Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2023 – 08:36 PM EDT

PDB ID	:	8G0W
Title	:	Crystal structure of human norovirus GII.4 P domain in complex with Nanobody M4
Authors	:	Hu, L.; Salmen, W.; Sankaran, B.; Prasad, B.V.V.
Deposited on	:	2023-02-01
Resolution	:	2.87 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:

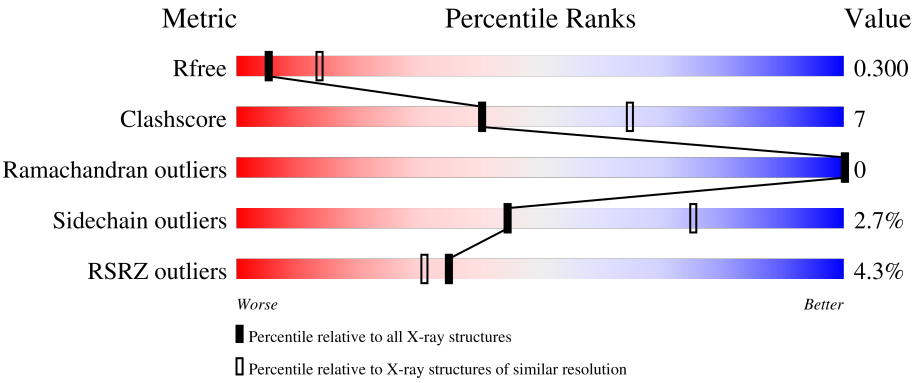
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 <=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	311	3% 79% 16% 5%
1	B	311	6% 72% 23%
1	E	311	2% 81% 12% 6%
1	F	311	4% 80% 17%
2	C	120	6% 71% 27%

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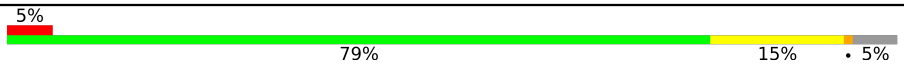
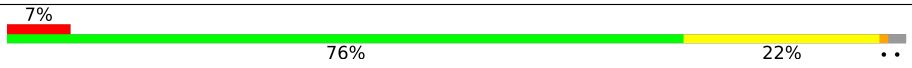
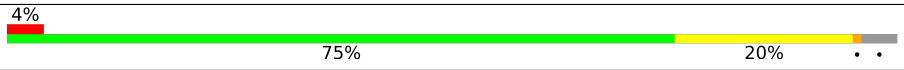
Mol	Chain	Length	Quality of chain
2	D	120	
2	G	120	
2	H	120	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12812 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	19	0	0
			2313	1472	392	439	10			
1	B	298	Total	C	N	O	S	0	0	0
			2331	1481	400	440	10			
1	E	291	Total	C	N	O	S	15	0	0
			2258	1440	377	431	10			
1	F	304	Total	C	N	O	S	70	0	0
			2362	1499	400	453	10			

- Molecule 2 is a protein called Nanobody M4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	117	Total	C	N	O	S	0	0	0
			894	550	165	176	3			
2	D	114	Total	C	N	O	S	9	0	0
			871	536	161	171	3			
2	G	118	Total	C	N	O	S	16	0	0
			901	555	166	177	3			
2	H	115	Total	C	N	O	S	12	0	0
			880	541	163	173	3			

- Molecule 3 is water.

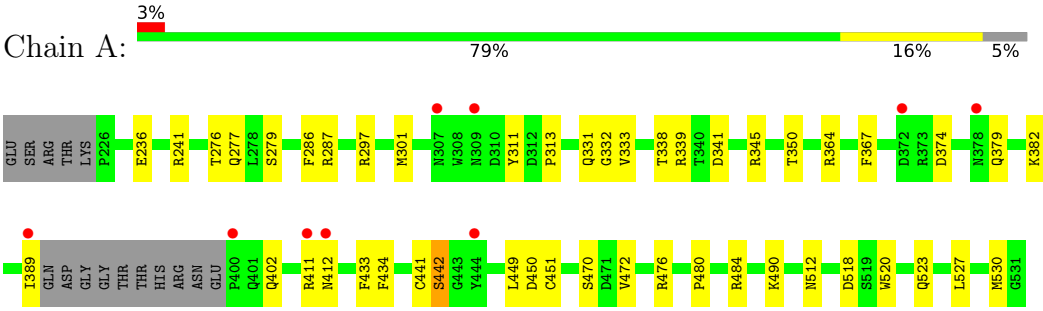
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		

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.

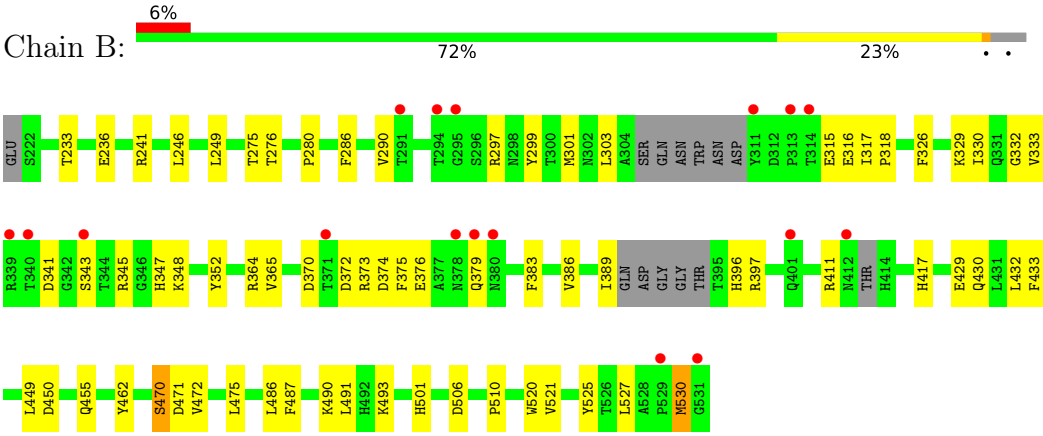
• Molecule 1: VP1

Chain A:



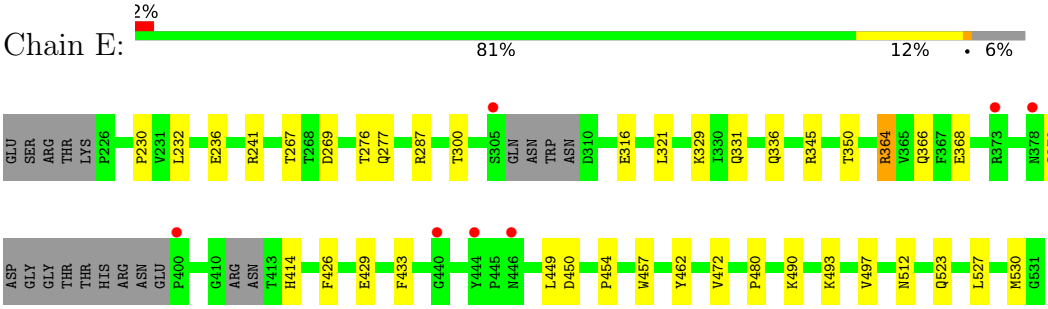
• Molecule 1: VP1

Chain B:



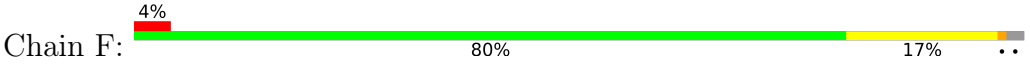
• Molecule 1: VP1

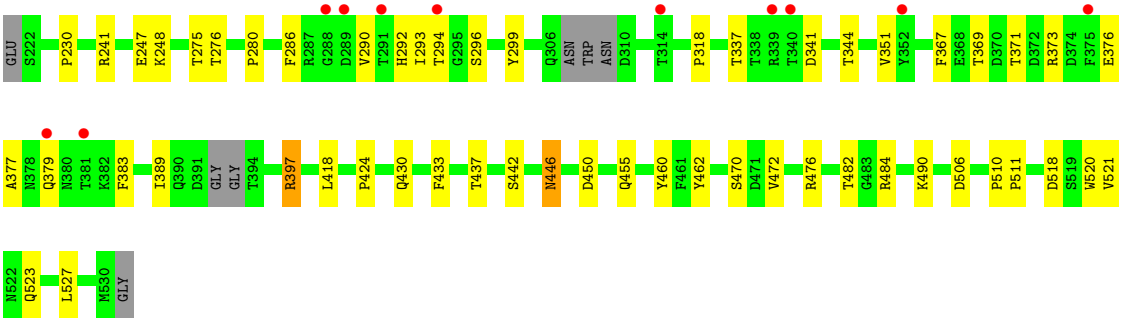
Chain E:



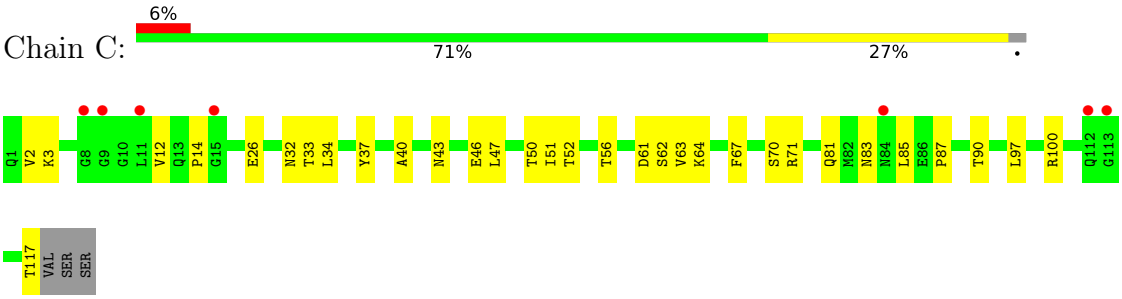
• Molecule 1: VP1

Chain F:

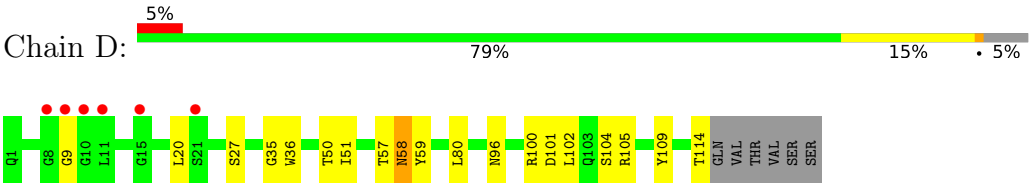




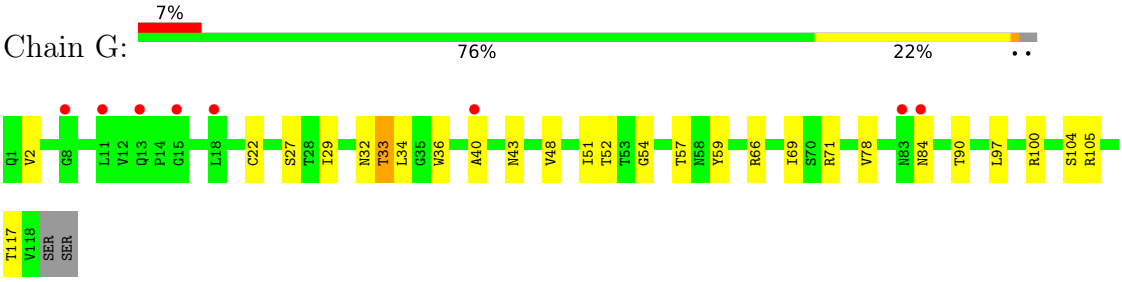
• Molecule 2: Nanobody M4



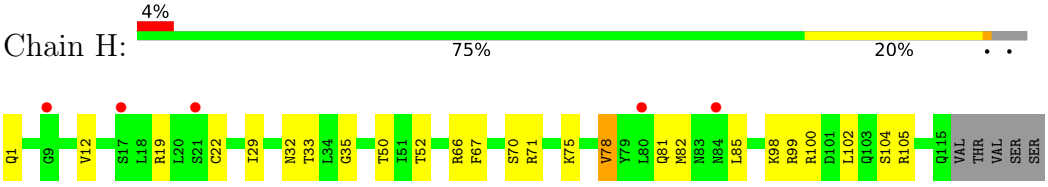
• Molecule 2: Nanobody M4



• Molecule 2: Nanobody M4



• Molecule 2: Nanobody M4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.51Å 90.67Å 107.21Å 90.00° 113.26° 90.00°	Depositor
Resolution (Å)	48.82 – 2.87 48.82 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.82-2.87) 98.7 (48.82-2.87)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.251 , 0.294 0.254 , 0.300	Depositor DCC
R_{free} test set	2006 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12812	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.93% 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

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	0.26	0/2381	0.51	0/3256
1	B	0.26	0/2396	0.51	0/3271
1	E	0.26	0/2323	0.48	0/3176
1	F	0.26	0/2428	0.50	0/3320
2	C	0.26	0/908	0.55	0/1229
2	D	0.25	0/885	0.53	0/1197
2	G	0.25	0/915	0.56	0/1239
2	H	0.25	0/894	0.55	0/1209
All	All	0.26	0/13130	0.51	0/17897

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	2313	0	2219	34	0
1	B	2331	0	2246	44	0
1	E	2258	0	2166	25	0
1	F	2362	0	2255	30	0
2	C	894	0	876	17	0
2	D	871	0	852	13	0
2	G	901	0	885	16	0
2	H	880	0	860	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	12812	0	12359	179	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 7.

All (179) 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:E:350:THR:OG1	1:E:368:GLU:OE1	1.98	0.82
1:B:345:ARG:NH1	1:B:374:ASP:O	2.17	0.77
1:B:389:ILE:HG13	1:B:442:SER:HB2	1.66	0.77
1:F:433:PHE:HB3	1:F:450:ASP:HB3	1.66	0.76
1:B:470:SER:HB3	1:B:520:TRP:HB3	1.67	0.74
1:E:433:PHE:HB3	1:E:450:ASP:HB3	1.71	0.73
2:D:9:GLY:HA3	2:D:114:THR:HG21	1.72	0.72
2:H:19:ARG:HH11	2:H:81:GLN:HE21	1.37	0.72
1:F:389:ILE:HG13	1:F:442:SER:HB3	1.70	0.72
1:B:286:PHE:HB2	1:B:383:PHE:HB3	1.70	0.71
1:A:276:THR:O	2:C:100:ARG:NH2	2.23	0.71
1:B:487:PHE:HB3	1:B:530:MET:HG2	1.71	0.71
1:F:369:THR:HG22	1:F:371:THR:H	1.55	0.70
1:A:331:GLN:HG3	1:A:350:THR:HG22	1.72	0.70
2:C:51:ILE:HD13	2:C:71:ARG:HB2	1.73	0.70
1:E:493:LYS:NZ	2:G:27:SER:O	2.24	0.69
1:E:364:ARG:NH2	1:E:366:GLN:OE1	2.27	0.68
1:B:433:PHE:HB3	1:B:450:ASP:HB3	1.74	0.68
2:G:32:ASN:OD1	2:G:71:ARG:NH2	2.27	0.67
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.77	0.67
1:A:382:LYS:HD3	1:A:384:THR:HG22	1.76	0.65
2:C:2:VAL:HG22	2:C:26:GLU:HG2	1.77	0.64
1:F:482:THR:HG23	1:F:484:ARG:H	1.63	0.64
2:G:90:THR:HG23	2:G:117:THR:HA	1.77	0.64
2:G:51:ILE:HD12	2:G:57:THR:HG22	1.79	0.63
1:F:276:THR:O	2:H:100:ARG:NH2	2.31	0.63
2:C:32:ASN:OD1	2:C:71:ARG:NH2	2.29	0.63
2:H:99:ARG:O	2:H:104:SER:OG	2.18	0.62
1:E:316:GLU:OE2	2:G:54:GLY:N	2.32	0.62
1:B:376:GLU:HB2	1:B:379:GLN:HG3	1.82	0.62
1:E:490:LYS:HG3	1:E:527:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:THR:O	2:G:100:ARG:NH2	2.32	0.61
1:F:247:GLU:OE1	1:F:437:THR:OG1	2.16	0.61
1:A:379:GLN:HE21	1:A:379:GLN:HA	1.66	0.61
1:B:280:PRO:HB3	1:B:455:GLN:HG2	1.83	0.61
2:H:35:GLY:HA3	2:H:50:THR:HG22	1.81	0.61
2:D:101:ASP:O	2:D:104:SER:OG	2.18	0.60
2:G:22:CYS:HB3	2:G:78:VAL:HG12	1.83	0.60
1:A:236:GLU:OE1	2:D:105:ARG:NH2	2.34	0.60
1:F:337:THR:HG23	1:F:344:THR:HG22	1.84	0.59
1:B:493:LYS:NZ	2:D:27:SER:O	2.32	0.59
1:A:332:GLY:HA2	1:A:386:VAL:HG23	1.86	0.58
2:C:90:THR:HG23	2:C:117:THR:HA	1.85	0.58
1:F:275:THR:HG23	1:F:318:PRO:HG2	1.86	0.58
2:D:35:GLY:HA3	2:D:50:THR:HG22	1.85	0.58
1:F:472:VAL:HG13	1:F:521:VAL:HG23	1.87	0.57
1:B:472:VAL:HG13	1:B:521:VAL:HG23	1.87	0.57
1:A:338:THR:OG1	1:A:341:ASP:OD1	2.22	0.56
1:B:462:TYR:OH	2:D:105:ARG:NH1	2.38	0.56
1:F:376:GLU:HB2	1:F:379:GLN:HG3	1.88	0.56
1:B:275:THR:HG23	1:B:318:PRO:HG2	1.86	0.56
1:E:472:VAL:HG11	1:E:490:LYS:HD3	1.88	0.56
1:F:397:ARG:HG3	1:F:446:ASN:HB2	1.88	0.56
1:F:341:ASP:OD1	1:F:341:ASP:N	2.40	0.55
1:F:280:PRO:HB3	1:F:455:GLN:HG2	1.87	0.54
2:G:66:ARG:HD2	2:G:84:ASN:HB2	1.88	0.54
1:E:490:LYS:O	1:E:497:VAL:HA	2.08	0.54
1:F:462:TYR:OH	2:H:105:ARG:NH1	2.40	0.54
1:B:475:LEU:HD11	1:B:491:LEU:HD22	1.90	0.54
1:A:402:GLN:HG3	1:A:449:LEU:HD12	1.90	0.54
1:A:286:PHE:HB3	1:A:301:MET:CE	2.38	0.53
1:B:490:LYS:HZ2	1:B:527:LEU:HG	1.73	0.53
1:B:290:VAL:CG2	1:B:299:TYR:HB3	2.38	0.53
1:A:472:VAL:HG11	1:A:490:LYS:HG2	1.91	0.53
1:A:389:ILE:HG23	1:A:442:SER:HB3	1.89	0.52
2:H:22:CYS:HB3	2:H:78:VAL:HG23	1.91	0.52
1:A:386:VAL:HG21	1:B:333:VAL:HG21	1.92	0.52
1:F:286:PHE:HB2	1:F:383:PHE:HB3	1.90	0.52
1:B:297:ARG:HD2	1:B:370:ASP:HA	1.91	0.52
1:B:315:GLU:HG2	1:B:317:ILE:HD13	1.91	0.52
2:C:81:GLN:NE2	2:C:83:ASN:OD1	2.37	0.52
2:H:29:ILE:HD12	2:H:29:ILE:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:TRP:O	2:G:48:VAL:HG22	2.10	0.51
2:D:102:LEU:HD12	2:D:105:ARG:HD2	1.93	0.51
1:B:345:ARG:NH1	1:B:376:GLU:HG3	2.25	0.51
1:E:336:GLN:NE2	1:E:379:GLN:HB2	2.26	0.51
1:E:331:GLN:HA	1:E:350:THR:HG22	1.94	0.50
1:F:377:ALA:O	1:F:379:GLN:HG2	2.10	0.50
1:B:286:PHE:HB3	1:B:301:MET:SD	2.51	0.50
1:A:472:VAL:HG21	1:A:490:LYS:HE2	1.93	0.50
1:A:339:ARG:HG3	1:A:379:GLN:HE22	1.77	0.50
1:A:286:PHE:HB2	1:A:383:PHE:HB3	1.94	0.49
1:A:470:SER:HB3	1:A:520:TRP:HB3	1.95	0.49
1:E:230:PRO:HB2	1:E:232:LEU:HD12	1.93	0.49
1:B:345:ARG:HH12	1:B:376:GLU:HG3	1.78	0.49
1:E:241:ARG:HB2	1:E:449:LEU:HD21	1.95	0.49
2:C:12:VAL:HG21	2:C:85:LEU:HD13	1.95	0.49
2:G:33:THR:HG23	2:G:52:THR:HG22	1.95	0.49
1:A:333:VAL:HG21	1:B:386:VAL:HG21	1.95	0.49
1:B:430:GLN:HE21	1:B:501:HIS:C	2.16	0.49
1:E:380:ASN:N	1:E:380:ASN:HD22	2.11	0.48
2:D:96:ASN:ND2	2:D:109:TYR:O	2.45	0.48
1:F:470:SER:HB3	1:F:520:TRP:HB3	1.95	0.48
1:B:429:GLU:OE2	1:B:490:LYS:NZ	2.35	0.47
1:A:379:GLN:HA	1:A:379:GLN:NE2	2.28	0.47
1:E:300:THR:OG1	1:E:364:ARG:NH2	2.47	0.47
1:A:277:GLN:NE2	1:A:279:SER:O	2.48	0.47
1:B:303:LEU:HD21	1:B:365:VAL:HG22	1.96	0.47
1:F:241:ARG:NH1	1:F:450:ASP:O	2.44	0.47
2:G:29:ILE:H	2:G:29:ILE:HD12	1.79	0.46
1:A:286:PHE:HB3	1:A:301:MET:HE3	1.97	0.46
1:E:462:TYR:OH	2:G:105:ARG:NH2	2.47	0.46
2:H:67:PHE:CD1	2:H:82:MET:HG2	2.50	0.46
2:C:47:LEU:HD11	2:C:50:THR:CG2	2.45	0.46
1:E:426:PHE:HB3	1:E:429:GLU:HG3	1.96	0.46
1:F:290:VAL:HG12	1:F:299:TYR:HD1	1.81	0.46
1:B:332:GLY:HA2	1:B:386:VAL:HG23	1.97	0.46
1:F:292:HIS:CE1	1:F:294:THR:HA	2.51	0.46
1:F:248:LYS:HD3	1:F:506:ASP:OD2	2.16	0.45
1:A:301:MET:HE1	1:A:367:PHE:HE2	1.82	0.45
1:B:276:THR:O	2:D:100:ARG:NH2	2.47	0.45
2:D:58:ASN:HD22	2:D:59:TYR:N	2.14	0.45
1:B:316:GLU:HB3	1:B:417:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:THR:HG23	2:H:52:THR:HG22	1.99	0.45
2:C:33:THR:HG23	2:C:52:THR:HG22	1.98	0.44
2:H:102:LEU:HD12	2:H:105:ARG:HD2	1.99	0.44
1:A:241:ARG:NH1	1:A:450:ASP:O	2.50	0.44
1:A:311:TYR:O	1:A:313:PRO:HD3	2.17	0.44
1:A:490:LYS:HG3	1:A:527:LEU:HD21	2.00	0.44
1:F:230:PRO:HG3	1:F:460:TYR:CD1	2.52	0.44
2:D:20:LEU:HD12	2:D:80:LEU:HD23	2.00	0.44
2:G:2:VAL:HG11	2:G:97:LEU:HD22	2.00	0.44
1:A:476:ARG:NH1	1:A:518:ASP:OD2	2.39	0.44
1:E:454:PRO:HG2	1:E:457:TRP:CD1	2.53	0.44
2:G:40:ALA:HB3	2:G:43:ASN:HB2	1.99	0.44
1:A:331:GLN:NE2	1:A:441:CYS:HB2	2.32	0.44
1:E:454:PRO:HG2	1:E:457:TRP:CG	2.53	0.43
1:A:286:PHE:HB3	1:A:301:MET:HE1	2.00	0.43
1:B:486:LEU:HD22	1:B:510:PRO:HD3	2.00	0.43
1:E:277:GLN:HB3	1:E:321:LEU:HD13	2.00	0.43
2:H:98:LYS:HE3	2:H:98:LYS:HB2	1.81	0.43
2:C:14:PRO:HG3	2:C:87:PRO:HG3	2.00	0.43
1:B:297:ARG:HG3	1:B:372:ASP:OD1	2.18	0.43
2:D:51:ILE:HD12	2:D:57:THR:HG22	2.01	0.43
1:B:329:LYS:HG3	1:B:352:TYR:CD1	2.54	0.43
1:B:233:THR:OG1	1:B:236:GLU:HG3	2.18	0.43
1:B:348:LYS:HD2	1:B:348:LYS:H	1.83	0.43
1:B:249:LEU:HB3	1:B:432:LEU:HD11	2.00	0.43
1:E:267:THR:OG1	1:E:269:ASP:OD1	2.28	0.43
2:H:32:ASN:OD1	2:H:71:ARG:NH2	2.52	0.42
1:A:297:ARG:HE	1:A:297:ARG:HB2	1.67	0.42
1:A:480:PRO:HD2	1:A:512:ASN:ND2	2.33	0.42
1:B:246:LEU:HA	1:B:436:SER:OG	2.19	0.42
2:C:37:TYR:CZ	2:C:47:LEU:HD12	2.55	0.42
1:E:523:GLN:N	1:E:523:GLN:OE1	2.48	0.42
1:F:318:PRO:HB3	1:F:418:LEU:HD23	2.01	0.42
2:C:63:VAL:HB	2:C:67:PHE:CG	2.54	0.42
1:F:523:GLN:H	1:F:523:GLN:CD	2.23	0.42
2:G:34:LEU:H	2:G:71:ARG:HH12	1.67	0.42
1:A:434:PHE:HB2	1:A:451:CYS:SG	2.60	0.42
1:B:470:SER:OG	1:B:471:ASP:N	2.53	0.42
1:B:525:TYR:HE2	1:B:527:LEU:HD23	1.84	0.42
2:C:3:LYS:HD2	2:C:3:LYS:HA	1.66	0.42
2:H:12:VAL:HG11	2:H:85:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:MET:HE2	1:A:301:MET:HB3	1.80	0.42
2:C:51:ILE:HA	2:C:56:THR:O	2.20	0.42
2:C:40:ALA:HB3	2:C:43:ASN:HB2	2.02	0.41
1:B:347:HIS:HB3	1:B:370:ASP:OD1	2.20	0.41
1:E:429:GLU:OE2	1:E:490:LYS:HE3	2.20	0.41
2:C:34:LEU:HD21	2:C:97:LEU:HD12	2.01	0.41
2:D:36:TRP:CD1	2:D:80:LEU:HB2	2.55	0.41
1:A:412:ASN:OD1	1:F:476:ARG:NH2	2.47	0.41
1:A:523:GLN:OE1	1:A:523:GLN:N	2.47	0.41
1:B:241:ARG:HB2	1:B:449:LEU:HD21	2.03	0.41
1:E:236:GLU:OE2	2:H:105:ARG:NH2	2.54	0.41
1:F:351:VAL:HB	1:F:367:PHE:CE2	2.56	0.41
2:G:59:TYR:OH	2:G:69:ILE:HG22	2.21	0.41
1:B:299:TYR:CE2	1:B:375:PHE:HB2	2.56	0.41
1:B:334:LEU:HD12	1:B:334:LEU:HA	1.95	0.41
2:C:61:ASP:HA	2:C:64:LYS:HG3	2.01	0.41
1:E:480:PRO:HD2	1:E:512:ASN:ND2	2.35	0.41
1:F:424:PRO:HG3	1:F:430:GLN:HA	2.02	0.41
1:B:290:VAL:HG23	1:B:299:TYR:HB3	2.02	0.41
1:B:326:PHE:CZ	1:B:330:ILE:HD11	2.56	0.41
1:F:510:PRO:HA	1:F:511:PRO:HD3	1.98	0.41
1:F:476:ARG:NH1	1:F:518:ASP:OD2	2.43	0.40
1:F:490:LYS:HG3	1:F:527:LEU:HD11	2.03	0.40
2:H:1:GLN:HB3	2:H:99:ARG:NH2	2.37	0.40
1:B:341:ASP:OD2	1:B:343:SER:OG	2.39	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	292/311 (94%)	281 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	290/311 (93%)	284 (98%)	6 (2%)	0	100	100
1	E	285/311 (92%)	273 (96%)	12 (4%)	0	100	100
1	F	298/311 (96%)	285 (96%)	13 (4%)	0	100	100
2	C	115/120 (96%)	115 (100%)	0	0	100	100
2	D	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
2	G	116/120 (97%)	115 (99%)	1 (1%)	0	100	100
2	H	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
All	All	1621/1724 (94%)	1575 (97%)	46 (3%)	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	257/270 (95%)	249 (97%)	8 (3%)	40	72
1	B	259/270 (96%)	251 (97%)	8 (3%)	40	72
1	E	251/270 (93%)	244 (97%)	7 (3%)	43	75
1	F	262/270 (97%)	257 (98%)	5 (2%)	57	82
2	C	95/98 (97%)	92 (97%)	3 (3%)	39	71
2	D	92/98 (94%)	91 (99%)	1 (1%)	73	90
2	G	96/98 (98%)	94 (98%)	2 (2%)	53	80
2	H	93/98 (95%)	89 (96%)	4 (4%)	29	60
All	All	1405/1472 (95%)	1367 (97%)	38 (3%)	44	75

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

Mol	Chain	Res	Type
1	A	287	ARG
1	A	345	ARG

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Mol	Chain	Res	Type
1	A	364	ARG
1	A	374	ASP
1	A	411	ARG
1	A	442	SER
1	A	484	ARG
1	A	530	MET
1	B	364	ARG
1	B	373	ARG
1	B	396	HIS
1	B	397	ARG
1	B	411	ARG
1	B	470	SER
1	B	506	ASP
1	B	530	MET
2	C	46	GLU
2	C	62	SER
2	C	70	SER
2	D	58	ASN
1	E	287	ARG
1	E	329	LYS
1	E	345	ARG
1	E	364	ARG
1	E	380	ASN
1	E	414	HIS
1	E	530	MET
1	F	293	ILE
1	F	296	SER
1	F	373	ARG
1	F	397	ARG
1	F	446	ASN
2	G	33	THR
2	G	104	SER
2	H	66	ARG
2	H	70	SER
2	H	75	LYS
2	H	78	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	GLN
1	A	379	GLN

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Mol	Chain	Res	Type
1	B	430	GLN
2	C	6	GLN
2	C	44	GLN
2	C	84	ASN
2	D	58	ASN
2	D	81	GLN
1	E	380	ASN
1	F	446	ASN
2	G	5	GLN
2	H	1	GLN
2	H	81	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 monosaccharides 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	293/311 (94%)	0.14	9 (3%)	49	45	14, 24, 53, 63	0
1	B	298/311 (95%)	0.36	18 (6%)	21	17	18, 36, 67, 89	0
1	E	289/311 (92%)	0.18	7 (2%)	59	57	13, 24, 48, 62	1 (0%)
1	F	296/311 (95%)	0.40	11 (3%)	41	37	17, 34, 62, 79	1 (0%)
2	C	117/120 (97%)	0.39	7 (5%)	21	17	16, 33, 54, 66	0
2	D	113/120 (94%)	0.40	6 (5%)	26	22	22, 38, 66, 75	0
2	G	116/120 (96%)	0.48	8 (6%)	16	13	17, 34, 50, 60	0
2	H	113/120 (94%)	0.50	5 (4%)	34	30	19, 38, 73, 87	0
All	All	1635/1724 (94%)	0.32	71 (4%)	35	31	13, 31, 59, 89	2 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	373	ARG	6.0
1	A	378	ASN	6.0
2	H	9	GLY	5.2
2	C	84	ASN	4.3
1	F	379	GLN	4.2
1	E	378	ASN	4.2
2	G	84	ASN	4.2
1	A	444	TYR	4.1
1	B	294	THR	4.0
1	F	314	THR	3.8
2	H	17	SER	3.6
2	C	11	LEU	3.5
1	F	339	ARG	3.5
1	B	379	GLN	3.5
1	B	378	ASN	3.3
1	F	291	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	371	THR	3.2
2	H	84	ASN	3.1
1	B	340	THR	3.1
1	B	337	THR	3.0
1	F	294	THR	3.0
2	D	8	GLY	2.9
2	G	8	GLY	2.9
1	E	444	TYR	2.9
2	D	15	GLY	2.8
1	F	375	PHE	2.6
1	A	307	ASN	2.6
2	G	18	LEU	2.6
1	B	291	THR	2.5
1	A	412	ASN	2.4
2	C	9	GLY	2.4
1	B	412	ASN	2.4
1	B	343	SER	2.4
1	B	313	PRO	2.4
2	G	83	ASN	2.4
2	G	15	GLY	2.3
1	B	314	THR	2.3
1	A	372	ASP	2.3
1	F	340	THR	2.3
1	E	305	SER	2.3
1	B	295	GLY	2.3
1	A	389	ILE	2.3
2	H	80	LEU	2.3
1	F	288	GLY	2.3
1	F	352	TYR	2.3
2	C	8	GLY	2.2
2	C	112	GLN	2.2
1	B	531	GLY	2.2
1	F	289	ASP	2.2
2	D	9	GLY	2.2
2	C	113	GLY	2.2
2	D	11	LEU	2.2
2	H	21	SER	2.1
1	B	529	PRO	2.1
1	F	381	THR	2.1
1	A	411	ARG	2.1
1	B	339	ARG	2.1
2	D	10	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	400	PRO	2.1
1	B	311	TYR	2.1
1	A	309	ASN	2.1
2	C	15	GLY	2.1
2	G	11	LEU	2.1
1	E	440	GLY	2.1
2	G	13	GLN	2.0
1	E	446	ASN	2.0
2	G	40	ALA	2.0
1	B	380	ASN	2.0
1	B	401	GLN	2.0
1	E	400	PRO	2.0
2	D	21	SER	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 monosaccharides 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.