Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:20 PM JST

PDB ID	:	5IQ0
Title	:	Crystal structure of Esterase mutant - F72G
Authors	:	Seok, S.-H.; Seo, M.-D.; Kim, J.; Ryu, Y.
Deposited on	:	2016-03-10
Resolution	:	1.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 1.80 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.
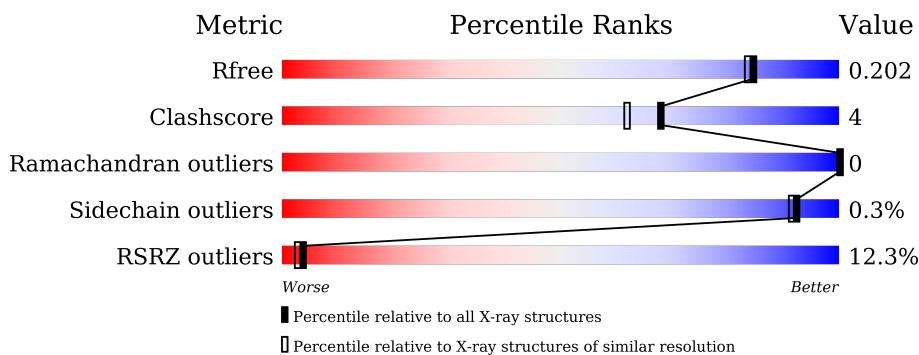
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	362	10% / 92% / 7% ·
1	B	362	15% / 92% / 6% ·
1	C	362	9% / 92% / 5% ··
1	D	362	15% / 89% / 9% ·
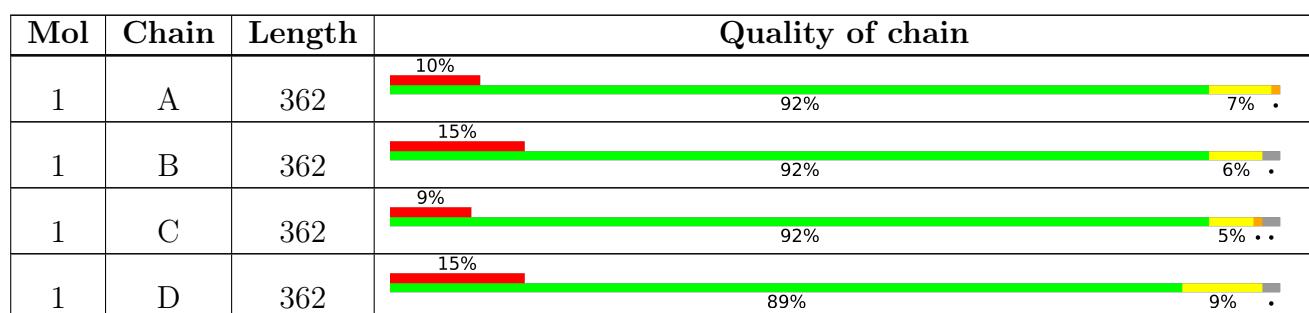
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 11515 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 Esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2683	1677	463	528	15			
1	B	355	Total	C	N	O	S	0	0	0
			2633	1648	454	517	14			
1	C	354	Total	C	N	O	S	0	0	0
			2624	1643	452	515	14			
1	D	355	Total	C	N	O	S	0	0	0
			2629	1646	453	516	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	GLY	PHE	engineered mutation	UNP Q4TZQ3
B	72	GLY	PHE	engineered mutation	UNP Q4TZQ3
C	72	GLY	PHE	engineered mutation	UNP Q4TZQ3
D	72	GLY	PHE	engineered mutation	UNP Q4TZQ3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	254	Total	O	0	0
			254	254		
2	B	230	Total	O	0	0
			230	230		
2	C	228	Total	O	0	0
			228	228		
2	D	234	Total	O	0	0
			234	234		

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: Esterase
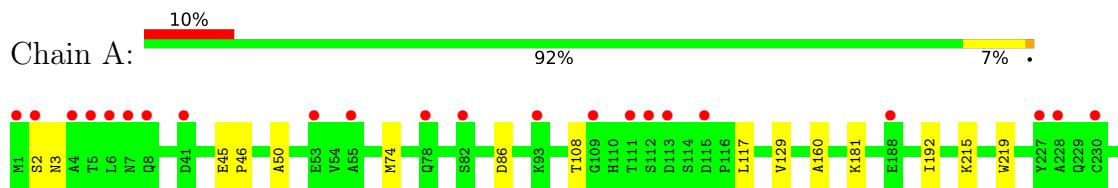
- Molecule 1: Esterase
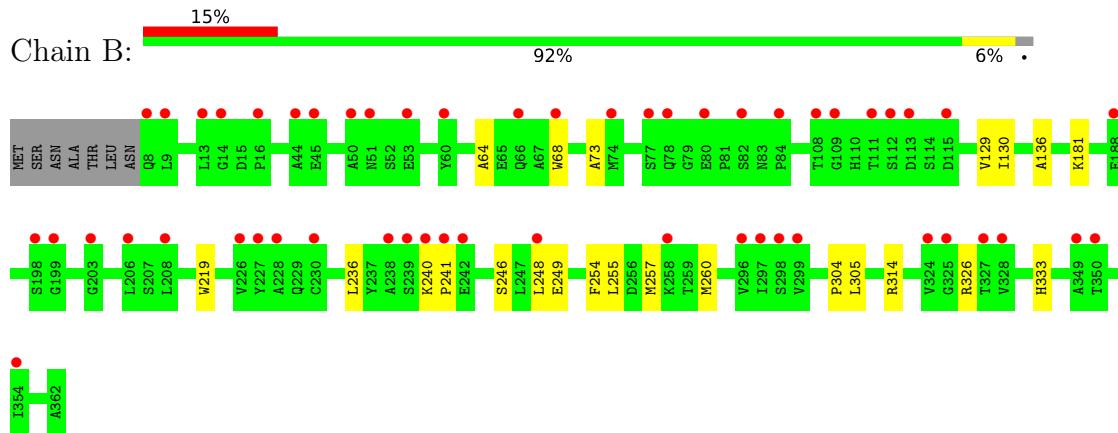
- Molecule 1: Esterase
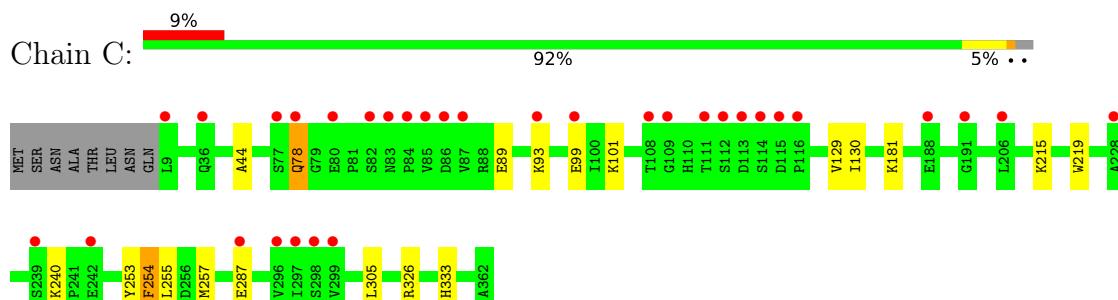
- Molecule 1: Esterase
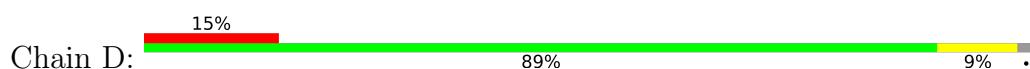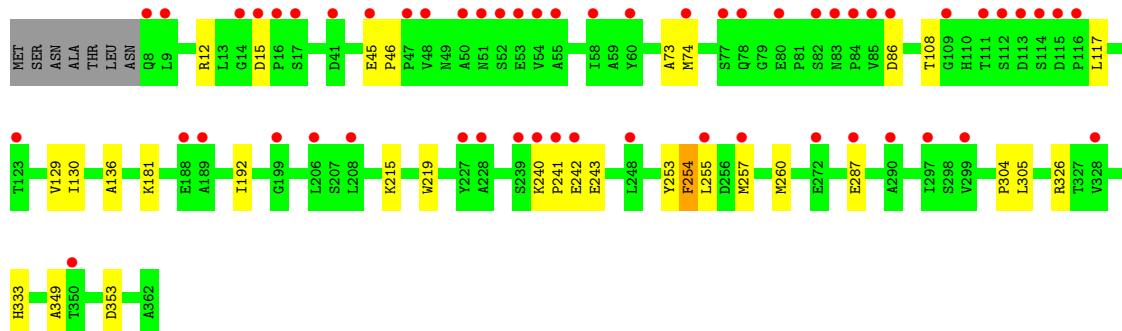
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.25Å 95.64Å 99.14Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	36.17 – 1.80 36.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.17-1.80) 97.5 (36.17-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.34 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.175 , 0.197 0.179 , 0.202	Depositor DCC
R_{free} test set	2000 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 50.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11515	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.41	0/2745	0.65	5/3747 (0.1%)
1	B	0.41	0/2695	0.59	0/3679
1	C	0.45	1/2686 (0.0%)	0.63	2/3667 (0.1%)
1	D	0.40	1/2691 (0.0%)	0.58	0/3674
All	All	0.42	2/10817 (0.0%)	0.61	7/14767 (0.0%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLN	CD-OE1	-5.24	1.12	1.24
1	D	242	GLU	CB-CG	5.01	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	LYS	CB-CG-CD	7.69	131.58	111.60
1	A	318	LYS	CD-CE-NZ	6.70	127.10	111.70
1	A	318	LYS	CA-CB-CG	6.50	127.71	113.40
1	A	318	LYS	CG-CD-CE	-6.29	93.02	111.90
1	C	44	ALA	C-N-CA	-5.62	107.66	121.70
1	C	255	LEU	CB-CG-CD1	5.61	120.53	111.00
1	A	240	LYS	CD-CE-NZ	-5.22	99.68	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	78	GLN	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	2683	0	2603	22	1
1	B	2633	0	2551	21	0
1	C	2624	0	2543	16	0
1	D	2629	0	2545	23	1
2	A	254	0	0	1	0
2	B	230	0	0	1	0
2	C	228	0	0	1	0
2	D	234	0	0	0	0
All	All	11515	0	10242	78	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 4.

All (78) 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:240:LYS:HZ1	1:A:257:MET:HG3	1.39	0.87
1:D:240:LYS:NZ	1:D:257:MET:SD	2.53	0.81
1:A:240:LYS:HZ1	1:A:257:MET:CG	1.96	0.79
1:B:240:LYS:NZ	1:B:257:MET:HG3	1.99	0.78
1:D:255:LEU:HB3	1:D:260:MET:HE2	1.68	0.75
1:B:68:TRP:HZ3	1:B:254:PHE:HE1	1.36	0.72
1:C:326:ARG:HH21	1:D:349:ALA:HB1	1.57	0.70
1:B:240:LYS:HZ1	1:B:257:MET:HG3	1.58	0.69
1:B:68:TRP:CZ3	1:B:254:PHE:HE1	2.12	0.67
1:C:240:LYS:HE2	1:C:257:MET:HG3	1.79	0.65
1:B:181:LYS:HE2	1:B:219:TRP:NE1	2.11	0.64
1:C:240:LYS:CE	1:C:257:MET:HG3	2.29	0.63
1:B:240:LYS:HD3	1:B:248:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HB2	1:A:243:GLU:HG2	1.85	0.59
1:B:255:LEU:HB3	1:B:260:MET:HE2	1.84	0.57
1:D:305:LEU:HD12	1:D:333:HIS:CE1	2.40	0.57
1:D:73:ALA:HA	1:D:136:ALA:HB3	1.87	0.57
1:D:240:LYS:HZ1	1:D:257:MET:CG	2.18	0.57
1:B:240:LYS:HZ3	1:B:257:MET:HG3	1.71	0.56
1:D:241:PRO:HB2	1:D:243:GLU:CD	2.25	0.56
1:C:287:GLU:OE1	1:C:287:GLU:N	2.32	0.55
1:C:305:LEU:HD12	1:C:333:HIS:CE1	2.41	0.55
1:B:64:ALA:O	1:B:68:TRP:HD1	1.90	0.55
1:A:181:LYS:HE2	1:A:219:TRP:NE1	2.22	0.55
1:C:240:LYS:NZ	2:C:402:HOH:O	2.33	0.55
1:B:73:ALA:HA	1:B:136:ALA:HB3	1.90	0.54
1:A:45:GLU:OE2	1:A:258:LYS:NZ	2.26	0.54
1:A:287:GLU:H	1:A:287:GLU:CD	2.11	0.53
1:A:318:LYS:HD3	2:A:617:HOH:O	2.09	0.53
1:C:326:ARG:NH2	1:D:349:ALA:HB1	2.23	0.53
1:D:215:LYS:NZ	1:D:287:GLU:O	2.42	0.53
1:C:181:LYS:HE2	1:C:219:TRP:NE1	2.24	0.53
1:B:181:LYS:HE2	1:B:219:TRP:CE2	2.43	0.52
1:A:181:LYS:HE2	1:A:219:TRP:CE2	2.44	0.52
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.75	0.52
1:C:89:GLU:OE1	1:C:101:LYS:NZ	2.39	0.51
1:A:3:ASN:OD1	1:B:314:ARG:NE	2.45	0.49
1:D:255:LEU:CB	1:D:260:MET:HE2	2.42	0.48
1:A:255:LEU:HB3	1:A:260:MET:HE2	1.93	0.48
1:B:326:ARG:HH11	1:B:326:ARG:HG2	1.78	0.48
1:A:117:LEU:O	1:A:192:ILE:HA	2.13	0.48
1:B:68:TRP:HZ3	1:B:254:PHE:CE1	2.24	0.48
1:A:45:GLU:HG2	1:A:46:PRO:HD2	1.96	0.48
1:D:86:ASP:OD1	1:D:108:THR:HG22	2.14	0.47
1:B:129:VAL:HG12	1:B:130:ILE:HG23	1.96	0.47
1:D:287:GLU:H	1:D:287:GLU:CD	2.17	0.47
1:C:129:VAL:HG12	1:C:130:ILE:HG23	1.96	0.47
1:D:45:GLU:HG3	1:D:46:PRO:HD2	1.97	0.47
1:A:50:ALA:O	1:A:265:LYS:NZ	2.38	0.46
1:A:240:LYS:NZ	1:A:257:MET:HG3	2.21	0.46
1:D:253:TYR:O	1:D:254:PHE:HB2	2.16	0.46
1:C:240:LYS:HE3	1:C:257:MET:HG3	1.97	0.46
1:A:240:LYS:HZ3	1:A:240:LYS:HG2	1.48	0.46
1:C:253:TYR:O	1:C:254:PHE:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:NZ	1:A:287:GLU:O	2.50	0.45
1:C:93:LYS:HE3	1:C:99:GLU:HG2	1.99	0.44
1:C:181:LYS:HE2	1:C:219:TRP:CE2	2.53	0.44
1:D:240:LYS:HZ1	1:D:257:MET:HG3	1.83	0.44
1:D:129:VAL:HG12	1:D:130:ILE:HG23	2.01	0.43
1:B:257:MET:HE3	1:B:304:PRO:HB2	2.00	0.43
1:C:215:LYS:NZ	1:C:287:GLU:O	2.52	0.42
1:D:257:MET:HE3	1:D:304:PRO:HB2	2.01	0.42
1:B:255:LEU:CB	1:B:260:MET:HE2	2.49	0.42
1:A:129:VAL:HG22	1:A:160:ALA:HB3	2.00	0.42
1:B:236:LEU:HD13	1:B:241:PRO:HG3	2.01	0.42
1:A:86:ASP:OD1	1:A:108:THR:HG22	2.20	0.42
1:B:240:LYS:HD3	1:B:248:LEU:CD2	2.50	0.41
1:A:2:SER:HB2	2:B:575:HOH:O	2.20	0.41
1:D:181:LYS:HE2	1:D:219:TRP:CD1	2.56	0.41
1:A:305:LEU:HD12	1:A:333:HIS:CE1	2.56	0.41
1:B:305:LEU:HD12	1:B:333:HIS:CE1	2.55	0.41
1:D:117:LEU:O	1:D:192:ILE:HA	2.21	0.41
1:D:240:LYS:NZ	1:D:257:MET:CG	2.82	0.41
1:C:326:ARG:NH1	1:D:326:ARG:NH1	2.69	0.41
1:D:326:ARG:HH12	1:D:353:ASP:CG	2.24	0.40
1:A:240:LYS:NZ	1:A:257:MET:SD	2.92	0.40
1:B:246:SER:HA	1:B:249:GLU:HB3	2.04	0.40
1:D:12:ARG:HA	1:D:15:ASP:O	2.21	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:A:74:MET:SD	1:D:74:MET:CE[4_455]	1.54	0.66

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	360/362 (99%)	350 (97%)	10 (3%)	0	100	100
1	B	353/362 (98%)	345 (98%)	8 (2%)	0	100	100
1	C	352/362 (97%)	342 (97%)	10 (3%)	0	100	100
1	D	353/362 (98%)	344 (98%)	9 (2%)	0	100	100
All	All	1418/1448 (98%)	1381 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	281/281 (100%)	280 (100%)	1 (0%)	91	89
1	B	275/281 (98%)	275 (100%)	0	100	100
1	C	274/281 (98%)	273 (100%)	1 (0%)	91	89
1	D	274/281 (98%)	273 (100%)	1 (0%)	91	89
All	All	1104/1124 (98%)	1101 (100%)	3 (0%)	92	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	PHE
1	C	254	PHE
1	D	254	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	78	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	362/362 (100%)	0.50	35 (9%)	7	6	18, 26, 45, 58	0
1	B	355/362 (98%)	0.77	53 (14%)	2	1	18, 28, 47, 62	0
1	C	354/362 (97%)	0.55	32 (9%)	9	7	19, 30, 46, 64	0
1	D	355/362 (98%)	0.78	56 (15%)	2	1	19, 29, 50, 64	0
All	All	1426/1448 (98%)	0.65	176 (12%)	4	3	18, 28, 47, 64	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	ALA	7.4
1	D	51	ASN	6.4
1	A	6	LEU	6.4
1	A	7	ASN	6.2
1	B	82	SER	6.0
1	D	109	GLY	5.9
1	D	111	THR	5.7
1	B	109	GLY	5.6
1	A	4	ALA	5.4
1	C	113	ASP	5.3
1	B	113	ASP	5.1
1	D	9	LEU	5.1
1	C	109	GLY	5.0
1	B	8	GLN	5.0
1	D	8	GLN	4.9
1	D	112	SER	4.8
1	D	113	ASP	4.6
1	D	242	GLU	4.5
1	B	242	GLU	4.4
1	B	51	ASN	4.4
1	B	112	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	52	SER	4.3
1	C	111	THR	4.3
1	C	82	SER	4.3
1	A	242	GLU	4.3
1	B	354	ILE	4.2
1	A	112	SER	4.2
1	A	113	ASP	4.1
1	D	54	VAL	4.1
1	A	82	SER	4.1
1	A	111	THR	4.0
1	B	111	THR	4.0
1	B	227	TYR	3.9
1	D	114	SER	3.8
1	D	78	GLN	3.8
1	B	299	VAL	3.8
1	C	242	GLU	3.8
1	B	14	GLY	3.7
1	D	53	GLU	3.7
1	C	116	PRO	3.6
1	C	112	SER	3.6
1	C	108	THR	3.6
1	B	248	LEU	3.5
1	B	78	GLN	3.5
1	B	238	ALA	3.5
1	C	115	ASP	3.4
1	B	228	ALA	3.4
1	B	45	GLU	3.4
1	D	14	GLY	3.3
1	D	82	SER	3.3
1	B	297	ILE	3.3
1	D	188	GLU	3.3
1	B	50	ALA	3.3
1	A	188	GLU	3.3
1	B	44	ALA	3.2
1	D	287	GLU	3.2
1	B	13	LEU	3.2
1	B	188	GLU	3.2
1	B	199	GLY	3.2
1	C	114	SER	3.1
1	D	115	ASP	3.1
1	C	84	PRO	3.1
1	D	84	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	80	GLU	3.1
1	B	350	THR	3.1
1	B	53	GLU	3.1
1	C	85	VAL	3.1
1	A	8	GLN	3.1
1	B	328	VAL	3.0
1	D	239	SER	3.0
1	B	239	SER	2.9
1	B	327	THR	2.9
1	B	66	GLN	2.9
1	C	287	GLU	2.9
1	A	328	VAL	2.9
1	C	78	GLN	2.9
1	D	257	MET	2.8
1	A	228	ALA	2.8
1	A	109	GLY	2.8
1	A	296	VAL	2.8
1	C	206	LEU	2.8
1	A	2	SER	2.8
1	D	227	TYR	2.8
1	D	241	PRO	2.8
1	B	84	PRO	2.7
1	A	5	THR	2.7
1	A	53	GLU	2.7
1	D	299	VAL	2.7
1	C	188	GLU	2.7
1	A	297	ILE	2.7
1	D	189	ALA	2.7
1	B	296	VAL	2.7
1	D	116	PRO	2.7
1	B	298	SER	2.7
1	C	299	VAL	2.7
1	C	239	SER	2.7
1	D	272	GLU	2.6
1	D	297	ILE	2.6
1	B	60	TYR	2.6
1	B	108	THR	2.6
1	C	83	ASN	2.6
1	C	228	ALA	2.6
1	D	85	VAL	2.6
1	B	9	LEU	2.6
1	B	115	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	255	LEU	2.6
1	D	16	PRO	2.6
1	A	55	ALA	2.6
1	D	86	ASP	2.6
1	A	354	ILE	2.6
1	A	115	ASP	2.5
1	C	9	LEU	2.5
1	A	227	TYR	2.5
1	B	80	GLU	2.5
1	A	93	LYS	2.5
1	D	15	ASP	2.5
1	D	41	ASP	2.5
1	A	299	VAL	2.5
1	A	298	SER	2.5
1	D	199	GLY	2.5
1	B	258	LYS	2.5
1	A	78	GLN	2.5
1	B	208	LEU	2.5
1	A	287	GLU	2.5
1	B	74	MET	2.5
1	C	80	GLU	2.5
1	D	208	LEU	2.5
1	C	36	GLN	2.5
1	B	77	SER	2.4
1	C	87	VAL	2.4
1	D	55	ALA	2.4
1	D	17	SER	2.4
1	D	77	SER	2.4
1	D	206	LEU	2.4
1	D	228	ALA	2.4
1	A	41	ASP	2.4
1	C	191	GLY	2.4
1	B	230	CYS	2.3
1	D	74	MET	2.3
1	B	349	ALA	2.3
1	C	86	ASP	2.3
1	D	248	LEU	2.3
1	C	93	LYS	2.3
1	B	68	TRP	2.3
1	D	83	ASN	2.3
1	B	240	LYS	2.3
1	C	99	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	198	SER	2.2
1	C	296	VAL	2.2
1	D	60	TYR	2.2
1	B	16	PRO	2.2
1	B	206	LEU	2.2
1	B	241	PRO	2.2
1	D	47	PRO	2.2
1	B	203	GLY	2.2
1	B	324	VAL	2.2
1	C	77	SER	2.2
1	C	297	ILE	2.2
1	A	349	ALA	2.2
1	A	1	MET	2.2
1	B	226	VAL	2.2
1	A	230	CYS	2.1
1	D	328	VAL	2.1
1	D	45	GLU	2.1
1	D	48	VAL	2.1
1	D	123	THR	2.1
1	B	325	GLY	2.1
1	C	298	SER	2.1
1	D	350	THR	2.1
1	D	290	ALA	2.1
1	D	58	ILE	2.1
1	A	272	GLU	2.1
1	A	239	SER	2.1
1	A	334	ALA	2.0
1	D	240	LYS	2.0
1	A	243	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.