

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 22, 2023 – 06:37 PM JST

PDB ID	:	7X4I
Title	:	Crystal structure of nanobody aSA3 in complex with dimer SARS-CoV-1 RBD
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Deposited on	:	2022-03-02
Resolution	:	3.38  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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.38 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\# { m Entries,\ resolution\ range}({ m \AA}))$		
$R_{free}$	130704	1691 (3.46-3.30)		
Clashscore	141614	1762 (3.46-3.30)		
Ramachandran outliers	138981	1732 (3.46-3.30)		
Sidechain outliers	138945	1731 (3.46-3.30)		
RSRZ outliers	127900	1635 (3.46-3.30)		

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	А	204	71%	20%	9%
1	В	204	9% 81%	14%	5%
1	С	204	7%	22%	8%
1	D	204	7%	15%	8%
2	Е	123	78%	21%	
2	F	123	5%	28%	



Mol	Chain	Length	Quality of chain		
2	G	123	77%	23%	•
2	Н	123	77%	20% ••	1



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9779 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	196	Total	С	Ν	0	$\mathbf{S}$	0	0 0	0
1	A	180	1478	953	243	273	9	0		0
1	р	104	Total	С	Ν	0	S	0	0	0
1	D	194	1542	995	253	285	9	0	0	0
1	C	188	Total	С	Ν	0	S	0	0	0
1			1497	966	246	276	9		0	0
1 D	197	Total	С	Ν	0	S	0	1	0	
	187	1494	962	248	275	9	0	1	0	

• Molecule 1 is a protein called Spike glycoprotein.

• Molecule 2 is a protein called nanobody aSA3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	F	192	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	Ľ	123	942	589	162	187	4	0		0
0	Б	123	Total	С	Ν	0	S	0	2	0
	2 F		948	593	162	189	4		2	0
0	C	192	Total	С	Ν	0	S	0	2	0
	2 G	123	946	592	162	188	4		2	U
0	о п	I 101	Total	С	Ν	0	S	0	2	0
	121	932	583	161	184	4	0		U	



## 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: Spike glycoprotein







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	101.70Å 112.01Å 151.04Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution(A)	75.52 - 3.38	Depositor
Resolution (A)	75.52 - 3.38	EDS
% Data completeness	99.0 (75.52-3.38)	Depositor
(in resolution range)	99.0 (75.52-3.38)	EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.57 (at 3.41 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_2481	Depositor
D D	0.267 , $0.321$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.267 , $0.321$	DCC
$R_{free}$ test set	1213 reflections $(4.94\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	85.9	Xtriage
Anisotropy	0.948	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 52.9	EDS
L-test for $twinning^2$	$ \langle L  \rangle = 0.45, \langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9779	wwPDB-VP
Average B, all atoms $(Å^2)$	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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	
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.31	0/1524	0.49	0/2079
1	В	0.34	0/1591	0.49	0/2173
1	С	0.31	0/1544	0.48	0/2106
1	D	0.32	0/1543	0.49	0/2104
2	Ε	0.34	0/964	0.57	0/1306
2	F	0.32	0/975	0.57	0/1319
2	G	0.35	0/974	0.53	0/1319
2	Н	0.33	0/959	0.54	0/1299
All	All	0.33	0/10074	0.51	0/13705

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	А	1478	0	1399	24	0
1	В	1542	0	1464	20	0
1	С	1497	0	1417	26	0
1	D	1494	0	1421	18	0
2	Е	942	0	880	18	0
2	F	948	0	890	29	0
2	G	946	0	886	18	0
2	Н	932	0	876	18	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9779	0	9233	162	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 9.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:409:ASN:HD21	1:A:441:ARG:H	1.17	0.89	
1:C:389:VAL:HG11	1:C:405:ILE:HD12	1.54	0.88	
1:D:440:TYR:OH	2:F:115:GLN:NE2	2.13	0.81	
2:G:24:ALA:HB3	2:G:76:ASN:HB3	1.63	0.78	
2:H:100:TRP:HH2	2:H:110:TYR:HA	1.56	0.70	
2:F:24:ALA:HB3	2:F:76:ASN:HB3	1.74	0.70	
2:H:71:ARG:HB3	2:H:78:VAL:HG12	1.73	0.69	
2:H:103:ARG:NH2	2:H:104:SER:O	2.28	0.67	
2:E:71:ARG:HG2	2:E:78:VAL:HG12	1.76	0.67	
2:G:2:VAL:HG13	2:G:26:GLY:HA3	1.77	0.66	
2:G:52:ASP:OD1	2:G:56:ASN:N	2.29	0.65	
1:B:440:TYR:OH	2:E:115:GLN:NE2	2.29	0.64	
1:C:346:SER:OG	1:C:381:ASN:ND2	2.31	0.64	
1:B:467:CYS:HB2	1:B:469:PRO:HD2	1.81	0.62	
2:E:52:ASP:O	2:E:71:ARG:NH1	2.32	0.62	
2:F:34:LEU:HD13	2:F:78:VAL:HG22	1.82	0.61	
2:E:98:GLY:HA3	2:E:100:TRP:CZ3	2.37	0.59	
1:B:363:THR:OG1	2:F:106:ASN:ND2	2.36	0.58	
1:B:489:ILE:N	2:F:44:GLU:OE2	2.37	0.57	
1:A:441:ARG:NH2	1:A:454:ASP:O	2.37	0.57	
1:B:399:PRO:HB3	1:B:414:ASP:HA	1.87	0.57	
1:B:418:GLY:HA2	1:B:501:PHE:HE2	1.71	0.56	
2:E:66:ARG:NH1	2:E:84:SER:O	2.37	0.56	
1:A:361:PHE:HA	1:A:423:TRP:HB3	1.87	0.56	
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.87	0.56	
2:F:52:ASP:OD1	2:F:56:ASN:N	2.38	0.56	
1:A:363:THR:HB	1:A:422:ALA:HB3	1.88	0.55	
1:B:441:ARG:NH2	1:B:454:ASP:O	2.39	0.54	
1:D:441:ARG:NH2	1:D:454:ASP:O	2.41	0.54	
2:F:100:TRP:HD1	2:F:102:GLY:H	1.54	0.54	
2:F:100:TRP:HD1	2:F:102:GLY:N	2.06	0.54	
1:B:388:VAL:HG22	1:B:495:ARG:HG2	1.90	0.53	
1:D:379:PHE:O	1:D:509:THR:N	2.42	0.53	



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:G:66:ARG:NH1	2:G:84:SER:O	2.42	0.53
2:E:33:ALA:HA	2:E:71:ARG:HH12	1.74	0.52
2:E:39:GLN:HB2	2:E:45:ARG:HB3	1.90	0.52
2:F:33:ALA:HA	2:F:71:ARG:HH12	1.73	0.52
1:C:385:ASP:OD2	1:C:410:TYR:OH	2.22	0.52
1:D:444:ARG:HH21	1:D:454:ASP:HB2	1.75	0.52
1:A:353:SER:HA	1:A:356:TYR:CE2	2.45	0.52
2:F:96:ALA:HB2	2:F:113:TRP:CE3	2.44	0.52
1:C:388:VAL:HG22	1:C:495:ARG:HG2	1.91	0.51
2:G:34:LEU:HD12	2:G:71:ARG:CZ	2.40	0.51
1:B:395:ARG:NE	2:F:108:PHE:O	2.43	0.51
2:E:5:VAL:O	2:E:22:CYS:HA	2.10	0.51
2:G:3:GLN:HB3	2:G:25[A]:SER:HB2	1.92	0.51
2:G:3:GLN:HB3	2:G:25[B]:SER:HB2	1.92	0.51
2:F:68:THR:O	2:F:81:GLN:N	2.34	0.51
2:F:5:VAL:O	2:F:22:CYS:HA	2.11	0.50
1:A:448:LEU:HD22	1:A:452:GLU:HB3	1.93	0.50
1:D:366:CYS:HA	1:D:419:CYS:HA	1.94	0.50
1:B:380:SER:HA	1:B:508:ALA:HA	1.93	0.50
2:F:24:ALA:HB1	2:F:27:PHE:CE1	2.46	0.50
2:G:71:ARG:HA	2:G:78:VAL:HA	1.94	0.50
1:C:328:VAL:HG22	1:C:343:LYS:HD3	1.92	0.50
2:H:71:ARG:CB	2:H:78:VAL:HG12	2.42	0.50
2:G:1:GLN:HA	2:G:27:PHE:HE2	1.77	0.49
1:C:379:PHE:O	1:C:509:THR:N	2.45	0.49
1:D:385:ASP:OD2	1:D:410:TYR:OH	2.26	0.49
1:D:353:SER:HA	1:D:356:TYR:CE2	2.47	0.49
1:A:366:CYS:HA	1:A:419:CYS:HA	1.95	0.49
1:A:399:PRO:HB3	1:A:414:ASP:HA	1.94	0.49
2:F:100:TRP:HZ3	2:F:109:ASP:O	1.95	0.49
2:H:52:ASP:OD1	2:H:103:ARG:HA	2.13	0.48
1:C:409:ASN:ND2	1:C:441:ARG:O	2.36	0.48
1:C:378:CYS:HA	1:C:511:CYS:HA	1.95	0.48
2:F:34:LEU:HD13	2:F:78:VAL:CG2	2.42	0.48
2:H:95:CYS:O	2:H:114:GLY:N	2.46	0.48
1:D:413:PRO:HD3	1:D:450:PRO:HB3	1.95	0.48
2:G:51:ILE:HD12	2:G:56:ASN:O	2.14	0.48
1:A:459:PRO:HG3	1:A:469:PRO:HG3	1.96	0.48
2:E:12:VAL:HG11	2:E:18:LEU:HG	1.94	0.48
1:C:396:GLN:HB3	1:C:406:ALA:HB2	1.96	0.48
2:E:52:ASP:OD1	2:E:53:SER:N	2.45	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:12:VAL:HG12	2:H:13:GLN:H	1.80	0.47
1:A:337:VAL:HA	1:A:387:PHE:HB2	1.97	0.47
1:C:413:PRO:HB2	1:C:415:ASP:OD1	2.15	0.47
2:E:39:GLN:NE2	2:E:43:LYS:O	2.48	0.47
1:B:385:ASP:OD2	1:B:410:TYR:OH	2.27	0.47
1:C:337:VAL:HG22	1:C:409:ASN:HB3	1.97	0.47
1:C:396:GLN:OE1	1:C:405:ILE:HG23	2.15	0.47
2:E:6:GLU:HG3	2:E:22:CYS:HB2	1.95	0.47
1:A:443:LEU:HD13	1:A:460:PHE:CD2	2.51	0.46
2:H:5:VAL:O	2:H:22:CYS:HA	2.14	0.46
2:F:75:LYS:HA	2:F:75:LYS:HD2	1.65	0.46
2:H:100:TRP:HE3	2:H:104:SER:HG	1.63	0.46
2:E:51:ILE:HG21	2:E:71:ARG:HG3	1.98	0.46
1:B:483:PHE:CE2	1:B:493:PRO:HB3	2.50	0.46
2:H:6:GLU:CD	2:H:115:GLN:H	2.18	0.46
1:C:320:THR:OG1	1:C:321:ASN:N	2.48	0.46
1:C:399:PRO:HB3	1:C:414:ASP:HA	1.98	0.46
2:E:96:ALA:HB2	2:E:113:TRP:CE3	2.51	0.46
1:A:483:PHE:CE2	1:A:493:PRO:HB3	2.51	0.45
1:A:398:ALA:HB3	1:A:401:GLN:HG3	1.99	0.45
1:A:459:PRO:CG	1:A:469:PRO:HG3	2.46	0.45
1:C:413:PRO:HA	2:F:28:THR:O	2.17	0.45
1:D:337:VAL:HA	1:D:387:PHE:HB2	1.99	0.45
2:E:51:ILE:HA	2:E:57:PRO:HA	1.99	0.45
1:D:459:PRO:HB2	1:D:467:CYS:O	2.17	0.44
1:A:337:VAL:HG22	1:A:409:ASN:HB3	2.00	0.44
1:D:321:ASN:ND2	1:D:347:ASN:O	2.40	0.44
1:A:406:ALA:HA	1:A:410:TYR:O	2.18	0.44
1:B:425:THR:HG21	1:B:495:ARG:HD2	2.00	0.44
1:C:337:VAL:HA	1:C:387:PHE:HB2	1.99	0.44
2:G:58:PHE:CE2	2:G:103:ARG:HG2	2.53	0.44
1:D:356:TYR:O	2:E:103:ARG:NH2	2.50	0.44
2:E:66:ARG:HH22	2:E:89:ASP:CG	2.21	0.44
2:F:3:GLN:HB3	2:F:25[B]:SER:HB2	2.00	0.44
2:H:4:LEU:HB2	2:H:114:GLY:HA2	1.99	0.44
1:A:393:ASP:HB3	1:A:405:ILE:HG13	2.00	0.44
1:A:363:THR:HG23	2:H:105:LEU:HG	1.99	0.43
2:H:22:CYS:HB3	2:H:78:VAL:CG2	2.48	0.43
2:H:66:ARG:NH1	2:H:84:SER:O	2.51	0.43
2:F:12:VAL:HG12	2:F:13:GLN:H	1.83	0.43
1:A:365:LYS:HG3	1:A:420:VAL:HB	2.01	0.43



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Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:11:LEU:HD11	2:F:122:SER:HB3	2.01	0.43
2:G:51:ILE:HD12	2:G:56:ASN:C	2.38	0.43
2:G:111:ASP:N	2:G:111:ASP:OD1	2.48	0.43
2:F:3:GLN:HB3	2:F:25[A]:SER:HB2	2.00	0.43
2:F:34:LEU:HD12	2:F:71:ARG:CZ	2.49	0.43
2:F:100:TRP:CZ3	2:F:109:ASP:O	2.71	0.43
2:G:100:TRP:HD1	2:G:102:GLY:N	2.15	0.43
2:F:1:GLN:HB3	2:F:2:VAL:H	1.70	0.43
1:B:336:SER:HB3	1:B:439:LYS:O	2.18	0.42
1:C:390:LYS:O	1:C:394:VAL:HG23	2.18	0.42
2:H:34:LEU:HB3	2:H:78:VAL:HG11	2.00	0.42
1:B:468:THR:N	1:B:469:PRO:CD	2.82	0.42
1:C:445:HIS:NE2	1:C:461:SER:O	2.50	0.42
1:C:399:PRO:HG3	1:C:416:PHE:HB3	2.01	0.42
1:A:445:HIS:NE2	1:A:461:SER:O	2.52	0.42
1:C:449:ARG:HG3	1:C:452:GLU:OE1	2.20	0.42
1:D:378:CYS:HA	1:D:511:CYS:HA	2.02	0.42
1:D:439:LYS:HD3	1:D:480:ASP:HB3	2.02	0.42
1:B:395:ARG:HH21	2:F:110:TYR:H	1.67	0.42
2:G:4:LEU:HD23	2:G:24:ALA:HA	2.02	0.42
2:H:61:ASP:HA	2:H:64:LYS:HG3	2.02	0.42
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.23	0.42
1:C:441:ARG:NH2	1:C:454:ASP:O	2.52	0.41
1:C:448:LEU:HD22	1:C:452:GLU:HB3	2.02	0.41
1:D:487:THR:HB	1:D:491:TYR:HB2	2.01	0.41
1:C:336:SER:HB3	1:C:439:LYS:O	2.21	0.41
1:C:366:CYS:HA	1:C:419:CYS:HA	2.02	0.41
1:C:483:PHE:CE2	1:C:493:PRO:HB3	2.54	0.41
2:G:96:ALA:HB2	2:G:113:TRP:CZ3	2.56	0.41
2:H:40:ALA:HB3	2:H:43:LYS:HD3	2.01	0.41
1:B:353:SER:HB3	1:B:375:ASN:ND2	2.35	0.41
1:A:385:ASP:OD2	1:A:410:TYR:OH	2.23	0.41
1:D:483:PHE:CE2	1:D:493:PRO:HB3	2.55	0.41
1:D:390:LYS:O	1:D:394:VAL:HG23	2.20	0.41
1:B:353:SER:N	1:B:375:ASN:OD1	2.54	0.41
2:E:104:SER:O	2:E:110:TYR:OH	2.25	0.41
1:B:334:PHE:HB3	1:B:388:VAL:HG23	2.03	0.41
2:G:68:THR:O	2:G:81:GLN:N	2.45	0.41
2:F:17:SER:HA	2:F:82:MET:O	2.20	0.41
1:B:461:SER:HB3	1:B:467:CYS:SG	2.61	0.40
1:C:352:TYR:N	1:C:375:ASN:OD1	2.54	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:SER:HA	1:D:356:TYR:CZ	2.56	0.40
2:G:51:ILE:HG12	2:G:71:ARG:HG3	2.03	0.40
1:A:378:CYS:HA	1:A:511:CYS:HA	2.02	0.40
1:A:421:LEU:O	1:A:496:VAL:HA	2.21	0.40
2:F:52:ASP:O	2:F:71:ARG:NH1	2.54	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	Perce	ntiles
1	А	182/204~(89%)	177 (97%)	5(3%)	0	100	100
1	В	192/204~(94%)	185 (96%)	7 (4%)	0	100	100
1	С	184/204~(90%)	178 (97%)	6 (3%)	0	100	100
1	D	184/204~(90%)	178 (97%)	6 (3%)	0	100	100
2	Е	121/123~(98%)	113 (93%)	8 (7%)	0	100	100
2	F	122/123~(99%)	112 (92%)	10 (8%)	0	100	100
2	G	123/123~(100%)	114 (93%)	9~(7%)	0	100	100
2	Н	121/123~(98%)	112 (93%)	9~(7%)	0	100	100
All	All	1229/1308~(94%)	1169 (95%)	60 (5%)	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 side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	162/179~(90%)	161~(99%)	1 (1%)	86 93
1	В	169/179~(94%)	169 (100%)	0	100 100
1	С	164/179~(92%)	163 (99%)	1 (1%)	86 93
1	D	164/179~(92%)	163 (99%)	1 (1%)	86 93
2	Е	98/98~(100%)	96~(98%)	2 (2%)	55 77
2	F	100/98~(102%)	99~(99%)	1 (1%)	76 87
2	G	99/98~(101%)	97~(98%)	2 (2%)	55 77
2	Н	97/98~(99%)	95~(98%)	2 (2%)	53 77
All	All	1053/1108~(95%)	1043 (99%)	10 (1%)	76 89

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	A	352	TYR
1	С	364	PHE
1	D	334	PHE
2	Е	22	CYS
2	Е	101	TYR
2	F	22	CYS
2	G	32	TYR
2	G	73	ASN
2	Н	22	CYS
2	Н	73	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	381	ASN
1	А	409	ASN
1	А	473	ASN
1	В	347	ASN
1	В	473	ASN
1	С	381	ASN
1	D	473	ASN
2	Е	81	GLN
2	Е	115	GLN



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Mol	Chain	Res	Type
2	F	13	GLN
2	F	76	ASN
2	F	106	ASN
2	F	115	GLN
2	G	81	GLN
2	Н	13	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 monosaccharides 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,  $95^{th}$  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	$<$ <b>RSRZ</b> $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	186/204 (91%)	0.88	24 (12%) 3 4	73, 95, 145, 155	0
1	В	194/204~(95%)	0.75	19 (9%) 7 9	72, 95, 141, 147	0
1	С	188/204~(92%)	0.70	15 (7%) 12 14	84, 101, 137, 153	0
1	D	187/204 (91%)	0.77	14 (7%) 14 17	80, 96, 137, 148	0
2	Е	123/123~(100%)	0.91	14 (11%) 5 6	76, 90, 105, 117	0
2	F	123/123~(100%)	0.82	6 (4%) 29 33	80, 94, 105, 118	0
2	G	123/123~(100%)	0.83	13 (10%) 6 8	83, 100, 114, 122	0
2	Н	121/123~(98%)	0.95	15 (12%) 4 5	92, 104, 114, 120	0
All	All	1245/1308 (95%)	0.81	120 (9%) 8 10	72, 97, 137, 155	0

Mol	Chain	Res	Type	RSRZ
2	Н	10	GLY	5.7
2	Е	54	ASP	5.5
1	В	511	CYS	5.0
2	Н	59	TYR	4.6
1	D	417	MET	4.6
1	В	393	ASP	4.5
2	Н	27	PHE	4.3
2	G	10	GLY	4.3
1	А	350	ALA	4.2
2	G	28	THR	4.1
1	D	356	TYR	3.9
1	D	446	GLY	3.7
1	С	350	ALA	3.6
1	D	429	ASP	3.5
2	G	88	GLU	3.5
1	В	484	TYR	3.5



Mol	Chain	Res	Type	RSRZ
2	Е	120	THR	3.5
1	А	487	THR	3.4
1	С	325	PHE	3.4
1	В	508	ALA	3.3
2	Н	70	SER	3.2
2	Н	44	GLU	3.2
1	В	468	THR	3.2
2	Н	37	PHE	3.2
1	С	499	LEU	3.1
2	F	79	TYR	3.1
1	А	421	LEU	3.1
1	А	367	TYR	3.1
1	D	483	PHE	3.1
1	А	369	VAL	3.1
1	А	363	THR	3.1
1	А	496	VAL	3.0
2	Н	60	ALA	2.9
1	А	352	TYR	2.9
1	D	508	ALA	2.9
1	В	483	PHE	2.9
1	А	419	CYS	2.8
1	А	366	CYS	2.8
1	D	444	ARG	2.8
2	Н	38	ARG	2.8
2	G	122	SER	2.8
2	Н	36	TRP	2.7
2	G	42	GLY	2.7
1	В	421	LEU	2.7
1	D	460	PHE	2.7
1	В	438	TYR	2.7
1	С	484	TYR	2.7
2	Е	80	LEU	2.6
1	В	394	VAL	2.6
1	С	483	PHE	2.6
2	E	97	ALA	2.6
1	С	419	CYS	2.6
1	В	497	VAL	2.6
1	С	498	VAL	2.6
1	В	412	LEU	2.6
1	С	468	THR	2.5
1	А	486	THR	2.5
1	D	481	TYR	2.5



Mol	Chain	Res	Type	RSRZ
1	D	422	ALA	2.5
1	D	418	GLY	2.4
2	G	50	CYS	2.4
1	А	417	MET	2.4
1	D	487	THR	2.4
2	Е	119	VAL	2.4
1	А	356	TYR	2.4
1	С	397	ILE	2.4
2	Е	10	GLY	2.4
1	А	509	THR	2.4
2	Е	55	GLY	2.4
1	С	329	PHE	2.4
1	А	381	ASN	2.3
1	А	438	TYR	2.3
1	В	500	SER	2.3
2	F	19	ARG	2.3
1	С	487	THR	2.3
2	G	120	THR	2.3
1	С	387	PHE	2.3
2	Е	45	ARG	2.3
1	В	417	MET	2.3
1	С	443	LEU	2.3
2	G	82	MET	2.3
1	В	452	GLU	2.3
2	Н	54	ASP	2.2
2	F	40	ALA	2.2
2	Н	106	ASN	2.2
2	Н	117	THR	2.2
1	В	487	THR	2.2
2	Н	61	ASP	2.2
1	С	476	TRP	2.2
2	G	37	PHE	2.2
2	Е	36	TRP	2.2
1	В	371	ALA	2.2
2	G	110	TYR	2.2
2	Е	56	ASN	2.2
2	G	74	ALA	2.2
2	F	69	GLY	2.1
1	А	484	TYR	2.1
2	F	113	TRP	2.1
2	Н	9	GLY	2.1
1	А	440	TYR	2.1



Mol	Chain	Res	Type	RSRZ
1	С	485	THR	2.1
1	А	389	VAL	2.1
1	D	376	ASP	2.1
1	А	320	THR	2.1
2	F	80	LEU	2.1
2	Е	44	GLU	2.1
2	Е	100	TRP	2.1
1	А	483	PHE	2.1
1	А	489	ILE	2.1
1	В	481	TYR	2.0
1	А	324	PRO	2.0
2	G	113	TRP	2.0
2	Н	39[A]	GLN	2.0
1	В	489	ILE	2.0
1	А	386	SER	2.0
1	D	445	HIS	2.0
2	G	27	PHE	2.0
2	Е	82	MET	2.0
1	В	471	ALA	2.0
2	Е	110	TYR	2.0

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### 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.

