



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 AM GMT

PDB ID : 2CYX
Title : Structure of human ubiquitin-conjugating enzyme E2 G2 (UBE2G2/UBC7)
Authors : Yoshikawa, S.; Arai, R.; Murayama, K.; Imai, Y.; Takahashi, R.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-08
Resolution : 2.56 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

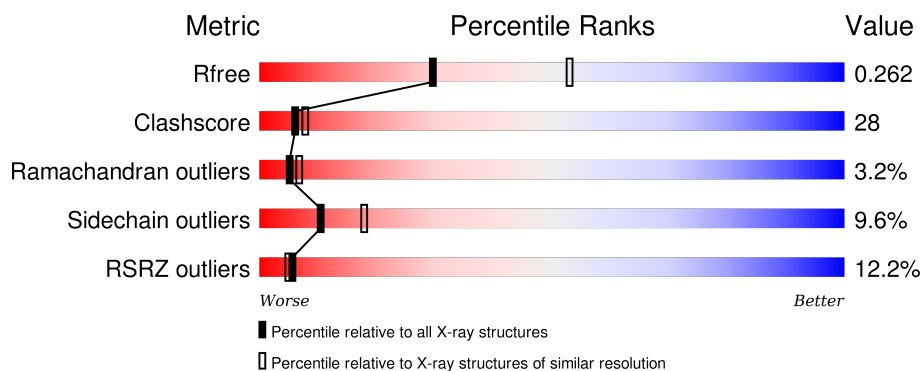
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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	170	<div> <div>9%</div> <div>51%</div> <div>39%</div> <div>9%</div> <div>..</div> </div>
1	B	170	<div> <div>8%</div> <div>62%</div> <div>32%</div> <div>5%</div> <div>..</div> </div>
1	C	170	<div> <div>19%</div> <div>52%</div> <div>39%</div> <div>8%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4019 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 Ubiquitin-conjugating enzyme E2 G2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1332	854	213	253	12			
1	B	169	Total	C	N	O	S	0	0	0
			1332	854	213	253	12			
1	C	169	Total	C	N	O	S	0	0	0
			1332	854	213	253	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP P60604
A	-4	GLY	-	CLONING ARTIFACT	UNP P60604
A	-3	SER	-	CLONING ARTIFACT	UNP P60604
A	-2	GLU	-	CLONING ARTIFACT	UNP P60604
A	-1	PHE	-	CLONING ARTIFACT	UNP P60604
B	-5	GLY	-	CLONING ARTIFACT	UNP P60604
B	-4	GLY	-	CLONING ARTIFACT	UNP P60604
B	-3	SER	-	CLONING ARTIFACT	UNP P60604
B	-2	GLU	-	CLONING ARTIFACT	UNP P60604
B	-1	PHE	-	CLONING ARTIFACT	UNP P60604
C	-5	GLY	-	CLONING ARTIFACT	UNP P60604
C	-4	GLY	-	CLONING ARTIFACT	UNP P60604
C	-3	SER	-	CLONING ARTIFACT	UNP P60604
C	-2	GLU	-	CLONING ARTIFACT	UNP P60604
C	-1	PHE	-	CLONING ARTIFACT	UNP P60604

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	12	Total	O	0	0
			12	12		

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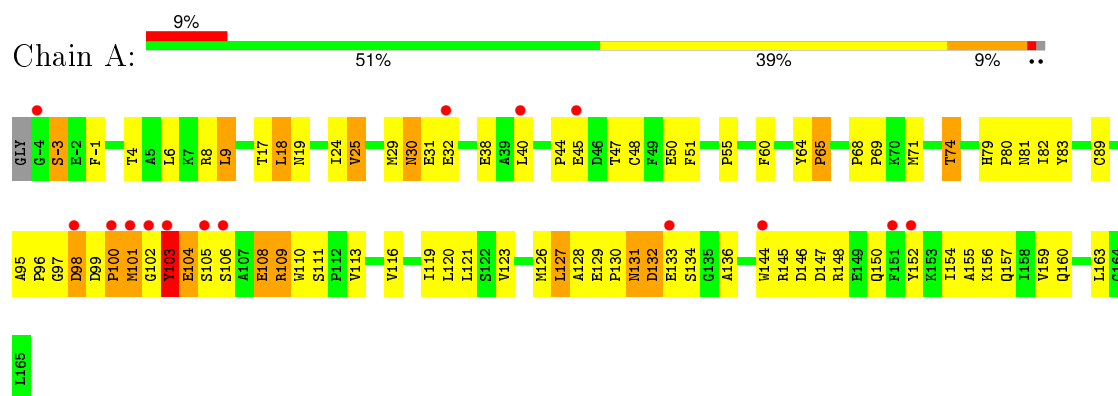
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total	O	0	0
			3	3		

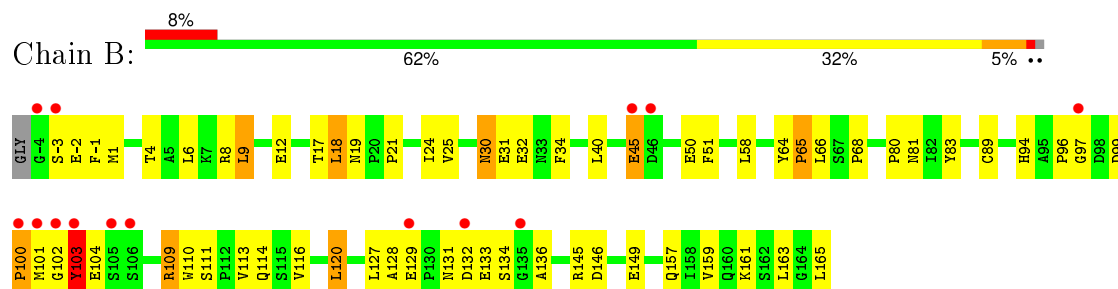
3 Residue-property plots [i](#)

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.

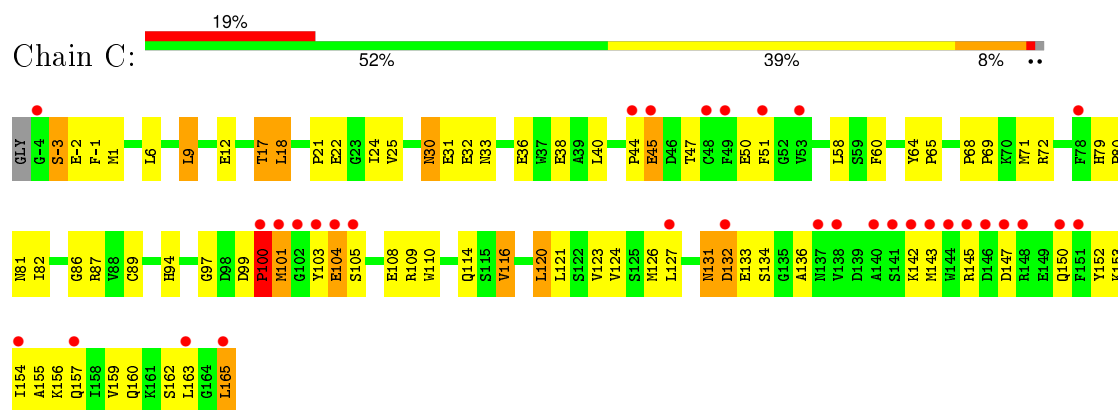
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.52Å 87.61Å 157.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.56 49.43 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.43-2.56) 97.6 (49.43-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.262 0.228 , 0.262	Depositor DCC
R_{free} test set	2861 reflections (10.08%)	DCC
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.880	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28405 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4019	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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 [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	0.49	0/1369	0.69	0/1855
1	B	0.45	0/1369	0.69	0/1855
1	C	0.43	0/1369	0.76	3/1855 (0.2%)
All	All	0.46	0/4107	0.71	3/5565 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-2	GLU	N-CA-C	-7.26	91.40	111.00
1	C	100	PRO	N-CA-C	6.43	128.82	112.10
1	C	104	GLU	N-CA-C	6.33	128.09	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	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	1332	0	1292	79	0
1	B	1332	0	1292	63	0
1	C	1332	0	1292	91	0
2	A	8	0	0	0	0
2	B	12	0	0	0	0
2	C	3	0	0	0	0
All	All	4019	0	3876	223	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 28.

All (223) 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:99:ASP:HB3	1:A:100:PRO:CD	1.87	1.03
1:A:99:ASP:CB	1:A:100:PRO:HD2	1.86	1.02
1:B:17:THR:HG22	1:B:18:LEU:HD13	1.42	1.02
1:A:99:ASP:HB3	1:A:100:PRO:HD2	0.99	0.98
1:B:97:GLY:HA2	1:B:100:PRO:HG3	1.48	0.95
1:B:101:MET:C	1:B:103:TYR:H	1.62	0.93
1:A:25:VAL:HG13	1:A:40:LEU:HB2	1.56	0.88
1:C:17:THR:HG22	1:C:18:LEU:HD13	1.57	0.86
1:C:100:PRO:HB3	1:C:109:ARG:HH12	1.42	0.85
1:A:148:ARG:HG2	1:A:152:TYR:CE1	2.11	0.84
1:A:95:ALA:O	1:A:98:ASP:HB2	1.78	0.83
1:B:145:ARG:HD2	1:B:146:ASP:OD2	1.81	0.80
1:B:101:MET:C	1:B:103:TYR:N	2.33	0.80
1:B:96:PRO:HA	1:B:109:ARG:HG2	1.62	0.80
1:A:55:PRO:HG2	1:A:74:THR:HG22	1.64	0.80
1:C:100:PRO:HB3	1:C:109:ARG:HH22	1.46	0.80
1:C:100:PRO:CB	1:C:109:ARG:HH12	1.93	0.80
1:C:100:PRO:HB3	1:C:109:ARG:NH1	2.01	0.75
1:A:145:ARG:HD2	1:A:146:ASP:OD2	1.87	0.74
1:B:25:VAL:CG1	1:B:40:LEU:HB2	2.17	0.74
1:B:-3:SER:HB2	1:C:31:GLU:HB3	1.69	0.73
1:B:1:MET:HG3	1:C:31:GLU:HG3	1.71	0.73
1:B:4:THR:HG22	1:C:17:THR:HG21	1.70	0.73
1:C:100:PRO:HB3	1:C:109:ARG:NH2	2.04	0.72
1:A:103:TYR:C	1:A:105:SER:H	1.91	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:CYS:HB3	1:A:152:TYR:HD2	1.55	0.71
1:B:102:GLY:C	1:B:104:GLU:H	1.94	0.70
1:B:81:ASN:HD22	1:B:134:SER:HB3	1.55	0.70
1:B:81:ASN:ND2	1:B:134:SER:HB3	2.06	0.70
1:B:110:TRP:CZ3	1:B:114:GLN:HB2	2.26	0.70
1:C:25:VAL:CG1	1:C:40:LEU:HB2	2.21	0.70
1:B:-3:SER:C	1:B:-1:PHE:H	1.94	0.70
1:C:156:LYS:O	1:C:159:VAL:HG22	1.91	0.70
1:B:17:THR:HG22	1:B:18:LEU:CD1	2.19	0.69
1:A:50:GLU:HG2	1:A:51:PHE:CD1	2.29	0.68
1:B:97:GLY:HA2	1:B:100:PRO:CG	2.22	0.67
1:B:4:THR:CG2	1:C:17:THR:HG21	2.23	0.67
1:B:80:PRO:O	1:B:136:ALA:HB3	1.94	0.67
1:A:105:SER:O	1:A:109:ARG:CG	2.43	0.67
1:A:17:THR:HG22	1:A:18:LEU:CD1	2.24	0.67
1:B:94:HIS:O	1:B:109:ARG:HG3	1.95	0.67
1:C:156:LYS:O	1:C:160:GLN:HG3	1.93	0.67
1:C:142:LYS:NZ	1:C:145:ARG:HH22	1.93	0.66
1:C:154:ILE:HA	1:C:157:GLN:NE2	2.09	0.66
1:A:-3:SER:C	1:A:-1:PHE:H	1.98	0.66
1:A:71:MET:CE	1:A:123:VAL:HG21	2.26	0.66
1:C:71:MET:HE1	1:C:123:VAL:HG21	1.78	0.65
1:A:105:SER:O	1:A:109:ARG:HG3	1.97	0.65
1:A:156:LYS:O	1:A:159:VAL:HG22	1.96	0.65
1:C:25:VAL:HG13	1:C:40:LEU:HB2	1.79	0.65
1:B:25:VAL:HG12	1:B:40:LEU:HB2	1.79	0.65
1:C:31:GLU:CD	1:C:31:GLU:H	2.00	0.65
1:A:97:GLY:O	1:A:98:ASP:C	2.35	0.64
1:A:17:THR:HG22	1:A:18:LEU:HD13	1.79	0.64
1:C:160:GLN:HB3	1:C:165:LEU:CD1	2.27	0.63
1:B:102:GLY:O	1:B:104:GLU:N	2.31	0.63
1:C:30:ASN:HD21	1:C:32:GLU:HB2	1.62	0.62
1:C:17:THR:CG2	1:C:18:LEU:HD13	2.29	0.62
1:B:12:GLU:OE1	1:B:116:VAL:HG13	2.00	0.62
1:A:81:ASN:HD22	1:A:134:SER:CB	2.14	0.61
1:A:103:TYR:C	1:A:105:SER:N	2.54	0.61
1:A:83:TYR:HE1	1:A:89:CYS:HB2	1.66	0.61
1:C:45:GLU:O	1:C:50:GLU:CD	2.39	0.61
1:A:4:THR:HG22	1:B:17:THR:HG21	1.83	0.60
1:C:100:PRO:CB	1:C:109:ARG:HH22	2.12	0.60
1:C:33:ASN:HD21	1:C:36:GLU:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PRO:HB3	1:C:109:ARG:CZ	2.31	0.59
1:B:-3:SER:HB2	1:C:31:GLU:CB	2.32	0.59
1:A:152:TYR:O	1:A:156:LYS:HG3	2.02	0.59
1:C:142:LYS:HZ3	1:C:145:ARG:HH22	1.49	0.59
1:A:131:ASN:OD1	1:A:133:GLU:HB2	2.03	0.59
1:C:160:GLN:HB3	1:C:165:LEU:HD11	1.84	0.58
1:C:97:GLY:C	1:C:100:PRO:HD3	2.24	0.58
1:B:111:SER:OG	1:B:113:VAL:HG12	2.03	0.57
1:C:152:TYR:O	1:C:156:LYS:HG3	2.04	0.57
1:A:103:TYR:O	1:A:105:SER:N	2.38	0.57
1:C:9:LEU:HD13	1:C:64:TYR:CE2	2.39	0.57
1:B:81:ASN:HD22	1:B:134:SER:CB	2.18	0.56
1:B:101:MET:O	1:B:103:TYR:N	2.37	0.56
1:C:101:MET:SD	1:C:104:GLU:HG3	2.45	0.56
1:B:81:ASN:ND2	1:B:134:SER:CB	2.69	0.56
1:A:102:GLY:HA3	1:A:105:SER:HB3	1.86	0.56
1:C:153:LYS:O	1:C:157:GLN:HG3	2.06	0.56
1:B:24:ILE:HD12	1:B:120:LEU:HB3	1.88	0.56
1:C:97:GLY:HA2	1:C:100:PRO:HG3	1.88	0.56
1:C:30:ASN:ND2	1:C:32:GLU:HB2	2.21	0.56
1:B:45:GLU:O	1:B:50:GLU:CD	2.44	0.56
1:A:25:VAL:CG1	1:A:40:LEU:HB2	2.32	0.56
1:A:83:TYR:CE1	1:A:89:CYS:HB2	2.41	0.56
1:C:71:MET:CE	1:C:123:VAL:HG21	2.35	0.55
1:C:22:GLU:O	1:C:24:ILE:HG12	2.06	0.55
1:A:81:ASN:HD22	1:A:134:SER:HB3	1.69	0.55
1:A:159:VAL:O	1:A:163:LEU:HG	2.06	0.55
1:C:89:CYS:SG	1:C:94:HIS:HE1	2.28	0.55
1:B:102:GLY:C	1:B:104:GLU:N	2.60	0.55
1:C:103:TYR:HE2	1:C:108:GLU:OE2	1.89	0.55
1:C:64:TYR:CD1	1:C:65:PRO:HA	2.41	0.55
1:A:119:ILE:O	1:A:123:VAL:HG23	2.07	0.55
1:C:17:THR:HG22	1:C:18:LEU:N	2.21	0.54
1:C:131:ASN:OD1	1:C:133:GLU:HB2	2.07	0.54
1:B:101:MET:HB2	1:B:103:TYR:HB2	1.90	0.54
1:C:110:TRP:CZ3	1:C:114:GLN:HB2	2.43	0.54
1:A:29:MET:HB3	1:A:38:GLU:HB2	1.89	0.54
1:C:12:GLU:OE1	1:C:116:VAL:HG13	2.07	0.54
1:C:100:PRO:HB2	1:C:109:ARG:HH12	1.73	0.53
1:C:30:ASN:OD1	1:C:32:GLU:HG2	2.09	0.53
1:A:45:GLU:O	1:A:50:GLU:CD	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PRO:CA	1:B:109:ARG:HG2	2.34	0.53
1:A:95:ALA:O	1:A:98:ASP:N	2.41	0.53
1:A:111:SER:OG	1:A:113:VAL:HG12	2.09	0.53
1:A:44:PRO:HB2	1:A:47:THR:OG1	2.09	0.53
1:A:80:PRO:O	1:A:136:ALA:HB3	2.08	0.52
1:C:33:ASN:ND2	1:C:36:GLU:HG2	2.24	0.52
1:A:159:VAL:CG2	1:A:160:GLN:N	2.73	0.52
1:A:97:GLY:O	1:A:98:ASP:O	2.27	0.51
1:C:81:ASN:ND2	1:C:134:SER:HB3	2.25	0.51
1:A:155:ALA:O	1:A:159:VAL:HG13	2.11	0.51
1:C:159:VAL:CG2	1:C:160:GLN:N	2.73	0.51
1:A:60:PHE:CD2	1:A:69:PRO:HB3	2.46	0.51
1:A:-3:SER:C	1:A:-1:PHE:N	2.64	0.51
1:B:-3:SER:C	1:B:-1:PHE:N	2.64	0.51
1:A:71:MET:HE1	1:A:123:VAL:HG21	1.92	0.50
1:C:132:ASP:OD2	1:C:145:ARG:HB2	2.12	0.50
1:A:4:THR:CG2	1:B:17:THR:HG21	2.41	0.50
1:C:60:PHE:CD2	1:C:69:PRO:HB3	2.47	0.50
1:A:79:HIS:ND1	1:A:80:PRO:HD2	2.26	0.50
1:C:103:TYR:CE2	1:C:108:GLU:OE2	2.64	0.50
1:C:58:LEU:CD1	1:C:71:MET:HG3	2.42	0.49
1:A:79:HIS:HB3	1:A:82:ILE:HG13	1.94	0.49
1:C:-3:SER:OG	1:C:1:MET:HG3	2.13	0.49
1:B:83:TYR:HE1	1:B:89:CYS:HB2	1.78	0.49
1:C:24:ILE:HG22	1:C:25:VAL:N	2.27	0.49
1:A:123:VAL:O	1:A:126:MET:HB3	2.11	0.49
1:B:96:PRO:HG3	1:B:109:ARG:HB3	1.95	0.49
1:A:81:ASN:ND2	1:A:134:SER:HB3	2.29	0.48
1:B:9:LEU:HD13	1:B:64:TYR:CD2	2.49	0.48
1:C:101:MET:CB	1:C:104:GLU:HG3	2.44	0.48
1:C:142:LYS:NZ	1:C:145:ARG:NH2	2.60	0.48
1:C:104:GLU:O	1:C:105:SER:C	2.52	0.48
1:C:159:VAL:O	1:C:162:SER:HB3	2.13	0.48
1:C:121:LEU:O	1:C:124:VAL:HB	2.13	0.47
1:B:159:VAL:O	1:B:163:LEU:HG	2.14	0.47
1:A:29:MET:CE	1:A:38:GLU:HB2	2.45	0.47
1:A:154:ILE:O	1:A:157:GLN:HB2	2.15	0.47
1:A:104:GLU:O	1:A:108:GLU:HG3	2.15	0.47
1:C:44:PRO:HB2	1:C:47:THR:CG2	2.44	0.47
1:C:154:ILE:O	1:C:157:GLN:HB2	2.13	0.47
1:A:96:PRO:C	1:A:98:ASP:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG23	1:C:160:GLN:N	2.30	0.47
1:C:50:GLU:HG2	1:C:51:PHE:CG	2.50	0.47
1:C:44:PRO:HB2	1:C:47:THR:HG21	1.96	0.47
1:A:95:ALA:O	1:A:98:ASP:CB	2.58	0.46
1:C:24:ILE:HD12	1:C:120:LEU:HB3	1.96	0.46
1:B:8:ARG:NH2	1:B:65:PRO:HG3	2.29	0.46
1:C:123:VAL:O	1:C:126:MET:HB3	2.15	0.46
1:A:81:ASN:ND2	1:A:134:SER:CB	2.78	0.46
1:A:9:LEU:HD13	1:A:64:TYR:CD2	2.50	0.46
1:A:64:TYR:CD1	1:A:65:PRO:HA	2.50	0.46
1:C:101:MET:HB2	1:C:104:GLU:HG3	1.97	0.46
1:C:101:MET:HB2	1:C:104:GLU:CG	2.46	0.46
1:B:1:MET:HG3	1:C:31:GLU:CG	2.44	0.46
1:A:71:MET:HE3	1:A:123:VAL:HG21	1.98	0.46
1:B:58:LEU:HD12	1:B:58:LEU:N	2.31	0.46
1:A:71:MET:HE2	1:A:71:MET:HB3	1.81	0.45
1:C:58:LEU:HD11	1:C:71:MET:HG3	1.98	0.45
1:A:147:ASP:OD1	1:A:150:GLN:HB2	2.16	0.45
1:B:131:ASN:OD1	1:B:131:ASN:O	2.34	0.45
1:C:100:PRO:CG	1:C:109:ARG:HH22	2.30	0.45
1:C:155:ALA:O	1:C:159:VAL:HG13	2.17	0.45
1:A:132:ASP:N	1:A:132:ASP:OD2	2.50	0.45
1:B:21:PRO:HG2	1:B:24:ILE:HB	1.99	0.45
1:C:97:GLY:HA2	1:C:100:PRO:CG	2.46	0.45
1:C:-3:SER:C	1:C:-1:PHE:H	2.03	0.45
1:B:97:GLY:C	1:B:100:PRO:HD3	2.37	0.44
1:A:24:ILE:HG22	1:A:25:VAL:N	2.32	0.44
1:A:30:ASN:OD1	1:A:32:GLU:HG2	2.17	0.44
1:C:101:MET:CG	1:C:104:GLU:HG3	2.47	0.44
1:B:131:ASN:C	1:B:133:GLU:H	2.19	0.44
1:A:102:GLY:CA	1:A:105:SER:HB3	2.47	0.44
1:C:97:GLY:CA	1:C:100:PRO:HG3	2.47	0.44
1:A:8:ARG:NH2	1:A:65:PRO:HG3	2.33	0.44
1:B:100:PRO:O	1:C:163:LEU:O	2.36	0.44
1:C:143:MET:SD	1:C:154:ILE:HD12	2.58	0.44
1:A:105:SER:O	1:A:109:ARG:HG2	2.18	0.44
1:B:30:ASN:OD1	1:B:32:GLU:HG2	2.19	0.43
1:C:21:PRO:HG2	1:C:24:ILE:HB	1.99	0.43
1:A:159:VAL:HG23	1:A:160:GLN:N	2.33	0.43
1:B:50:GLU:HG2	1:B:51:PHE:CG	2.54	0.43
1:B:17:THR:CG2	1:B:18:LEU:HD13	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:C	1:B:136:ALA:H	2.22	0.43
1:A:68:PRO:HB3	1:A:110:TRP:CG	2.54	0.43
1:C:105:SER:HA	1:C:109:ARG:HG3	1.99	0.42
1:C:99:ASP:N	1:C:100:PRO:HD3	2.34	0.42
1:B:50:GLU:O	1:B:51:PHE:HB2	2.18	0.42
1:B:128:ALA:O	1:B:129:GLU:HG2	2.20	0.42
1:C:116:VAL:HG23	1:C:120:LEU:HD22	2.02	0.42
1:C:58:LEU:N	1:C:58:LEU:HD12	2.34	0.42
1:A:134:SER:C	1:A:136:ALA:H	2.22	0.42
1:A:68:PRO:HB3	1:A:110:TRP:CD2	2.54	0.42
1:C:68:PRO:HB3	1:C:110:TRP:CG	2.55	0.42
1:B:83:TYR:CE1	1:B:89:CYS:HB2	2.55	0.42
1:C:79:HIS:HB3	1:C:82:ILE:HG13	2.01	0.42
1:B:31:GLU:H	1:B:31:GLU:CD	2.23	0.42
1:A:101:MET:HB2	1:B:165:LEU:HD21	2.02	0.42
1:B:68:PRO:HB3	1:B:110:TRP:CG	2.54	0.42
1:C:71:MET:HE1	1:C:123:VAL:CG2	2.49	0.41
1:A:100:PRO:O	1:A:101:MET:C	2.59	0.41
1:A:128:ALA:O	1:A:129:GLU:HG2	2.20	0.41
1:A:127:LEU:HD12	1:A:127:LEU:HA	1.88	0.41
1:B:68:PRO:HB3	1:B:110:TRP:CD2	2.55	0.41
1:B:157:GLN:O	1:B:161:LYS:HG3	2.20	0.41
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.89	0.41
1:C:72:ARG:HG3	1:C:87:ARG:N	2.34	0.41
1:B:99:ASP:N	1:B:100:PRO:HD3	2.36	0.41
1:B:110:TRP:CZ3	1:B:114:GLN:CB	3.02	0.41
1:A:44:PRO:CB	1:A:128:ALA:HB2	2.51	0.41
1:C:147:ASP:OD1	1:C:150:GLN:NE2	2.39	0.41
1:C:80:PRO:O	1:C:136:ALA:HB3	2.21	0.41
1:A:79:HIS:HA	1:A:80:PRO:HD3	1.97	0.40
1:A:130:PRO:HD2	1:A:144:TRP:CZ2	2.56	0.40
1:A:47:THR:HG21	1:A:128:ALA:HA	2.04	0.40
1:C:72:ARG:HG3	1:C:86:GLY:C	2.42	0.40
1:A:24:ILE:CG2	1:A:25:VAL:N	2.85	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	167/170 (98%)	147 (88%)	13 (8%)	7 (4%)	3	4
1	B	167/170 (98%)	151 (90%)	11 (7%)	5 (3%)	5	7
1	C	167/170 (98%)	151 (90%)	12 (7%)	4 (2%)	7	12
All	All	501/510 (98%)	449 (90%)	36 (7%)	16 (3%)	5	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	B	103	TYR
1	C	45	GLU
1	A	30	ASN
1	A	98	ASP
1	A	101	MET
1	A	104	GLU
1	B	30	ASN
1	B	132	ASP
1	C	30	ASN
1	C	100	PRO
1	A	132	ASP
1	B	45	GLU
1	A	-3	SER
1	B	-2	GLU
1	C	132	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	146/146 (100%)	129 (88%)	17 (12%)	7	11
1	B	146/146 (100%)	134 (92%)	12 (8%)	14	25
1	C	146/146 (100%)	133 (91%)	13 (9%)	12	21
All	All	438/438 (100%)	396 (90%)	42 (10%)	10	18

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	9	LEU
1	A	18	LEU
1	A	19	ASN
1	A	25	VAL
1	A	31	GLU
1	A	65	PRO
1	A	74	THR
1	A	103	TYR
1	A	106	SER
1	A	108	GLU
1	A	109	ARG
1	A	116	VAL
1	A	120	LEU
1	A	121	LEU
1	A	127	LEU
1	A	131	ASN
1	B	6	LEU
1	B	9	LEU
1	B	18	LEU
1	B	19	ASN
1	B	34	PHE
1	B	65	PRO
1	B	100	PRO
1	B	103	TYR
1	B	109	ARG
1	B	120	LEU
1	B	127	LEU
1	B	149	GLU
1	C	-3	SER
1	C	6	LEU
1	C	9	LEU

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Mol	Chain	Res	Type
1	C	17	THR
1	C	18	LEU
1	C	38	GLU
1	C	100	PRO
1	C	101	MET
1	C	116	VAL
1	C	120	LEU
1	C	127	LEU
1	C	131	ASN
1	C	165	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	94	HIS
1	A	150	GLN
1	A	160	GLN
1	B	94	HIS
1	B	150	GLN
1	C	81	ASN
1	C	94	HIS
1	C	157	GLN
1	C	160	GLN

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

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	169/170 (99%)	0.78	15 (8%)	12 10	41, 64, 142, 162	0
1	B	169/170 (99%)	0.76	14 (8%)	14 12	39, 59, 147, 165	0
1	C	169/170 (99%)	1.11	33 (19%)	1 1	43, 76, 145, 173	0
All	All	507/510 (99%)	0.88	62 (12%)	5 5	39, 66, 146, 173	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	MET	14.3
1	C	151	PHE	6.7
1	C	103	TYR	5.3
1	B	105	SER	5.3
1	A	102	GLY	5.3
1	C	154	ILE	5.1
1	C	104	GLU	5.0
1	C	147	ASP	4.7
1	C	-4	GLY	4.6
1	C	146	ASP	4.6
1	C	105	SER	4.5
1	B	102	GLY	4.5
1	C	165	LEU	4.2
1	C	44	PRO	4.1
1	C	142	LYS	4.1
1	C	145	ARG	4.0
1	C	163	LEU	3.9
1	B	100	PRO	3.9
1	B	101	MET	3.9
1	C	143	MET	3.9
1	C	100	PRO	3.9
1	A	106	SER	3.8
1	B	-3	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	138	VAL	3.6
1	C	150	GLN	3.5
1	A	103	TYR	3.4
1	B	132	ASP	3.3
1	A	105	SER	3.2
1	A	-4	GLY	3.0
1	C	51	PHE	3.0
1	C	132	ASP	3.0
1	B	103	TYR	2.8
1	C	127	LEU	2.8
1	C	78	PHE	2.7
1	B	-4	GLY	2.7
1	C	101	MET	2.7
1	B	45	GLU	2.6
1	C	140	ALA	2.6
1	B	135	GLY	2.5
1	C	148	ARG	2.5
1	A	144	TRP	2.5
1	C	48	CYS	2.4
1	A	151	PHE	2.4
1	A	133	GLU	2.4
1	A	152	TYR	2.4
1	C	141	SER	2.3
1	C	137	ASN	2.3
1	C	49	PHE	2.3
1	A	32	GLU	2.3
1	A	45	GLU	2.3
1	C	157	GLN	2.2
1	C	102	GLY	2.2
1	A	100	PRO	2.2
1	C	53	VAL	2.2
1	A	98	ASP	2.2
1	B	106	SER	2.1
1	C	45	GLU	2.1
1	B	46	ASP	2.1
1	B	97	GLY	2.0
1	C	144	TRP	2.0
1	A	40	LEU	2.0
1	B	129	GLU	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.