



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:27 AM GMT

PDB ID : 3IJ2
Title : Ligand-receptor structure
Authors : Feng, D.; Garcia, K.C.
Deposited on : 2009-08-03
Resolution : 3.75 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

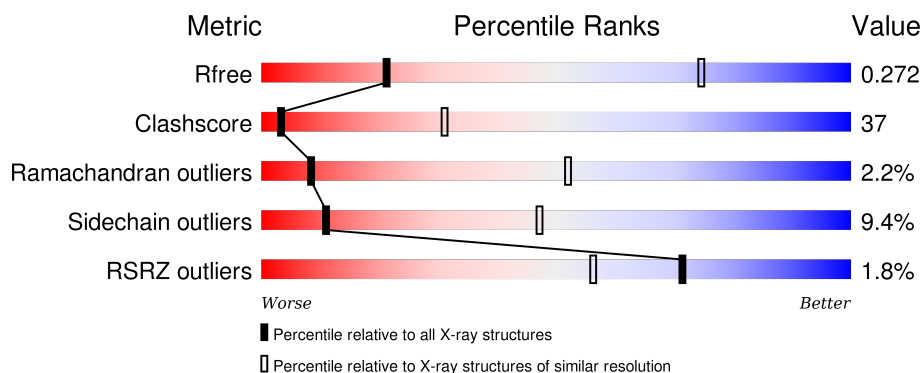
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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 $\leq 5\%$. 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	230	<div> <div>2%</div> <div>20%</div> <div>23%</div> <div>• •</div> <div>52%</div> </div>
1	B	230	<div> <div>2%</div> <div>20%</div> <div>24%</div> <div>•</div> <div>52%</div> </div>
2	X	171	<div> <div>%</div> <div>45%</div> <div>43%</div> <div>7%</div> <div>5%</div> </div>
2	Y	171	<div> <div>%</div> <div>44%</div> <div>42%</div> <div>7%</div> <div>6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4092 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 Beta-nerve growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			864	540	152	165	7			
1	B	110	Total	C	N	O	S	0	0	0
			864	540	152	165	7			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-72	ALA	ARG	ENGINEERED	UNP P01139
A	-71	ALA	ARG	ENGINEERED	UNP P01139
A	-42	ALA	LYS	ENGINEERED	UNP P01139
A	-41	ALA	ARG	ENGINEERED	UNP P01139
A	-1	ALA	LYS	ENGINEERED	UNP P01139
A	0	ALA	ARG	ENGINEERED	UNP P01139
A	118	ALA	ARG	ENGINEERED	UNP P01139
A	119	ALA	ARG	ENGINEERED	UNP P01139
A	121	HIS	-	EXPRESSION TAG	UNP P01139
A	122	HIS	-	EXPRESSION TAG	UNP P01139
A	123	HIS	-	EXPRESSION TAG	UNP P01139
A	124	HIS	-	EXPRESSION TAG	UNP P01139
A	125	HIS	-	EXPRESSION TAG	UNP P01139
A	126	HIS	-	EXPRESSION TAG	UNP P01139
A	127	HIS	-	EXPRESSION TAG	UNP P01139
B	118	ALA	ARG	ENGINEERED	UNP P01139
B	-72	ALA	ARG	ENGINEERED	UNP P01139
B	-71	ALA	ARG	ENGINEERED	UNP P01139
B	-42	ALA	LYS	ENGINEERED	UNP P01139
B	-41	ALA	ARG	ENGINEERED	UNP P01139
B	-1	ALA	LYS	ENGINEERED	UNP P01139
B	0	ALA	ARG	ENGINEERED	UNP P01139
B	118	ALA	ARG	ENGINEERED	UNP P01139
B	119	ALA	ARG	ENGINEERED	UNP P01139
B	121	HIS	-	EXPRESSION TAG	UNP P01139

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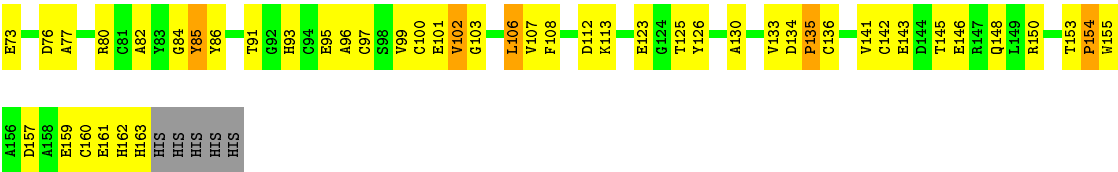
Chain	Residue	Modelled	Actual	Comment	Reference
B	122	HIS	-	EXPRESSION TAG	UNP P01139
B	123	HIS	-	EXPRESSION TAG	UNP P01139
B	124	HIS	-	EXPRESSION TAG	UNP P01139
B	125	HIS	-	EXPRESSION TAG	UNP P01139
B	126	HIS	-	EXPRESSION TAG	UNP P01139
B	127	HIS	-	EXPRESSION TAG	UNP P01139

- Molecule 2 is a protein called Nerve growth factor receptor (TNFR superfamily, member 16).

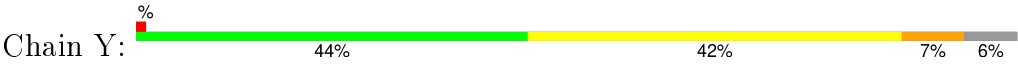
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	162	Total	C	N	O	S	0	0	0
			1192	709	195	263	25			
2	Y	160	Total	C	N	O	S	0	0	0
			1172	697	189	261	25			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	ALA	-	EXPRESSION TAG	UNP P07174
X	-1	ASP	-	EXPRESSION TAG	UNP P07174
X	0	PRO	-	EXPRESSION TAG	UNP P07174
X	32	ASP	ASN	ENGINEERED	UNP P07174
X	42	SER	ASN	CONFLICT	UNP P07174
X	162	HIS	-	EXPRESSION TAG	UNP P07174
X	163	HIS	-	EXPRESSION TAG	UNP P07174
X	164	HIS	-	EXPRESSION TAG	UNP P07174
X	165	HIS	-	EXPRESSION TAG	UNP P07174
X	166	HIS	-	EXPRESSION TAG	UNP P07174
X	167	HIS	-	EXPRESSION TAG	UNP P07174
X	168	HIS	-	EXPRESSION TAG	UNP P07174
Y	-2	ALA	-	EXPRESSION TAG	UNP P07174
Y	-1	ASP	-	EXPRESSION TAG	UNP P07174
Y	0	PRO	-	EXPRESSION TAG	UNP P07174
Y	32	ASP	ASN	ENGINEERED	UNP P07174
Y	42	SER	ASN	CONFLICT	UNP P07174
Y	162	HIS	-	EXPRESSION TAG	UNP P07174
Y	163	HIS	-	EXPRESSION TAG	UNP P07174
Y	164	HIS	-	EXPRESSION TAG	UNP P07174
Y	165	HIS	-	EXPRESSION TAG	UNP P07174
Y	166	HIS	-	EXPRESSION TAG	UNP P07174
Y	167	HIS	-	EXPRESSION TAG	UNP P07174
Y	168	HIS	-	EXPRESSION TAG	UNP P07174



● Molecule 2: Nerve growth factor receptor (TNFR superfamily, member 16)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.41Å 145.41Å 114.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.59 – 3.75 47.60 – 3.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.59-3.75) 100.0 (47.60-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_153)	Depositor
R, R_{free}	0.256 , 0.274 0.247 , 0.272	Depositor DCC
R_{free} test set	736 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	120.1	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 120.3	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 14762 reflections (0.027%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4092	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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, 0.375 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	0.86	3/881 (0.3%)	0.88	4/1193 (0.3%)
1	B	0.80	2/881 (0.2%)	1.03	5/1193 (0.4%)
2	X	0.64	0/1214	0.70	0/1655
2	Y	0.46	0/1192	0.62	0/1625
All	All	0.69	5/4168 (0.1%)	0.80	9/5666 (0.2%)

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
1	A	0	2
1	B	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	35	GLU	CD-OE2	-8.80	1.16	1.25
1	A	35	GLU	CD-OE1	-8.55	1.16	1.25
1	A	35	GLU	CD-OE2	-7.56	1.17	1.25
1	B	35	GLU	CD-OE1	-7.45	1.17	1.25
1	A	9	MET	N-CA	-6.19	1.33	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	MET	N-CA-C	-15.90	68.08	111.00
1	B	9	MET	N-CA-CB	-10.62	91.48	110.60
1	B	35	GLU	OE1-CD-OE2	-10.43	110.79	123.30
1	A	35	GLU	OE1-CD-OE2	-10.11	111.17	123.30
1	A	9	MET	CA-CB-CG	-7.18	101.09	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	MET	CA-CB-CG	6.98	125.17	113.30
1	B	9	MET	CB-CA-C	6.85	124.10	110.40
1	A	9	MET	CB-CA-C	6.77	123.94	110.40
1	A	9	MET	N-CA-CB	-5.26	101.12	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	HIS	Peptide
1	A	9	MET	Peptide
1	B	116	ALA	Peptide
1	B	9	MET	Mainchain,Peptide

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	864	0	837	74	0
1	B	864	0	837	62	1
2	X	1192	0	1035	89	1
2	Y	1172	0	1021	96	0
All	All	4092	0	3730	290	1

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 37.

All (290) 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:A:9:MET:O	2:Y:108:PHE:CE2	2.02	1.11
2:X:108:PHE:HE2	1:B:9:MET:O	1.30	1.09
1:B:116:ALA:O	1:B:117:THR:HG22	1.56	1.04
2:X:108:PHE:CE2	1:B:9:MET:O	2.09	1.03
1:A:47:SER:HB3	2:Y:40:LEU:HD21	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:MET:O	2:Y:108:PHE:HE2	1.46	0.97
1:A:8:HIS:C	1:A:9:MET:HG2	1.89	0.90
2:Y:106:LEU:HD12	2:Y:107:VAL:N	1.91	0.86
2:X:106:LEU:HD12	2:X:107:VAL:N	1.91	0.85
1:A:30:ASP:HB3	1:A:34:LYS:H	1.40	0.85
1:A:81:THR:HG22	1:A:82:THR:N	1.92	0.84
2:Y:20:ASN:HA	2:Y:49:VAL:HG12	1.59	0.84
1:A:116:ALA:O	1:A:117:THR:HG22	1.77	0.84
1:A:9:MET:C	2:Y:108:PHE:CE2	2.51	0.84
1:B:30:ASP:HB3	1:B:34:LYS:H	1.43	0.84
2:X:21:LEU:H	2:X:21:LEU:HD22	1.43	0.83
2:Y:145:THR:HG22	2:Y:146:GLU:H	1.44	0.83
1:B:8:HIS:O	1:B:10:GLY:HA3	1.78	0.83
1:B:81:THR:HG22	1:B:82:THR:N	1.95	0.81
2:X:20:ASN:HA	2:X:49:VAL:HG12	1.60	0.81
2:X:106:LEU:HD12	2:X:107:VAL:H	1.45	0.81
1:A:8:HIS:N	1:A:9:MET:HG2	1.95	0.80
2:X:162:HIS:CG	2:X:163:HIS:H	2.00	0.80
1:A:47:SER:CB	2:Y:40:LEU:HD21	2.12	0.79
1:A:9:MET:C	2:Y:108:PHE:HE2	1.85	0.78
1:B:116:ALA:O	1:B:117:THR:CG2	2.32	0.78
1:A:81:THR:HG22	1:A:82:THR:H	1.49	0.78
1:B:14:VAL:HG12	1:B:68:CYS:HB3	1.65	0.78
2:X:41:ASP:O	2:X:42:SER:HB2	1.84	0.77
2:Y:44:THR:HB	2:Y:55:CYS:HB3	1.65	0.77
1:A:69:ARG:O	1:B:112:LEU:HD11	1.84	0.77
2:X:44:THR:HB	2:X:55:CYS:HB3	1.68	0.75
2:Y:106:LEU:HD12	2:Y:107:VAL:H	1.52	0.75
1:B:81:THR:HG22	1:B:82:THR:H	1.52	0.75
1:A:14:VAL:HG12	1:A:68:CYS:HB3	1.67	0.75
1:A:112:LEU:HD11	1:B:69:ARG:O	1.85	0.74
1:B:36:VAL:HG22	1:B:37:THR:H	1.53	0.73
1:A:71:ILE:HA	1:B:71:ILE:HA	1.70	0.72
2:X:106:LEU:H	2:X:135:PRO:HA	1.54	0.72
2:Y:41:ASP:O	2:Y:42:SER:HB2	1.91	0.71
2:X:71:CYS:HB2	2:X:77:ALA:HB2	1.71	0.71
2:Y:71:CYS:HB2	2:Y:77:ALA:HB2	1.73	0.71
2:X:133:VAL:HG23	2:X:134:ASP:OD1	1.91	0.71
2:X:27:GLN:HB3	2:X:35:VAL:CG1	2.20	0.70
2:X:101:GLU:HA	2:X:130:ALA:CB	2.22	0.70
2:Y:106:LEU:H	2:Y:135:PRO:HA	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:101:GLU:HA	2:Y:130:ALA:CB	2.21	0.70
1:A:36:VAL:HG22	1:A:37:THR:H	1.56	0.69
2:Y:27:GLN:HB3	2:Y:35:VAL:CG1	2.23	0.68
2:Y:21:LEU:H	2:Y:21:LEU:HD22	1.59	0.68
1:B:103:ARG:O	1:B:103:ARG:HG2	1.94	0.67
2:X:103:GLY:HA2	2:X:154:PRO:O	1.95	0.67
1:A:38:VAL:HG12	1:A:39:LEU:H	1.59	0.67
1:A:8:HIS:CA	1:A:9:MET:HG2	2.25	0.67
2:Y:133:VAL:HG23	2:Y:134:ASP:OD1	1.95	0.66
2:X:40:LEU:HD21	1:B:47:SER:CB	2.26	0.66
2:Y:84:GLY:O	2:Y:97:CYS:SG	2.54	0.66
2:X:66:SER:OG	2:X:82:ALA:HA	1.96	0.66
1:A:81:THR:CG2	1:A:82:THR:N	2.59	0.65
1:B:30:ASP:HB3	1:B:34:LYS:N	2.11	0.65
1:A:103:ARG:O	1:A:103:ARG:HG2	1.97	0.64
1:B:39:LEU:HB3	1:B:42:VAL:CG2	2.28	0.64
1:B:81:THR:CG2	1:B:82:THR:H	2.10	0.64
2:Y:103:GLY:HA2	2:Y:154:PRO:O	1.97	0.64
1:A:30:ASP:HB3	1:A:34:LYS:N	2.10	0.64
2:X:162:HIS:CG	2:X:163:HIS:N	2.66	0.64
2:X:40:LEU:HD21	1:B:47:SER:HB3	1.78	0.64
1:B:38:VAL:HG12	1:B:39:LEU:H	1.63	0.64
2:Y:85:TYR:HB3	2:Y:95:GLU:O	1.98	0.64
1:A:81:THR:CG2	1:A:82:THR:H	2.10	0.64
2:X:84:GLY:O	2:X:97:CYS:SG	2.56	0.63
2:X:25:VAL:H	2:X:54:PRO:HA	1.64	0.63
1:B:81:THR:CG2	1:B:82:THR:N	2.60	0.63
1:A:9:MET:O	2:Y:108:PHE:CZ	2.50	0.62
2:Y:101:GLU:HA	2:Y:130:ALA:HB2	1.80	0.62
2:X:10:THR:CG2	2:X:14:GLU:HB2	2.28	0.62
2:X:22:GLY:HA2	2:X:73:GLU:HB3	1.81	0.62
2:X:85:TYR:HB3	2:X:95:GLU:O	1.98	0.62
2:Y:160:CYS:O	2:Y:161:GLU:HB3	2.00	0.61
2:X:146:GLU:HG2	2:X:162:HIS:HB2	1.82	0.61
1:A:112:LEU:HD21	1:B:14:VAL:HG22	1.82	0.61
2:Y:145:THR:HG22	2:Y:146:GLU:N	2.15	0.61
1:B:36:VAL:HG22	1:B:37:THR:N	2.15	0.61
2:X:85:TYR:CD1	2:X:85:TYR:N	2.68	0.61
2:Y:22:GLY:HA2	2:Y:73:GLU:HB3	1.83	0.60
2:X:27:GLN:HB3	2:X:35:VAL:HG12	1.83	0.60
1:B:30:ASP:HB2	1:B:34:LYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:26:ALA:HB2	2:Y:37:GLU:HG3	1.82	0.60
2:Y:27:GLN:HB3	2:Y:35:VAL:HG12	1.83	0.60
1:A:39:LEU:HB3	1:A:42:VAL:CG2	2.31	0.60
1:A:30:ASP:HB2	1:A:34:LYS:O	2.02	0.59
2:X:101:GLU:HA	2:X:130:ALA:HB2	1.83	0.59
2:Y:66:SER:OG	2:Y:82:ALA:HA	2.00	0.59
1:B:44:ILE:O	1:B:45:ASN:HB2	2.03	0.59
2:X:21:LEU:H	2:X:21:LEU:CD2	2.14	0.59
1:A:49:PHE:O	2:Y:42:SER:CB	2.51	0.59
2:Y:6:THR:HG21	2:Y:51:ALA:HB3	1.84	0.59
2:X:21:LEU:HD22	2:X:21:LEU:N	2.15	0.59
2:X:26:ALA:HB2	2:X:37:GLU:HG3	1.84	0.59
2:X:19:CYS:O	2:X:49:VAL:HA	2.03	0.59
2:X:6:THR:HG21	2:X:51:ALA:HB3	1.85	0.59
2:X:20:ASN:HD22	2:X:20:ASN:N	2.00	0.58
2:Y:100:CYS:O	2:Y:130:ALA:HA	2.03	0.58
1:A:44:ILE:O	1:A:45:ASN:HB2	2.03	0.58
2:X:162:HIS:ND1	2:X:163:HIS:N	2.49	0.58
1:A:68:CYS:SG	1:A:78:SER:HB2	2.43	0.58
2:Y:10:THR:CG2	2:Y:14:GLU:HB2	2.33	0.58
1:A:91:THR:OG1	1:A:100:ARG:HD2	2.04	0.58
1:A:49:PHE:O	1:A:50:ARG:HB2	2.03	0.57
2:Y:41:ASP:O	2:Y:42:SER:CB	2.51	0.57
1:A:36:VAL:HG22	1:A:37:THR:N	2.18	0.57
1:B:39:LEU:HB3	1:B:42:VAL:HG21	1.85	0.57
1:B:49:PHE:O	1:B:50:ARG:HB2	2.04	0.57
2:Y:62:LEU:N	2:Y:65:GLN:HB2	2.19	0.57
2:X:20:ASN:ND2	2:X:20:ASN:H	2.03	0.57
2:Y:19:CYS:O	2:Y:49:VAL:HA	2.03	0.57
1:A:8:HIS:C	1:A:9:MET:CG	2.68	0.57
2:Y:85:TYR:CD1	2:Y:85:TYR:N	2.73	0.57
2:X:45:PHE:CE1	2:X:76:ASP:HB2	2.40	0.56
1:A:8:HIS:HA	1:A:11:GLU:OE1	2.05	0.56
1:A:39:LEU:HB3	1:A:42:VAL:HG21	1.87	0.56
1:A:53:PHE:HE1	1:A:102:ILE:HD11	1.70	0.56
1:A:76:TRP:CZ3	1:A:114:ARG:HG3	2.40	0.56
2:Y:48:VAL:HG22	2:Y:49:VAL:N	2.21	0.56
1:A:9:MET:HA	2:Y:108:PHE:HE2	1.71	0.56
2:Y:25:VAL:H	2:Y:54:PRO:HA	1.71	0.56
2:X:20:ASN:N	2:X:20:ASN:ND2	2.54	0.55
2:X:142:CYS:O	2:X:143:GLU:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:62:LEU:N	2:X:65:GLN:HB2	2.20	0.55
2:X:91:THR:O	2:X:91:THR:HG22	2.07	0.55
1:A:38:VAL:HG12	1:A:39:LEU:N	2.20	0.55
2:Y:142:CYS:O	2:Y:143:GLU:HG3	2.06	0.55
2:X:20:ASN:ND2	2:X:23:GLU:HB2	2.22	0.55
1:B:38:VAL:HG12	1:B:39:LEU:N	2.22	0.55
2:Y:45:PHE:CE1	2:Y:76:ASP:HB2	2.41	0.55
1:B:68:CYS:SG	1:B:78:SER:HB2	2.48	0.54
2:X:27:GLN:H	2:X:35:VAL:HG13	1.72	0.54
2:Y:91:THR:O	2:Y:91:THR:HG22	2.09	0.53
1:B:79:TYR:CE1	1:B:111:VAL:HB	2.43	0.53
2:Y:22:GLY:O	2:Y:38:PRO:HA	2.08	0.53
1:A:14:VAL:HG22	1:B:112:LEU:HD21	1.90	0.53
2:X:10:THR:HG21	2:X:14:GLU:HB2	1.90	0.53
2:X:91:THR:HG22	2:X:93:HIS:HB3	1.91	0.53
2:X:125:THR:HB	2:X:136:CYS:HB3	1.90	0.53
2:Y:91:THR:HG22	2:Y:93:HIS:HB3	1.89	0.53
1:B:37:THR:OG1	1:B:92:THR:HG23	2.09	0.53
1:B:114:ARG:NH1	2:Y:136:CYS:HB2	2.23	0.53
2:Y:125:THR:HB	2:Y:136:CYS:HB3	1.91	0.53
1:B:53:PHE:HE1	1:B:102:ILE:HD11	1.74	0.52
2:X:100:CYS:O	2:X:130:ALA:HA	2.08	0.52
2:Y:20:ASN:HD22	2:Y:20:ASN:N	2.07	0.52
2:Y:20:ASN:ND2	2:Y:23:GLU:HB2	2.24	0.52
1:A:53:PHE:CE1	1:A:102:ILE:HD11	2.44	0.52
1:B:87:VAL:O	1:B:101:PHE:HA	2.10	0.52
2:X:20:ASN:HD22	2:X:23:GLU:HB2	1.74	0.52
2:X:48:VAL:HG22	2:X:49:VAL:N	2.24	0.52
2:Y:48:VAL:HG22	2:Y:49:VAL:H	1.75	0.52
1:A:21:TRP:NE1	2:Y:68:SER:O	2.43	0.52
2:Y:27:GLN:H	2:Y:35:VAL:HG13	1.74	0.51
2:Y:20:ASN:HD22	2:Y:23:GLU:HB2	1.73	0.51
2:X:101:GLU:HA	2:X:130:ALA:HB1	1.92	0.51
1:B:91:THR:OG1	1:B:100:ARG:HD2	2.11	0.51
2:Y:150:ARG:NH1	2:Y:159:GLU:CD	2.64	0.51
2:Y:101:GLU:HA	2:Y:130:ALA:HB1	1.92	0.51
2:X:25:VAL:N	2:X:54:PRO:HA	2.24	0.51
1:B:20:VAL:CG2	1:B:21:TRP:N	2.73	0.51
1:B:53:PHE:CE1	1:B:102:ILE:HD11	2.47	0.51
2:Y:21:LEU:N	2:Y:21:LEU:HD22	2.24	0.50
2:X:22:GLY:O	2:X:38:PRO:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:10:THR:HG21	2:Y:14:GLU:HB2	1.94	0.50
2:Y:146:GLU:HA	2:Y:161:GLU:O	2.11	0.50
2:X:153:THR:O	2:X:155:TRP:N	2.45	0.50
2:X:126:TYR:CZ	2:X:157:ASP:HB2	2.47	0.50
1:B:76:TRP:CZ3	1:B:114:ARG:HG3	2.46	0.50
1:A:22:VAL:HG12	1:A:25:LYS:HB2	1.94	0.50
1:B:52:TYR:N	1:B:52:TYR:CD2	2.80	0.49
1:B:44:ILE:O	1:B:45:ASN:CB	2.60	0.49
2:Y:56:LYS:HB3	2:Y:57:PRO:HD2	1.94	0.49
2:Y:153:THR:O	2:Y:155:TRP:N	2.46	0.49
2:X:150:ARG:NH1	2:X:159:GLU:CD	2.65	0.49
2:Y:20:ASN:ND2	2:Y:20:ASN:H	2.09	0.49
2:X:40:LEU:HD21	1:B:47:SER:HB2	1.92	0.49
1:A:79:TYR:CE1	1:A:111:VAL:HB	2.48	0.49
2:Y:20:ASN:ND2	2:Y:20:ASN:N	2.60	0.49
2:X:48:VAL:HG22	2:X:49:VAL:H	1.78	0.49
2:Y:71:CYS:N	2:Y:77:ALA:HB2	2.28	0.49
1:A:44:ILE:O	1:A:45:ASN:CB	2.61	0.49
1:A:51:GLN:OE1	1:A:90:LEU:HB3	2.13	0.49
2:Y:80:ARG:NH1	2:Y:112:ASP:HB3	2.27	0.49
2:X:102:VAL:HG12	2:X:103:GLY:N	2.28	0.48
2:Y:91:THR:C	2:Y:93:HIS:H	2.16	0.48
1:A:20:VAL:CG2	1:A:21:TRP:N	2.76	0.48
2:Y:25:VAL:HG21	2:Y:52:THR:C	2.34	0.48
2:X:62:LEU:H	2:X:65:GLN:HB2	1.79	0.48
2:Y:62:LEU:H	2:Y:65:GLN:HB2	1.78	0.48
2:X:80:ARG:NH1	2:X:112:ASP:HB3	2.28	0.48
2:Y:146:GLU:CD	2:Y:161:GLU:HA	2.34	0.48
1:B:22:VAL:HG12	1:B:25:LYS:HB2	1.95	0.48
1:A:49:PHE:O	1:A:50:ARG:CB	2.61	0.48
2:Y:71:CYS:HB2	2:Y:77:ALA:CB	2.42	0.48
1:B:51:GLN:OE1	1:B:90:LEU:HB3	2.14	0.48
2:X:135:PRO:HB3	1:B:12:PHE:CE1	2.48	0.48
2:Y:21:LEU:H	2:Y:21:LEU:CD2	2.26	0.48
2:Y:26:ALA:HB2	2:Y:37:GLU:CG	2.43	0.48
1:B:49:PHE:O	1:B:50:ARG:CB	2.61	0.48
2:Y:6:THR:HG21	2:Y:51:ALA:CB	2.44	0.47
2:X:91:THR:C	2:X:93:HIS:N	2.68	0.47
2:X:153:THR:C	2:X:155:TRP:H	2.17	0.47
2:X:91:THR:C	2:X:93:HIS:H	2.18	0.47
2:Y:91:THR:C	2:Y:93:HIS:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:25:VAL:N	2:Y:54:PRO:HA	2.29	0.47
2:X:56:LYS:HB3	2:X:57:PRO:HD2	1.97	0.47
2:Y:91:THR:HG22	2:Y:93:HIS:CB	2.44	0.47
2:Y:146:GLU:HA	2:Y:161:GLU:C	2.35	0.46
2:X:71:CYS:HB2	2:X:77:ALA:CB	2.44	0.46
2:X:65:GLN:OE1	2:X:65:GLN:HA	2.15	0.46
1:A:12:PHE:CE1	2:Y:135:PRO:HB3	2.50	0.46
2:X:6:THR:HG21	2:X:51:ALA:CB	2.45	0.46
2:X:25:VAL:HG21	2:X:52:THR:C	2.36	0.46
2:X:91:THR:HG22	2:X:93:HIS:CB	2.46	0.46
1:B:85:THR:HG22	1:B:106:THR:HB	1.97	0.46
1:A:37:THR:OG1	1:A:92:THR:HG23	2.15	0.46
1:B:84:HIS:HB3	1:B:103:ARG:HG3	1.96	0.46
1:A:9:MET:HA	2:Y:108:PHE:CE2	2.51	0.46
1:A:52:TYR:CD2	1:A:52:TYR:N	2.84	0.45
2:X:85:TYR:CD2	2:X:96:ALA:HB2	2.51	0.45
1:A:85:THR:HG22	1:A:106:THR:HB	1.99	0.45
1:B:68:CYS:HB2	1:B:71:ILE:HG23	1.98	0.45
1:A:57:LYS:HE2	1:A:105:ASP:OD1	2.16	0.45
2:Y:133:VAL:HG23	2:Y:134:ASP:N	2.32	0.45
1:B:15:CYS:HB3	1:B:108:CYS:SG	2.57	0.45
2:X:27:GLN:HB3	2:X:35:VAL:HG11	1.99	0.44
2:X:25:VAL:HG23	2:X:53:GLU:O	2.17	0.44
1:A:15:CYS:HB3	1:A:108:CYS:SG	2.57	0.44
2:X:133:VAL:HG21	1:B:59:ARG:HH11	1.82	0.44
1:A:87:VAL:O	1:A:101:PHE:HA	2.18	0.44
1:A:9:MET:CA	2:Y:108:PHE:HE2	2.30	0.44
1:A:112:LEU:HD21	1:B:14:VAL:CG2	2.46	0.44
1:B:77:ASN:OD1	1:B:115:LYS:HE2	2.17	0.44
1:A:53:PHE:N	1:A:53:PHE:CD2	2.86	0.44
2:X:143:GLU:C	2:X:145:THR:H	2.21	0.44
1:A:64:VAL:HG12	1:A:65:GLU:N	2.33	0.43
2:Y:65:GLN:OE1	2:Y:65:GLN:HA	2.19	0.43
2:X:71:CYS:N	2:X:77:ALA:HB2	2.34	0.43
2:X:133:VAL:HG23	2:X:134:ASP:N	2.33	0.43
2:X:27:GLN:N	2:X:35:VAL:HG13	2.32	0.43
2:X:26:ALA:HB2	2:X:37:GLU:CG	2.47	0.43
2:X:108:PHE:CD2	1:B:9:MET:O	2.68	0.43
2:Y:160:CYS:O	2:Y:161:GLU:CB	2.66	0.43
1:A:30:ASP:OD2	1:A:32:LYS:HB2	2.19	0.43
2:X:161:GLU:HG3	2:X:162:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:8:LEU:HD11	2:X:52:THR:HG22	2.01	0.42
1:B:45:ASN:O	1:B:46:ASN:HB2	2.20	0.42
2:X:86:TYR:N	2:X:86:TYR:CD2	2.87	0.42
2:Y:126:TYR:CZ	2:Y:157:ASP:HB2	2.54	0.42
1:A:49:PHE:O	2:Y:42:SER:OG	2.35	0.42
2:Y:86:TYR:CE1	2:Y:115:ASN:HB2	2.54	0.42
1:A:52:TYR:CE1	2:Y:67:MET:CE	3.02	0.42
1:A:92:THR:HA	1:A:97:ALA:HA	2.02	0.42
2:Y:72:VAL:HG12	2:Y:73:GLU:N	2.35	0.42
2:X:153:THR:C	2:X:155:TRP:N	2.73	0.42
1:A:52:TYR:HE1	2:Y:67:MET:CE	2.32	0.42
1:A:27:THR:HG23	1:A:35:GLU:OE2	2.19	0.42
2:Y:102:VAL:HG12	2:Y:103:GLY:N	2.34	0.42
2:X:143:GLU:C	2:X:145:THR:N	2.73	0.42
2:Y:85:TYR:CD2	2:Y:96:ALA:HB2	2.54	0.42
2:Y:25:VAL:HG23	2:Y:53:GLU:O	2.20	0.42
2:X:123:GLU:OE1	2:X:123:GLU:HA	2.20	0.42
1:B:57:LYS:HE2	1:B:105:ASP:OD1	2.20	0.42
1:A:45:ASN:O	1:A:46:ASN:HB2	2.20	0.41
1:A:8:HIS:N	1:A:9:MET:CG	2.76	0.41
1:B:74:LYS:O	1:B:74:LYS:HG3	2.19	0.41
1:B:27:THR:CG2	1:B:28:ALA:N	2.83	0.41
1:B:8:HIS:C	1:B:10:GLY:HA3	2.39	0.41
1:A:22:VAL:O	1:A:22:VAL:HG12	2.21	0.41
2:Y:153:THR:C	2:Y:155:TRP:H	2.23	0.41
1:A:69:ARG:HH11	1:A:69:ARG:HG3	1.85	0.41
1:B:92:THR:HA	1:B:97:ALA:HA	2.02	0.41
2:Y:27:GLN:N	2:Y:35:VAL:HG13	2.35	0.41
2:X:91:THR:O	2:X:93:HIS:N	2.54	0.41
2:X:10:THR:HG22	2:X:14:GLU:O	2.21	0.41
2:Y:128:ASP:HB3	2:Y:129:GLU:CD	2.41	0.41
1:B:42:VAL:O	1:B:42:VAL:HG12	2.21	0.41
1:A:74:LYS:HG3	1:A:74:LYS:O	2.21	0.41
2:Y:91:THR:O	2:Y:93:HIS:N	2.53	0.40
2:X:150:ARG:HH11	2:X:159:GLU:CD	2.24	0.40
1:B:69:ARG:HH11	1:B:69:ARG:HG3	1.86	0.40
1:A:104:ILE:HG13	1:A:104:ILE:O	2.20	0.40
1:A:71:ILE:HG12	1:A:72:ASP:N	2.37	0.40
2:Y:8:LEU:HD11	2:Y:52:THR:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:9:TYR:O	1:B:117:THR:CG2[5_665]	2.07	0.13

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	108/230 (47%)	95 (88%)	11 (10%)	2 (2%)	10	55
1	B	108/230 (47%)	94 (87%)	11 (10%)	3 (3%)	6	47
2	X	160/171 (94%)	136 (85%)	19 (12%)	5 (3%)	5	45
2	Y	158/171 (92%)	133 (84%)	23 (15%)	2 (1%)	15	61
All	All	534/802 (67%)	458 (86%)	64 (12%)	12 (2%)	8	52

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	ASN
1	A	50	ARG
1	B	50	ARG
2	Y	102	VAL
2	X	12	SER
2	X	154	PRO
2	Y	154	PRO
1	B	43	ASN
2	X	135	PRO
2	X	102	VAL
2	X	54	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	97/197 (49%)	90 (93%)	7 (7%)	18	59
1	B	97/197 (49%)	91 (94%)	6 (6%)	23	64
2	X	139/147 (95%)	123 (88%)	16 (12%)	7	37
2	Y	137/147 (93%)	122 (89%)	15 (11%)	8	40
All	All	470/688 (68%)	426 (91%)	44 (9%)	11	47

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	19	SER
1	A	20	VAL
1	A	29	THR
1	A	71	ILE
1	A	92	THR
1	A	117	THR
2	X	5	SER
2	X	20	ASN
2	X	21	LEU
2	X	34	THR
2	X	37	GLU
2	X	49	VAL
2	X	56	LYS
2	X	62	LEU
2	X	68	SER
2	X	85	TYR
2	X	99	VAL
2	X	106	LEU
2	X	113	LYS
2	X	141	VAL
2	X	148	GLN
2	X	160	CYS
1	B	9	MET
1	B	20	VAL
1	B	29	THR
1	B	71	ILE
1	B	92	THR

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Mol	Chain	Res	Type
1	B	117	THR
2	Y	5	SER
2	Y	20	ASN
2	Y	21	LEU
2	Y	37	GLU
2	Y	42	SER
2	Y	56	LYS
2	Y	62	LEU
2	Y	68	SER
2	Y	85	TYR
2	Y	99	VAL
2	Y	106	LEU
2	Y	113	LYS
2	Y	141	VAL
2	Y	148	GLN
2	Y	160	CYS

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

Mol	Chain	Res	Type
1	A	43	ASN
2	X	20	ASN
1	B	43	ASN
2	Y	20	ASN

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 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 [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, 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	110/230 (47%)	0.29	4 (3%)	46 32	70, 136, 268, 306	0
1	B	110/230 (47%)	0.23	4 (3%)	46 32	84, 148, 255, 286	0
2	X	162/171 (94%)	-0.35	1 (0%)	90 82	89, 143, 210, 265	3 (1%)
2	Y	160/171 (93%)	-0.14	1 (0%)	90 82	104, 200, 284, 317	3 (1%)
All	All	542/802 (67%)	-0.04	10 (1%)	71 56	70, 153, 265, 317	6 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	SER	4.6
1	B	43	ASN	4.2
1	A	41	GLU	3.8
1	A	47	SER	3.5
1	B	46	ASN	3.0
1	A	42	VAL	2.8
2	Y	6	THR	2.6
1	A	43	ASN	2.5
2	X	2	GLU	2.4
1	B	93	ASP	2.3

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.