



# Full wwPDB X-ray Structure Validation Report i

Feb 4, 2024 – 04:52 PM EST

PDB ID : 1RJW

Title : CRYSTAL STRUCTURE OF NAD(+) -DEPENDENT ALCOHOL DEHYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS STRAIN LLD-R

Authors : Ceccarelli, C.; Bahnsen, B.J.

Deposited on : 2003-11-20

Resolution : 2.35 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](mailto: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 i symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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

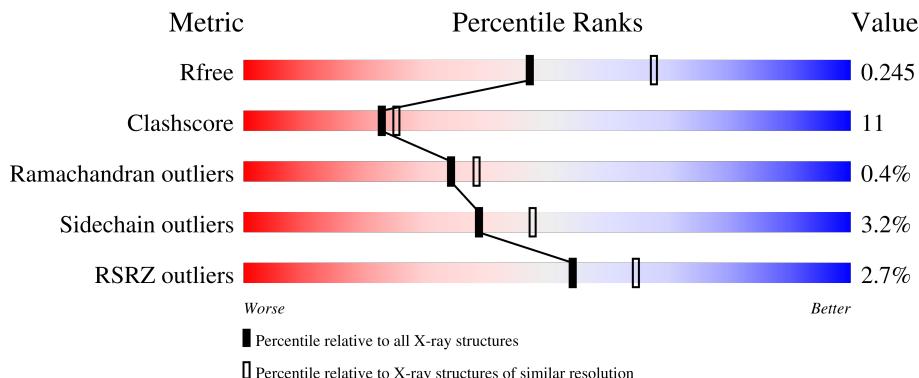
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

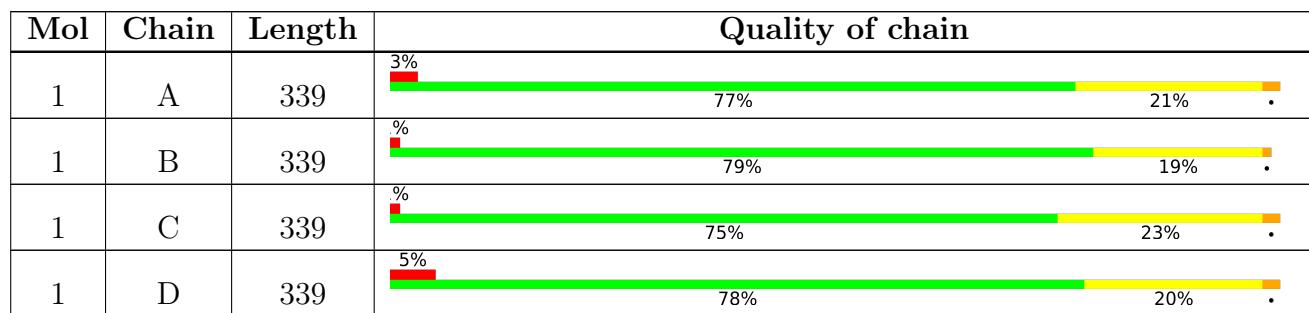
The reported resolution of this entry is 2.35 Å.

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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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.



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ETF	A	607	-	-	X	-

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10634 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.

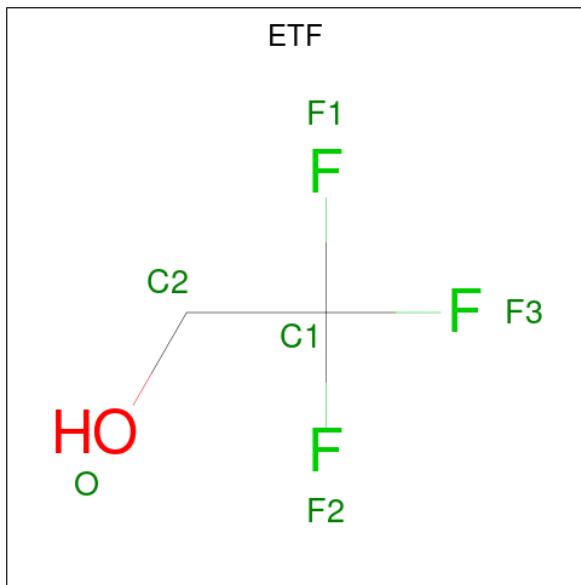
- Molecule 1 is a protein called Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total 2554	C 1637	N 430	O 473	S 14	0	0	0
1	B	339	Total 2554	C 1637	N 430	O 473	S 14	0	0	0
1	C	339	Total 2554	C 1637	N 430	O 473	S 14	0	0	0
1	D	339	Total 2554	C 1637	N 430	O 473	S 14	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0

- Molecule 3 is TRIFLUOROETHANOL (three-letter code: ETF) (formula: C<sub>2</sub>H<sub>3</sub>F<sub>3</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O 6 2 3 1	0	0
3	A	1	Total C F O 6 2 3 1	0	0
3	B	1	Total C F O 6 2 3 1	0	0
3	B	1	Total C F O 6 2 3 1	0	0
3	B	1	Total C F O 6 2 3 1	0	0
3	B	1	Total C F O 6 2 3 1	0	0
3	C	1	Total C F O 6 2 3 1	0	0
3	C	1	Total C F O 6 2 3 1	0	0
3	C	1	Total C F O 6 2 3 1	0	0
3	D	1	Total C F O 6 2 3 1	0	0
3	D	1	Total C F O 6 2 3 1	0	0
3	D	1	Total C F O 6 2 3 1	0	0
3	D	1	Total C F O 6 2 3 1	0	0

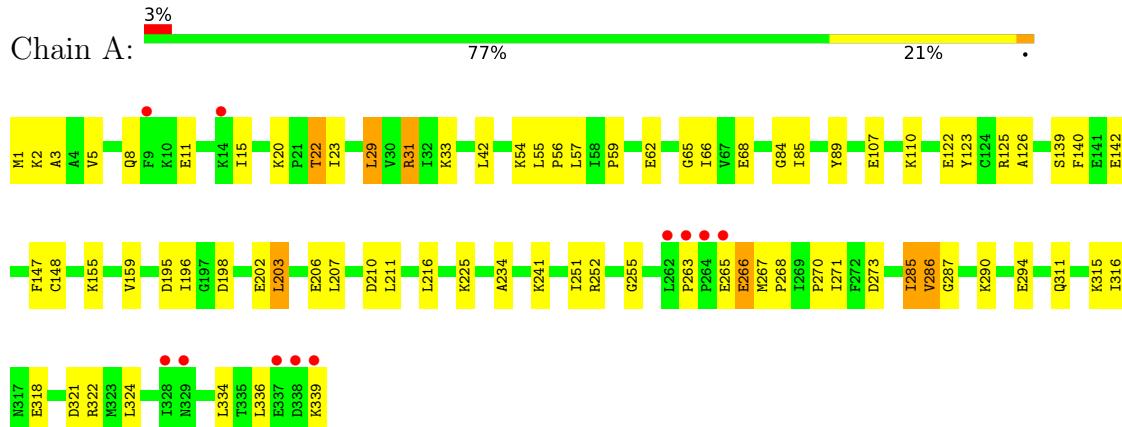
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	79	Total O 79 79	0	0
4	B	103	Total O 103 103	0	0
4	C	72	Total O 72 72	0	0
4	D	78	Total O 78 78	0	0

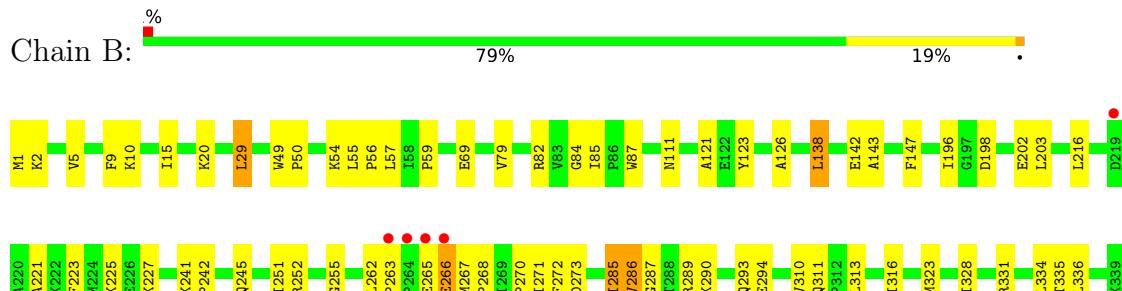
### 3 Residue-property plots (i)

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.

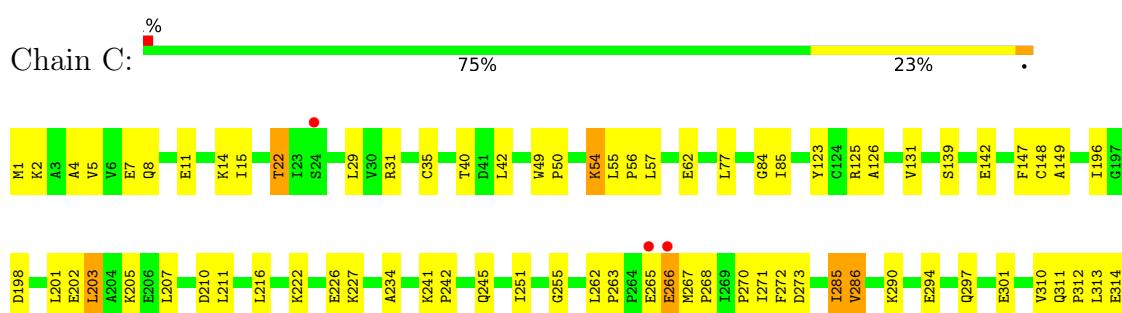
- Molecule 1: Alcohol dehydrogenase



- Molecule 1: Alcohol dehydrogenase

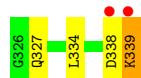
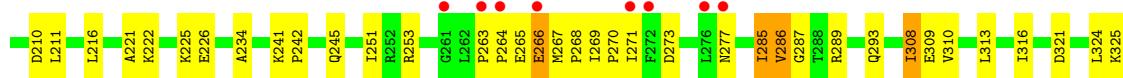
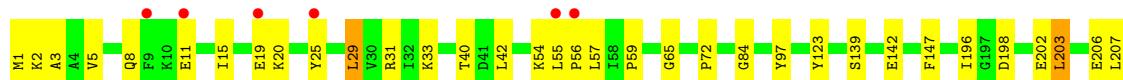
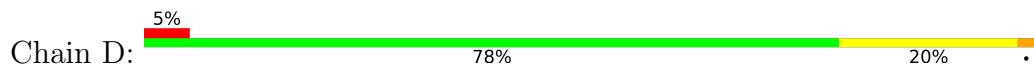


- Molecule 1: Alcohol dehydrogenase





- Molecule 1: Alcohol dehydrogenase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.32 Å   138.22 Å   158.68 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	41.44 – 2.35 41.44 – 2.35	Depositor EDS
% Data completeness (in resolution range)	81.1 (41.44-2.35) 81.2 (41.44-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	6.64 (at 2.34 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
$R$ , $R_{free}$	0.214 , 0.252 0.208 , 0.245	Depositor DCC
$R_{free}$ test set	2596 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.5	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.47$ , $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10634	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 i

### 5.1 Standard geometry i

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

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	0.36	0/2605	0.60	0/3530
1	B	0.36	0/2605	0.60	0/3530
1	C	0.35	0/2605	0.60	0/3530
1	D	0.36	0/2605	0.60	0/3530
All	All	0.36	0/10420	0.60	0/14120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2554	0	2605	66	0
1	B	2554	0	2605	64	0
1	C	2554	0	2605	72	0
1	D	2554	0	2605	70	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	12	0	5	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	11	0	0
3	C	18	0	8	1	0
3	D	24	0	11	1	0
4	A	79	0	0	0	0
4	B	103	0	0	3	0
4	C	72	0	0	1	0
4	D	78	0	0	4	0
All	All	10634	0	10455	238	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 11.

All (238) 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:323:MET:HG3	1:B:328:ILE:HD12	1.34	1.08
1:D:8:GLN:HB2	1:D:11:GLU:HG3	1.56	0.86
1:A:271:ILE:HD11	1:D:267:MET:HG2	1.63	0.79
1:B:82:ARG:HD3	4:B:1016:HOH:O	1.86	0.75
1:B:323:MET:HG3	1:B:328:ILE:CD1	2.16	0.74
1:C:323:MET:HG2	1:C:328:ILE:HD12	1.71	0.73
1:A:202:GLU:O	1:A:206:GLU:HG3	1.90	0.72
1:A:267:MET:HG2	1:D:271:ILE:HD11	1.71	0.71
1:A:62:GLU:OE2	1:A:148:CYS:HB3	1.91	0.70
1:B:267:MET:HG2	1:C:271:ILE:HD11	1.73	0.70
1:C:8:GLN:HB2	1:C:11:GLU:HG3	1.74	0.69
1:A:196:ILE:HG22	1:A:216:LEU:HD13	1.76	0.68
1:D:8:GLN:CB	1:D:11:GLU:HG3	2.24	0.67
1:B:331:ARG:HG3	1:B:331:ARG:HH11	1.61	0.66
1:C:310:VAL:HG13	1:C:335:THR:HG23	1.78	0.66
1:A:33:LYS:CE	1:A:66:ILE:HD13	2.26	0.65
1:A:33:LYS:HE3	1:A:66:ILE:HD13	1.79	0.65
1:A:23:ILE:HG22	1:A:125:ARG:HG3	1.79	0.65
1:C:321:ASP:O	1:C:325:LYS:HD3	1.96	0.65
1:D:19:GLU:HG2	4:D:1317:HOH:O	1.96	0.65
1:C:297:GLN:O	1:C:301:GLU:HG3	1.95	0.65
1:C:311:GLN:OE1	1:C:315:LYS:HD2	1.97	0.65
1:D:2:LYS:HD3	1:D:313:LEU:HD23	1.80	0.64
1:B:271:ILE:HD12	1:C:263:PRO:HG2	1.79	0.63
1:D:308:ILE:HD12	1:D:309:GLU:N	2.13	0.63
1:B:121:ALA:O	1:B:336:LEU:HD22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PRO:HG2	1:C:271:ILE:HD12	1.81	0.62
1:B:196:ILE:HG22	1:B:216:LEU:HD13	1.81	0.62
1:C:196:ILE:HG22	1:C:216:LEU:HD13	1.81	0.62
1:B:267:MET:CG	1:C:271:ILE:HD11	2.30	0.61
1:C:316:ILE:HD13	1:C:334:LEU:HD11	1.82	0.61
1:A:54:LYS:O	1:A:57:LEU:HB2	2.01	0.60
1:C:149:ALA:HB2	1:C:331:ARG:NH2	2.16	0.60
1:B:138:LEU:HD12	1:B:143:ALA:HB2	1.83	0.60
1:C:270:PRO:HB2	1:C:273:ASP:HB2	1.83	0.60
1:C:2:LYS:NZ	1:C:2:LYS:HB3	2.16	0.60
1:A:265:GLU:HG2	1:A:266:GLU:H	1.67	0.59
1:A:271:ILE:CD1	1:D:267:MET:HG2	2.33	0.59
1:B:271:ILE:CD1	1:C:263:PRO:HG2	2.32	0.59
1:D:196:ILE:HG22	1:D:216:LEU:HD13	1.85	0.59
1:B:271:ILE:HD11	1:C:267:MET:HG2	1.83	0.59
1:A:196:ILE:HG23	3:A:607:ETF:H21	1.85	0.59
1:B:221:ALA:O	1:B:225:LYS:HG2	2.03	0.59
1:B:272:PHE:CD1	1:C:262:LEU:HD22	2.37	0.59
1:A:84:GLY:HA3	1:A:147:PHE:CE2	2.38	0.59
1:B:323:MET:CG	1:B:328:ILE:HD12	2.20	0.58
1:A:107:GLU:HG2	1:D:253:ARG:NH2	2.19	0.58
1:D:84:GLY:HA3	1:D:147:PHE:CE2	2.38	0.58
1:B:265:GLU:HG2	1:B:266:GLU:H	1.69	0.57
1:B:310:VAL:HG13	1:B:335:THR:HG23	1.85	0.57
1:A:271:ILE:HD11	1:D:267:MET:CG	2.34	0.57
1:D:264:PRO:HD2	4:D:1146:HOH:O	2.02	0.57
1:B:54:LYS:O	1:B:57:LEU:HB2	2.03	0.57
1:D:210:ASP:O	1:D:211:LEU:HD12	2.05	0.57
1:C:54:LYS:O	1:C:57:LEU:HB2	2.05	0.57
1:C:198:ASP:O	1:C:202:GLU:HG3	2.04	0.57
1:D:263:PRO:HB2	4:D:1146:HOH:O	2.05	0.57
1:D:308:ILE:HD11	1:D:310:VAL:CG2	2.35	0.56
1:C:84:GLY:HA3	1:C:147:PHE:CE2	2.41	0.56
1:A:22:THR:O	1:A:125:ARG:HD3	2.05	0.56
1:A:66:ILE:N	1:A:66:ILE:HD12	2.21	0.56
1:A:139:SER:OG	1:A:142:GLU:HG3	2.06	0.56
1:B:84:GLY:HA3	1:B:147:PHE:CE2	2.40	0.56
1:B:263:PRO:HG2	1:C:271:ILE:CD1	2.36	0.55
1:D:25:TYR:CD1	1:D:72:PRO:HB2	2.41	0.55
1:C:222:LYS:O	1:C:226:GLU:HG3	2.07	0.55
1:D:1:MET:SD	1:D:123:TYR:HB2	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:123:TYR:HB2	2.47	0.54
1:D:265:GLU:HG2	1:D:266:GLU:H	1.71	0.54
1:B:198:ASP:O	1:B:202:GLU:HG3	2.08	0.54
1:A:210:ASP:O	1:A:211:LEU:HD12	2.08	0.53
1:B:270:PRO:HB2	1:B:273:ASP:HB2	1.89	0.53
1:D:202:GLU:O	1:D:206:GLU:HG3	2.09	0.53
1:D:270:PRO:HB2	1:D:273:ASP:HB2	1.90	0.53
1:A:66:ILE:HD11	1:A:140:PHE:CZ	2.44	0.52
1:A:265:GLU:HG2	1:A:266:GLU:N	2.23	0.52
1:B:271:ILE:HD11	1:C:267:MET:CG	2.40	0.52
1:B:79:VAL:HG23	4:B:1074:HOH:O	2.09	0.52
1:A:84:GLY:HA3	1:A:147:PHE:CZ	2.44	0.52
1:D:308:ILE:HD11	1:D:310:VAL:HG23	1.92	0.52
1:B:271:ILE:CG2	1:C:263:PRO:HD2	2.41	0.51
1:C:265:GLU:HG2	1:C:266:GLU:H	1.74	0.51
1:A:65:GLY:C	1:A:66:ILE:HD12	2.32	0.51
1:B:223:PHE:O	1:B:227:LYS:HD3	2.11	0.50
1:D:308:ILE:HD12	1:D:309:GLU:C	2.31	0.50
1:D:54:LYS:O	1:D:57:LEU:HB2	2.11	0.50
1:C:40:THR:HG21	3:C:501:ETF:H22	1.94	0.50
1:A:89:TYR:HB3	1:A:110:LYS:O	2.12	0.50
1:B:265:GLU:HG2	1:B:266:GLU:N	2.27	0.50
1:A:122:GLU:OE2	1:A:339:LYS:HA	2.12	0.50
1:B:121:ALA:C	1:B:336:LEU:HD22	2.32	0.50
1:B:138:LEU:HD13	1:B:142:GLU:HB2	1.93	0.50
1:C:85:ILE:HD13	1:C:126:ALA:HB2	1.94	0.50
1:D:265:GLU:HG2	1:D:266:GLU:N	2.27	0.50
1:B:271:ILE:HG21	1:C:263:PRO:HD2	1.93	0.50
1:C:251:ILE:CG2	1:C:255:GLY:HA3	2.42	0.50
1:A:251:ILE:CG2	1:A:255:GLY:HA3	2.42	0.50
1:B:316:ILE:HD13	1:B:334:LEU:HD11	1.94	0.49
1:A:196:ILE:HG23	3:A:607:ETF:C2	2.41	0.49
1:B:1:MET:SD	1:B:123:TYR:HB2	2.52	0.49
1:C:290:LYS:HD2	1:C:294:GLU:OE2	2.12	0.49
1:D:84:GLY:HA3	1:D:147:PHE:CZ	2.47	0.49
1:D:198:ASP:O	1:D:202:GLU:HG3	2.13	0.49
1:A:33:LYS:HE2	1:A:66:ILE:HD13	1.94	0.49
1:A:318:GLU:O	1:A:322:ARG:HG3	2.12	0.49
1:A:271:ILE:HD11	1:D:267:MET:HE2	1.95	0.48
1:A:263:PRO:HG2	1:D:271:ILE:CD1	2.43	0.48
1:B:251:ILE:CG2	1:B:255:GLY:HA3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLU:HG2	1:C:266:GLU:N	2.29	0.48
1:D:42:LEU:HD21	1:D:324:LEU:CD2	2.44	0.48
1:D:222:LYS:HG2	1:D:226:GLU:OE2	2.14	0.48
1:B:49:TRP:HB3	1:B:50:PRO:HD2	1.96	0.48
1:D:31:ARG:HG3	1:D:123:TYR:CE1	2.49	0.48
1:A:267:MET:HG2	1:D:271:ILE:CD1	2.40	0.48
1:D:339:LYS:HE3	1:D:339:LYS:HA	1.95	0.48
1:C:1:MET:SD	1:C:123:TYR:HB2	2.54	0.47
1:A:315:LYS:HG2	1:A:318:GLU:OE2	2.13	0.47
1:A:311:GLN:O	1:A:334:LEU:HA	2.14	0.47
1:B:15:ILE:HD12	1:B:15:ILE:N	2.29	0.47
1:A:198:ASP:O	1:A:202:GLU:HG3	2.14	0.47
1:A:271:ILE:HD11	1:D:267:MET:CE	2.44	0.47
1:D:55:LEU:HA	1:D:56:PRO:C	2.33	0.47
1:A:234:ALA:HB3	1:A:251:ILE:HD11	1.97	0.47
1:A:316:ILE:HD13	1:A:334:LEU:HD11	1.96	0.47
1:C:7:GLU:O	1:C:8:GLN:NE2	2.47	0.47
1:A:55:LEU:HA	1:A:56:PRO:C	2.36	0.47
1:A:203:LEU:HD22	1:A:207:LEU:HG	1.96	0.47
1:C:234:ALA:HB3	1:C:251:ILE:HD11	1.96	0.47
1:D:2:LYS:HG2	1:D:3:ALA:N	2.29	0.47
1:A:85:ILE:HD13	1:A:126:ALA:HB2	1.96	0.47
1:D:316:ILE:HD13	1:D:334:LEU:HD11	1.96	0.47
1:A:241:LYS:HZ2	1:A:268:PRO:CD	2.28	0.46
1:C:227:LYS:NZ	4:C:1275:HOH:O	2.49	0.46
1:C:310:VAL:CG1	1:C:335:THR:HG23	2.44	0.46
1:A:8:GLN:O	1:A:11:GLU:HB2	2.15	0.46
1:C:4:ALA:HB2	1:C:313:LEU:HD11	1.98	0.46
1:A:270:PRO:HB2	1:A:273:ASP:HB2	1.97	0.46
1:B:289:ARG:O	1:B:293:GLN:HG3	2.16	0.46
1:D:203:LEU:HD22	1:D:207:LEU:HG	1.98	0.46
1:B:84:GLY:HA3	1:B:147:PHE:CZ	2.50	0.46
1:B:55:LEU:HA	1:B:56:PRO:C	2.36	0.46
1:B:271:ILE:HD11	1:C:267:MET:CE	2.46	0.46
1:A:285:ILE:HG23	1:A:286:VAL:HG22	1.98	0.46
1:B:9:PHE:O	1:B:10:LYS:HB2	2.16	0.46
1:C:210:ASP:O	1:C:211:LEU:HD12	2.16	0.46
1:D:325:LYS:HB2	1:D:327:GLN:HG3	1.98	0.46
1:B:267:MET:SD	1:C:271:ILE:HD11	2.55	0.46
1:D:40:THR:HG21	3:D:501:ETF:H22	1.98	0.46
1:D:273:ASP:O	1:D:277:ASN:CG	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:GLN:O	1:C:334:LEU:HA	2.16	0.45
1:B:69:GLU:HB3	4:B:1028:HOH:O	2.16	0.45
1:B:85:ILE:HD13	1:B:126:ALA:HB2	1.98	0.45
1:C:241:LYS:HZ1	1:C:268:PRO:HG2	1.82	0.45
1:D:241:LYS:HZ1	1:D:268:PRO:HG2	1.80	0.45
1:D:234:ALA:HB3	1:D:251:ILE:HD11	1.98	0.45
1:A:252:ARG:HB2	1:D:97:TYR:OH	2.15	0.45
1:C:15:ILE:N	1:C:15:ILE:HD12	2.31	0.45
1:C:84:GLY:HA3	1:C:147:PHE:CZ	2.52	0.45
1:D:33:LYS:HG2	1:D:65:GLY:HA2	1.99	0.45
1:B:286:VAL:HG23	1:B:287:GLY:N	2.32	0.45
1:A:271:ILE:CG1	1:D:267:MET:HG2	2.47	0.45
1:C:201:LEU:O	1:C:205:LYS:HG3	2.16	0.45
1:B:267:MET:HG2	1:C:271:ILE:CD1	2.44	0.45
1:D:139:SER:OG	1:D:142:GLU:HG3	2.17	0.44
1:A:336:LEU:N	1:A:336:LEU:HD12	2.31	0.44
1:C:241:LYS:N	1:C:242:PRO:HD2	2.33	0.44
1:C:325:LYS:HD2	1:C:325:LYS:N	2.32	0.44
1:D:221:ALA:O	1:D:225:LYS:HG3	2.18	0.44
1:A:290:LYS:HD2	1:A:294:GLU:OE2	2.17	0.44
1:A:271:ILE:CD1	1:D:263:PRO:HG2	2.48	0.44
1:D:285:ILE:HG23	1:D:286:VAL:HG22	2.00	0.44
1:A:241:LYS:HZ2	1:A:268:PRO:HD3	1.82	0.44
1:A:286:VAL:HG23	1:A:287:GLY:N	2.32	0.44
1:B:241:LYS:N	1:B:242:PRO:HD2	2.33	0.44
1:C:62:GLU:OE2	1:C:148:CYS:HB3	2.18	0.44
1:D:20:LYS:HE2	1:D:29:LEU:HD11	2.00	0.44
1:B:331:ARG:HG3	1:B:331:ARG:NH1	2.29	0.44
1:D:245:GLN:NE2	4:D:1294:HOH:O	2.51	0.44
1:D:269:ILE:HG13	1:D:269:ILE:O	2.19	0.43
1:A:2:LYS:HG2	1:A:3:ALA:N	2.32	0.43
1:A:42:LEU:HD21	1:A:324:LEU:CD2	2.49	0.43
1:B:271:ILE:HD11	1:C:267:MET:SD	2.59	0.43
1:D:210:ASP:C	1:D:211:LEU:HD12	2.38	0.43
1:A:263:PRO:HG2	1:D:271:ILE:HD13	2.00	0.43
1:C:311:GLN:OE1	1:C:312:PRO:HD2	2.18	0.43
1:C:285:ILE:HG23	1:C:286:VAL:HG22	2.00	0.43
1:B:57:LEU:O	1:B:59:PRO:HD3	2.19	0.43
1:C:35:CYS:HA	1:C:62:GLU:O	2.19	0.43
1:C:55:LEU:HA	1:C:56:PRO:C	2.37	0.43
1:C:241:LYS:HZ2	1:C:268:PRO:CD	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HD2	1:B:313:LEU:HD23	2.00	0.42
1:C:2:LYS:HB3	1:C:2:LYS:HZ3	1.81	0.42
1:C:42:LEU:HD21	1:C:324:LEU:CD2	2.49	0.42
1:C:139:SER:OG	1:C:142:GLU:HG3	2.18	0.42
1:A:15:ILE:N	1:A:15:ILE:HD12	2.34	0.42
1:A:57:LEU:O	1:A:59:PRO:HD3	2.20	0.42
1:B:251:ILE:HG22	1:B:252:ARG:O	2.19	0.42
1:D:57:LEU:HD13	1:D:57:LEU:C	2.40	0.42
1:D:241:LYS:HZ2	1:D:268:PRO:HD3	1.84	0.42
1:A:195:ASP:HA	3:A:607:ETF:H22	2.01	0.42
1:C:7:GLU:OE1	1:C:14:LYS:HD2	2.20	0.42
1:D:308:ILE:HD11	1:D:310:VAL:HG22	2.00	0.42
1:C:203:LEU:HD22	1:C:207:LEU:HG	2.02	0.42
1:B:87:TRP:O	1:B:111:ASN:HA	2.20	0.42
1:B:290:LYS:HD2	1:B:294:GLU:OE2	2.20	0.42
1:D:8:GLN:NE2	1:D:11:GLU:OE2	2.53	0.42
1:D:273:ASP:O	1:D:277:ASN:ND2	2.53	0.42
1:B:263:PRO:HD2	1:C:271:ILE:CG2	2.50	0.42
1:B:285:ILE:HG23	1:B:286:VAL:HG22	2.02	0.42
1:C:15:ILE:HG12	1:C:314:GLU:HA	2.01	0.42
1:D:241:LYS:N	1:D:242:PRO:HD2	2.35	0.42
1:C:77:LEU:HD11	1:C:131:VAL:CG2	2.50	0.41
1:C:337:GLU:OE1	1:C:337:GLU:HA	2.20	0.41
1:D:15:ILE:N	1:D:15:ILE:HD12	2.34	0.41
1:D:286:VAL:HG23	1:D:287:GLY:N	2.35	0.41
1:D:2:LYS:CD	1:D:313:LEU:HD23	2.48	0.41
1:A:31:ARG:HB2	1:A:68:GLU:CG	2.50	0.41
1:A:196:ILE:CG2	1:A:216:LEU:HD13	2.47	0.41
1:B:20:LYS:HE2	1:B:29:LEU:HD11	2.03	0.41
1:B:311:GLN:O	1:B:334:LEU:HA	2.21	0.41
1:B:241:LYS:HZ1	1:B:268:PRO:HG2	1.85	0.41
1:B:245:GLN:HE21	1:B:245:GLN:HB3	1.64	0.41
1:B:267:MET:CE	1:C:271:ILE:HD11	2.51	0.41
1:C:22:THR:O	1:C:125:ARG:HD3	2.21	0.41
1:A:263:PRO:HD2	1:D:271:ILE:HG21	2.03	0.41
1:A:267:MET:HE2	1:D:271:ILE:HD11	2.03	0.41
1:C:49:TRP:HB3	1:C:50:PRO:HD2	2.02	0.41
1:C:241:LYS:HZ2	1:C:268:PRO:HD3	1.85	0.41
1:A:20:LYS:HE2	1:A:29:LEU:HD11	2.03	0.41
1:A:155:LYS:O	1:A:159:VAL:HG23	2.21	0.41
1:B:262:LEU:HD22	1:C:272:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:O	1:D:59:PRO:HD3	2.21	0.40
1:C:54:LYS:H	1:C:54:LYS:HG3	1.66	0.40
1:B:241:LYS:HZ2	1:B:268:PRO:HD3	1.86	0.40
1:B:196:ILE:CG2	1:B:216:LEU:HD13	2.49	0.40
1:C:54:LYS:HD2	1:C:57:LEU:HD23	2.03	0.40
1:A:107:GLU:HG2	1:D:253:ARG:HH21	1.85	0.40
1:D:289:ARG:O	1:D:293:GLN:HG3	2.22	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	337/339 (99%)	327 (97%)	9 (3%)	1 (0%)	41 47
1	B	337/339 (99%)	328 (97%)	8 (2%)	1 (0%)	41 47
1	C	337/339 (99%)	327 (97%)	8 (2%)	2 (1%)	25 27
1	D	337/339 (99%)	326 (97%)	10 (3%)	1 (0%)	41 47
All	All	1348/1356 (99%)	1308 (97%)	35 (3%)	5 (0%)	34 38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	ASP
1	D	286	VAL
1	A	286	VAL
1	B	286	VAL
1	C	286	VAL

### 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	269/269 (100%)	260 (97%)	9 (3%)	38   46
1	B	269/269 (100%)	263 (98%)	6 (2%)	52   63
1	C	269/269 (100%)	259 (96%)	10 (4%)	34   42
1	D	269/269 (100%)	260 (97%)	9 (3%)	38   46
All	All	1076/1076 (100%)	1042 (97%)	34 (3%)	39   47

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	22	THR
1	A	29	LEU
1	A	31	ARG
1	A	203	LEU
1	A	225	LYS
1	A	266	GLU
1	A	285	ILE
1	A	321	ASP
1	B	5	VAL
1	B	29	LEU
1	B	138	LEU
1	B	203	LEU
1	B	266	GLU
1	B	285	ILE
1	C	5	VAL
1	C	22	THR
1	C	29	LEU
1	C	31	ARG
1	C	54	LYS
1	C	203	LEU
1	C	245	GLN
1	C	266	GLU
1	C	285	ILE

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Mol	Chain	Res	Type
1	C	325	LYS
1	D	5	VAL
1	D	29	LEU
1	D	203	LEU
1	D	266	GLU
1	D	285	ILE
1	D	308	ILE
1	D	321	ASP
1	D	338	ASP
1	D	339	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	249	ASN
1	A	293	GLN
1	B	8	GLN
1	B	245	GLN
1	B	249	ASN
1	B	293	GLN
1	C	94	HIS
1	C	249	ASN
1	C	293	GLN
1	D	8	GLN
1	D	249	ASN

### 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)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ETF	A	607	-	5,5,5	0.37	0	7,7,7	0.50	0
3	ETF	A	501	2	5,5,5	0.43	0	7,7,7	0.45	0
3	ETF	B	603	-	5,5,5	0.39	0	7,7,7	0.43	0
3	ETF	D	501	2	5,5,5	0.32	0	7,7,7	0.45	0
3	ETF	C	609	-	5,5,5	0.33	0	7,7,7	0.42	0
3	ETF	D	608	-	5,5,5	0.45	0	7,7,7	0.50	0
3	ETF	D	601	-	5,5,5	0.28	0	7,7,7	0.40	0
3	ETF	B	606	-	5,5,5	0.37	0	7,7,7	0.44	0
3	ETF	C	604	-	5,5,5	0.38	0	7,7,7	0.43	0
3	ETF	B	501	2	5,5,5	0.53	0	7,7,7	0.43	0
3	ETF	D	602	-	5,5,5	0.46	0	7,7,7	0.46	0
3	ETF	B	605	-	5,5,5	0.30	0	7,7,7	0.42	0
3	ETF	C	501	2	5,5,5	0.33	0	7,7,7	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ETF	A	607	-	-	3/3/3/3	-
3	ETF	A	501	2	-	3/3/3/3	-
3	ETF	B	603	-	-	3/3/3/3	-
3	ETF	D	501	2	-	3/3/3/3	-
3	ETF	C	609	-	-	0/3/3/3	-
3	ETF	D	608	-	-	3/3/3/3	-
3	ETF	D	601	-	-	3/3/3/3	-
3	ETF	B	606	-	-	2/3/3/3	-
3	ETF	C	604	-	-	0/3/3/3	-
3	ETF	B	501	2	-	3/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ETF	D	602	-	-	0/3/3/3	-
3	ETF	B	605	-	-	3/3/3/3	-
3	ETF	C	501	2	-	3/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ETF	F3-C1-C2-O
3	D	608	ETF	F1-C1-C2-O
3	C	501	ETF	F1-C1-C2-O
3	D	501	ETF	F1-C1-C2-O
3	A	501	ETF	F2-C1-C2-O
3	B	501	ETF	F3-C1-C2-O
3	D	501	ETF	F3-C1-C2-O
3	A	501	ETF	F1-C1-C2-O
3	D	501	ETF	F2-C1-C2-O
3	D	608	ETF	F3-C1-C2-O
3	B	501	ETF	F2-C1-C2-O
3	C	501	ETF	F2-C1-C2-O
3	D	608	ETF	F2-C1-C2-O
3	B	501	ETF	F1-C1-C2-O
3	B	603	ETF	F3-C1-C2-O
3	B	605	ETF	F2-C1-C2-O
3	B	605	ETF	F3-C1-C2-O
3	C	501	ETF	F3-C1-C2-O
3	A	607	ETF	F2-C1-C2-O
3	B	603	ETF	F2-C1-C2-O
3	B	605	ETF	F1-C1-C2-O
3	B	603	ETF	F1-C1-C2-O
3	A	607	ETF	F1-C1-C2-O
3	D	601	ETF	F2-C1-C2-O
3	D	601	ETF	F3-C1-C2-O
3	A	607	ETF	F3-C1-C2-O
3	B	606	ETF	F2-C1-C2-O
3	B	606	ETF	F3-C1-C2-O
3	D	601	ETF	F1-C1-C2-O

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	607	ETF	3	0
3	D	501	ETF	1	0
3	C	501	ETF	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	339/339 (100%)	0.07	11 (3%) 47 59	19, 34, 61, 83	0
1	B	339/339 (100%)	0.03	5 (1%) 73 81	18, 33, 57, 81	0
1	C	339/339 (100%)	-0.13	4 (1%) 79 86	19, 35, 58, 80	0
1	D	339/339 (100%)	0.03	16 (4%) 31 44	20, 33, 59, 80	0
All	All	1356/1356 (100%)	0.00	36 (2%) 54 64	18, 34, 59, 83	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	PHE	6.5
1	B	264	PRO	6.5
1	D	263	PRO	6.0
1	A	264	PRO	5.2
1	D	271	ILE	4.7
1	A	339	LYS	4.3
1	D	55	LEU	4.1
1	D	9	PHE	3.9
1	B	265	GLU	3.8
1	A	263	PRO	3.8
1	D	276	LEU	3.7
1	A	338	ASP	3.7
1	B	263	PRO	3.5
1	D	277	ASN	3.3
1	A	328	ILE	3.2
1	D	264	PRO	3.2
1	D	266	GLU	3.1
1	A	262	LEU	3.0
1	A	329	ASN	3.0
1	A	9	PHE	3.0
1	D	338	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	25	TYR	2.7
1	D	339	LYS	2.7
1	A	14	LYS	2.6
1	B	266	GLU	2.5
1	C	338	ASP	2.4
1	A	265	GLU	2.4
1	C	266	GLU	2.4
1	B	219	ASP	2.3
1	A	337	GLU	2.3
1	D	261	GLY	2.3
1	D	56	PRO	2.3
1	C	24	SER	2.2
1	D	19	GLU	2.1
1	D	11	GLU	2.1
1	C	265	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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	ETF	D	608	6/6	0.61	0.21	74,76,77,78	0
3	ETF	A	501	6/6	0.84	0.21	75,76,77,77	0
3	ETF	B	605	6/6	0.88	0.28	65,67,67,68	0
3	ETF	B	606	6/6	0.88	0.20	70,70,71,71	0
3	ETF	B	501	6/6	0.88	0.20	53,58,60,61	0
3	ETF	C	501	6/6	0.89	0.20	62,65,67,67	0
3	ETF	C	609	6/6	0.89	0.17	79,81,81,82	0
3	ETF	A	607	6/6	0.89	0.22	72,73,73,74	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ETF	D	501	6/6	0.92	0.14	55,57,59,60	0
3	ETF	D	602	6/6	0.94	0.14	54,55,56,56	0
3	ETF	B	603	6/6	0.94	0.15	62,64,65,66	0
3	ETF	D	601	6/6	0.95	0.13	47,48,50,50	0
3	ETF	C	604	6/6	0.97	0.11	66,67,67,67	0
2	ZN	C	402	1/1	0.97	0.06	57,57,57,57	0
2	ZN	A	402	1/1	0.98	0.08	56,56,56,56	0
2	ZN	D	402	1/1	0.99	0.07	38,38,38,38	0
2	ZN	C	401	1/1	0.99	0.07	25,25,25,25	0
2	ZN	B	401	1/1	1.00	0.10	22,22,22,22	0
2	ZN	D	401	1/1	1.00	0.10	21,21,21,21	0
2	ZN	B	402	1/1	1.00	0.08	29,29,29,29	0
2	ZN	A	401	1/1	1.00	0.08	29,29,29,29	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.