	2.9
1	G	276	ASN	2.8
2	B	297	ASN	2.8
1	G	359	THR	2.8
1	G	303	VAL	2.8
1	A	304	SER	2.8
1	A	360	LYS	2.8
1	A	268	HIS	2.8
1	G	342	GLN	2.8
2	B	269	GLU	2.8
3	E	6	PHE	2.8
2	H	297	ASN	2.8
1	G	289	THR	2.8
1	A	444	SER	2.7
1	A	329	PRO	2.7
1	G	300	TYR	2.7
1	G	321	CYS	2.7
2	H	290	LYS	2.7
1	G	335	THR	2.7
1	A	287	ALA	2.6
1	A	293	GLU	2.6
1	A	355	ARG	2.6
1	G	338	LYS	2.6
3	E	39	CYS	2.6
1	G	295	GLN	2.6
1	G	332	ILE	2.5
1	G	355	ARG	2.5
2	B	362	GLN	2.5
1	G	360	LYS	2.5
1	G	415	SER	2.5
1	G	326	LYS	2.5
2	B	270	ASP	2.5
1	A	282	VAL	2.5
2	B	290	LYS	2.5
1	G	242	LEU	2.4
1	G	267	SER	2.4
2	B	237	GLY	2.4
1	A	262	VAL	2.4
3	J	6	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	299	THR	2.4
2	H	366	TRP	2.4
1	G	340	LYS	2.4
1	G	260	THR	2.4
1	G	293	GLU	2.4
1	A	281	GLY	2.4
1	G	302	VAL	2.4
2	H	269	GLU	2.3
2	H	291	PRO	2.3
1	G	279	VAL	2.3
1	G	268	HIS	2.3
1	A	320	LYS	2.3
3	I	6	PHE	2.3
2	B	300	TYR	2.3
2	H	237	GLY	2.3
1	A	330	ALA	2.3
2	B	416	ARG	2.3
2	H	270	ASP	2.3
1	A	278	TYR	2.2
1	G	331	PRO	2.2
1	A	306	LEU	2.2
1	A	274	LYS	2.2
1	A	301	ARG	2.2
1	G	239	SER	2.2
1	A	340	LYS	2.2
1	G	266	VAL	2.2
1	G	269	GLU	2.1
1	A	307	THR	2.1
2	H	292	ARG	2.1
2	B	271	PRO	2.1
1	A	263	VAL	2.1
2	H	298	SER	2.1
2	B	299	THR	2.1
2	H	329	PRO	2.1
2	B	266	VAL	2.1
2	B	359	THR	2.1
1	A	328	LEU	2.1
2	B	268	HIS	2.1
1	A	273	VAL	2.1
2	H	294	GLU	2.1
1	G	274	LYS	2.1
1	G	259	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLU	2.0
1	G	294	GLU	2.0
3	J	36	ARG	2.0
1	G	339	ALA	2.0
2	H	359	THR	2.0
2	B	295	GLN	2.0
1	A	236	GLY	2.0
2	B	292	ARG	2.0
1	G	318	GLU	2.0
2	B	289	THR	2.0
1	A	276	ASN	2.0
1	G	263	VAL	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 oligosaccharides 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.