



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2022 – 05:01 PM EST

PDB ID : 3UW6
Title : Crystal Structure of Engineered Protein, Northeast Structural Genomics Consortium Target OR120
Authors : Seetharaman, J.; Lew, S.; Nivon, L.; Baker, D.; Bjelic, S.; Ciccocanti, C.; Sahdev, S.; Xiao, R.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-11-30
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
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) : 2.26

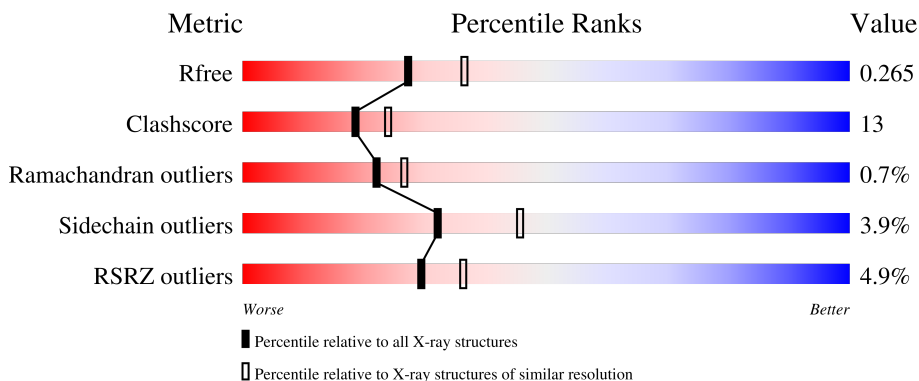
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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 $\leq 5\%$. 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	390	 3% 73% 20% • 5%
1	B	390	 4% 71% 22% •• 5%
1	C	390	 7% 71% 22% •• 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8977 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 Alanine racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	372	Total 2929	C 1876	N 520	O 519	S 4	Se 10	0	0	0
1	B	371	Total 2914	C 1867	N 516	O 518	S 4	Se 9	0	0	0
1	C	370	Total 2900	C 1858	N 515	O 514	S 4	Se 9	0	0	0

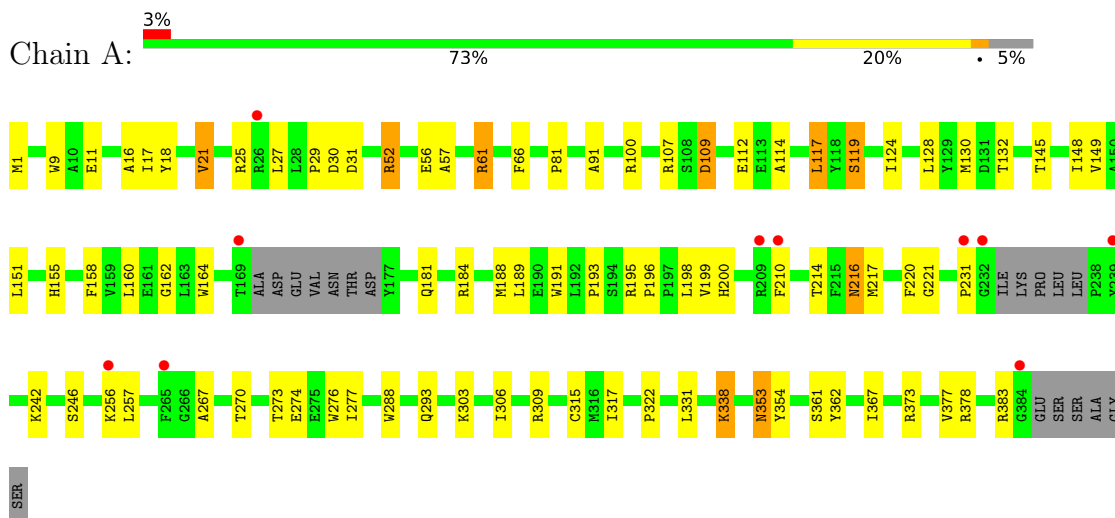
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total 80	O 80	0	0
2	B	80	Total 80	O 80	0	0
2	C	74	Total 74	O 74	0	0

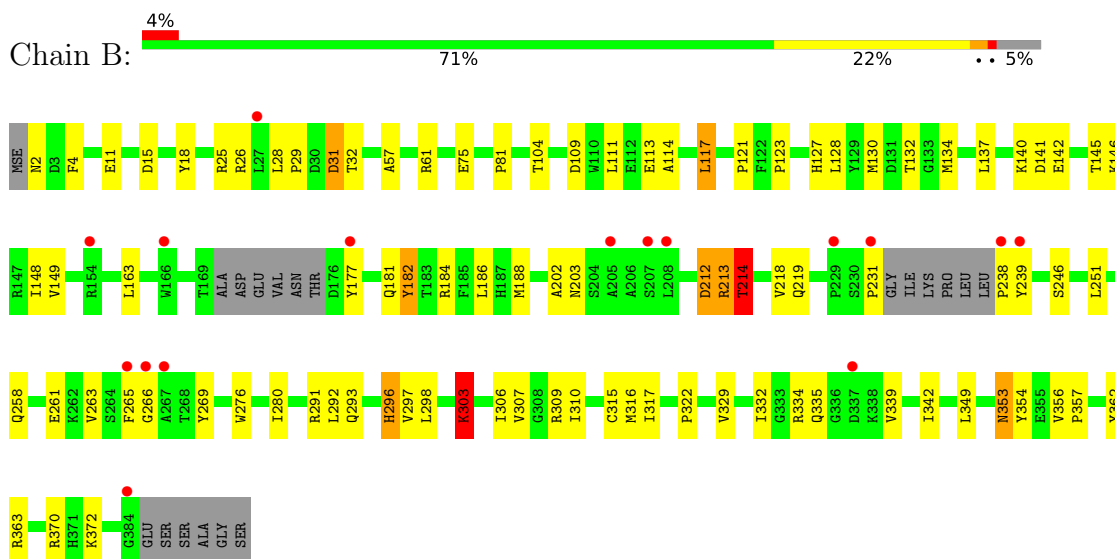
3 Residue-property plots [i](#)

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: Alanine racemase

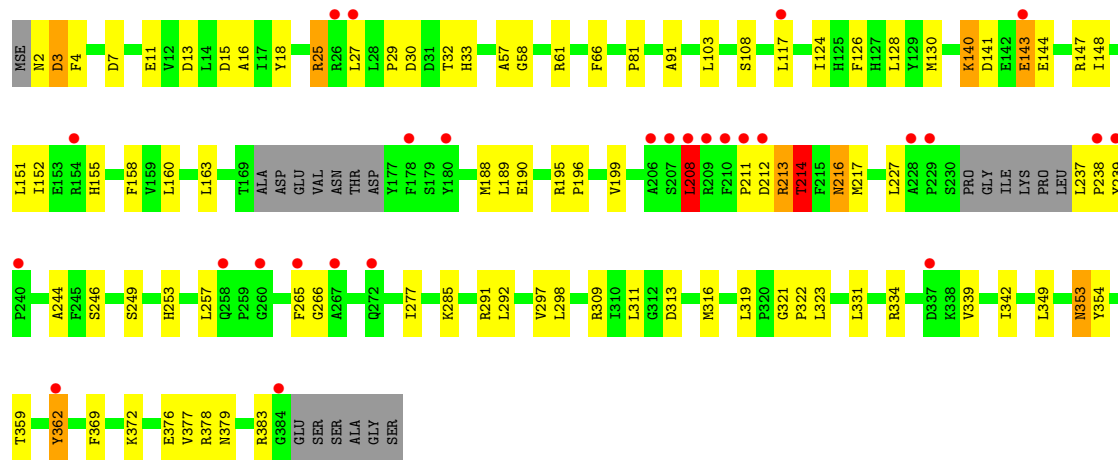


- Molecule 1: Alanine racemase



- Molecule 1: Alanine racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.35Å 112.35Å 237.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.47 – 2.30 37.66 – 2.13	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.47-2.30) 98.1 (37.66-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 2.14Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.259 0.227 , 0.265	Depositor DCC
R_{free} test set	12039 reflections (7.48%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	3/2995 (0.1%)	0.65	5/4051 (0.1%)
1	B	0.80	14/2980 (0.5%)	0.65	2/4035 (0.0%)
1	C	1.15	37/2965 (1.2%)	0.74	8/4014 (0.2%)
All	All	0.86	54/8940 (0.6%)	0.68	15/12100 (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
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	LYS	CB-CG	-14.42	1.13	1.52
1	B	213	ARG	CA-CB	-14.06	1.23	1.53
1	C	376	GLU	CD-OE1	-13.63	1.10	1.25
1	C	376	GLU	CD-OE2	-13.24	1.11	1.25
1	C	377	VAL	CB-CG2	-13.19	1.25	1.52
1	C	3	ASP	CB-CG	-12.28	1.25	1.51
1	B	214	THR	CB-CG2	-11.77	1.13	1.52
1	C	4	PHE	CD2-CE2	-11.74	1.15	1.39
1	C	4	PHE	CD1-CE1	-11.27	1.16	1.39
1	C	379	ASN	C-O	-10.99	1.02	1.23
1	C	377	VAL	CB-CG1	-10.77	1.30	1.52
1	C	4	PHE	CE2-CZ	-10.21	1.18	1.37
1	C	376	GLU	C-O	-9.28	1.05	1.23
1	C	2	ASN	C-O	-9.27	1.05	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	PHE	CG-CD2	-9.15	1.25	1.38
1	C	4	PHE	CE1-CZ	-9.10	1.20	1.37
1	C	378	ARG	CZ-NH2	-9.01	1.21	1.33
1	B	214	THR	C-O	-9.01	1.06	1.23
1	B	213	ARG	C-O	-8.81	1.06	1.23
1	C	3	ASP	C-O	-8.79	1.06	1.23
1	C	379	ASN	CG-ND2	-8.71	1.11	1.32
1	C	3	ASP	CG-OD2	-8.53	1.05	1.25
1	C	378	ARG	CZ-NH1	-8.27	1.22	1.33
1	A	119	SER	C-O	-8.09	1.07	1.23
1	C	379	ASN	CG-OD1	-8.08	1.06	1.24
1	B	296	HIS	C-O	-7.94	1.08	1.23
1	C	378	ARG	C-O	-7.75	1.08	1.23
1	C	3	ASP	CG-OD1	-7.74	1.07	1.25
1	C	4	PHE	C-O	-7.64	1.08	1.23
1	B	303	LYS	CA-CB	-7.57	1.37	1.53
1	C	377	VAL	C-O	-7.57	1.08	1.23
1	B	212	ASP	CG-OD2	-7.41	1.08	1.25
1	B	212	ASP	C-O	-7.37	1.09	1.23
1	C	214	THR	CB-CG2	-7.30	1.28	1.52
1	B	303	LYS	CG-CD	-7.19	1.28	1.52
1	A	119	SER	CA-CB	-7.15	1.42	1.52
1	C	4	PHE	CG-CD1	-7.08	1.28	1.38
1	C	211	PRO	CA-C	-7.05	1.38	1.52
1	C	378	ARG	CB-CG	-6.88	1.33	1.52
1	A	119	SER	CB-OG	-6.66	1.33	1.42
1	C	208	LEU	N-CA	-6.64	1.33	1.46
1	B	303	LYS	C-O	-6.45	1.11	1.23
1	C	376	GLU	CG-CD	-6.19	1.42	1.51
1	C	213	ARG	C-O	-5.91	1.12	1.23
1	B	212	ASP	CG-OD1	-5.87	1.11	1.25
1	C	211	PRO	N-CA	-5.87	1.37	1.47
1	C	377	VAL	CA-CB	-5.78	1.42	1.54
1	C	211	PRO	C-O	-5.74	1.11	1.23
1	C	2	ASN	CG-OD1	-5.74	1.11	1.24
1	C	214	THR	CA-CB	-5.70	1.38	1.53
1	B	214	THR	N-CA	-5.55	1.35	1.46
1	C	4	PHE	CB-CG	-5.40	1.42	1.51
1	B	303	LYS	N-CA	-5.08	1.36	1.46
1	C	214	THR	C-O	-5.05	1.13	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	378	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	B	212	ASP	CB-CG-OD1	8.48	125.93	118.30
1	A	378	ARG	N-CA-CB	-8.10	96.03	110.60
1	C	3	ASP	CB-CG-OD1	7.63	125.17	118.30
1	C	378	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	C	2	ASN	N-CA-C	7.57	131.43	111.00
1	C	376	GLU	OE1-CD-OE2	-6.19	115.88	123.30
1	C	378	ARG	CG-CD-NE	6.04	124.48	111.80
1	A	377	VAL	N-CA-C	-6.01	94.77	111.00
1	A	378	ARG	N-CA-C	-5.80	95.34	111.00
1	B	231	PRO	N-CA-CB	5.62	110.04	103.30
1	A	231	PRO	N-CA-CB	5.49	109.89	103.30
1	A	377	VAL	CB-CA-C	-5.38	101.17	111.40
1	C	214	THR	CA-CB-CG2	-5.18	105.14	112.40
1	C	208	LEU	CA-CB-CG	-5.07	103.65	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	362	TYR	Sidechain
1	B	362	TYR	Sidechain
1	C	213	ARG	Peptide
1	C	362	TYR	Sidechain

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	2929	0	2900	66	0
1	B	2914	0	2865	72	0
1	C	2900	0	2861	97	1
2	A	80	0	0	4	1
2	B	80	0	0	1	0
2	C	74	0	0	2	0
All	All	8977	0	8626	229	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 13.

All (229) 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:B:296:HIS:ND1	1:B:303:LYS:HE2	1.20	1.46
1:B:296:HIS:CE1	1:B:303:LYS:HE2	1.72	1.23
1:C:91:ALA:HA	1:C:117:LEU:CD2	1.71	1.19
1:C:208:LEU:CD2	1:C:239:TYR:OH	1.94	1.15
1:B:296:HIS:ND1	1:B:303:LYS:CE	2.13	1.11
1:B:296:HIS:CE1	1:B:303:LYS:CE	2.39	1.06
1:C:91:ALA:HA	1:C:117:LEU:HD21	1.38	1.04
1:B:296:HIS:CE1	1:B:303:LYS:NZ	2.38	0.92
1:C:199:VAL:H	1:C:216:ASN:HD21	1.15	0.90
1:C:208:LEU:HD21	1:C:239:TYR:OH	1.70	0.90
1:C:91:ALA:HA	1:C:117:LEU:HD23	1.52	0.89
1:A:25:ARG:O	1:A:25:ARG:HD3	1.74	0.88
1:A:353:ASN:HD22	1:A:354:TYR:H	1.16	0.88
1:C:128:LEU:HD21	1:C:148:ILE:HG21	1.54	0.87
1:A:216:ASN:HD22	1:A:216:ASN:H	1.18	0.87
1:A:199:VAL:H	1:A:216:ASN:HD21	1.20	0.86
1:A:132:THR:HG23	1:A:184:ARG:CG	2.07	0.84
1:A:132:THR:HG22	1:A:132:THR:O	1.76	0.83
1:A:17:ILE:O	1:A:21:VAL:HG12	1.79	0.83
1:B:25:ARG:O	1:B:25:ARG:HD3	1.78	0.82
1:A:130:MSE:HE3	1:A:188:MSE:HB3	1.64	0.80
1:A:353:ASN:HD22	1:A:354:TYR:N	1.82	0.78
1:C:208:LEU:HD22	1:C:239:TYR:OH	1.82	0.77
1:B:296:HIS:HE1	1:B:303:LYS:NZ	1.82	0.75
1:C:322:PRO:O	1:C:323:LEU:HD12	1.85	0.75
1:C:128:LEU:CD2	1:C:148:ILE:HG21	2.16	0.75
1:A:114:ALA:HA	1:A:117:LEU:HD22	1.68	0.75
1:C:353:ASN:HD22	1:C:354:TYR:H	1.35	0.74
1:C:91:ALA:CA	1:C:117:LEU:CD2	2.61	0.74
1:C:163:LEU:HG	1:C:196:PRO:HG3	1.70	0.73
1:B:212:ASP:OD1	1:B:214:THR:CG2	2.36	0.72
1:A:132:THR:HG21	1:A:181:GLN:HA	1.72	0.72
1:C:216:ASN:H	1:C:216:ASN:HD22	1.36	0.71
1:C:91:ALA:CA	1:C:117:LEU:HD21	2.19	0.71
1:B:266:GLY:HA3	1:B:309:ARG:HB2	1.72	0.71
1:C:208:LEU:HD21	1:C:239:TYR:HH	1.55	0.71
1:B:332:ILE:HD13	1:B:342:ILE:HD13	1.72	0.71
1:B:130:MSE:SE	1:B:163:LEU:HD21	2.41	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:THR:O	1:B:184:ARG:HG2	1.91	0.70
1:A:216:ASN:H	1:A:216:ASN:ND2	1.88	0.70
1:B:334:ARG:HB2	1:B:339:VAL:HG12	1.75	0.68
1:A:52:ARG:HD2	2:A:400:HOH:O	1.93	0.68
1:A:132:THR:HG23	1:A:184:ARG:HB3	1.75	0.68
1:A:132:THR:CG2	1:A:184:ARG:HB3	2.24	0.68
1:C:195:ARG:NH2	1:C:199:VAL:HG21	2.08	0.68
1:C:124:ILE:HD13	1:C:126:PHE:CZ	2.29	0.68
1:B:353:ASN:HD22	1:B:354:TYR:H	1.43	0.67
1:A:91:ALA:HA	1:A:117:LEU:HD11	1.76	0.67
1:C:29:PRO:HG2	1:C:32:THR:HG23	1.77	0.67
1:A:61:ARG:HG3	1:A:81:PRO:HB2	1.76	0.67
1:C:321:GLY:O	1:C:323:LEU:HD13	1.95	0.67
1:A:107:ARG:NH1	1:A:109:ASP:HB2	2.10	0.66
1:A:256:LYS:HD3	1:A:276:TRP:CZ2	2.31	0.66
1:B:296:HIS:HE1	1:B:303:LYS:HZ1	1.43	0.65
1:C:199:VAL:H	1:C:216:ASN:ND2	1.90	0.65
1:B:297:VAL:HG11	1:B:329:VAL:CG1	2.27	0.65
1:B:212:ASP:O	1:B:213:ARG:CB	2.30	0.64
1:A:353:ASN:ND2	1:A:354:TYR:H	1.94	0.64
1:A:132:THR:HG23	1:A:184:ARG:CB	2.28	0.64
1:A:199:VAL:H	1:A:216:ASN:ND2	1.96	0.62
1:C:147:ARG:O	1:C:151:LEU:HD23	2.00	0.62
1:C:353:ASN:HD22	1:C:354:TYR:N	1.98	0.61
1:C:216:ASN:HD22	1:C:216:ASN:N	1.95	0.61
1:C:334:ARG:HB2	1:C:339:VAL:HG12	1.82	0.61
1:A:61:ARG:HD2	1:A:217:MSE:HE1	1.82	0.60
1:B:353:ASN:HD22	1:B:354:TYR:N	1.99	0.60
1:C:216:ASN:H	1:C:216:ASN:ND2	2.00	0.60
1:A:132:THR:O	1:A:132:THR:CG2	2.48	0.60
1:A:257:LEU:HD11	1:A:277:ILE:HD12	1.84	0.59
1:B:145:THR:O	1:B:149:VAL:HG23	2.02	0.59
1:C:27:LEU:HD21	1:C:238:PRO:HG2	1.83	0.59
1:B:114:ALA:HA	1:B:117:LEU:CD2	2.33	0.58
1:B:291:ARG:HE	1:C:291:ARG:NE	2.01	0.58
1:A:100:ARG:HG3	1:A:100:ARG:HH11	1.68	0.58
1:B:363:ARG:HG2	1:C:66:PHE:HZ	1.67	0.58
1:C:128:LEU:HD21	1:C:148:ILE:CG2	2.29	0.58
1:B:184:ARG:O	1:B:188:MSE:HG3	2.03	0.58
1:C:124:ILE:HG23	1:C:124:ILE:O	2.04	0.57
1:C:311:LEU:HD21	1:C:316:MSE:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:HIS:CE1	1:B:303:LYS:HZ3	2.22	0.57
1:C:297:VAL:CG2	1:C:331:LEU:HD13	2.34	0.57
1:B:61:ARG:HG2	1:B:81:PRO:HB2	1.86	0.57
1:B:251:LEU:HD21	1:B:317:ILE:HD11	1.87	0.56
1:C:208:LEU:CD2	1:C:239:TYR:HH	2.09	0.56
1:C:266:GLY:HA3	1:C:309:ARG:HB2	1.85	0.56
1:C:297:VAL:HG22	1:C:298:LEU:H	1.71	0.56
1:B:291:ARG:NE	1:C:291:ARG:NE	2.54	0.56
1:C:227:LEU:HD21	1:C:342:ILE:HD12	1.88	0.56
1:B:356:VAL:HB	1:B:357:PRO:HD3	1.87	0.56
1:C:322:PRO:C	1:C:323:LEU:HD12	2.26	0.56
1:C:297:VAL:HG23	1:C:331:LEU:HD13	1.87	0.55
1:A:216:ASN:HD22	1:A:216:ASN:N	1.83	0.55
1:A:130:MSE:CE	1:A:188:MSE:HB3	2.36	0.55
1:C:163:LEU:HD12	1:C:163:LEU:O	2.07	0.55
1:A:132:THR:HG23	1:A:184:ARG:HG3	1.87	0.55
1:C:128:LEU:HG	1:C:160:LEU:HD11	1.90	0.54
1:A:52:ARG:O	1:A:56:GLU:HG3	2.06	0.54
1:A:353:ASN:ND2	1:A:354:TYR:N	2.55	0.54
1:B:212:ASP:OD1	1:B:214:THR:HG23	2.07	0.54
1:B:297:VAL:HG12	1:B:298:LEU:N	2.22	0.54
1:C:3:ASP:OD2	1:C:3:ASP:N	2.34	0.54
1:C:238:PRO:HG2	1:C:239:TYR:HD1	1.73	0.53
1:B:142:GLU:O	1:B:146:LYS:HG2	2.08	0.53
1:A:267:ALA:HB2	1:A:309:ARG:HD2	1.91	0.53
1:C:141:ASP:OD2	1:C:143:GLU:HB2	2.09	0.53
1:B:114:ALA:HA	1:B:117:LEU:HD22	1.90	0.53
1:C:292:LEU:HG	1:C:349:LEU:HD21	1.90	0.52
1:A:293:GLN:O	1:A:306:ILE:O	2.27	0.52
1:A:184:ARG:O	1:A:188:MSE:HG3	2.09	0.52
1:B:263:VAL:HG23	1:B:269:TYR:HB3	1.92	0.52
1:A:124:ILE:HD12	2:A:409:HOH:O	2.09	0.52
1:A:315:CYS:HB2	2:A:401:HOH:O	2.09	0.51
1:A:160:LEU:HD22	1:A:196:PRO:HB3	1.91	0.51
1:C:309:ARG:HG2	1:C:309:ARG:HH11	1.76	0.51
1:A:128:LEU:HD11	1:A:148:ILE:HG21	1.92	0.51
1:B:181:GLN:O	1:B:182:TYR:HB2	2.10	0.51
1:C:316:MSE:SE	1:C:316:MSE:N	2.94	0.50
1:B:306:ILE:HG21	1:B:310:ILE:HD11	1.93	0.50
1:C:33:HIS:O	1:C:217:MSE:HA	2.12	0.50
1:B:75:GLU:OE1	1:C:383:ARG:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HH22	1:C:199:VAL:HG21	1.75	0.50
1:B:28:LEU:HD11	1:B:218:VAL:HG21	1.94	0.50
1:C:297:VAL:HG22	1:C:298:LEU:N	2.26	0.50
1:A:29:PRO:HG2	1:A:31:ASP:OD1	2.13	0.49
1:C:237:LEU:N	1:C:238:PRO:HD2	2.27	0.49
1:B:32:THR:HG21	1:B:218:VAL:HG13	1.94	0.49
1:C:25:ARG:HG3	1:C:58:GLY:HA3	1.94	0.49
1:A:27:LEU:C	1:A:27:LEU:HD23	2.33	0.48
1:B:113:GLU:O	1:B:117:LEU:HD22	2.13	0.48
1:B:128:LEU:HB2	1:B:163:LEU:HD23	1.95	0.48
1:C:130:MSE:HE3	1:C:188:MSE:HE2	1.94	0.48
1:B:266:GLY:C	1:B:309:ARG:HD2	2.34	0.48
1:C:103:LEU:HD12	1:C:124:ILE:HD11	1.94	0.48
1:B:18:TYR:CD1	1:B:57:ALA:HB2	2.49	0.48
1:B:238:PRO:HG2	1:B:239:TYR:CD1	2.49	0.47
1:A:288:TRP:CE2	1:A:331:LEU:HD23	2.49	0.47
1:C:199:VAL:HG23	1:C:199:VAL:O	2.15	0.47
1:C:11:GLU:HB2	1:C:246:SER:OG	2.15	0.47
1:C:334:ARG:CB	1:C:339:VAL:HG12	2.45	0.47
1:C:128:LEU:O	1:C:163:LEU:HA	2.14	0.47
1:C:257:LEU:HD11	1:C:277:ILE:HD12	1.95	0.47
1:A:132:THR:HG23	1:A:184:ARG:HG2	1.94	0.47
1:A:155:HIS:HB3	1:A:158:PHE:HB2	1.96	0.46
1:B:128:LEU:HD21	1:B:148:ILE:HG21	1.98	0.46
1:B:297:VAL:CG1	1:B:329:VAL:CG1	2.94	0.46
1:C:334:ARG:HB2	1:C:334:ARG:HH11	1.80	0.46
1:B:316:MSE:SE	1:B:316:MSE:N	2.98	0.46
1:A:303:LYS:HE2	1:A:338:LYS:HG3	1.97	0.46
1:A:61:ARG:CD	1:A:217:MSE:HE1	2.46	0.46
1:B:291:ARG:C	1:B:293:GLN:H	2.19	0.46
1:C:11:GLU:HG2	1:C:369:PHE:HE1	1.80	0.46
1:B:140:LYS:HG3	1:B:141:ASP:OD1	2.16	0.46
1:A:107:ARG:HH12	1:A:109:ASP:HB2	1.80	0.46
1:B:128:LEU:HB2	1:B:163:LEU:CD2	2.47	0.46
1:C:152:ILE:HG23	1:C:158:PHE:HB3	1.98	0.45
1:A:195:ARG:NH2	1:A:214:THR:O	2.49	0.45
1:A:1:MSE:HG2	1:A:383:ARG:HB2	1.98	0.45
1:C:124:ILE:HG23	1:C:126:PHE:CE2	2.52	0.45
1:A:91:ALA:CA	1:A:117:LEU:HD11	2.45	0.45
1:A:117:LEU:C	1:A:117:LEU:HD23	2.37	0.45
1:B:15:ASP:OD2	1:B:370:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ALA:HB2	1:B:219:GLN:OE1	2.17	0.45
1:B:266:GLY:CA	1:B:309:ARG:HB2	2.44	0.45
1:C:353:ASN:HD22	1:C:353:ASN:N	2.15	0.45
1:A:164:TRP:HA	1:A:200:HIS:O	2.17	0.44
1:A:9:TRP:CD1	1:A:367:ILE:HD12	2.52	0.44
1:B:137:LEU:HB2	1:C:253:HIS:CD2	2.52	0.44
1:B:182:TYR:O	1:B:186:LEU:HG	2.17	0.44
1:B:269:TYR:CE2	1:B:307:VAL:HB	2.52	0.44
1:C:7:ASP:O	1:C:249:SER:HA	2.17	0.44
1:A:162:GLY:HA2	1:A:198:LEU:O	2.18	0.44
1:B:26:ARG:HH11	1:B:26:ARG:HB3	1.83	0.44
1:C:16:ALA:HB3	1:C:244:ALA:HB2	2.00	0.44
1:C:362:TYR:N	1:C:362:TYR:CD1	2.84	0.44
1:C:140:LYS:H	1:C:140:LYS:HD3	1.82	0.44
1:B:276:TRP:CE3	1:B:322:PRO:HB3	2.53	0.44
1:C:238:PRO:HG2	1:C:239:TYR:CD1	2.53	0.44
1:A:188:MSE:HA	1:A:191:TRP:CD2	2.53	0.44
1:C:155:HIS:HB3	1:C:158:PHE:HB2	2.00	0.44
1:B:296:HIS:CD2	1:B:296:HIS:H	2.34	0.43
1:C:32:THR:HA	1:C:216:ASN:O	2.18	0.43
1:C:61:ARG:HG2	1:C:61:ARG:HH11	1.83	0.43
1:C:124:ILE:CG2	1:C:126:PHE:CE2	3.02	0.43
1:B:104:THR:HA	1:B:127:HIS:O	2.18	0.43
1:B:263:VAL:HG23	1:B:263:VAL:O	2.19	0.43
1:C:13:ASP:OD1	1:C:15:ASP:HB2	2.18	0.43
1:C:334:ARG:HB2	1:C:334:ARG:NH1	2.33	0.43
1:A:306:ILE:HA	1:A:317:ILE:HG22	2.00	0.43
1:B:276:TRP:CZ3	1:B:322:PRO:HB3	2.53	0.43
1:B:26:ARG:HB3	1:B:26:ARG:NH1	2.33	0.43
1:C:61:ARG:HD3	1:C:81:PRO:HB2	2.00	0.43
1:A:276:TRP:CZ2	1:A:322:PRO:HB3	2.54	0.43
1:C:195:ARG:NH2	1:C:214:THR:O	2.51	0.43
1:C:29:PRO:HG2	1:C:32:THR:CG2	2.47	0.43
1:C:353:ASN:N	1:C:353:ASN:ND2	2.65	0.43
1:C:237:LEU:N	1:C:238:PRO:CD	2.82	0.43
1:B:280:ILE:HD11	1:B:315:CYS:SG	2.59	0.42
1:B:292:LEU:HG	1:B:349:LEU:HD21	1.99	0.42
1:A:257:LEU:CD1	1:A:277:ILE:HD12	2.50	0.42
1:C:18:TYR:CD1	1:C:57:ALA:HB2	2.55	0.42
1:C:25:ARG:O	1:C:25:ARG:HD3	2.19	0.42
1:C:27:LEU:HD12	1:C:27:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:SER:HB3	1:C:144:GLU:HG3	2.00	0.42
1:B:4:PHE:HB2	2:C:399:HOH:O	2.19	0.42
1:B:134:MSE:HE1	1:B:177:TYR:CZ	2.55	0.42
1:A:18:TYR:CD1	1:A:57:ALA:HB2	2.55	0.42
1:A:273:THR:OG1	1:A:274:GLU:N	2.52	0.42
1:C:353:ASN:ND2	1:C:354:TYR:H	2.11	0.42
1:C:359:THR:HB	2:C:413:HOH:O	2.20	0.42
1:A:25:ARG:HD3	1:A:25:ARG:C	2.34	0.42
1:C:311:LEU:CD2	1:C:316:MSE:HE1	2.50	0.41
1:A:11:GLU:HB2	1:A:246:SER:OG	2.20	0.41
1:B:11:GLU:HB2	1:B:246:SER:OG	2.20	0.41
1:B:29:PRO:C	1:B:31:ASP:H	2.24	0.41
1:C:124:ILE:O	1:C:124:ILE:CG2	2.67	0.41
1:C:319:LEU:HD13	1:C:323:LEU:HB2	2.02	0.41
1:A:16:ALA:HB1	1:A:242:LYS:HG3	2.02	0.41
1:C:285:LYS:HE2	1:C:313:ASP:OD1	2.20	0.41
1:A:145:THR:O	1:A:149:VAL:HG23	2.20	0.41
1:B:258:GLN:O	1:B:261:GLU:HB2	2.21	0.41
1:B:363:ARG:HG2	1:C:66:PHE:CZ	2.52	0.41
1:C:189:LEU:HD23	1:C:189:LEU:O	2.21	0.41
1:A:66:PHE:HB2	2:A:398:HOH:O	2.20	0.40
1:A:373:ARG:NH1	1:A:373:ARG:HB2	2.35	0.40
1:B:332:ILE:HD13	1:B:342:ILE:CD1	2.46	0.40
1:C:297:VAL:HG21	1:C:331:LEU:HD13	2.03	0.40
1:A:112:GLU:HG2	1:A:151:LEU:HD11	2.03	0.40
1:B:123:PRO:HB3	2:B:469:HOH:O	2.20	0.40
1:C:353:ASN:ND2	1:C:354:TYR:N	2.68	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)
1:C:117:LEU:CD1	2:A:443:HOH:O[8_654]	2.18	0.02

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	366/390 (94%)	355 (97%)	9 (2%)	2 (0%)	29	35
1	B	365/390 (94%)	347 (95%)	16 (4%)	2 (0%)	29	35
1	C	364/390 (93%)	351 (96%)	9 (2%)	4 (1%)	14	15
All	All	1095/1170 (94%)	1053 (96%)	34 (3%)	8 (1%)	22	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	PHE
1	C	212	ASP
1	C	214	THR
1	B	182	TYR
1	C	265	PHE
1	C	30	ASP
1	A	221	GLY
1	A	193	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	304/314 (97%)	289 (95%)	15 (5%)	25	35
1	B	300/314 (96%)	288 (96%)	12 (4%)	31	44
1	C	299/314 (95%)	291 (97%)	8 (3%)	44	61
All	All	903/942 (96%)	868 (96%)	35 (4%)	32	46

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL

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Mol	Chain	Res	Type
1	A	30	ASP
1	A	52	ARG
1	A	61	ARG
1	A	109	ASP
1	A	117	LEU
1	A	119	SER
1	A	189	LEU
1	A	210	PHE
1	A	216	ASN
1	A	220	PHE
1	A	270	THR
1	A	338	LYS
1	A	353	ASN
1	A	361	SER
1	B	2	ASN
1	B	31	ASP
1	B	109	ASP
1	B	111	LEU
1	B	117	LEU
1	B	121	PRO
1	B	203	ASN
1	B	214	THR
1	B	303	LYS
1	B	335	GLN
1	B	353	ASN
1	B	372	LYS
1	C	25	ARG
1	C	140	LYS
1	C	143	GLU
1	C	190	GLU
1	C	208	LEU
1	C	216	ASN
1	C	353	ASN
1	C	372	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	99	GLN
1	A	181	GLN
1	A	203	ASN

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Mol	Chain	Res	Type
1	A	216	ASN
1	A	258	GLN
1	A	293	GLN
1	A	348	HIS
1	A	353	ASN
1	B	5	HIS
1	B	157	HIS
1	B	203	ASN
1	B	293	GLN
1	B	296	HIS
1	B	348	HIS
1	B	353	ASN
1	C	23	ASN
1	C	33	HIS
1	C	125	HIS
1	C	216	ASN
1	C	272	GLN
1	C	353	ASN

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

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, 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	362/390 (92%)	0.06	10 (2%) 53 60	20, 37, 64, 78	0
1	B	362/390 (92%)	0.21	16 (4%) 34 41	23, 39, 66, 82	0
1	C	361/390 (92%)	0.27	27 (7%) 14 19	25, 44, 74, 82	0
All	All	1085/1170 (92%)	0.18	53 (4%) 29 36	20, 40, 69, 82	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	SER	9.1
1	B	266	GLY	7.5
1	C	210	PHE	6.0
1	B	239	TYR	5.6
1	B	238	PRO	4.8
1	A	209	ARG	4.7
1	C	260	GLY	4.7
1	C	209	ARG	4.5
1	C	272	GLN	4.3
1	B	267	ALA	4.3
1	B	208	LEU	4.1
1	C	208	LEU	4.0
1	A	210	PHE	3.8
1	C	117	LEU	3.8
1	B	205	ALA	3.8
1	A	169	THR	3.7
1	C	27	LEU	3.6
1	B	265	PHE	3.3
1	C	207	SER	3.2
1	B	384	GLY	3.1
1	A	26	ARG	3.1
1	A	265	PHE	3.1
1	C	238	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	229	PRO	3.0
1	B	337	ASP	3.0
1	B	177	TYR	2.9
1	A	384	GLY	2.8
1	C	154	ARG	2.8
1	C	384	GLY	2.7
1	A	239	TYR	2.7
1	C	178	PHE	2.7
1	B	27	LEU	2.7
1	A	232	GLY	2.7
1	C	206	ALA	2.7
1	C	240	PRO	2.6
1	C	212	ASP	2.5
1	C	229	PRO	2.4
1	A	231	PRO	2.4
1	C	267	ALA	2.4
1	C	239	TYR	2.3
1	B	231	PRO	2.3
1	C	26	ARG	2.3
1	C	228	ALA	2.3
1	C	180	TYR	2.2
1	B	166	TRP	2.1
1	C	258	GLN	2.1
1	C	362	TYR	2.1
1	C	211	PRO	2.1
1	C	337	ASP	2.0
1	B	154	ARG	2.0
1	C	265	PHE	2.0
1	C	143	GLU	2.0
1	A	256	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.