



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2026 – 12:16 PM JST

PDB ID : 26QV / pdb_000026qv
Title : Crystal structure of monoalkyl phthalate hydrolase from Rhodococcus sp. EG-5
Authors : Aggarwal, S.; Jangid, K.; Singh, S.; Sharma, A.K.; Kumar, P.
Deposited on : 2026-05-11
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

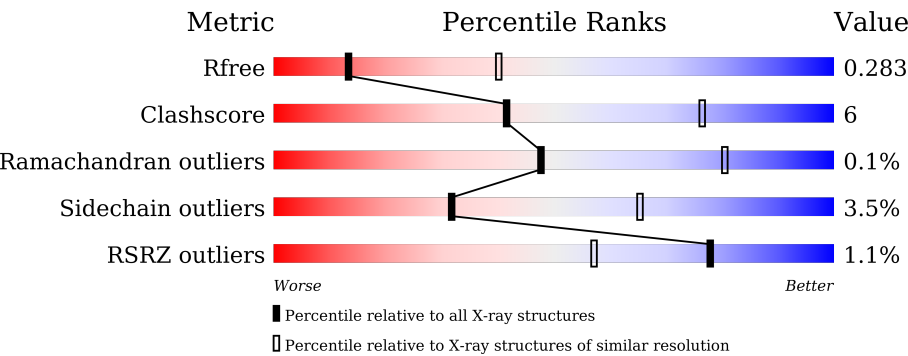
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	303	<div><div>%</div><div>80%14%5%</div></div>
1	B	303	<div><div>81%14%5%</div></div>
1	C	303	<div><div>%</div><div>78%15%6%</div></div>
1	D	303	<div><div>81%11%6%</div></div>
1	E	303	<div><div>%</div><div>80%13%5%</div></div>
1	F	303	<div><div>%</div><div>79%13%6%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	303	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>80%</div><div>13%</div><div>• 5%</div></div></div>
1	H	303	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>80%</div><div>13%</div><div>• 6%</div></div></div>
1	I	303	<div><div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>14%</div><div>• 6%</div></div></div>
1	J	303	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>77%</div><div>16%</div><div>• •</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43983 atoms, of which 21807 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 Mono-ethylhexylphthalate hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	H	N	O	S	59	0	0
			4392	1404	2189	378	415	6			
1	B	288	Total	C	H	N	O	S	59	0	0
			4389	1403	2187	378	415	6			
1	C	286	Total	C	H	N	O	S	59	0	0
			4358	1386	2178	377	410	7			
1	D	285	Total	C	H	N	O	S	57	0	0
			4349	1391	2169	375	408	6			
1	E	288	Total	C	H	N	O	S	60	0	0
			4388	1402	2188	378	414	6			
1	F	285	Total	C	H	N	O	S	58	0	0
			4348	1390	2170	375	407	6			
1	G	288	Total	C	H	N	O	S	60	0	0
			4388	1402	2188	378	414	6			
1	H	286	Total	C	H	N	O	S	58	0	0
			4360	1394	2174	376	410	6			
1	I	284	Total	C	H	N	O	S	57	0	0
			4342	1389	2166	374	407	6			
1	J	290	Total	C	H	N	O	S	60	0	0
			4415	1411	2198	380	420	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	27	Total	O	0	0
			27	27		
2	C	36	Total	O	0	0
			36	36		
2	D	26	Total	O	0	0
			26	26		

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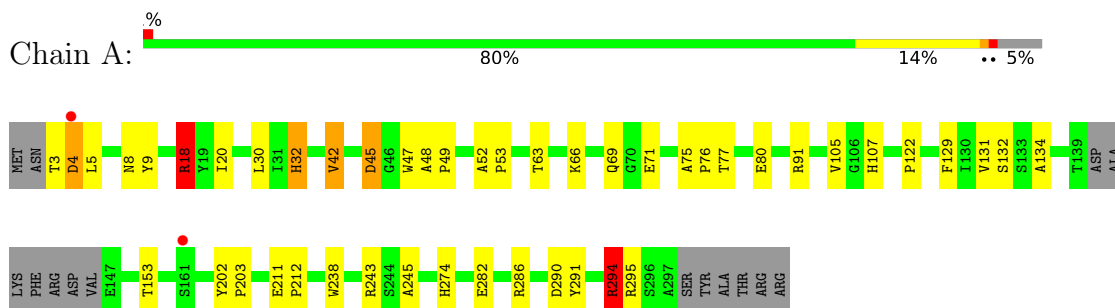
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	23	Total 23	O 23	0	0
2	F	24	Total 24	O 24	0	0
2	G	29	Total 29	O 29	0	0
2	H	32	Total 32	O 32	0	0
2	I	16	Total 16	O 16	0	0
2	J	27	Total 27	O 27	0	0

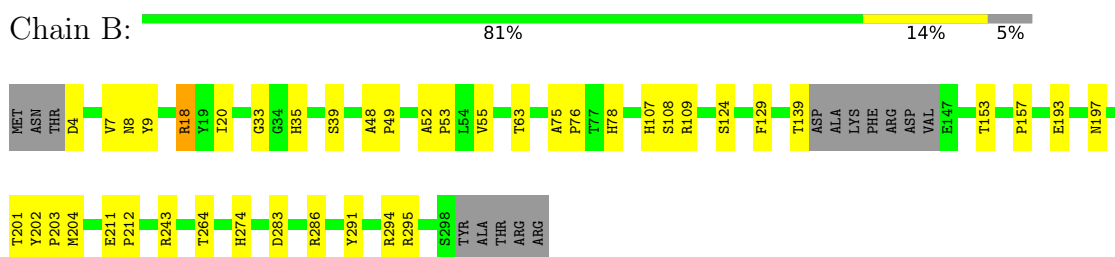
3 Residue-property plots

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.

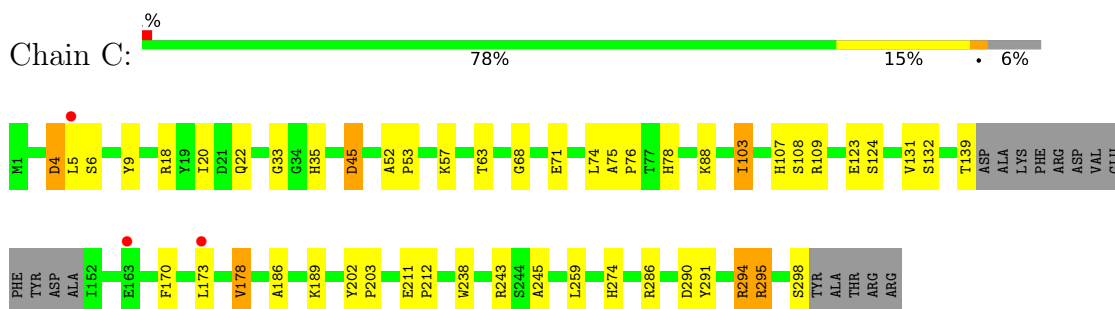
- Molecule 1: Mono-ethylhexylphthalate hydrolase



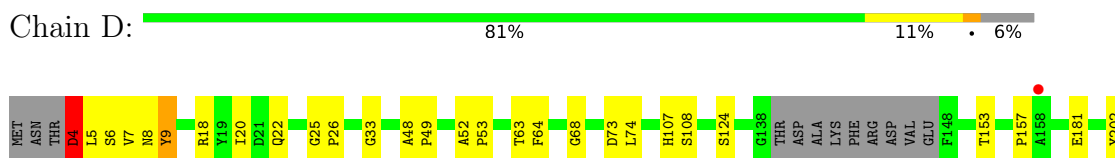
- Molecule 1: Mono-ethylhexylphthalate hydrolase



- Molecule 1: Mono-ethylhexylphthalate hydrolase

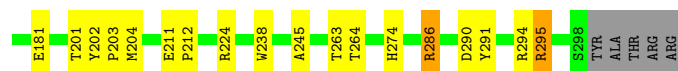
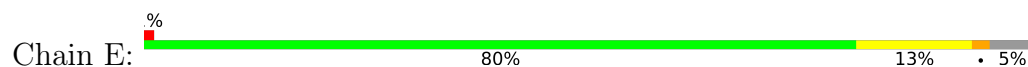


- Molecule 1: Mono-ethylhexylphthalate hydrolase

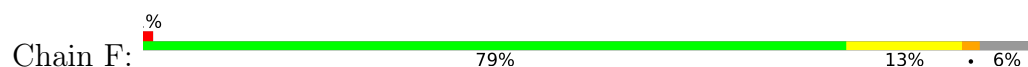




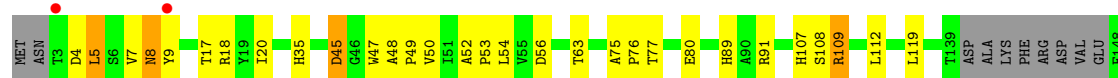
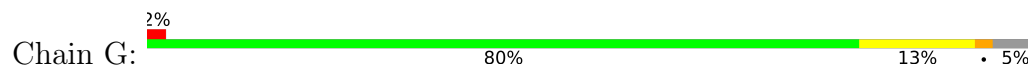
• Molecule 1: Mono-ethylhexylphthalate hydrolase



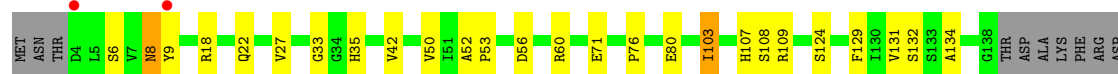
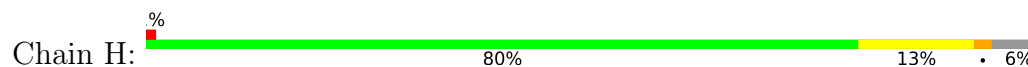
• Molecule 1: Mono-ethylhexylphthalate hydrolase



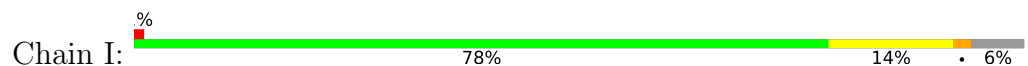
• Molecule 1: Mono-ethylhexylphthalate hydrolase

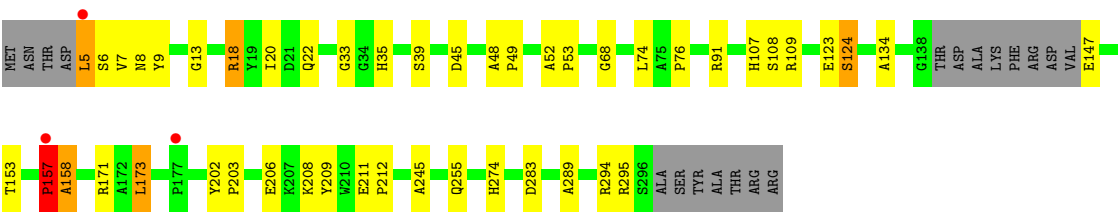


• Molecule 1: Mono-ethylhexylphthalate hydrolase

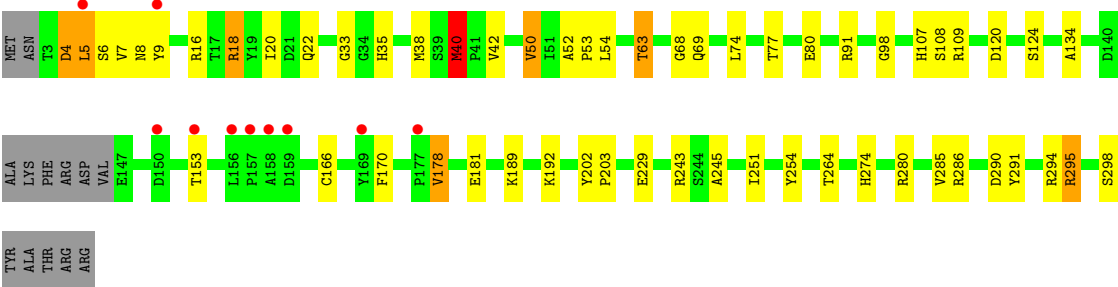
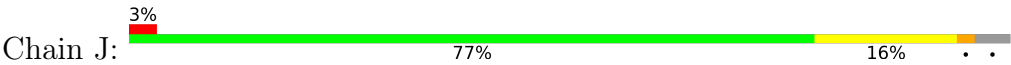


• Molecule 1: Mono-ethylhexylphthalate hydrolase





● Molecule 1: Mono-ethylhexylphthalate hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	177.61Å 245.49Å 191.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.38 – 3.00 27.38 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.38-3.00) 99.7 (27.38-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.83 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.251 , 0.294 0.242 , 0.283	Depositor DCC
R_{free} test set	4208 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	43983	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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	0.62	0/2252	1.09	6/3060 (0.2%)
1	B	0.62	0/2251	1.05	1/3058 (0.0%)
1	C	0.63	0/2227	1.08	3/3025 (0.1%)
1	D	0.61	0/2229	1.11	6/3028 (0.2%)
1	E	0.61	0/2249	1.09	4/3056 (0.1%)
1	F	0.60	0/2227	1.10	5/3025 (0.2%)
1	G	0.61	0/2249	1.07	1/3056 (0.0%)
1	H	0.61	0/2235	1.08	5/3036 (0.2%)
1	I	0.58	0/2225	1.07	2/3022 (0.1%)
1	J	0.60	0/2266	1.09	7/3079 (0.2%)
All	All	0.61	0/22410	1.08	40/30445 (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	3
1	B	0	1
1	C	0	2
1	D	0	4
1	E	0	3
1	F	0	1
1	G	0	2
1	H	0	1
1	I	0	4
1	J	0	3
All	All	0	24

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	ASP	CA-CB-CG	8.10	120.70	112.60
1	D	4	ASP	CB-CA-C	7.58	124.49	110.10
1	J	63	THR	CA-CB-OG1	-7.30	98.65	109.60
1	J	294	ARG	CG-CD-NE	-6.57	97.55	112.00
1	E	153	THR	CA-CB-OG1	-6.55	99.77	109.60

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Sidechain
1	A	243	ARG	Sidechain
1	A	294	ARG	Sidechain
1	B	18	ARG	Sidechain
1	C	243	ARG	Sidechain

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	2203	2189	2179	26	0
1	B	2202	2187	2177	25	0
1	C	2180	2178	2169	34	0
1	D	2180	2169	2159	25	0
1	E	2200	2188	2178	22	0
1	F	2178	2170	2160	26	2
1	G	2200	2188	2178	40	0
1	H	2186	2174	2164	25	0
1	I	2176	2166	2156	29	0
1	J	2217	2198	2188	42	2
2	A	14	0	0	1	0
2	B	27	0	0	2	0
2	C	36	0	0	2	0
2	D	26	0	0	4	0
2	E	23	0	0	1	0
2	F	24	0	0	0	0
2	G	29	0	0	1	0
2	H	32	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	16	0	0	2	0
2	J	27	0	0	1	0
All	All	22176	21807	21708	278	2

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 6.

The worst 5 of 278 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:D:204:MET:O	1:D:208:LYS:HE3	1.53	1.08
1:J:40:MET:HE2	1:J:40:MET:HA	1.39	1.03
1:G:254:TYR:CE1	1:G:264:THR:HG22	1.93	1.03
1:J:254:TYR:CE1	1:J:264:THR:HG22	1.95	1.01
1:C:9:TYR:OH	1:C:71:GLU:HB3	1.67	0.92

All (2) 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:F:243:ARG:HH12	1:J:229:GLU:OE1[4_554]	1.34	0.26
1:F:243:ARG:NH1	1:J:229:GLU:OE1[4_554]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	284/303 (94%)	273 (96%)	11 (4%)	0	100 100
1	B	284/303 (94%)	276 (97%)	8 (3%)	0	100 100
1	C	282/303 (93%)	271 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	281/303 (93%)	272 (97%)	9 (3%)	0	100	100
1	E	284/303 (94%)	276 (97%)	7 (2%)	1 (0%)	30	65
1	F	281/303 (93%)	271 (96%)	9 (3%)	1 (0%)	30	65
1	G	284/303 (94%)	274 (96%)	10 (4%)	0	100	100
1	H	282/303 (93%)	270 (96%)	11 (4%)	1 (0%)	30	65
1	I	280/303 (92%)	273 (98%)	6 (2%)	1 (0%)	30	65
1	J	286/303 (94%)	277 (97%)	9 (3%)	0	100	100
All	All	2828/3030 (93%)	2733 (97%)	91 (3%)	4 (0%)	48	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5	LEU
1	F	134	ALA
1	I	158	ALA
1	H	158	ALA

5.3.2 Protein sidechains ⓘ

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	228/241 (95%)	220 (96%)	8 (4%)	32	65
1	B	228/241 (95%)	222 (97%)	6 (3%)	40	72
1	C	227/241 (94%)	222 (98%)	5 (2%)	45	74
1	D	225/241 (93%)	215 (96%)	10 (4%)	25	60
1	E	228/241 (95%)	220 (96%)	8 (4%)	32	65
1	F	225/241 (93%)	217 (96%)	8 (4%)	31	65
1	G	228/241 (95%)	220 (96%)	8 (4%)	32	65
1	H	226/241 (94%)	217 (96%)	9 (4%)	28	62
1	I	225/241 (93%)	217 (96%)	8 (4%)	31	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	230/241 (95%)	221 (96%)	9 (4%)	28 62
All	All	2270/2410 (94%)	2191 (96%)	79 (4%)	32 65

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	153	THR
1	J	16	ARG
1	H	230	VAL
1	I	147	GLU
1	J	178	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	89	HIS
1	J	89	HIS
1	G	107	HIS
1	J	35	HIS
1	I	107	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 oligosaccharides 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	288/303 (95%)	-0.02	2 (0%) 84 66	5, 15, 29, 39	0
1	B	288/303 (95%)	-0.21	0 100 100	4, 12, 27, 39	0
1	C	286/303 (94%)	-0.05	3 (1%) 79 59	6, 14, 30, 51	0
1	D	285/303 (94%)	-0.10	1 (0%) 88 76	3, 13, 30, 44	0
1	E	288/303 (95%)	-0.04	4 (1%) 73 51	5, 15, 33, 44	0
1	F	285/303 (94%)	-0.06	2 (0%) 84 66	5, 16, 34, 51	0
1	G	288/303 (95%)	0.09	5 (1%) 69 45	8, 18, 37, 52	0
1	H	286/303 (94%)	-0.01	2 (0%) 84 66	7, 16, 32, 50	0
1	I	284/303 (93%)	0.01	3 (1%) 78 57	9, 18, 30, 54	0
1	J	290/303 (95%)	0.17	10 (3%) 48 27	8, 19, 48, 71	0
All	All	2868/3030 (94%)	-0.02	32 (1%) 78 57	3, 16, 34, 71	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	THR	3.4
1	I	157	PRO	3.1
1	G	9	TYR	3.0
1	E	4	ASP	2.9
1	H	4	ASP	2.9

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 oligosaccharides 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.