



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 06:58 PM EDT

PDB ID : 4H05
Title : Crystal structure of aminoglycoside-3'-phosphotransferase of type VIII
Authors : Boyko, K.M.; Gorbacheva, M.A.; Danilenko, V.N.; Alekseeva, M.G.; Korzhenevskiy, D.A.; Dorovatovskiy, P.V.; Lipkin, A.V.; Popov, V.O.
Deposited on : 2012-09-07
Resolution : 2.15 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

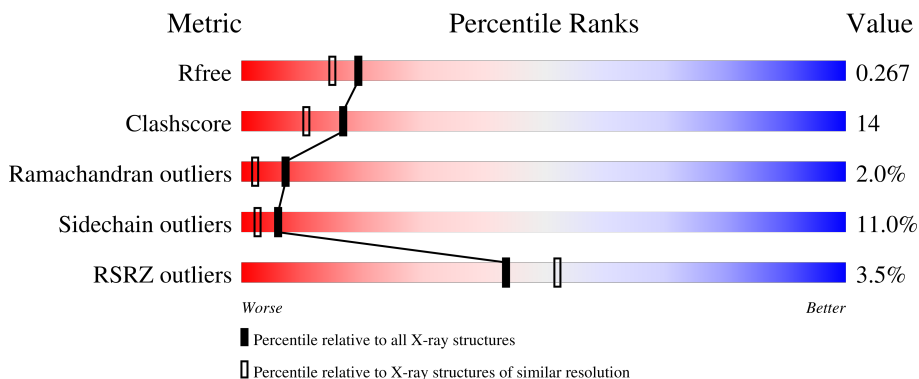
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

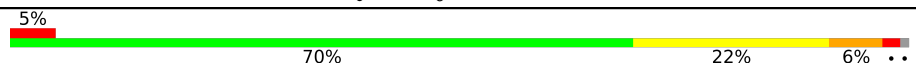

The reported resolution of this entry is 2.15 Å.

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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	273	 5% 70% 22% 6% ..
1	B	273	 2% 69% 26% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4232 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 Aminoglycoside-O-phosphotransferase VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	Total	C	N	O	S	0	2	0
			2061	1292	379	382	8			
1	B	271	Total	C	N	O	S	0	5	0
			2077	1297	384	388	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9F9M5
A	-4	HIS	-	expression tag	UNP Q9F9M5
A	-3	HIS	-	expression tag	UNP Q9F9M5
A	-2	HIS	-	expression tag	UNP Q9F9M5
A	-1	HIS	-	expression tag	UNP Q9F9M5
A	0	HIS	-	expression tag	UNP Q9F9M5
B	-5	HIS	-	expression tag	UNP Q9F9M5
B	-4	HIS	-	expression tag	UNP Q9F9M5
B	-3	HIS	-	expression tag	UNP Q9F9M5
B	-2	HIS	-	expression tag	UNP Q9F9M5
B	-1	HIS	-	expression tag	UNP Q9F9M5
B	0	HIS	-	expression tag	UNP Q9F9M5

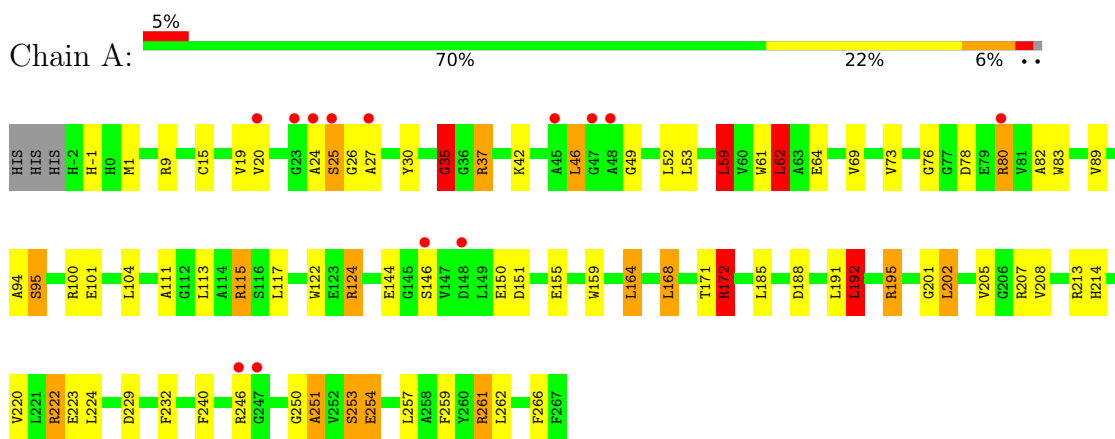
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		
2	B	48	Total	O	0	0
			48	48		

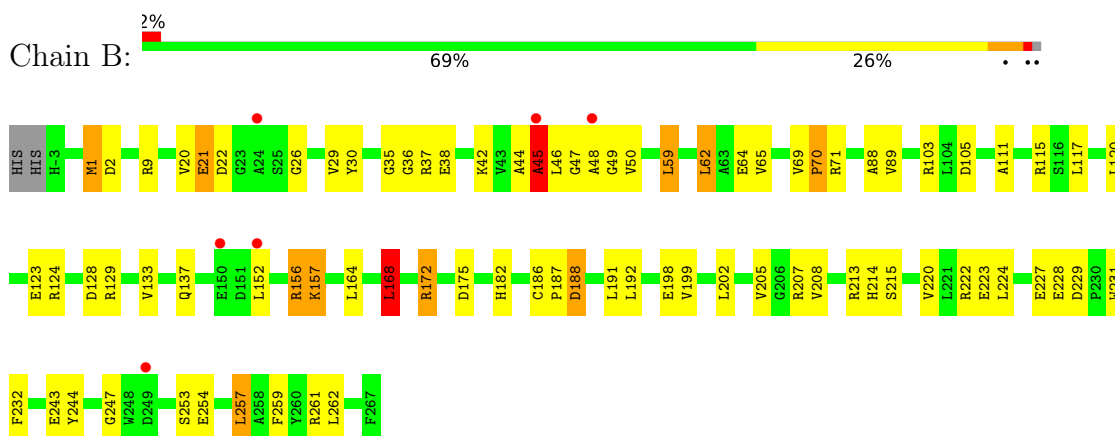
3 Residue-property plots [i](#)

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: Aminoglycoside-O-phosphotransferase VIII



- Molecule 1: Aminoglycoside-O-phosphotransferase VIII



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.34Å 103.34Å 53.68Å 90.00° 94.36° 90.00°	Depositor
Resolution (Å)	28.97 – 2.15 28.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.97-2.15) 100.0 (28.97-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.16Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.268 0.198 , 0.267	Depositor DCC
R_{free} test set	1536 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.059	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.044 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4232	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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	1.09	4/2114 (0.2%)	1.29	23/2875 (0.8%)
1	B	1.07	0/2145	1.30	22/2913 (0.8%)
All	All	1.08	4/4259 (0.1%)	1.30	45/5788 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	TRP	CD2-CE2	6.29	1.48	1.41
1	A	83	TRP	CD2-CE2	5.88	1.48	1.41
1	A	159	TRP	CD2-CE2	5.49	1.48	1.41
1	A	61	TRP	CD2-CE2	5.46	1.47	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	B	172	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	A	222	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	B	261	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	A	222	ARG	NE-CZ-NH2	-10.45	115.07	120.30
1	A	192	LEU	CA-CB-CG	9.39	136.90	115.30
1	B	261	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	B	156	ARG	NE-CZ-NH2	-8.56	116.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	129	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	B	45	ALA	N-CA-C	-7.82	89.88	111.00
1	B	207	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	A	207	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	B	129	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	35	GLY	N-CA-C	7.04	130.70	113.10
1	A	115	ARG	CA-CB-CG	7.02	128.85	113.40
1	B	117	LEU	CB-CG-CD2	-6.97	99.15	111.00
1	A	202	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	B	175	ASP	N-CA-CB	-6.78	98.39	110.60
1	A	59	LEU	CB-CG-CD1	6.73	122.44	111.00
1	A	261	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	9	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	62	LEU	CB-CG-CD1	6.29	121.69	111.00
1	A	229	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	117	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	213	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	207	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	172	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	95	SER	N-CA-CB	-5.59	102.11	110.50
1	B	257	LEU	CB-CG-CD1	5.40	120.19	111.00
1	B	71	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	128	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	207	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	261	ARG	CG-CD-NE	-5.31	100.65	111.80
1	B	257	LEU	CA-CB-CG	5.28	127.43	115.30
1	B	168	LEU	CB-CG-CD2	5.27	119.95	111.00
1	A	213	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	195	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	62	LEU	CA-CB-CG	5.14	127.11	115.30
1	B	105	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	195	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	124	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	213	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	59	LEU	CA-CB-CG	5.03	126.87	115.30
1	A	202	LEU	CB-CA-C	-5.02	100.65	110.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	ARG	Peptide
1	A	35	GLY	Peptide
1	B	228	GLU	Peptide
1	B	247	GLY	Peptide

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	2061	0	1983	48	0
1	B	2077	0	2001	68	0
2	A	46	0	0	2	0
2	B	48	0	0	1	0
All	All	4232	0	3984	115	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 (115) 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:59:LEU:HD12	1:B:69:VAL:CG1	1.83	1.08
1:B:59:LEU:HD12	1:B:69:VAL:HG11	1.33	1.07
1:A:113:LEU:HD21	1:A:202:LEU:HD21	1.09	1.06
1:A:24:ALA:HB3	1:A:27:ALA:HB3	1.34	1.05
1:A:59:LEU:HD13	1:A:205:VAL:CG2	1.88	1.03
1:A:113:LEU:CD2	1:A:202:LEU:HD21	1.89	1.03
1:A:254[A]:GLU:OE2	2:A:322:HOH:O	1.78	1.01
1:B:168:LEU:HD22	1:B:259:PHE:CE1	2.04	0.93
1:B:44:ALA:HB1	1:B:45:ALA:CB	1.98	0.92
1:A:59:LEU:HD13	1:A:205:VAL:HG22	1.56	0.87
1:B:168:LEU:CD2	1:B:259:PHE:CE1	2.58	0.87
1:B:44:ALA:HB1	1:B:45:ALA:HB2	1.54	0.86
1:A:59:LEU:HD13	1:A:205:VAL:HG21	1.56	0.85
1:A:76:GLY:O	1:A:82:ALA:HB1	1.77	0.84
1:B:59:LEU:HD13	1:B:205:VAL:CG2	2.06	0.84
1:B:59:LEU:HD13	1:B:205:VAL:HG21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ALA:HB3	1:A:27:ALA:CB	2.10	0.82
1:A:250:GLY:HA2	1:A:251:ALA:HB2	1.62	0.82
1:A:250:GLY:CA	1:A:251:ALA:CB	2.60	0.79
1:A:1:MET:HG2	1:A:25:SER:HB2	1.63	0.78
1:B:222:ARG:NH1	1:B:223:GLU:OE2	2.16	0.78
1:B:45:ALA:HB3	1:B:48:ALA:HB3	1.64	0.78
1:B:59:LEU:CD1	1:B:69:VAL:CG1	2.62	0.77
1:A:164:LEU:HD13	1:A:266:PHE:CZ	2.23	0.73
1:A:73:VAL:HG13	1:B:64:GLU:HG2	1.69	0.73
1:B:229:ASP:HB2	1:B:231:TRP:CZ3	2.24	0.72
1:B:44:ALA:CB	1:B:45:ALA:HB2	2.19	0.72
1:B:172:ARG:HD3	2:B:336:HOH:O	1.90	0.71
1:B:192:LEU:HD23	1:B:199:VAL:HA	1.73	0.70
1:B:168:LEU:HD22	1:B:259:PHE:HE1	1.55	0.69
1:A:250:GLY:HA2	1:A:251:ALA:CB	2.23	0.69
1:A:168:LEU:HD22	1:A:259:PHE:CE1	2.29	0.68
1:A:46:LEU:HA	1:A:80:ARG:HA	1.74	0.67
1:A:113:LEU:HD21	1:A:202:LEU:CD2	2.05	0.67
1:A:76:GLY:O	1:A:82:ALA:CB	2.43	0.66
1:A:42:LYS:HE2	1:A:52:LEU:HD21	1.78	0.65
1:B:44:ALA:HB1	1:B:45:ALA:HB3	1.76	0.64
1:A:250:GLY:CA	1:A:251:ALA:HB3	2.29	0.63
1:B:168:LEU:HD22	1:B:259:PHE:CZ	2.34	0.63
1:A:250:GLY:HA3	1:A:251:ALA:HB3	1.80	0.63
1:B:65:VAL:CG1	1:B:120:LEU:HD21	2.28	0.63
1:B:164:LEU:HD23	1:B:262:LEU:HD11	1.82	0.62
1:B:59:LEU:HD13	1:B:205:VAL:HG22	1.81	0.61
1:B:65:VAL:CG1	1:B:65:VAL:O	2.49	0.60
1:B:69:VAL:CG1	1:B:70:PRO:HD2	2.32	0.60
1:B:187:PRO:HD2	1:B:223:GLU:HG2	1.85	0.59
1:A:46:LEU:N	1:A:80:ARG:O	2.32	0.58
1:A:62:LEU:HD21	1:A:208:VAL:HG21	1.86	0.58
1:A:59:LEU:CD1	1:A:205:VAL:HG21	2.30	0.57
1:B:69:VAL:HG13	1:B:70:PRO:HD2	1.85	0.57
1:A:89:VAL:HG11	1:A:201:GLY:HA3	1.86	0.57
1:A:164:LEU:HD13	1:A:266:PHE:CE2	2.40	0.57
1:B:65:VAL:CG1	1:B:120:LEU:CD2	2.82	0.57
1:B:156:ARG:O	1:B:157:LYS:O	2.23	0.57
1:A:26:GLY:O	1:A:30:TYR:OH	2.21	0.56
1:B:65:VAL:HG11	1:B:120:LEU:HD22	1.87	0.56
1:A:214:HIS:CE1	1:A:253:SER:H	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASP:HA	2:A:338:HOH:O	2.06	0.55
1:A:164:LEU:HD22	1:A:262:LEU:HD11	1.89	0.54
1:B:214:HIS:CE1	1:B:253:SER:H	2.26	0.54
1:B:168:LEU:CD2	1:B:259:PHE:CZ	2.91	0.54
1:B:20:VAL:O	1:B:21:GLU:C	2.45	0.53
1:B:65:VAL:O	1:B:65:VAL:HG12	2.09	0.53
1:B:182:HIS:HA	1:B:208:VAL:HG22	1.91	0.52
1:B:192:LEU:HD23	1:B:199:VAL:CA	2.39	0.52
1:B:65:VAL:HG11	1:B:120:LEU:CD2	2.40	0.52
1:B:168:LEU:HD23	1:B:259:PHE:CE1	2.42	0.52
1:B:115[A]:ARG:HD3	1:B:244:TYR:O	2.11	0.51
1:B:224:LEU:HD23	1:B:232:PHE:CD2	2.45	0.51
1:A:46:LEU:HA	1:A:80:ARG:CA	2.41	0.50
1:B:227:GLU:O	1:B:231:TRP:HA	2.12	0.49
1:A:254[B]:GLU:OE2	1:A:261:ARG:NH2	2.43	0.49
1:A:224:LEU:HD23	1:A:232:PHE:CD1	2.48	0.49
1:B:115[A]:ARG:HG2	1:B:244:TYR:CD1	2.48	0.49
1:B:44:ALA:CA	1:B:45:ALA:HB2	2.44	0.47
1:B:65:VAL:HG22	1:B:124:ARG:NH2	2.29	0.47
1:A:214:HIS:HE1	1:A:253:SER:H	1.61	0.47
1:B:1:MET:HE2	1:B:1:MET:HB3	1.62	0.46
1:B:26:GLY:O	1:B:30:TYR:OH	2.25	0.46
1:A:49:GLY:O	1:A:53:LEU:HD13	2.16	0.46
1:B:156:ARG:O	1:B:157:LYS:C	2.54	0.46
1:A:15:CYS:SG	1:A:37:ARG:NH2	2.88	0.46
1:B:214:HIS:HE1	1:B:253:SER:H	1.63	0.46
1:B:229:ASP:HB3	1:B:231:TRP:CH2	2.51	0.45
1:A:172:ARG:HA	1:A:259:PHE:CE1	2.50	0.45
1:B:29:VAL:HG22	1:B:42:LYS:HG2	1.97	0.45
1:A:171:THR:O	1:A:172:ARG:C	2.54	0.45
1:B:224:LEU:HD23	1:B:232:PHE:CG	2.51	0.45
1:B:164:LEU:HD23	1:B:262:LEU:CD1	2.47	0.45
1:B:20:VAL:O	1:B:29:VAL:O	2.36	0.44
1:B:89:VAL:HB	1:B:191:LEU:HD12	1.99	0.44
1:A:49:GLY:O	1:A:53:LEU:CD1	2.66	0.44
1:B:47:GLY:H	1:B:49:GLY:H	1.65	0.44
1:A:89:VAL:CG1	1:A:201:GLY:HA3	2.48	0.44
1:A:224:LEU:HD23	1:A:232:PHE:CG	2.53	0.44
1:B:229:ASP:CB	1:B:231:TRP:CH2	3.00	0.44
1:B:20:VAL:O	1:B:21:GLU:O	2.36	0.43
1:B:115[A]:ARG:NH1	1:B:244:TYR:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASP:CB	1:B:231:TRP:CZ3	3.00	0.43
1:A:222:ARG:HD2	1:A:223:GLU:OE2	2.18	0.43
1:B:111:ALA:HB3	1:B:243:GLU:HG2	2.01	0.42
1:A:111:ALA:HA	1:A:240:PHE:CE2	2.55	0.42
1:B:35:GLY:HA2	1:B:36:GLY:HA2	1.79	0.42
1:B:186[A]:CYS:SG	1:B:188:ASP:HB2	2.59	0.42
1:B:44:ALA:CB	1:B:45:ALA:CB	2.81	0.42
1:A:19:VAL:HG22	1:A:30:TYR:CE1	2.56	0.41
1:B:152:LEU:CD2	1:B:164:LEU:HD11	2.51	0.41
1:A:185:LEU:O	1:A:220:VAL:HG23	2.20	0.41
1:A:42:LYS:HE2	1:A:52:LEU:CD2	2.48	0.41
1:B:103:ARG:HD3	1:B:231:TRP:O	2.21	0.41
1:A:94:ALA:HB2	1:A:192:LEU:HD21	2.03	0.40
1:B:192:LEU:HD23	1:B:199:VAL:N	2.37	0.40
1:B:152:LEU:HD21	1:B:164:LEU:HD11	2.03	0.40
1:B:38:GLU:HG2	1:B:88:ALA:HB2	2.02	0.40
1:B:133:VAL:O	1:B:137:GLN:HG3	2.21	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	270/273 (99%)	247 (92%)	17 (6%)	6 (2%)	6 2
1	B	274/273 (100%)	255 (93%)	14 (5%)	5 (2%)	8 3
All	All	544/546 (100%)	502 (92%)	31 (6%)	11 (2%)	7 2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER

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Mol	Chain	Res	Type
1	A	46	LEU
1	A	251	ALA
1	B	21	GLU
1	B	45	ALA
1	B	46	LEU
1	B	157	LYS
1	B	22	ASP
1	A	-1	HIS
1	A	80	ARG
1	A	35	GLY

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	201/211 (95%)	172 (86%)	29 (14%)	3 1
1	B	205/211 (97%)	188 (92%)	17 (8%)	11 6
All	All	406/422 (96%)	360 (89%)	46 (11%)	6 2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	20	VAL
1	A	37	ARG
1	A	59	LEU
1	A	62	LEU
1	A	64	GLU
1	A	69	VAL
1	A	78	ASP
1	A	95	SER
1	A	100	ARG
1	A	101	GLU
1	A	104	LEU
1	A	115	ARG

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Mol	Chain	Res	Type
1	A	124	ARG
1	A	144	GLU
1	A	146	SER
1	A	150	GLU
1	A	155	GLU
1	A	164	LEU
1	A	168	LEU
1	A	172	ARG
1	A	188	ASP
1	A	191	LEU
1	A	192	LEU
1	A	195	ARG
1	A	253	SER
1	A	254[A]	GLU
1	A	254[B]	GLU
1	A	257	LEU
1	B	1	MET
1	B	2	ASP
1	B	37	ARG
1	B	50	VAL
1	B	59	LEU
1	B	62	LEU
1	B	70	PRO
1	B	123	GLU
1	B	168	LEU
1	B	188	ASP
1	B	198	GLU
1	B	202	LEU
1	B	215[A]	SER
1	B	215[B]	SER
1	B	220	VAL
1	B	254	GLU
1	B	257	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	214	HIS
1	B	214	HIS

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 [i](#)

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	270/273 (98%)	0.16	13 (4%) 30 39	21, 35, 68, 101	0
1	B	271/273 (99%)	0.09	6 (2%) 62 69	21, 37, 64, 79	0
All	All	541/546 (99%)	0.13	19 (3%) 44 52	21, 36, 67, 101	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	ALA	4.4
1	A	48	ALA	3.8
1	A	47	GLY	3.6
1	A	23	GLY	3.4
1	A	24	ALA	3.3
1	B	249	ASP	3.0
1	A	25	SER	3.0
1	A	45	ALA	3.0
1	B	45	ALA	2.7
1	B	150	GLU	2.6
1	A	246	ARG	2.5
1	A	27	ALA	2.4
1	A	80	ARG	2.3
1	B	24	ALA	2.2
1	A	146	SER	2.2
1	A	148	ASP	2.2
1	A	247	GLY	2.1
1	B	152	LEU	2.0
1	A	20	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 monosaccharides 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.