



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:48 PM GMT

PDB ID : 1FVC  
Title : X-RAY STRUCTURES OF THE ANTIGEN-BINDING DOMAINS FROM  
THREE VARIANTS OF HUMANIZED ANTI-P185-HER2 ANTIBODY 4D5  
AND COMPARISON WITH MOLECULAR MODELING  
Authors : Eigenbrot, C.; Randal, M.; Kossiakoff, A.A.; Presta, L.  
Deposited on : 1992-10-20  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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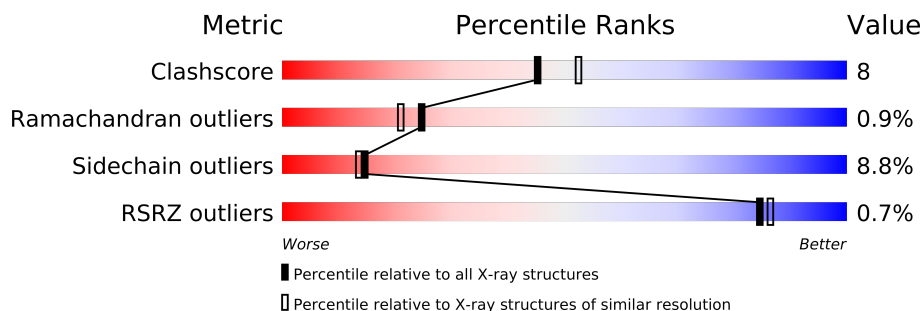
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	109	
1	C	109	
2	B	120	
2	D	120	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3647 atoms, of which 0 are hydrogen and 0 are deuterium.

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 IGG1-KAPPA 4D5 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			835	526	139	167	3			
1	C	108	Total	C	N	O	S	4	0	0
			828	522	138	165	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	SER	CONFLICT	GB 185985
A	29	VAL	ILE	CONFLICT	GB 185985
A	30	ASN	SER	CONFLICT	GB 185985
A	31	THR	SER	CONFLICT	GB 185985
A	32	ALA	TYR	CONFLICT	GB 185985
A	33	VAL	LEU	CONFLICT	GB 185985
A	34	ALA	ASN	CONFLICT	GB 185985
A	50	SER	ALA	CONFLICT	GB 185985
A	53	PHE	SER	CONFLICT	GB 185985
A	55	TYR	GLN	CONFLICT	GB 185985
A	66	ARG	GLY	CONFLICT	GB 185985
A	91	HIS	SER	CONFLICT	GB 185985
A	93	THR	SER	CONFLICT	GB 185985
A	?	-	TRP	DELETION	GB 185985
C	28	ASP	SER	CONFLICT	GB 185985
C	29	VAL	ILE	CONFLICT	GB 185985
C	30	ASN	SER	CONFLICT	GB 185985
C	31	THR	SER	CONFLICT	GB 185985
C	32	ALA	TYR	CONFLICT	GB 185985
C	33	VAL	LEU	CONFLICT	GB 185985
C	34	ALA	ASN	CONFLICT	GB 185985
C	50	SER	ALA	CONFLICT	GB 185985
C	53	PHE	SER	CONFLICT	GB 185985
C	55	TYR	GLN	CONFLICT	GB 185985
C	66	ARG	GLY	CONFLICT	GB 185985

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Chain	Residue	Modelled	Actual	Comment	Reference
C	91	HIS	SER	CONFLICT	GB 185985
C	93	THR	SER	CONFLICT	GB 185985
C	?	-	TRP	DELETION	GB 185985

- Molecule 2 is a protein called IGG1-KAPPA 4D5 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	4	0	0
			929	586	160	179	4			
2	D	120	Total	C	N	O	S	0	0	0
			929	586	160	179	4			

- Molecule 3 is water.

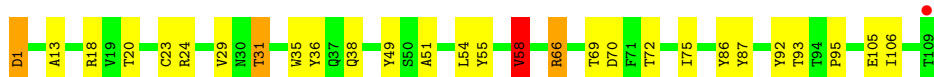
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	23	Total	O	0	0
			23	23		
3	C	31	Total	O	0	0
			31	31		
3	D	25	Total	O	0	0
			25	25		

### 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.

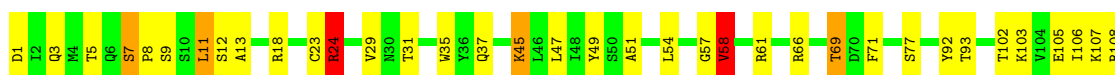
- Molecule 1: IGG1-KAPPA 4D5 FV (LIGHT CHAIN)

Chain A: 



- Molecule 1: IGG1-KAPPA 4D5 FV (LIGHT CHAIN)

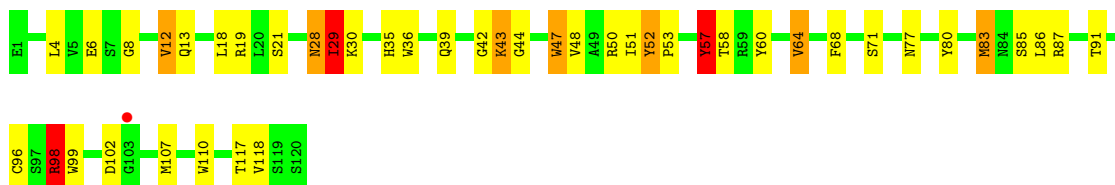
Chain C: 



THR

- Molecule 2: IGG1-KAPPA 4D5 FV (HEAVY CHAIN)

Chain B: 



- Molecule 2: IGG1-KAPPA 4D5 FV (HEAVY CHAIN)

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.60Å 63.40Å 90.20Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 9.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 80.5 (9.96-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.183 , (Not available) 0.177 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 17110 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.00% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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	0.89	1/855 (0.1%)	1.71	21/1164 (1.8%)
1	C	0.86	0/848	1.70	18/1154 (1.6%)
2	B	0.89	0/952	1.84	27/1291 (2.1%)
2	D	0.96	0/952	1.80	24/1291 (1.9%)
All	All	0.90	1/3607 (0.0%)	1.77	90/4900 (1.8%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	VAL	CB-CG1	-5.04	1.42	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	LEU	CA-CB-CG	10.58	139.63	115.30
1	A	35	TRP	CD1-CG-CD2	10.45	114.66	106.30
2	D	57	TYR	CB-CG-CD2	-9.61	115.23	121.00
2	D	47	TRP	CD1-CG-CD2	9.04	113.53	106.30
1	A	35	TRP	CG-CD2-CE3	8.91	141.91	133.90
2	D	59	ARG	NE-CZ-NH1	8.64	124.62	120.30
2	B	80	TYR	CB-CG-CD1	-8.55	115.87	121.00
1	C	24	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	B	83	MET	CG-SD-CE	-8.46	86.66	100.20
1	A	35	TRP	CE2-CD2-CG	-8.34	100.62	107.30
2	B	98	ARG	NE-CZ-NH2	-8.03	116.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	D	110	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	C	35	TRP	CD1-CG-CD2	7.73	112.48	106.30
2	B	52	TYR	CB-CG-CD2	-7.70	116.38	121.00
2	B	19	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	B	98	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	D	110	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	B	47	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	C	92	TYR	CB-CG-CD2	-7.32	116.61	121.00
2	B	64	VAL	N-CA-CB	-7.27	95.51	111.50
1	C	35	TRP	CE2-CD2-CG	-7.25	101.50	107.30
2	D	38	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	35	TRP	CG-CD1-NE1	-7.15	102.95	110.10
2	D	33	TYR	CB-CG-CD2	-7.14	116.72	121.00
2	B	47	TRP	CG-CD2-CE3	7.13	140.32	133.90
2	D	99	TRP	CD1-CG-CD2	6.95	111.86	106.30
2	B	36	TRP	CD1-CG-CD2	6.93	111.85	106.30
1	A	23	CYS	CA-CB-SG	-6.88	101.63	114.00
2	B	99	TRP	CD1-CG-CD2	6.86	111.79	106.30
2	B	47	TRP	CD1-CG-CD2	6.86	111.79	106.30
2	D	60	TYR	CB-CG-CD1	-6.82	116.91	121.00
2	B	36	TRP	CE2-CD2-CG	-6.74	101.91	107.30
2	D	47	TRP	CG-CD1-NE1	-6.71	103.39	110.10
1	A	18	ARG	NE-CZ-NH2	-6.69	116.95	120.30
2	D	80	TYR	CB-CG-CD2	-6.66	117.00	121.00
2	B	110	TRP	CD1-CG-CD2	6.62	111.59	106.30
2	B	48	VAL	CG1-CB-CG2	-6.59	100.35	110.90
2	D	110	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	C	29	VAL	N-CA-CB	-6.56	97.07	111.50
2	B	19	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	24	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	D	47	TRP	CE2-CD2-CG	-6.40	102.18	107.30
2	D	99	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	A	69	THR	N-CA-CB	-6.30	98.32	110.30
2	B	29	ILE	CA-CB-CG1	-6.21	99.19	111.00
2	B	99	TRP	CE2-CD2-CG	-6.19	102.35	107.30
2	B	110	TRP	CE2-CD2-CG	-6.17	102.37	107.30
1	C	49	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	A	1	ASP	CA-C-N	-6.13	103.71	117.20
2	B	57	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	A	86	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	C	35	TRP	CG-CD2-CE3	6.05	139.35	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	GLY	CA-C-N	6.04	130.50	117.20
2	B	43	LYS	N-CA-C	6.04	127.31	111.00
1	A	66	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	D	110	TRP	CB-CG-CD1	-6.02	119.18	127.00
1	A	31	THR	N-CA-CB	-5.93	99.03	110.30
2	D	59	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	C	35	TRP	CB-CG-CD1	-5.91	119.32	127.00
2	D	68	PHE	CB-CG-CD2	-5.89	116.67	120.80
1	A	49	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	C	24	ARG	CA-CB-CG	5.72	125.98	113.40
1	C	69	THR	CA-CB-CG2	5.71	120.39	112.40
1	C	69	THR	N-CA-CB	-5.61	99.64	110.30
2	B	4	LEU	CA-CB-CG	5.60	128.18	115.30
2	B	102	ASP	CA-C-N	-5.58	105.05	116.20
1	C	35	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	A	35	TRP	CB-CG-CD1	-5.48	119.88	127.00
2	D	57	TYR	CB-CG-CD1	5.46	124.28	121.00
1	A	87	TYR	CD1-CG-CD2	5.46	123.90	117.90
2	D	36	TRP	CD1-CG-CD2	5.37	110.59	106.30
2	B	13	GLN	CB-CG-CD	5.25	125.26	111.60
1	A	75	ILE	N-CA-C	-5.25	96.81	111.00
1	C	58	VAL	CG1-CB-CG2	5.19	119.21	110.90
1	C	45	LYS	CA-CB-CG	5.16	124.75	113.40
2	D	19	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	87	TYR	CG-CD1-CE1	-5.14	117.19	121.30
2	D	36	TRP	CE2-CD2-CG	-5.12	103.20	107.30
2	D	2	VAL	CA-CB-CG1	-5.11	103.23	110.90
1	A	58	VAL	CG1-CB-CG2	-5.11	102.73	110.90
2	B	60	TYR	CB-CA-C	-5.09	100.22	110.40
1	A	92	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	36	TYR	CB-CG-CD1	-5.07	117.96	121.00
2	B	36	TRP	CG-CD2-CE3	5.06	138.46	133.90
2	B	47	TRP	CB-CG-CD1	-5.06	120.42	127.00
1	A	92	TYR	N-CA-CB	-5.06	101.50	110.60
1	C	18	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	D	114	THR	CA-CB-CG2	-5.04	105.35	112.40
2	D	101	GLY	O-C-N	5.02	130.73	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	57	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	835	0	810	9	0
1	C	828	0	803	12	0
2	B	929	0	885	21	0
2	D	929	0	885	18	0
3	A	47	0	0	1	0
3	B	23	0	0	0	0
3	C	31	0	0	0	0
3	D	25	0	0	0	0
All	All	3647	0	3383	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:51:ILE:HG13	2:D:58:THR:HG22	1.63	0.80
2:D:35:HIS:HD2	2:D:47:TRP:HE1	1.30	0.77
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.32	0.75
1:A:38:GLN:HE22	2:B:39:GLN:HE22	1.42	0.68
2:D:11:LEU:HD21	2:D:119:SER:HB3	1.78	0.64
1:C:7:SER:HB2	1:C:24:ARG:HH22	1.64	0.62
2:B:91:THR:HG23	2:B:117:THR:HA	1.85	0.58
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.86	0.57
2:D:30:LYS:HB3	2:D:54:THR:HG23	1.85	0.57
2:B:51:ILE:HA	2:B:57:TYR:O	2.05	0.56
2:D:28:ASN:HB3	2:D:30:LYS:HE3	1.89	0.55
1:A:54:LEU:HD22	1:A:58:VAL:HG22	1.88	0.55
2:B:6:GLU:HA	2:B:21:SER:O	2.07	0.54
1:C:66:ARG:HG3	1:C:71:PHE:CE1	2.43	0.53
2:D:62:ASP:HA	2:D:65:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:12:VAL:HG21	2:D:18:LEU:HD22	1.90	0.52
2:B:28:ASN:HA	2:B:77:ASN:HD21	1.75	0.52
2:B:35:HIS:HD2	2:B:47:TRP:NE1	2.06	0.51
1:C:107:LYS:HG3	1:C:108:ARG:N	2.26	0.51
1:C:31:THR:HG22	1:C:66:ARG:HD2	1.93	0.50
1:A:95:PRO:HB3	2:B:47:TRP:CE3	2.46	0.50
1:C:5:THR:O	1:C:23:CYS:HA	2.12	0.49
1:C:12:SER:HA	1:C:105:GLU:O	2.12	0.49
2:B:29:ILE:HG23	2:B:53:PRO:HG2	1.95	0.49
1:A:13:ALA:O	1:A:106:ILE:HA	2.13	0.48
2:B:42:GLY:H	2:B:43:LYS:NZ	2.10	0.48
2:D:52:TYR:HB3	2:D:55:ASN:HD21	1.78	0.48
2:D:35:HIS:CD2	2:D:47:TRP:HE1	2.20	0.48
2:B:30:LYS:HA	2:B:53:PRO:HB2	1.95	0.48
2:D:43:LYS:HD2	2:D:43:LYS:N	2.28	0.48
2:B:35:HIS:O	2:B:96:CYS:HA	2.13	0.47
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.97	0.47
2:D:94:TYR:O	2:D:113:GLY:HA2	2.15	0.47
1:C:61:ARG:HD2	1:C:77:SER:O	2.15	0.47
2:B:50:ARG:O	2:B:58:THR:HA	2.15	0.47
1:A:1:ASP:HB2	1:A:95:PRO:HD2	1.97	0.46
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.98	0.46
1:A:54:LEU:CD2	1:A:58:VAL:HG22	2.45	0.46
1:A:20:THR:HG23	1:A:72:THR:HG23	1.98	0.45
3:A:129:HOH:O	2:B:44:GLY:HA3	2.17	0.45
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.82	0.44
2:B:12:VAL:O	2:B:118:VAL:HA	2.18	0.44
2:B:51:ILE:HG12	2:B:52:TYR:N	2.33	0.44
2:B:8:GLY:O	2:B:18:LEU:HD22	2.17	0.43
1:A:55:TYR:O	1:A:58:VAL:HG12	2.18	0.43
2:D:85:SER:HB3	2:D:87:ARG:NH1	2.34	0.43
1:C:13:ALA:O	1:C:106:ILE:HA	2.18	0.43
2:D:6:GLU:HA	2:D:21:SER:O	2.19	0.43
2:B:98:ARG:O	2:B:107:MET:HA	2.19	0.42
2:B:64:VAL:HG22	2:B:68:PHE:CE2	2.55	0.42
2:D:76:LYS:HE2	2:D:76:LYS:HB3	1.86	0.42
1:C:54:LEU:HG	1:C:58:VAL:HG22	2.01	0.42
1:A:1:ASP:HB2	1:A:95:PRO:CD	2.51	0.41
2:B:64:VAL:HG13	2:B:68:PHE:HB2	2.01	0.41
2:D:58:THR:O	2:D:59:ARG:HD3	2.21	0.40
1:C:107:LYS:HG3	1:C:108:ARG:H	1.86	0.40
1:C:9:SER:O	1:C:102:THR:HA	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:68:PHE:CD1	2:D:68:PHE:N	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	107/109 (98%)	102 (95%)	4 (4%)	1 (1%)	25	21
1	C	106/109 (97%)	98 (92%)	7 (7%)	1 (1%)	25	21
2	B	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
2	D	118/120 (98%)	110 (93%)	6 (5%)	2 (2%)	14	8
All	All	449/458 (98%)	422 (94%)	23 (5%)	4 (1%)	25	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	ALA
2	D	2	VAL
2	D	102	ASP
1	A	51	ALA

### 5.3.2 Protein sidechains ⓘ

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	94/95 (99%)	86 (92%)	8 (8%)	15	14
1	C	93/95 (98%)	82 (88%)	11 (12%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	95/95 (100%)	88 (93%)	7 (7%)	20	19
2	D	95/95 (100%)	88 (93%)	7 (7%)	20	19
All	All	377/380 (99%)	344 (91%)	33 (9%)	14	13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	29	VAL
1	A	31	THR
1	A	58	VAL
1	A	66	ARG
1	A	70	ASP
1	A	93	THR
1	A	105	GLU
2	B	12	VAL
2	B	28	ASN
2	B	29	ILE
2	B	71	SER
2	B	85	SER
2	B	87	ARG
2	B	98	ARG
1	C	1	ASP
1	C	3	GLN
1	C	7	SER
1	C	8	PRO
1	C	11	LEU
1	C	24	ARG
1	C	45	LYS
1	C	58	VAL
1	C	69	THR
1	C	93	THR
1	C	103	LYS
2	D	11	LEU
2	D	30	LYS
2	D	43	LYS
2	D	54	THR
2	D	55	ASN
2	D	98	ARG
2	D	114	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	28	ASN
2	B	35	HIS
2	B	39	GLN
2	D	3	GLN
2	D	35	HIS
2	D	55	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	109/109 (100%)	-0.69	1 (0%) 81 82	7, 18, 39, 70	0
1	C	108/109 (99%)	-0.71	0 100 100	7, 19, 36, 47	1 (0%)
2	B	120/120 (100%)	-0.37	1 (0%) 83 85	10, 25, 50, 72	1 (0%)
2	D	120/120 (100%)	-0.42	1 (0%) 83 85	8, 26, 51, 65	0
All	All	457/458 (99%)	-0.54	3 (0%) 84 86	7, 22, 46, 72	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	THR	2.6
2	D	120	SER	2.3
2	B	103	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.