



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:26 am BST

PDB ID : 2ES4  
Title : Crystal structure of the Burkholderia glumae lipase-specific foldase in complex with its cognate lipase  
Authors : Pauwels, K.; Wyns, L.; Tommassen, J.; Savvides, S.N.; Van Gelder, P.  
Deposited on : 2005-10-25  
Resolution : 1.85 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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

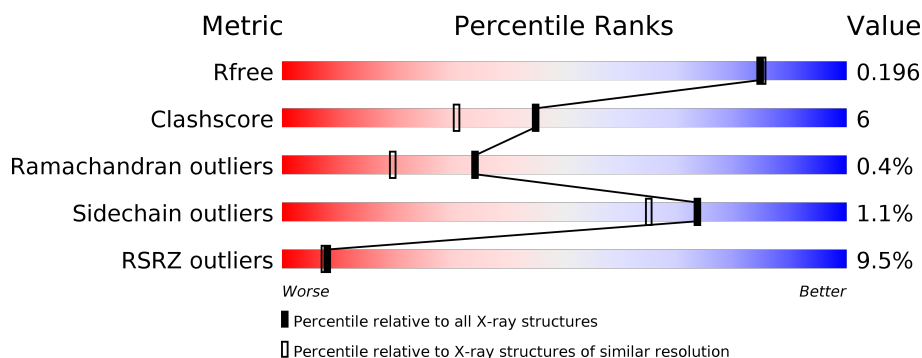
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on 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.

Mol	Chain	Length	Quality of chain
1	A	319	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>••</div> </div> </div>
1	B	319	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>7%</div> <div>•</div> </div> </div>
2	D	332	<div> <div>15%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>19%</div> </div> </div>
2	E	332	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9463 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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2303	1434	404	462	3			
1	B	314	Total	C	N	O	S	0	0	0
			2292	1426	403	460	3			

- Molecule 2 is a protein called Lipase chaperone.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	270	Total	C	N	O	S	0	0	0
			1992	1229	377	381	5			
2	E	278	Total	C	N	O	S	0	0	0
			2023	1251	381	386	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	GLY	-	CLONING ARTIFACT	UNP Q05490
D	2	HIS	-	EXPRESSION TAG	UNP Q05490
D	3	HIS	-	EXPRESSION TAG	UNP Q05490
D	4	HIS	-	EXPRESSION TAG	UNP Q05490
D	5	HIS	-	EXPRESSION TAG	UNP Q05490
D	6	HIS	-	EXPRESSION TAG	UNP Q05490
D	7	HIS	-	EXPRESSION TAG	UNP Q05490
D	8	HIS	-	EXPRESSION TAG	UNP Q05490
D	9	HIS	-	EXPRESSION TAG	UNP Q05490
D	10	HIS	-	EXPRESSION TAG	UNP Q05490
D	11	HIS	-	EXPRESSION TAG	UNP Q05490
D	12	SER	-	CLONING ARTIFACT	UNP Q05490
D	13	SER	-	CLONING ARTIFACT	UNP Q05490
D	14	GLY	-	CLONING ARTIFACT	UNP Q05490
D	15	HIS	-	CLONING ARTIFACT	UNP Q05490
D	16	ILE	-	CLONING ARTIFACT	UNP Q05490

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Chain	Residue	Modelled	Actual	Comment	Reference
D	17	GLU	-	CLONING ARTIFACT	UNP Q05490
D	18	GLY	-	CLONING ARTIFACT	UNP Q05490
D	19	ARG	-	CLONING ARTIFACT	UNP Q05490
D	20	HIS	-	CLONING ARTIFACT	UNP Q05490
D	21	MET	-	CLONING ARTIFACT	UNP Q05490
D	92	CSO	CYS	MODIFIED RESIDUE	UNP Q05490
E	1	GLY	-	CLONING ARTIFACT	UNP Q05490
E	2	HIS	-	EXPRESSION TAG	UNP Q05490
E	3	HIS	-	EXPRESSION TAG	UNP Q05490
E	4	HIS	-	EXPRESSION TAG	UNP Q05490
E	5	HIS	-	EXPRESSION TAG	UNP Q05490
E	6	HIS	-	EXPRESSION TAG	UNP Q05490
E	7	HIS	-	EXPRESSION TAG	UNP Q05490
E	8	HIS	-	EXPRESSION TAG	UNP Q05490
E	9	HIS	-	EXPRESSION TAG	UNP Q05490
E	10	HIS	-	EXPRESSION TAG	UNP Q05490
E	11	HIS	-	EXPRESSION TAG	UNP Q05490
E	12	SER	-	CLONING ARTIFACT	UNP Q05490
E	13	SER	-	CLONING ARTIFACT	UNP Q05490
E	14	GLY	-	CLONING ARTIFACT	UNP Q05490
E	15	HIS	-	CLONING ARTIFACT	UNP Q05490
E	16	ILE	-	CLONING ARTIFACT	UNP Q05490
E	17	GLU	-	CLONING ARTIFACT	UNP Q05490
E	18	GLY	-	CLONING ARTIFACT	UNP Q05490
E	19	ARG	-	CLONING ARTIFACT	UNP Q05490
E	20	HIS	-	CLONING ARTIFACT	UNP Q05490
E	21	MET	-	CLONING ARTIFACT	UNP Q05490
E	92	CSO	CYS	MODIFIED RESIDUE	UNP Q05490

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total I 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total I 1 1	0	0
4	E	3	Total I 3 3	0	0

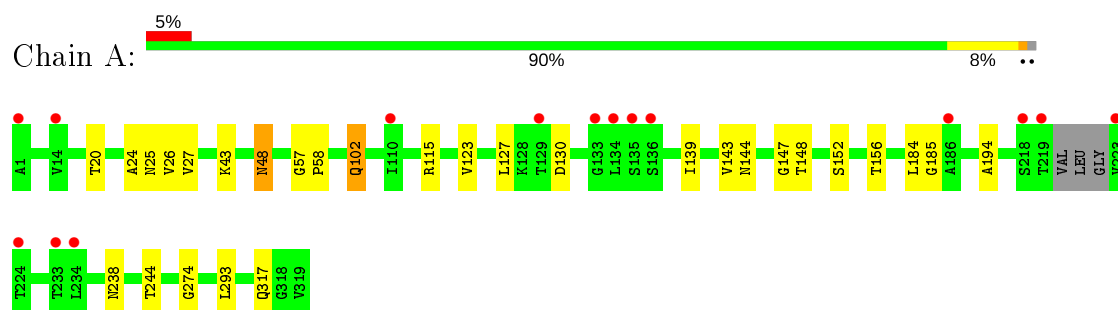
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	184	Total O 184 184	0	0
5	D	169	Total O 169 169	0	0
5	B	298	Total O 298 298	0	0
5	E	192	Total O 192 192	0	0

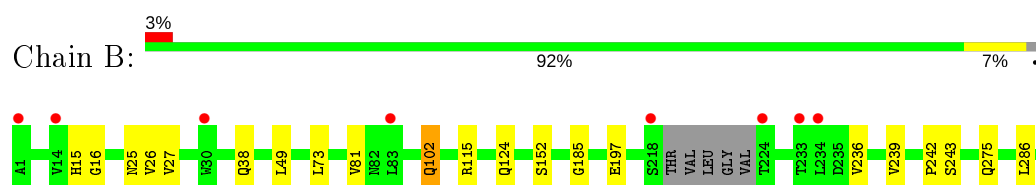
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

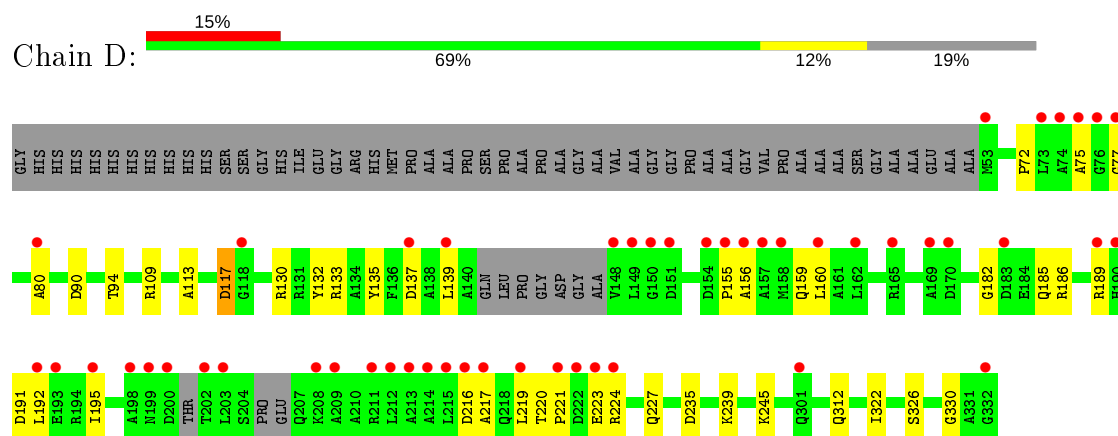
#### • Molecule 1: Lipase



#### • Molecule 1: Lipase

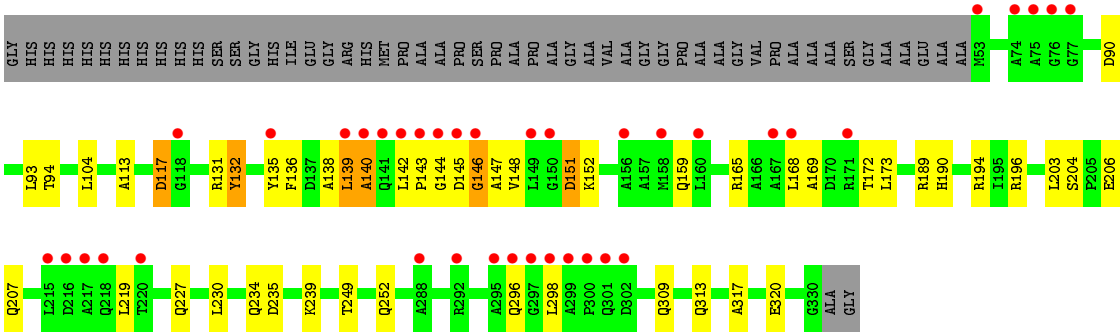


#### • Molecule 2: Lipase chaperone



#### • Molecule 2: Lipase chaperone





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.00Å 75.70Å 116.60Å 90.00° 117.60° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 38.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.85) 97.3 (38.83-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.199 , 0.219 0.196 , 0.196	Depositor DCC
$R_{free}$ test set	6407 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9463	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, IOD, CA

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	0.46	0/2343	0.59	0/3203
1	B	0.48	0/2332	0.60	0/3187
2	D	0.43	0/2014	0.51	0/2733
2	E	0.42	0/2049	0.53	1/2788 (0.0%)
All	All	0.45	0/8738	0.56	1/11911 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	143	PRO	N-CA-CB	5.50	109.90	103.30

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	2303	0	2251	23	0
1	B	2292	0	2239	21	0
2	D	1992	0	1904	35	0
2	E	2023	0	1915	41	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	2	0
4	D	1	0	0	0	0
4	E	3	0	0	0	0
5	A	184	0	0	3	0
5	B	298	0	0	3	0
5	D	169	0	0	2	0
5	E	192	0	0	2	1
All	All	9463	0	8309	110	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 6.

All (110) 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:25:ASN:HD21	1:B:152:SER:H	1.06	0.99
1:B:15:HIS:HE1	1:B:49:LEU:H	1.18	0.92
1:B:25:ASN:ND2	1:B:152:SER:H	1.79	0.79
1:B:197:GLU:HG3	4:B:904:IOD:I	2.54	0.78
1:A:102:GLN:NE2	1:A:102:GLN:H	1.82	0.76
2:D:159:GLN:HE22	2:D:189:ARG:NH1	1.84	0.76
1:A:102:GLN:HE21	1:A:102:GLN:H	1.32	0.74
1:B:239:VAL:HG21	2:E:144:GLY:O	1.87	0.74
1:B:15:HIS:CE1	1:B:49:LEU:H	2.07	0.71
2:E:159:GLN:HG3	2:E:196:ARG:HH22	1.56	0.70
1:B:102:GLN:NE2	1:B:102:GLN:H	1.89	0.70
1:B:102:GLN:HE21	1:B:102:GLN:H	1.37	0.70
2:E:135:TYR:HB2	2:E:173:LEU:CD2	2.24	0.68
4:B:903:IOD:I	2:E:234:GLN:HG2	2.66	0.66
2:E:139:LEU:O	2:E:139:LEU:HD22	1.97	0.63
2:E:298:LEU:HD13	5:E:1073:HOH:O	2.00	0.61
2:E:139:LEU:HD13	2:E:140:ALA:N	2.15	0.61
2:D:159:GLN:HE22	2:D:189:ARG:HH11	1.47	0.60
1:A:20:THR:HA	1:A:48:ASN:ND2	2.17	0.60
1:A:27:VAL:HG11	1:A:293:LEU:HD21	1.83	0.58
2:D:72:PRO:HB2	2:D:80:ALA:HB3	1.87	0.57
2:E:204:SER:H	2:E:207:GLN:HE21	1.52	0.57
2:D:132:TYR:O	2:D:135:TYR:HB3	2.05	0.57
1:A:43:LYS:HE3	5:A:1158:HOH:O	2.05	0.57
2:E:93:LEU:HD23	2:E:104:LEU:HD21	1.87	0.57
2:E:159:GLN:CG	2:E:196:ARG:HH22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:230:LEU:O	2:E:234:GLN:HG3	2.05	0.56
2:E:219:LEU:HD21	2:E:227:GLN:NE2	2.22	0.54
2:D:235:ASP:O	2:D:239:LYS:HG3	2.09	0.53
1:A:127:LEU:HA	1:A:130:ASP:O	2.09	0.52
2:E:159:GLN:HG3	2:E:196:ARG:NH2	2.23	0.52
2:D:159:GLN:NE2	2:D:189:ARG:HH11	2.07	0.52
2:D:220:THR:HG22	2:D:223:GLU:HG2	1.91	0.52
2:D:217:ALA:HA	2:D:224:ARG:HH22	1.75	0.52
2:E:309:GLN:O	2:E:313:GLN:HG3	2.09	0.52
2:E:136:PHE:O	2:E:139:LEU:HD12	2.09	0.51
2:E:151:ASP:CG	2:E:152:LYS:H	2.12	0.51
2:E:190:HIS:CE1	2:E:194:ARG:HD2	2.46	0.51
2:D:159:GLN:NE2	2:D:189:ARG:NH1	2.58	0.51
1:A:20:THR:HA	1:A:48:ASN:HD22	1.74	0.51
2:D:139:LEU:HD23	2:D:139:LEU:O	2.10	0.51
2:E:168:LEU:O	2:E:172:THR:HG22	2.12	0.50
2:E:169:ALA:HA	2:E:172:THR:HG22	1.93	0.50
2:E:249:THR:OG1	2:E:252:GLN:HG3	2.12	0.49
2:E:90:ASP:O	2:E:94:THR:HG23	2.12	0.49
2:D:220:THR:OG1	2:D:221:PRO:HD2	2.13	0.49
2:D:155:PRO:O	2:D:159:GLN:HB2	2.14	0.48
1:A:144:ASN:O	1:A:148:THR:HG23	2.13	0.48
2:E:135:TYR:HB2	2:E:173:LEU:HD21	1.95	0.48
1:B:15:HIS:HD2	1:B:16:GLY:O	1.96	0.48
5:A:1127:HOH:O	2:D:322:ILE:HD12	2.12	0.48
1:B:243:SER:CB	1:B:286:LEU:HD12	2.44	0.48
1:A:293:LEU:HD11	2:D:195:ILE:CD1	2.44	0.48
2:E:113:ALA:O	2:E:117:ASP:HB2	2.15	0.47
2:E:172:THR:HG23	2:E:173:LEU:HD23	1.95	0.47
1:B:236:VAL:CG1	2:E:165:ARG:HH11	2.27	0.47
2:D:90:ASP:O	2:D:94:THR:HG23	2.14	0.47
2:D:216:ASP:OD2	2:E:206:GLU:HB3	2.14	0.47
2:D:220:THR:HG23	2:D:223:GLU:H	1.80	0.47
1:A:123:VAL:O	1:A:127:LEU:HD13	2.15	0.46
1:A:238:ASN:ND2	1:A:244:THR:HG21	2.30	0.46
1:B:26:VAL:HG13	1:B:27:VAL:HG23	1.95	0.46
1:A:293:LEU:HD11	2:D:195:ILE:HD12	1.97	0.46
2:D:113:ALA:O	2:D:117:ASP:HB2	2.14	0.46
2:E:235:ASP:O	2:E:239:LYS:HG3	2.16	0.46
2:E:132:TYR:O	2:E:135:TYR:HB3	2.16	0.46
2:E:148:VAL:HB	2:E:151:ASP:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD21	1:B:81:VAL:HG13	1.99	0.45
1:A:317:GLN:HG2	5:A:1041:HOH:O	2.16	0.45
2:D:223:GLU:O	2:D:227:GLN:HG3	2.17	0.45
2:E:131:ARG:HG2	2:E:173:LEU:HA	1.99	0.45
2:D:191:ASP:O	2:D:195:ILE:HG13	2.17	0.45
2:E:138:ALA:HB1	2:E:168:LEU:HD11	1.98	0.45
2:D:130:ARG:O	2:D:133:ARG:HG2	2.17	0.44
1:A:58:PRO:HD2	2:D:330:GLY:HA3	1.99	0.44
1:B:239:VAL:HG22	2:E:147:ALA:HB2	1.99	0.44
1:B:124:GLN:NE2	5:B:1092:HOH:O	2.43	0.44
2:E:206:GLU:CD	2:E:206:GLU:H	2.19	0.44
2:E:296:GLN:HB2	2:E:298:LEU:HG	2.00	0.44
1:A:139:ILE:O	1:A:143:VAL:HG23	2.18	0.44
1:B:115:ARG:NH2	1:B:185:GLY:O	2.51	0.44
2:E:146:GLY:O	2:E:147:ALA:HB3	2.17	0.43
2:D:220:THR:HG22	2:D:223:GLU:CG	2.48	0.43
1:A:115:ARG:NH2	1:A:185:GLY:O	2.52	0.43
1:A:115:ARG:NH2	1:A:184:LEU:HB3	2.33	0.43
2:E:204:SER:H	2:E:207:GLN:NE2	2.16	0.43
1:A:25:ASN:HD21	1:A:152:SER:H	1.67	0.43
1:A:194:ALA:O	1:A:274:GLY:HA2	2.19	0.43
2:D:185:GLN:O	2:D:189:ARG:HG3	2.19	0.43
2:D:109:ARG:NH2	5:D:993:HOH:O	2.51	0.42
1:A:24:ALA:O	1:A:26:VAL:HG23	2.19	0.42
1:B:242:PRO:HA	5:B:1291:HOH:O	2.19	0.42
2:D:219:LEU:N	2:D:219:LEU:HD22	2.34	0.42
2:D:75:ALA:C	2:D:77:GLY:H	2.22	0.42
2:E:159:GLN:HE22	2:E:189:ARG:HG2	1.84	0.42
2:D:156:ALA:O	2:D:160:LEU:HG	2.19	0.42
2:E:317:ALA:HB3	2:E:320:GLU:CD	2.39	0.42
2:D:220:THR:HG22	2:D:223:GLU:OE2	2.19	0.42
1:B:298:ALA:HB2	2:E:139:LEU:HD21	2.02	0.42
1:A:57:GLY:HA2	2:D:326:SER:O	2.20	0.41
2:D:216:ASP:O	2:D:219:LEU:HD23	2.20	0.41
2:D:245:LYS:HG3	5:D:1038:HOH:O	2.19	0.41
1:A:147:GLY:O	1:A:156:THR:HB	2.21	0.41
2:E:203:LEU:HA	2:E:207:GLN:NE2	2.35	0.41
1:B:275:GLN:NE2	5:B:1031:HOH:O	2.30	0.41
2:D:182:GLY:O	2:D:186:ARG:HG3	2.20	0.41
1:A:102:GLN:N	1:A:102:GLN:HE21	2.10	0.41
2:D:155:PRO:HA	2:D:192:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ALA:HB2	2:E:139:LEU:CD2	2.51	0.41
1:B:38:GLN:HG2	5:E:939:HOH: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)
5:E:1079:HOH:O	5:E:1079:HOH:O[2_555]	2.11	0.09

## 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	312/319 (98%)	303 (97%)	9 (3%)	0	100	100
1	B	310/319 (97%)	301 (97%)	9 (3%)	0	100	100
2	D	261/332 (79%)	254 (97%)	7 (3%)	0	100	100
2	E	275/332 (83%)	262 (95%)	8 (3%)	5 (2%)	8	2
All	All	1158/1302 (89%)	1120 (97%)	33 (3%)	5 (0%)	34	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	140	ALA
2	E	146	GLY
2	E	151	ASP
2	E	142	LEU
2	E	145	ASP

### 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	243/248 (98%)	241 (99%)	2 (1%)	81	76
1	B	242/248 (98%)	241 (100%)	1 (0%)	91	89
2	D	173/226 (76%)	170 (98%)	3 (2%)	60	47
2	E	170/226 (75%)	167 (98%)	3 (2%)	59	45
All	All	828/948 (87%)	819 (99%)	9 (1%)	73	65

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	102	GLN
2	D	117	ASP
2	D	137	ASP
2	D	312	GLN
1	B	102	GLN
2	E	117	ASP
2	E	132	TYR
2	E	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	48	ASN
1	A	71	GLN
1	A	102	GLN
1	A	178	ASN
1	A	238	ASN
2	D	159	GLN
2	D	164	GLN
2	D	185	GLN
2	D	227	GLN

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Mol	Chain	Res	Type
2	D	233	GLN
2	D	244	GLN
1	B	15	HIS
1	B	25	ASN
1	B	38	GLN
1	B	59	ASN
1	B	71	GLN
1	B	102	GLN
1	B	144	ASN
1	B	178	ASN
1	B	191	GLN
1	B	238	ASN
2	E	159	GLN
2	E	185	GLN
2	E	207	GLN
2	E	227	GLN
2	E	244	GLN
2	E	313	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
2	CSO	E	92	2	3,6,7	0.61	0	0,6,8	0.00	-
2	CSO	D	92	2	3,6,7	0.59	0	0,6,8	0.00	-

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
2	CSO	E	92	2	-	0/1/5/7	-
2	CSO	D	92	2	-	0/1/5/7	-

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.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 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, 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	316/319 (99%)	0.27	15 (4%) 31 30	15, 28, 55, 65	0
1	B	314/319 (98%)	-0.00	8 (2%) 57 56	14, 22, 39, 51	0
2	D	269/332 (81%)	0.69	51 (18%) 1 1	17, 37, 79, 96	0
2	E	277/332 (83%)	0.60	38 (13%) 3 3	19, 40, 73, 83	0
All	All	1176/1302 (90%)	0.37	112 (9%) 8 7	14, 30, 69, 96	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	149	LEU	8.5
2	D	75	ALA	7.8
2	E	300	PRO	7.7
2	D	53	MET	7.2
2	E	299	ALA	7.2
2	E	140	ALA	7.1
2	E	298	LEU	6.6
2	D	148	VAL	6.4
2	E	75	ALA	6.3
2	E	297	GLY	6.0
1	A	233	THR	5.7
1	A	223	VAL	5.6
2	D	216	ASP	5.6
2	E	145	ASP	5.5
1	A	219	THR	5.5
2	E	150	GLY	5.4
1	A	234	LEU	5.3
2	D	160	LEU	5.3
2	D	213	ALA	5.2
2	D	215	LEU	5.2
1	A	218	SER	5.1

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Mol	Chain	Res	Type	RSRZ
2	E	295	ALA	4.8
2	D	202	THR	4.7
2	D	156	ALA	4.7
2	D	150	GLY	4.6
2	D	212	LEU	4.6
2	D	332	GLY	4.4
1	B	233	THR	4.3
2	D	76	GLY	3.9
2	E	135	TYR	3.9
2	D	214	ALA	3.7
2	E	53	MET	3.7
2	E	139	LEU	3.7
1	A	134	LEU	3.6
1	A	1	ALA	3.5
2	E	76	GLY	3.5
2	E	142	LEU	3.5
2	D	217	ALA	3.4
2	E	144	GLY	3.4
2	E	74	ALA	3.4
2	D	139	LEU	3.4
2	E	301	GLN	3.3
2	D	77	GLY	3.3
2	D	198	ALA	3.3
2	E	168	LEU	3.3
2	D	200	ASP	3.3
2	E	77	GLY	3.2
1	A	224	THR	3.2
2	D	162	LEU	3.2
2	E	146	GLY	3.2
2	D	199	ASN	3.2
2	D	158	MET	3.1
1	B	224	THR	3.1
2	D	169	ALA	3.1
2	E	143	PRO	3.0
1	A	135	SER	3.0
2	D	195	ILE	3.0
1	B	234	LEU	3.0
1	B	218	SER	2.9
2	D	155	PRO	2.9
2	E	156	ALA	2.9
1	A	133	GLY	2.9
2	D	193	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	224	ARG	2.8
2	D	301	GLN	2.8
2	D	137	ASP	2.8
2	D	209	ALA	2.8
2	D	118	GLY	2.8
2	E	118	GLY	2.7
2	E	296	GLN	2.7
1	A	136	SER	2.7
2	D	74	ALA	2.7
2	D	211	ARG	2.7
2	E	141	GLN	2.6
2	D	219	LEU	2.6
2	D	151	ASP	2.6
1	A	129	THR	2.5
2	E	149	LEU	2.5
2	D	73	LEU	2.5
2	E	220	THR	2.5
2	D	170	ASP	2.4
2	D	189	ARG	2.4
1	A	110	ILE	2.4
1	B	14	VAL	2.4
1	B	1	ALA	2.4
2	D	154	ASP	2.3
2	E	292	ARG	2.3
2	E	218	GLN	2.3
1	A	186	ALA	2.3
2	E	171	ARG	2.3
2	D	165	ARG	2.3
2	D	157	ALA	2.3
2	D	192	LEU	2.2
2	D	183	ASP	2.2
2	D	222	ASP	2.2
2	D	223	GLU	2.2
1	A	14	VAL	2.2
2	E	158	MET	2.2
2	E	160	LEU	2.1
1	B	30	TRP	2.1
2	E	167	ALA	2.1
2	E	288	ALA	2.1
2	E	302	ASP	2.1
2	D	203	LEU	2.1
2	E	215	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	190	HIS	2.1
2	E	217	ALA	2.1
2	E	216	ASP	2.1
2	D	208	LYS	2.1
2	D	221	PRO	2.0
1	B	83	LEU	2.0
2	D	80	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSO	E	92	7/8	0.91	0.20	33,42,44,46	0
2	CSO	D	92	7/8	0.96	0.14	33,42,44,46	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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
4	IOD	D	905	1/1	0.96	0.08	57,57,57,57	0
4	IOD	B	906	1/1	0.96	0.08	66,66,66,66	0
4	IOD	B	904	1/1	0.97	0.10	50,50,50,50	0
4	IOD	E	901	1/1	0.98	0.06	30,30,30,30	0
4	IOD	E	908	1/1	0.98	0.05	49,49,49,49	0
3	CA	A	999	1/1	0.98	0.06	31,31,31,31	0
4	IOD	B	907	1/1	0.98	0.09	53,53,53,53	0
4	IOD	B	903	1/1	0.99	0.04	40,40,40,40	0
4	IOD	E	902	1/1	0.99	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CA	B	998	1/1	1.00	0.06	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.