Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:49 AM GMT

PDB ID	:	3G5X
Title	:	Antibodies Specifically Targeting a Locally Misfolded Region of Tumor Associated EGFR
Authors	:	Garrett, T.P.J.; Burgess, A.W.
Deposited on	:	2009-02-05
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

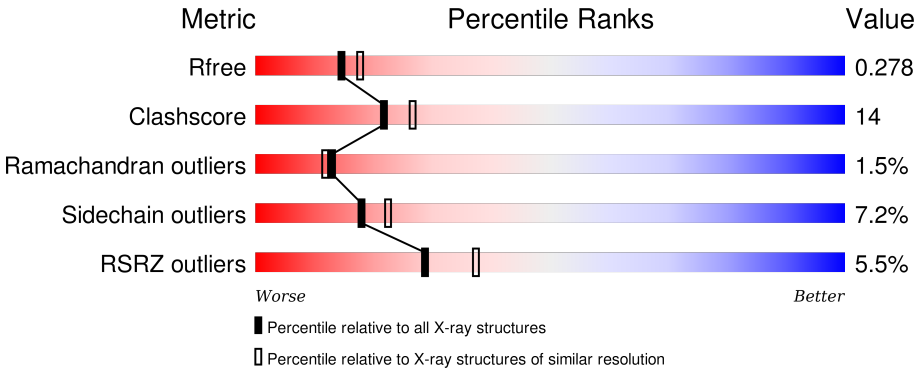
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 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	214	3% 70% 28%
1	C	214	5% 66% 30%
2	B	216	7% 75% 21%
2	D	216	6% 72% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6788 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 806 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1655	1028	273	346	8			
1	C	214	Total	C	N	O	S	0	0	0
			1655	1028	273	346	8			

- Molecule 2 is a protein called 806 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1635	1035	264	329	7			
2	D	216	Total	C	N	O	S	0	0	0
			1635	1035	264	329	7			

- Molecule 3 is water.

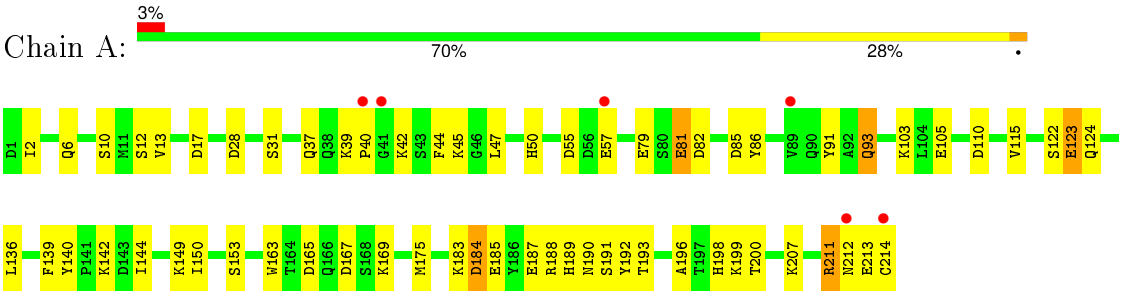
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	48	Total	O	0	0
			48	48		
3	C	54	Total	O	0	0
			54	54		
3	D	46	Total	O	0	0
			46	46		

3 Residue-property plots (i)

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.

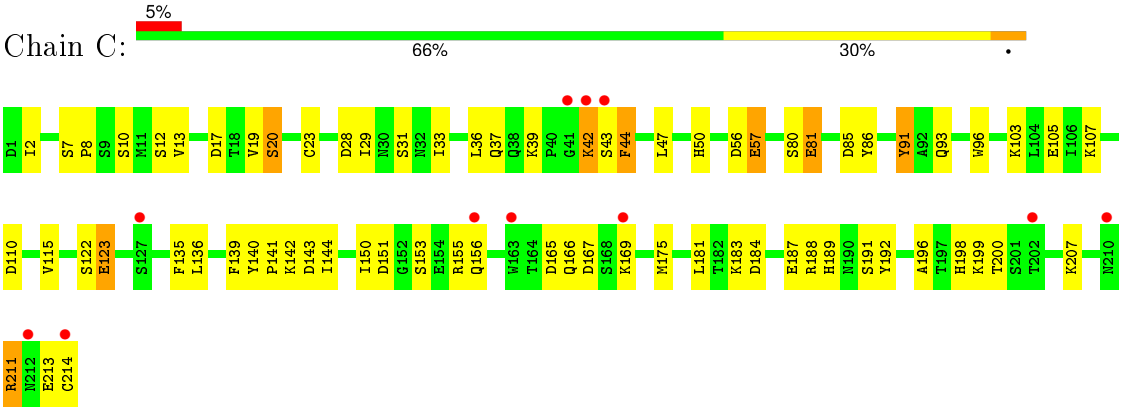
- Molecule 1: 806 light chain

Chain A:



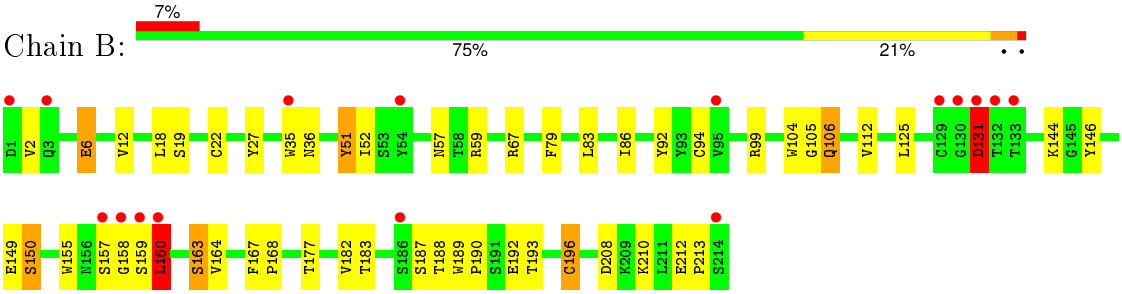
- Molecule 1: 806 light chain

Chain C:



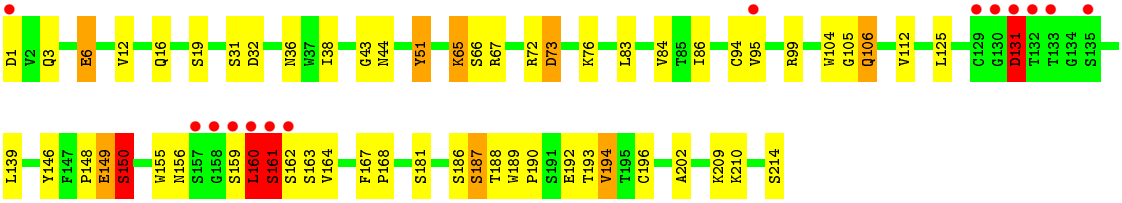
- Molecule 2: 806 heavy chain

Chain B:



- Molecule 2: 806 heavy chain

Chain D:


D1 V2 Q3 E6 V12 Q16 S19 S31 D32 N36 W37 I38 G43 N44 Y51 K65 S66 R67 R72 D73 K76 L83 V84 T85 I86 C94 V95 R99 W104 G105 Q106 V112 L125 C129 G130 D131 T132 T133 G134 S135
L139 Y146 F147 P148 E149 S150 W155 N156 S157 G158 S159 L160 S161 S162 S163 V164 F167 P168 S181 S186 S187 T188 W189 P190 S191 E192 T193 V194 T195 C196 A202 K209 K210 S214

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.37Å 74.62Å 83.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.30) 99.0 (19.98-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.225 , 0.289 0.219 , 0.278	Depositor DCC
R_{free} test set	2011 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 39408 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6788	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.27 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.9893e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

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	1.11	6/1693 (0.4%)	0.97	5/2296 (0.2%)
1	C	1.13	8/1693 (0.5%)	0.92	2/2296 (0.1%)
2	B	1.07	4/1680 (0.2%)	0.91	1/2302 (0.0%)
2	D	1.08	2/1680 (0.1%)	0.91	2/2302 (0.1%)
All	All	1.10	20/6746 (0.3%)	0.93	10/9196 (0.1%)

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	2
2	D	0	2
All	All	0	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	91	TYR	CE2-CZ	-10.82	1.24	1.38
1	C	192	TYR	CE2-CZ	-7.57	1.28	1.38
1	A	139	PHE	CE2-CZ	-6.96	1.24	1.37
2	B	35	TRP	CB-CG	6.60	1.62	1.50
1	C	91	TYR	CG-CD1	-6.56	1.30	1.39
2	B	146	TYR	CE2-CZ	-6.28	1.30	1.38
1	A	192	TYR	CG-CD1	-6.20	1.31	1.39
1	A	192	TYR	CE1-CZ	-6.14	1.30	1.38
1	A	91	TYR	CE1-CZ	-6.07	1.30	1.38
1	A	192	TYR	CG-CD2	-5.92	1.31	1.39
1	C	139	PHE	CE2-CZ	-5.69	1.26	1.37
1	C	91	TYR	CE1-CZ	-5.34	1.31	1.38
1	C	44	PHE	CB-CG	-5.31	1.42	1.51
1	C	192	TYR	CE1-CZ	-5.29	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	PHE	CG-CD1	-5.26	1.30	1.38
2	D	146	TYR	CE2-CZ	-5.22	1.31	1.38
2	B	22	CYS	CB-SG	-5.19	1.73	1.81
2	D	146	TYR	CE1-CZ	-5.12	1.31	1.38
1	C	91	TYR	CG-CD2	-5.06	1.32	1.39
2	B	92	TYR	CE1-CZ	-5.01	1.32	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	17	ASP	CB-CG-OD2	7.20	124.78	118.30
1	C	151	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	184	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	82	ASP	CB-CG-OD2	5.77	123.49	118.30
2	B	208	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	165	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	17	ASP	CB-CG-OD2	5.16	122.95	118.30
2	D	73	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	72	ARG	NE-CZ-NH1	-5.06	117.77	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	160	LEU	Peptide
2	B	83	LEU	Mainchain
2	D	150	SER	Peptide
2	D	83	LEU	Mainchain

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	1655	0	1556	46	0
1	C	1655	0	1556	55	0
2	B	1635	0	1586	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1635	0	1586	42	0
3	A	60	0	0	8	0
3	B	48	0	0	1	0
3	C	54	0	0	6	0
3	D	46	0	0	7	0
All	All	6788	0	6284	180	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 14.

All (180) 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:C:122:SER:O	1:C:123:GLU:HG3	1.58	1.01
2:D:6:GLU:HG2	2:D:106:GLN:NE2	1.78	0.97
2:D:160:LEU:O	2:D:160:LEU:HG	1.66	0.93
1:C:211:ARG:HH11	1:C:211:ARG:HG3	1.33	0.92
1:A:184:ASP:OD1	1:A:188:ARG:NH2	2.05	0.90
1:A:211:ARG:HH11	1:A:211:ARG:HG3	1.38	0.88
1:C:188:ARG:O	1:C:189:HIS:HD2	1.57	0.87
2:D:6:GLU:HG2	2:D:106:GLN:HE22	1.36	0.86
1:C:42:LYS:HB3	3:C:234:HOH:O	1.77	0.85
1:C:122:SER:O	1:C:123:GLU:CG	2.25	0.84
1:C:150:ILE:HG21	1:C:189:HIS:ND1	1.92	0.82
2:B:188:THR:O	2:B:192:GLU:HB2	1.80	0.82
2:B:193:THR:HG23	2:B:210:LYS:HD2	1.61	0.81
1:C:211:ARG:CG	1:C:211:ARG:HH11	1.90	0.81
2:D:214:SER:OG	3:D:625:HOH:O	1.99	0.81
2:D:188:THR:O	2:D:192:GLU:HB2	1.81	0.80
2:D:193:THR:HG23	2:D:210:LYS:HD2	1.63	0.80
2:D:65:LYS:HB3	3:D:627:HOH:O	1.82	0.79
1:A:211:ARG:CG	1:A:211:ARG:HH11	2.00	0.75
1:C:122:SER:O	1:C:123:GLU:CB	2.33	0.74
2:D:86:ILE:HG22	2:D:112:VAL:O	1.88	0.73
2:B:6:GLU:HG2	2:B:106:GLN:NE2	2.03	0.73
1:A:28:ASP:HB3	3:A:251:HOH:O	1.88	0.73
2:D:66:SER:N	3:D:627:HOH:O	2.22	0.72
2:B:149:GLU:O	2:B:150:SER:HB2	1.90	0.72
1:A:184:ASP:HB2	3:A:257:HOH:O	1.90	0.71
1:A:39:LYS:HD3	1:A:81:GLU:O	1.92	0.69
2:B:86:ILE:HG22	2:B:112:VAL:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:GLU:O	2:D:150:SER:HB2	1.92	0.69
1:A:189:HIS:O	1:A:211:ARG:NH1	2.25	0.68
1:A:122:SER:O	1:A:123:GLU:HG3	1.94	0.67
1:A:105:GLU:HB3	3:A:262:HOH:O	1.95	0.67
1:C:39:LYS:HD3	1:C:81:GLU:O	1.94	0.66
2:D:139:LEU:HD12	2:D:194:VAL:HG11	1.77	0.66
1:A:213:GLU:O	1:A:214:CYS:HB2	1.95	0.66
1:C:44:PHE:HB2	2:D:104:TRP:CD2	2.30	0.66
1:C:189:HIS:O	1:C:211:ARG:NH1	2.29	0.65
2:B:6:GLU:CG	2:B:106:GLN:NE2	2.60	0.65
1:A:185:GLU:OE1	3:A:271:HOH:O	2.15	0.65
2:D:3:GLN:HG2	3:D:612:HOH:O	1.96	0.64
1:C:188:ARG:O	1:C:189:HIS:CD2	2.47	0.64
2:B:158:GLY:C	2:B:160:LEU:H	1.99	0.64
1:A:85:ASP:OD1	1:A:103:LYS:HG2	1.98	0.64
2:B:189:TRP:CG	2:B:190:PRO:HA	2.33	0.63
1:A:39:LYS:HB3	1:A:40:PRO:HD2	1.79	0.63
1:C:31:SER:HB3	1:C:50:HIS:HD2	1.63	0.63
2:D:6:GLU:CG	2:D:106:GLN:NE2	2.58	0.63
1:A:163:TRP:HB3	3:A:227:HOH:O	1.97	0.62
1:C:85:ASP:OD1	1:C:103:LYS:HG2	1.99	0.62
2:B:149:GLU:HG3	2:B:150:SER:N	2.16	0.61
1:A:122:SER:O	1:A:123:GLU:CB	2.49	0.60
2:B:196:CYS:SG	2:B:196:CYS:O	2.60	0.60
1:C:122:SER:O	1:C:123:GLU:HB2	2.02	0.59
1:C:150:ILE:CG2	1:C:189:HIS:ND1	2.64	0.59
1:C:211:ARG:NH1	1:C:211:ARG:CG	2.56	0.59
2:B:210:LYS:HE3	2:B:212:GLU:OE2	2.03	0.59
1:C:2:ILE:CD1	1:C:93:GLN:HG2	2.32	0.59
2:B:158:GLY:C	2:B:160:LEU:N	2.55	0.58
2:D:189:TRP:CG	2:D:190:PRO:HA	2.38	0.58
1:A:6:GLN:NE2	1:A:86:TYR:O	2.32	0.58
2:D:6:GLU:CG	2:D:106:GLN:HE22	2.12	0.58
1:A:85:ASP:HB3	3:A:241:HOH:O	2.04	0.57
1:C:188:ARG:C	1:C:189:HIS:HD2	2.08	0.56
1:A:44:PHE:HB2	2:B:104:TRP:CD2	2.40	0.56
1:C:110:ASP:HB3	1:C:200:THR:HG22	1.88	0.56
2:B:164:VAL:HG22	2:B:182:VAL:HG23	1.88	0.55
1:C:188:ARG:C	1:C:189:HIS:CD2	2.80	0.55
1:C:20:SER:HB2	3:C:215:HOH:O	2.07	0.55
1:C:123:GLU:OE1	2:D:209:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:O	1:A:123:GLU:CG	2.55	0.54
1:C:213:GLU:O	1:C:214:CYS:HB2	2.06	0.54
1:A:188:ARG:C	1:A:189:HIS:HD2	2.11	0.54
1:A:2:ILE:CD1	1:A:93:GLN:HG2	2.37	0.54
2:B:36:ASN:O	2:B:94:CYS:HA	2.08	0.53
1:C:167:ASP:OD2	1:C:169:LYS:HG3	2.08	0.53
2:D:38:ILE:HD12	2:D:95:VAL:HG21	1.89	0.53
1:C:183:LYS:O	1:C:187:GLU:HG2	2.08	0.53
2:B:51:TYR:CD1	2:B:51:TYR:C	2.81	0.53
1:C:107:LYS:HA	1:C:140:TYR:OH	2.09	0.53
1:C:144:ILE:HG23	1:C:175:MET:CE	2.38	0.53
2:B:6:GLU:HG2	2:B:106:GLN:HE22	1.72	0.53
1:A:150:ILE:CG2	1:A:189:HIS:ND1	2.72	0.52
1:A:211:ARG:NH1	1:A:211:ARG:CG	2.63	0.52
1:C:144:ILE:CG2	1:C:175:MET:CE	2.88	0.52
1:C:20:SER:CB	3:C:215:HOH:O	2.57	0.52
1:A:122:SER:O	1:A:123:GLU:HB2	2.10	0.52
2:D:139:LEU:CD1	2:D:194:VAL:HG11	2.39	0.52
1:C:136:LEU:HD21	1:C:196:ALA:HB2	1.92	0.52
2:B:6:GLU:HG3	2:B:106:GLN:HE21	1.76	0.51
1:A:150:ILE:HG21	1:A:189:HIS:ND1	2.25	0.51
1:C:2:ILE:HD11	1:C:93:GLN:HG2	1.90	0.51
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.93	0.51
2:D:186:SER:O	2:D:187:SER:HB3	2.08	0.51
1:C:28:ASP:HB3	3:C:227:HOH:O	2.09	0.51
2:D:65:LYS:CB	3:D:627:HOH:O	2.49	0.51
1:A:183:LYS:O	1:A:187:GLU:HG2	2.11	0.51
1:C:56:ASP:O	1:C:57:GLU:HB2	2.12	0.50
2:D:6:GLU:HG2	2:D:106:GLN:HE21	1.72	0.49
2:B:144:LYS:HG2	2:B:177:THR:HG23	1.94	0.49
2:B:59:ARG:NE	3:B:602:HOH:O	2.45	0.49
1:C:115:VAL:O	1:C:207:LYS:HE3	2.13	0.49
2:B:6:GLU:H	2:B:106:GLN:HE22	1.61	0.48
1:C:211:ARG:NH1	1:C:211:ARG:CB	2.76	0.48
2:B:6:GLU:CG	2:B:106:GLN:HE21	2.25	0.48
1:A:144:ILE:HG23	1:A:175:MET:CE	2.42	0.48
2:D:36:ASN:O	2:D:94:CYS:HA	2.12	0.48
2:D:159:SER:C	2:D:161:SER:N	2.67	0.48
2:B:12:VAL:O	2:B:112:VAL:HA	2.12	0.48
2:B:18:LEU:HD23	2:B:18:LEU:C	2.34	0.48
2:B:164:VAL:CG2	2:B:182:VAL:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:TYR:CG	1:C:141:PRO:HA	2.49	0.48
2:B:51:TYR:C	2:B:51:TYR:HD1	2.18	0.47
2:B:189:TRP:CD1	2:B:190:PRO:HA	2.50	0.47
2:D:51:TYR:C	2:D:51:TYR:CD1	2.87	0.47
1:A:188:ARG:C	1:A:189:HIS:CD2	2.88	0.47
1:A:2:ILE:HD12	1:A:93:GLN:HG2	1.95	0.47
1:C:136:LEU:CD2	1:C:196:ALA:HB2	2.44	0.47
1:C:105:GLU:OE1	1:C:142:LYS:NZ	2.44	0.47
2:D:12:VAL:O	2:D:112:VAL:HA	2.15	0.47
2:B:182:VAL:O	2:B:182:VAL:HG13	2.13	0.47
2:D:73:ASP:OD2	2:D:76:LYS:HG3	2.14	0.47
1:C:43:SER:OG	2:D:105:GLY:O	2.24	0.46
1:A:124:GLN:OE1	3:A:240:HOH:O	2.20	0.46
2:D:31:SER:O	2:D:32:ASP:HB2	2.15	0.46
2:B:144:LYS:HB3	2:B:144:LYS:HE2	1.68	0.45
2:B:149:GLU:HG3	2:B:150:SER:H	1.81	0.45
2:B:2:VAL:HG22	2:B:27:TYR:HB2	1.99	0.45
2:D:16:GLN:O	2:D:84:VAL:HG22	2.17	0.45
2:D:160:LEU:O	2:D:162:SER:N	2.49	0.45
2:B:6:GLU:OE2	2:B:105:GLY:HA3	2.16	0.45
1:C:155:ARG:NH2	1:C:181:LEU:HD22	2.32	0.45
1:C:140:TYR:O	1:C:198:HIS:HE1	2.00	0.44
2:D:43:GLY:O	2:D:44:ASN:HB2	2.17	0.44
1:A:115:VAL:O	1:A:207:LYS:HE3	2.17	0.44
2:B:6:GLU:H	2:B:6:GLU:HG2	1.26	0.44
1:A:149:LYS:HB2	1:A:193:THR:HB	1.98	0.44
1:C:31:SER:O	1:C:50:HIS:HA	2.17	0.44
1:C:135:PHE:CE2	2:D:181:SER:HB3	2.53	0.44
1:C:29:ILE:HD12	1:C:33:ILE:HB	2.00	0.44
2:B:52:ILE:HA	2:B:57:ASN:O	2.18	0.44
1:A:188:ARG:HB3	1:A:189:HIS:HD2	1.82	0.44
2:B:155:TRP:CZ3	2:B:196:CYS:HB3	2.53	0.44
2:B:182:VAL:O	2:B:182:VAL:CG1	2.66	0.43
1:C:91:TYR:HA	1:C:96:TRP:CD1	2.54	0.43
1:A:37:GLN:HB2	1:A:47:LEU:HD11	2.00	0.43
1:A:167:ASP:OD2	1:A:169:LYS:HG3	2.19	0.43
1:A:31:SER:O	1:A:50:HIS:HA	2.19	0.43
2:D:131:ASP:OD1	2:D:131:ASP:N	2.52	0.43
2:D:6:GLU:HG2	2:D:6:GLU:H	1.36	0.42
2:B:212:GLU:HA	2:B:213:PRO:HD2	1.83	0.42
2:B:131:ASP:N	2:B:131:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:O	1:C:86:TYR:HA	2.20	0.42
1:A:150:ILE:HG22	1:A:189:HIS:ND1	2.35	0.42
1:C:43:SER:N	3:C:234:HOH:O	2.42	0.42
2:B:79:PHE:CZ	2:B:94:CYS:HB2	2.55	0.42
2:D:186:SER:O	2:D:187:SER:CB	2.68	0.41
1:A:211:ARG:CZ	1:A:211:ARG:HB3	2.50	0.41
1:C:39:LYS:HE2	3:C:250:HOH:O	2.20	0.41
1:C:7:SER:HA	1:C:8:PRO:HA	1.89	0.41
1:A:79:GLU:OE1	1:A:81:GLU:OE2	2.38	0.41
1:C:81:GLU:HG3	1:C:81:GLU:H	1.46	0.41
2:B:167:PHE:HA	2:B:168:PRO:HD3	1.90	0.41
2:D:155:TRP:CZ3	2:D:196:CYS:HB3	2.55	0.41
1:A:136:LEU:HD21	1:A:196:ALA:HB2	2.02	0.41
1:C:211:ARG:HB3	1:C:211:ARG:CZ	2.50	0.41
2:D:1:ASP:C	3:D:612:HOH:O	2.59	0.41
2:D:196:CYS:O	2:D:196:CYS:SG	2.78	0.41
1:C:110:ASP:HB3	1:C:200:THR:CG2	2.49	0.41
1:A:81:GLU:HG3	1:A:81:GLU:H	1.13	0.41
1:A:136:LEU:CD2	1:A:196:ALA:HB2	2.51	0.41
2:B:149:GLU:CG	2:B:150:SER:N	2.83	0.41
1:A:140:TYR:O	1:A:198:HIS:HE1	2.04	0.41
1:A:110:ASP:HB3	1:A:200:THR:HG22	2.03	0.41
1:A:45:LYS:HE2	3:A:258:HOH:O	2.21	0.40
2:D:148:PRO:HD2	2:D:202:ALA:CB	2.52	0.40
1:C:165:ASP:O	1:C:166:GLN:C	2.60	0.40
1:A:190:ASN:HB3	1:A:212:ASN:OD1	2.21	0.40
2:B:163:SER:HB3	2:B:183:THR:HB	2.02	0.40
2:D:167:PHE:HA	2:D:168:PRO:HD3	1.87	0.40
2:D:65:LYS:CA	3:D:627:HOH:O	2.68	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	212/214 (99%)	201 (95%)	10 (5%)	1 (0%)	34 41
1	C	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	34 41
2	B	214/216 (99%)	196 (92%)	15 (7%)	3 (1%)	14 13
2	D	214/216 (99%)	193 (90%)	13 (6%)	8 (4%)	4 2
All	All	852/860 (99%)	792 (93%)	47 (6%)	13 (2%)	13 12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	187	SER
1	C	123	GLU
2	D	161	SER
2	D	164	VAL
2	D	187	SER
2	D	194	VAL
2	B	150	SER
2	D	150	SER
2	D	156	ASN
2	D	160	LEU
2	D	131	ASP
2	B	131	ASP

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	191/191 (100%)	179 (94%)	12 (6%)	22 29
1	C	191/191 (100%)	174 (91%)	17 (9%)	12 14
2	B	191/191 (100%)	178 (93%)	13 (7%)	20 25
2	D	191/191 (100%)	178 (93%)	13 (7%)	20 25
All	All	764/764 (100%)	709 (93%)	55 (7%)	18 22

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	SER
1	A	13	VAL
1	A	42	LYS
1	A	57	GLU
1	A	81	GLU
1	A	93	GLN
1	A	142	LYS
1	A	153	SER
1	A	191	SER
1	A	199	LYS
1	A	211	ARG
2	B	6	GLU
2	B	19	SER
2	B	51	TYR
2	B	67	ARG
2	B	99	ARG
2	B	106	GLN
2	B	125	LEU
2	B	131	ASP
2	B	157	SER
2	B	159	SER
2	B	160	LEU
2	B	163	SER
2	B	196	CYS
1	C	10	SER
1	C	12	SER
1	C	13	VAL
1	C	19	VAL
1	C	20	SER
1	C	23	CYS
1	C	42	LYS
1	C	57	GLU
1	C	80	SER
1	C	81	GLU
1	C	143	ASP
1	C	153	SER
1	C	156	GLN
1	C	184	ASP
1	C	191	SER
1	C	199	LYS
1	C	211	ARG
2	D	6	GLU

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Mol	Chain	Res	Type
2	D	19	SER
2	D	51	TYR
2	D	65	LYS
2	D	67	ARG
2	D	99	ARG
2	D	106	GLN
2	D	125	LEU
2	D	131	ASP
2	D	149	GLU
2	D	160	LEU
2	D	161	SER
2	D	163	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	GLN
2	B	156	ASN
1	C	189	HIS
2	D	106	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	214/214 (100%)	0.19	6 (2%)	56	66	22, 39, 61, 91	0
1	C	214/214 (100%)	0.15	11 (5%)	32	41	22, 39, 61, 91	0
2	B	216/216 (100%)	0.28	16 (7%)	17	25	21, 37, 76, 96	0
2	D	216/216 (100%)	0.33	14 (6%)	22	30	21, 37, 77, 95	0
All	All	860/860 (100%)	0.24	47 (5%)	29	37	21, 38, 67, 96	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	158	GLY	9.0
1	A	214	CYS	7.1
2	B	159	SER	6.8
2	D	131	ASP	6.8
2	B	131	ASP	5.4
2	D	161	SER	5.4
2	D	157	SER	5.2
1	C	169	LYS	4.9
2	D	129	CYS	4.7
2	B	132	THR	4.6
1	C	214	CYS	4.5
2	B	158	GLY	4.5
2	D	133	THR	4.5
1	A	40	PRO	4.1
2	D	160	LEU	3.8
2	D	130	GLY	3.7
2	D	132	THR	3.6
2	B	130	GLY	3.5
2	B	157	SER	3.4
2	D	159	SER	3.4
2	D	162	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	1	ASP	3.4
2	B	1	ASP	3.3
2	D	135	SER	3.3
1	A	41	GLY	3.3
1	A	57	GLU	3.1
2	B	214	SER	2.9
2	B	35	TRP	2.9
2	B	133	THR	2.8
2	B	129	CYS	2.8
1	A	89	VAL	2.8
1	A	212	ASN	2.7
1	C	210	ASN	2.6
1	C	156	GLN	2.6
1	C	202	THR	2.5
2	B	54	TYR	2.4
1	C	127	SER	2.4
1	C	43	SER	2.4
2	B	186	SER	2.4
1	C	212	ASN	2.3
1	C	42	LYS	2.2
2	B	95	VAL	2.2
2	B	160	LEU	2.2
1	C	41	GLY	2.2
2	B	3	GLN	2.1
1	C	163	TRP	2.0
2	D	95	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 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.