wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 05:17 PM EST

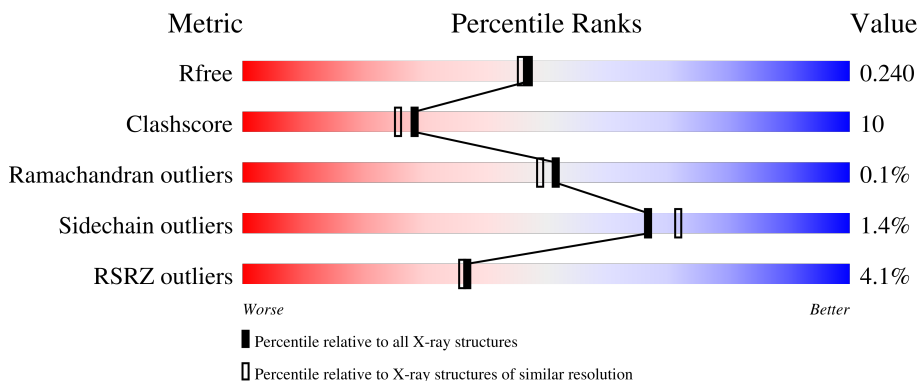|		
PDB ID	:	3AXG
Title	:	Structure of 6-aminohexanoate-oligomer hydrolase
Authors	:	Negoro, S.; Shibata, N.; Tanaka, Y.; Yasuhira, K.; Shibata, H.; Hashimoto, H.; Lee, Y.H.; Ohshima, S.; Santa, R.; Mochiji, K.; Goto, Y.; Ikegami, T.; Nagai, K.; Kato, D.; Takeo, M.; Higuchi, Y.
Deposited on	:	2011-04-04
Resolution	:	2.00 Å(reported)

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 2.00 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		10
Ramachandran outliers		0.1%
Sidechain outliers		1.4%
RSRZ outliers		4.1%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	355	3% / 81% / 16% ·
1	B	355	6% / 74% / 23% ··
1	C	355	3% / 81% / 15% ··
1	D	355	4% / 79% / 18% ·
1	E	355	7% / 78% / 19% ·

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Mol	Chain	Length	Quality of chain
1	F	355	5% / 77% / 20%
1	G	355	3% / 78% / 18%
1	H	355	8% / 79% / 17%
1	I	355	8% / 74% / 22%
1	J	355	5% / 81% / 15%
1	K	355	4% / 78% / 17%
1	L	355	3% / 80% / 16%
1	M	355	% / 85% / 12%
1	N	355	85% / 11%
1	O	355	87% / 10%

2 Entity composition (i)

There are 3 unique types of molecules in this entry. The entry contains 40681 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 Endotype 6-aminohexanoat-oligomer hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	B	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	C	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	D	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	E	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	F	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	G	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	H	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	I	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	J	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	K	342	Total 2511	C 1571	N 449	O 483	S 8	0	0	0
1	L	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	M	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	N	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0
1	O	344	Total 2522	C 1578	N 451	O 485	S 8	0	0	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Na 1	0	0
2	K	1	Total 1	Na 1	0	0
2	L	1	Total 1	Na 1	0	0
2	M	1	Total 1	Na 1	0	0
2	N	1	Total 1	Na 1	0	0
2	O	1	Total 1	Na 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total 188	O 188	0	0
3	B	104	Total 104	O 104	0	0
3	C	194	Total 194	O 194	0	0
3	D	165	Total 165	O 165	0	0
3	E	99	Total 99	O 99	0	0
3	F	182	Total 182	O 182	0	0
3	G	161	Total 161	O 161	0	0
3	H	116	Total 116	O 116	0	0
3	I	117	Total 117	O 117	0	0
3	J	170	Total 170	O 170	0	0
3	K	217	Total 217	O 217	0	0
3	L	174	Total 174	O 174	0	0
3	M	333	Total 333	O 333	0	0
3	N	318	Total 318	O 318	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	318	Total O 318 318		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: Endotype 6-aminohexanoat-oligomer hydrolase

- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

- Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

G339 K355

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain D:

4%

79%　　　　　18%

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain E:

7%

78%　　　　　19%

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain F:

5%

77%　　　　　20%

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain G:

3%

78%　　　　　18%

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain H:

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase
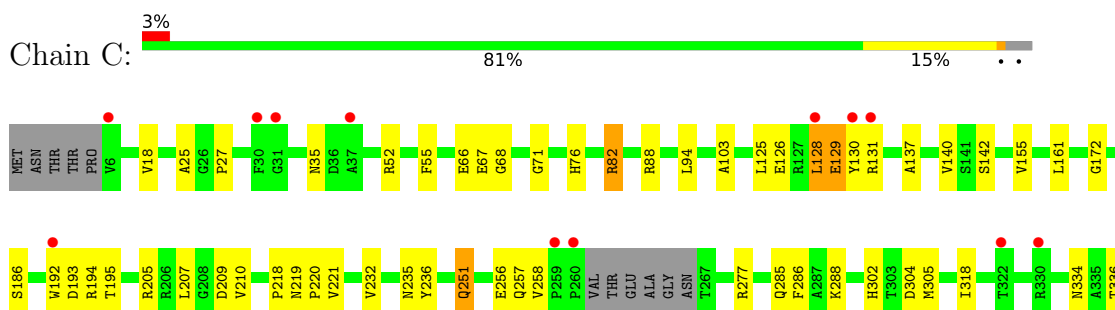
Chain I:

• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain J:

H302 T303 D304 M305 D306 G307 D308 A312 T322 R330 T336 G339 K355

● Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain K:

4%
78% 17%

MET ASN THR PRO V6 L9 I12 V18 P22 N35 R52 F55 E67 G68 H76 R82 A87 R88 G89 G90 A91 VAL GLY L94 E115 E126 R127 L128 E129 Y130 F134 S142 T153 A154 V155 Y156 P157 L161 V170 E173

K189 V190 D191 R194 R205 R206 L207 P218 N219 P220 V221 D226 V232 Y236 R244 V247 F248 Q251 E252 A253 V258 P259 P260 VAL THR GLU ALA GLY ASN T267 I272 R277 N284 Q285 F286 A287 K288 Q289 H302 T303 D304 M305 A312

D316 P321 T322 G325 S326 T336 G339 K355

● Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain L:

3%
80% 16%

MET ASN THR PRO V6 L9 I12 V18 P22 F30 G31 F38 D39 L40 S45 R52 F53 D54 F55 Y65 E66 E67 R82 R88 A118 G119 Y146 D147 F148 S152 T153 A154 V155 K159 G172 A179 K189 W192 D193 R194

A202 R205 R206 L207 G208 D209 V210 R211 A214 V215 V216 V217 P218 N219 P220 V221 V232 N235 Y236 D237 A238 Q251 E256 Q257 V258 P259 P260 VAL THR GLU ALA GLY ASN T267 I272 R277 Q285 F286 A287 K288 D304 M305 D306 G307 D308 D316 E317
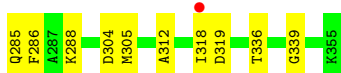
L320 P321 T322 T323 R328 G329 R330 G339 K355

● Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain M:

%
85% 12%

MET ASN THR PRO V6 V18 D39 L40 R52 F55 I60 Y65 G68 P69 H76 R88 G133 F134 A135 E136 T153 P157 L161 V170 P171 G172 E173 F174 G180 M183 R194 P218 N219 P220 V221 V232 N235 V247

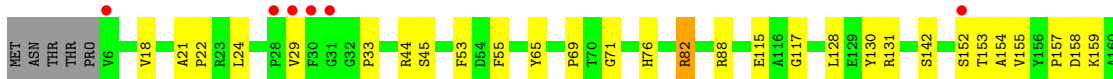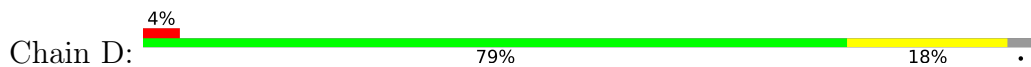Q251 P260 VAL THR GLU ALA GLY ASN T267 I272 V273 T274 R277 V281 F286 A287 K288 M305 A312 V313 T314 D319 G339 K355

● Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain N:

85% 11%

MET ASN THR PRO V6 V18 D19 P20 A21 P22 F30 M50 F55 I60 G68 R82 R88 F134 T153 P157 L161 V170 E173 F174 G180 M183 W192 D193 R194 P218 N219 P220 V221 V232 N235 Y236 D237 A238

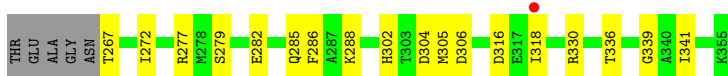R244 P260 VAL THR GLU ALA GLY ASN T267 I272 R277 F286 A287 K288 M305 A312 D319 T323 G339 A340 K355
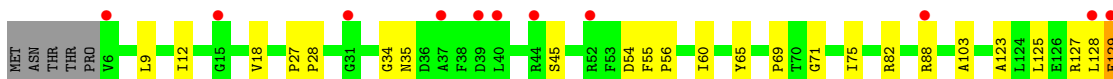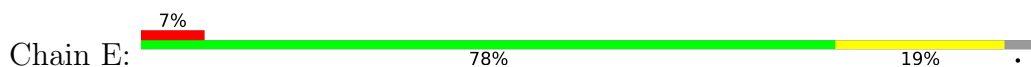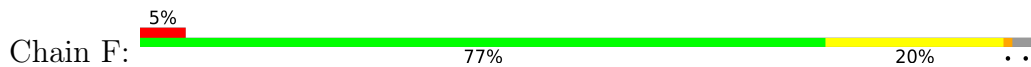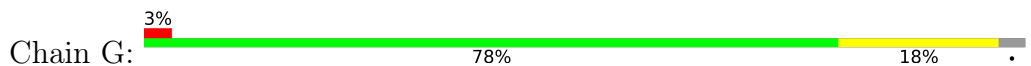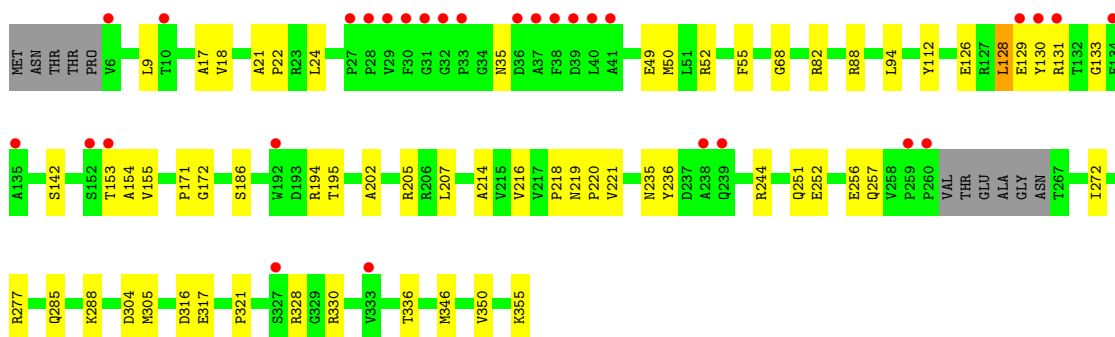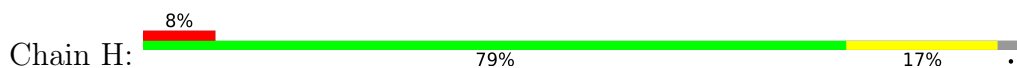
• Molecule 1: Endotype 6-aminohexanoat-oligomer hydrolase

Chain O:

87% 10%

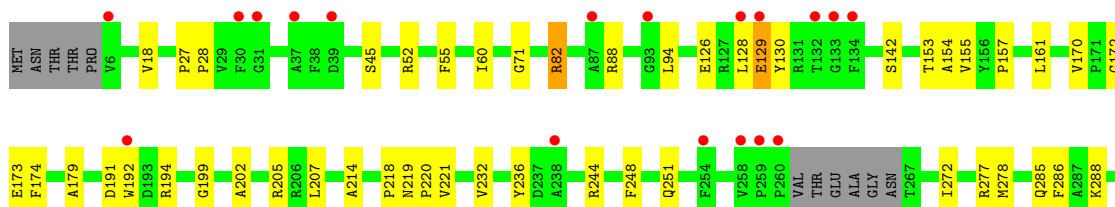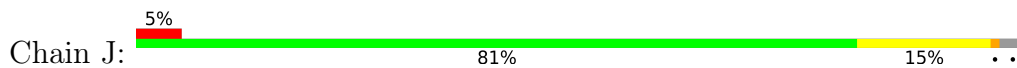MET ASN THR THR PRO V6 V18 A21 P22 N35 R52 F55 I60 H76 R82 R88 E126 Y130 V155 V170 P171 G172 E173 F174 R205 R206 L207 P218 N219 P220 V221 V232 Y236 P260 VAL THR GLU ALA GLY ASN T267

I272 R277 M278 F286 A287 K288 H302 M305 A312 D319 G339 K355

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	155.86Å 214.45Å 478.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.00 49.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.99-2.00) 94.2 (49.99-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.240 0.211 , 0.240	Depositor DCC
R_{free} test set	50323 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 64.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	40681	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.35% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.33	0/2576	0.50	0/3505
1	B	0.31	0/2576	0.47	0/3505
1	C	0.34	0/2576	0.48	0/3505
1	D	0.33	0/2576	0.48	0/3505
1	E	0.31	0/2576	0.47	0/3505
1	F	0.33	0/2576	0.48	0/3505
1	G	0.33	0/2576	0.48	0/3505
1	H	0.32	0/2576	0.47	0/3505
1	I	0.31	0/2576	0.46	0/3505
1	J	0.33	0/2576	0.48	0/3505
1	K	0.33	0/2564	0.49	0/3487
1	L	0.33	0/2576	0.47	0/3505
1	M	0.39	0/2576	0.53	0/3505
1	N	0.39	1/2576 (0.0%)	0.54	0/3505
1	O	0.36	0/2576	0.51	0/3505
All	All	0.34	1/38628 (0.0%)	0.49	0/52557

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	340	ALA	CA-CB	5.36	1.63	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2522	0	2454	55	0
1	B	2522	0	2454	76	0
1	C	2522	0	2454	55	0
1	D	2522	0	2454	62	0
1	E	2522	0	2454	62	0
1	F	2522	0	2454	62	0
1	G	2522	0	2454	61	0
1	H	2522	0	2454	62	0
1	I	2522	0	2454	77	0
1	J	2522	0	2454	60	0
1	K	2511	0	2441	65	0
1	L	2522	0	2454	51	0
1	M	2522	0	2454	33	0
1	N	2522	0	2454	31	0
1	O	2522	0	2454	28	0
2	A	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
3	A	188	0	0	2	0
3	B	104	0	0	3	0
3	C	194	0	0	2	0
3	D	165	0	0	7	0
3	E	99	0	0	1	0
3	F	182	0	0	3	0
3	G	161	0	0	2	0
3	H	116	0	0	2	0
3	I	117	0	0	4	0
3	J	170	0	0	2	0
3	K	217	0	0	6	0
3	L	174	0	0	1	0
3	M	333	0	0	7	0
3	N	318	0	0	3	0
3	O	318	0	0	3	0
All	All	40681	0	36797	730	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 10.

The worst 5 of 730 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:E:153:THR:HG22	1:E:155:VAL:H	1.29	0.95
1:J:153:THR:HG22	1:J:155:VAL:H	1.32	0.95
1:I:257:GLN:HE21	1:K:326:SER:HA	1.31	0.93
1:F:276:VAL:HG22	1:F:318:ILE:HD11	1.52	0.92
1:N:88:ARG:HH12	1:N:288:LYS:HB3	1.35	0.91

There are no symmetry-related clashes.

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	340/355 (96%)	326 (96%)	14 (4%)	0	100	100
1	B	340/355 (96%)	324 (95%)	16 (5%)	0	100	100
1	C	340/355 (96%)	327 (96%)	12 (4%)	1 (0%)	41	37
1	D	340/355 (96%)	329 (97%)	11 (3%)	0	100	100
1	E	340/355 (96%)	321 (94%)	19 (6%)	0	100	100
1	F	340/355 (96%)	327 (96%)	11 (3%)	2 (1%)	25	19
1	G	340/355 (96%)	327 (96%)	13 (4%)	0	100	100
1	H	340/355 (96%)	322 (95%)	17 (5%)	1 (0%)	41	37
1	I	340/355 (96%)	326 (96%)	14 (4%)	0	100	100
1	J	340/355 (96%)	320 (94%)	20 (6%)	0	100	100
1	K	336/355 (95%)	319 (95%)	16 (5%)	1 (0%)	41	37
1	L	340/355 (96%)	322 (95%)	18 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	340/355 (96%)	327 (96%)	13 (4%)	0	100	100
1	N	340/355 (96%)	326 (96%)	13 (4%)	1 (0%)	41	37
1	O	340/355 (96%)	326 (96%)	14 (4%)	0	100	100
All	All	5096/5325 (96%)	4869 (96%)	221 (4%)	6 (0%)	51	49

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	89	GLY
1	C	68	GLY
1	F	68	GLY
1	F	89	GLY
1	N	68	GLY

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	252/261 (97%)	250 (99%)	2 (1%)	81	86
1	B	252/261 (97%)	248 (98%)	4 (2%)	62	67
1	C	252/261 (97%)	245 (97%)	7 (3%)	43	44
1	D	252/261 (97%)	250 (99%)	2 (1%)	81	86
1	E	252/261 (97%)	249 (99%)	3 (1%)	71	76
1	F	252/261 (97%)	248 (98%)	4 (2%)	62	67
1	G	252/261 (97%)	249 (99%)	3 (1%)	71	76
1	H	252/261 (97%)	249 (99%)	3 (1%)	71	76
1	I	252/261 (97%)	247 (98%)	5 (2%)	55	58
1	J	252/261 (97%)	248 (98%)	4 (2%)	62	67
1	K	251/261 (96%)	247 (98%)	4 (2%)	62	67
1	L	252/261 (97%)	246 (98%)	6 (2%)	49	51
1	M	252/261 (97%)	249 (99%)	3 (1%)	71	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	252/261 (97%)	251 (100%)	1 (0%)	91	93
1	O	252/261 (97%)	250 (99%)	2 (1%)	81	86
All	All	3779/3915 (96%)	3726 (99%)	53 (1%)	67	72

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	52	ARG
1	J	129	GLU
1	M	305	MET
1	I	55	PHE
1	I	277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	176	GLN
1	J	257	GLN
1	J	76	HIS
1	L	257	GLN
1	C	334	ASN

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 ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	344/355 (96%)	0.04	10 (2%)	51	50	18, 31, 50, 71	0
1	B	344/355 (96%)	0.34	22 (6%)	19	18	22, 40, 60, 70	0
1	C	344/355 (96%)	0.02	12 (3%)	44	43	18, 30, 51, 64	0
1	D	344/355 (96%)	0.10	13 (3%)	40	39	18, 32, 53, 74	0
1	E	344/355 (96%)	0.41	25 (7%)	15	14	21, 39, 60, 83	0
1	F	344/355 (96%)	0.16	18 (5%)	27	26	21, 32, 54, 77	0
1	G	344/355 (96%)	-0.04	11 (3%)	47	46	18, 31, 53, 69	0
1	H	344/355 (96%)	0.50	29 (8%)	11	10	20, 37, 59, 74	0
1	I	344/355 (96%)	0.57	27 (7%)	13	12	25, 38, 55, 67	0
1	J	344/355 (96%)	0.18	19 (5%)	25	24	19, 30, 56, 71	0
1	K	342/355 (96%)	0.03	13 (3%)	40	39	19, 30, 49, 64	0
1	L	344/355 (96%)	0.15	11 (3%)	47	46	20, 32, 51, 63	0
1	M	344/355 (96%)	-0.44	2 (0%)	89	88	10, 18, 35, 57	0
1	N	344/355 (96%)	-0.50	1 (0%)	94	93	10, 19, 33, 49	0
1	O	344/355 (96%)	-0.46	1 (0%)	94	93	13, 21, 34, 45	0
All	All	5158/5325 (96%)	0.07	214 (4%)	37	36	10, 31, 54, 83	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	134	PHE	8.0
1	J	134	PHE	7.7
1	A	134	PHE	7.4
1	H	31	GLY	7.0
1	D	30	PHE	6.5

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NA	O	3004	1/1	0.94	0.08	34,34,34,34	0
2	NA	L	3006	1/1	0.96	0.15	44,44,44,44	0
2	NA	K	3001	1/1	0.96	0.10	28,28,28,28	0
2	NA	M	3003	1/1	0.97	0.06	32,32,32,32	0
2	NA	A	3005	1/1	0.97	0.09	32,32,32,32	0
2	NA	N	3002	1/1	0.99	0.10	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.

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