



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 12:19 AM EDT

PDB ID : 4EHB  
Title : Crystal structure of the CFTR inhibitory factor Cif with the D129S mutation bound to epoxyhexane  
Authors : Hvorecny, K.L.; Bahl, C.D.; Madden, D.R.  
Deposited on : 2012-04-02  
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.

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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

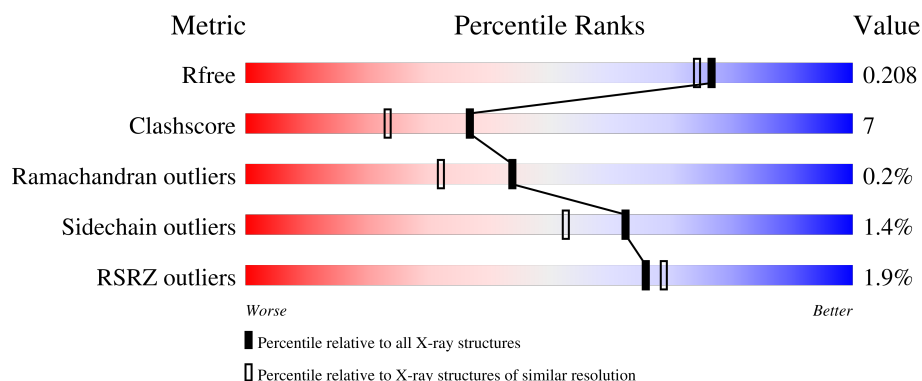
# 1 Overall quality at a glance

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))
$R_{free}$	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (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 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.

Mol	Chain	Length	Quality of chain
1	A	301	<div> <div>0%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	301	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
1	C	301	<div> <div>2%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	D	301	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10738 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 Putative hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	8	0
			2402	1545	412	434	11			
1	B	297	Total	C	N	O	S	0	2	0
			2383	1532	415	425	11			
1	C	297	Total	C	N	O	S	0	8	0
			2420	1557	420	432	11			
1	D	297	Total	C	N	O	S	0	11	0
			2446	1574	430	430	12			

There are 28 discrepancies between the modelled and reference sequences:

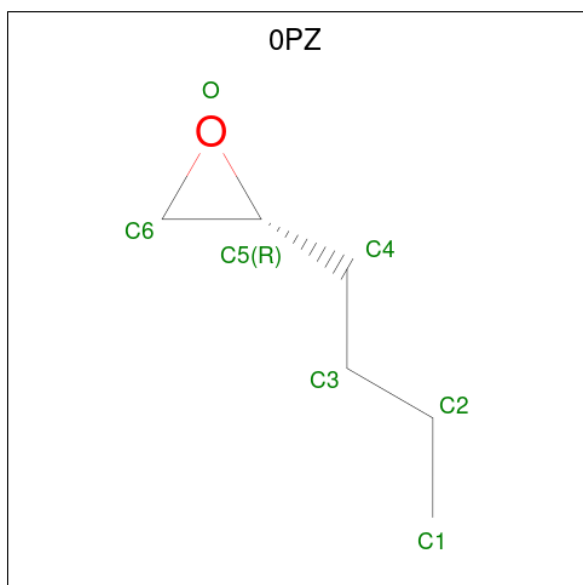
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	ASP	engineered mutation	UNP Q02P97
A	320	HIS	-	expression tag	UNP Q02P97
A	321	HIS	-	expression tag	UNP Q02P97
A	322	HIS	-	expression tag	UNP Q02P97
A	323	HIS	-	expression tag	UNP Q02P97
A	324	HIS	-	expression tag	UNP Q02P97
A	325	HIS	-	expression tag	UNP Q02P97
B	129	SER	ASP	engineered mutation	UNP Q02P97
B	320	HIS	-	expression tag	UNP Q02P97
B	321	HIS	-	expression tag	UNP Q02P97
B	322	HIS	-	expression tag	UNP Q02P97
B	323	HIS	-	expression tag	UNP Q02P97
B	324	HIS	-	expression tag	UNP Q02P97
B	325	HIS	-	expression tag	UNP Q02P97
C	129	SER	ASP	engineered mutation	UNP Q02P97
C	320	HIS	-	expression tag	UNP Q02P97
C	321	HIS	-	expression tag	UNP Q02P97
C	322	HIS	-	expression tag	UNP Q02P97
C	323	HIS	-	expression tag	UNP Q02P97
C	324	HIS	-	expression tag	UNP Q02P97
C	325	HIS	-	expression tag	UNP Q02P97

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Chain	Residue	Modelled	Actual	Comment	Reference
D	129	SER	ASP	engineered mutation	UNP Q02P97
D	320	HIS	-	expression tag	UNP Q02P97
D	321	HIS	-	expression tag	UNP Q02P97
D	322	HIS	-	expression tag	UNP Q02P97
D	323	HIS	-	expression tag	UNP Q02P97
D	324	HIS	-	expression tag	UNP Q02P97
D	325	HIS	-	expression tag	UNP Q02P97

- Molecule 2 is (2R)-2-butyloxirane (three-letter code: 0PZ) (formula: C<sub>6</sub>H<sub>12</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 6 1	0	0
2	B	1	Total C O 7 6 1	0	0
2	C	1	Total C O 7 6 1	0	0
2	D	1	Total C O 7 6 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	272	Total O 272 272	0	0
3	B	245	Total O 245 245	0	0

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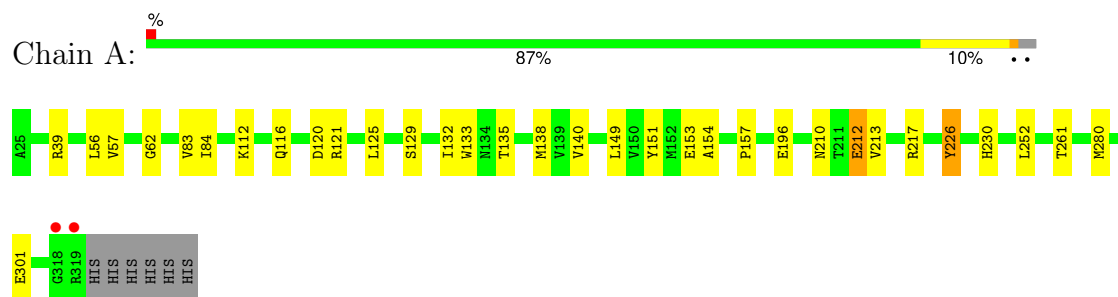
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	286	Total 286	O 286	0	0
3	D	256	Total 256	O 256	0	0

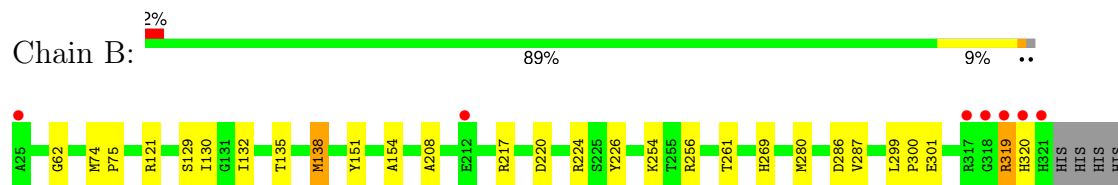
### 3 Residue-property plots

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.

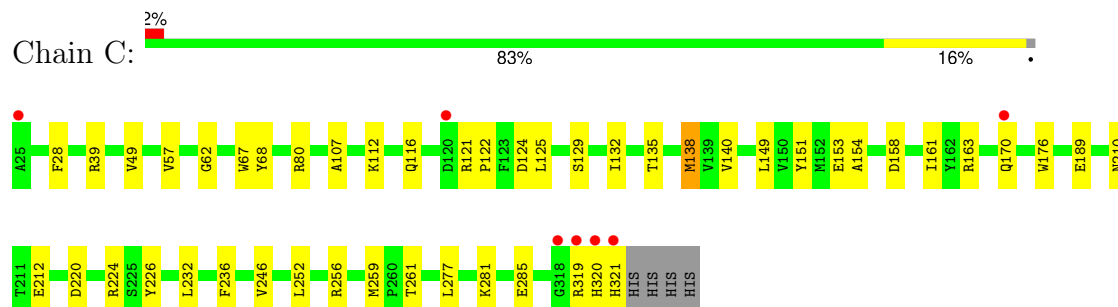
#### • Molecule 1: Putative hydrolase



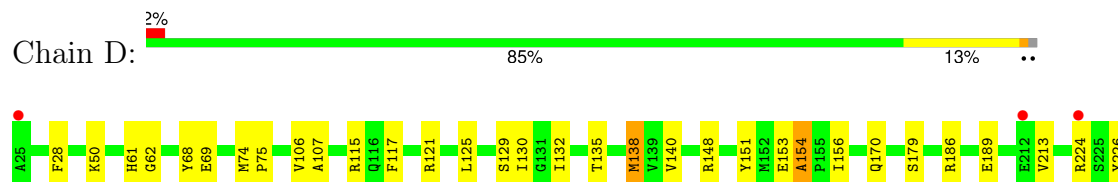
#### • Molecule 1: Putative hydrolase

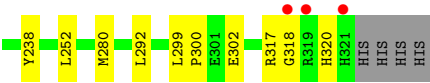


#### • Molecule 1: Putative hydrolase



#### • Molecule 1: Putative hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.43Å 83.92Å 88.74Å 90.00° 100.31° 90.00°	Depositor
Resolution (Å)	43.43 – 1.85 43.43 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.43-1.85) 96.9 (43.43-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 1.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.177 , 0.214 0.171 , 0.208	Depositor DCC
$R_{free}$ test set	4990 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: 0PZ

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	0.34	0/2491	0.51	0/3379
1	B	0.34	0/2462	0.51	0/3341
1	C	0.35	0/2517	0.51	0/3414
1	D	0.35	0/2546	0.51	0/3451
All	All	0.35	0/10016	0.51	0/13585

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	2402	0	2328	34	0
1	B	2383	0	2305	21	0
1	C	2420	0	2352	40	0
1	D	2446	0	2396	39	0
2	A	7	0	12	1	0
2	B	7	0	12	0	0
2	C	7	0	12	0	0
2	D	7	0	12	0	0
3	A	272	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	245	0	0	3	0
3	C	286	0	0	4	0
3	D	256	0	0	2	0
All	All	10738	0	9429	133	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 7.

All (133) 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:C:121[B]:ARG:HH11	1:C:122:PRO:HD2	1.37	0.89
1:C:121[B]:ARG:NH1	1:C:122:PRO:HD2	1.88	0.88
1:D:224[B]:ARG:HH21	1:D:224[B]:ARG:HG3	1.42	0.84
1:B:62:GLY:HA3	1:B:129:SER:HB3	1.61	0.83
1:A:62:GLY:HA3	1:A:129:SER:HB3	1.61	0.83
1:A:39:ARG:NE	1:A:116:GLN:HE22	1.81	0.77
1:C:62:GLY:HA3	1:C:129:SER:HB3	1.66	0.76
1:D:62:GLY:HA3	1:D:129:SER:HB3	1.68	0.75
1:A:210[B]:ASN:ND2	1:A:213:VAL:HG13	2.03	0.72
1:B:132:ILE:HD12	1:B:154:ALA:HB3	1.71	0.72
1:A:261[A]:THR:HG21	1:A:280:MET:CE	2.21	0.70
1:A:261[A]:THR:HG21	1:A:280:MET:HE3	1.74	0.70
1:A:210[B]:ASN:OD1	1:C:170[B]:GLN:HG2	1.94	0.67
1:A:210[B]:ASN:HD21	1:A:213:VAL:HG13	1.59	0.67
1:D:148[A]:ARG:NH2	1:D:317:ARG:HB2	2.11	0.66
1:C:121[B]:ARG:HH21	1:C:319:ARG:HH12	1.43	0.65
1:D:132[B]:ILE:CG2	1:D:156[B]:ILE:HD13	2.27	0.65
1:A:230:HIS:HE1	3:A:540:HOH:O	1.80	0.64
1:A:149:LEU:HB3	1:A:261[B]:THR:HG22	1.78	0.64
1:D:224[B]:ARG:HG3	1:D:224[B]:ARG:NH2	2.13	0.63
1:C:129:SER:HA	1:C:154:ALA:HB2	1.80	0.63
1:C:112:LYS:O	1:C:116:GLN:HG3	2.01	0.61
1:D:170:GLN:NE2	3:D:628:HOH:O	2.34	0.61
1:D:148[A]:ARG:HH22	1:D:317:ARG:HB2	1.68	0.59
2:A:401:OPZ:H1	3:A:544:HOH:O	2.03	0.59
1:A:132:ILE:HD12	1:A:154:ALA:HB3	1.84	0.59
1:C:39:ARG:NE	1:C:116:GLN:OE1	2.36	0.59
3:A:674:HOH:O	1:C:170[A]:GLN:HG2	2.02	0.57
1:C:132:ILE:HD12	1:C:154:ALA:HB3	1.86	0.57
1:A:129:SER:HA	1:A:154:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ARG:HD3	1:C:320:HIS:CD2	2.40	0.57
1:B:129:SER:HA	1:B:154:ALA:HB2	1.86	0.57
1:D:129:SER:HA	1:D:154:ALA:HB2	1.87	0.56
1:B:121[B]:ARG:NH2	1:B:319:ARG:HH11	2.04	0.56
1:D:148[A]:ARG:NH2	1:D:318:GLY:N	2.54	0.56
1:C:277:LEU:HG	1:C:281:LYS:HE3	1.88	0.55
1:A:210[B]:ASN:ND2	1:A:212[B]:GLU:OE1	2.40	0.55
1:B:151:TYR:HD2	1:B:280:MET:HE1	1.72	0.54
1:C:163[B]:ARG:HD3	3:C:704:HOH:O	2.08	0.54
1:C:121[B]:ARG:HH11	1:C:121[B]:ARG:HB3	1.73	0.52
1:B:220:ASP:O	1:B:224:ARG:HG3	2.10	0.52
1:C:220:ASP:O	1:C:224:ARG:HG3	2.09	0.52
1:A:210[B]:ASN:ND2	1:A:212[B]:GLU:CD	2.62	0.52
1:D:148[A]:ARG:HH22	1:D:318:GLY:N	2.08	0.52
1:C:189[A]:GLU:HG3	1:C:236:PHE:HD2	1.74	0.52
1:C:158:ASP:O	1:C:161:ILE:HG12	2.10	0.52
1:C:256:ARG:HD3	1:C:285:GLU:OE2	2.10	0.51
1:C:121[B]:ARG:HH21	1:C:319:ARG:NH1	2.08	0.51
1:D:151:TYR:CD2	1:D:280:MET:HE3	2.46	0.51
1:D:318:GLY:O	1:D:320:HIS:HD2	1.93	0.51
1:D:186[B]:ARG:HD2	1:D:189:GLU:CD	2.32	0.50
1:C:210[B]:ASN:OD1	1:C:212[B]:GLU:CD	2.49	0.50
1:A:261[A]:THR:HG21	1:A:280:MET:HE2	1.93	0.50
1:C:125:LEU:HD21	1:C:135:THR:HB	1.94	0.50
1:D:186[B]:ARG:HD2	1:D:189:GLU:OE2	2.12	0.49
1:A:56:LEU:HD11	1:A:84[A]:ILE:HG12	1.94	0.49
1:C:259:MET:O	1:C:261:THR:HG23	2.13	0.49
1:D:151:TYR:HD2	1:D:280:MET:HE3	1.78	0.49
1:B:151:TYR:CD2	1:B:280:MET:HE1	2.48	0.49
1:B:121[B]:ARG:NH1	1:B:319:ARG:HE	2.11	0.48
1:D:148[A]:ARG:HH22	1:D:317:ARG:CA	2.26	0.48
1:A:140:VAL:HG11	1:A:252:LEU:HB3	1.95	0.48
1:B:299:LEU:HB2	1:B:300:PRO:HD3	1.96	0.47
1:A:133:TRP:CD1	1:A:157:PRO:HD3	2.49	0.47
1:D:153:GLU:O	1:D:154:ALA:HB2	2.13	0.47
1:B:280:MET:HE2	3:B:637:HOH:O	2.14	0.47
1:D:148[A]:ARG:HH12	1:D:317:ARG:C	2.17	0.47
1:D:299:LEU:HB2	1:D:300:PRO:HD3	1.96	0.47
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.79	0.47
1:C:189[A]:GLU:HG3	1:C:236:PHE:CD2	2.50	0.47
1:A:153:GLU:O	1:A:154:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148[A]:ARG:NH2	1:D:318:GLY:H	2.13	0.47
1:C:189[B]:GLU:HG3	1:C:232:LEU:HD23	1.97	0.46
1:C:121[B]:ARG:NH1	3:C:702:HOH:O	2.49	0.46
1:D:148[A]:ARG:HH22	1:D:317:ARG:CB	2.29	0.46
1:A:39:ARG:CG	1:A:116:GLN:HE22	2.28	0.46
1:C:39:ARG:NH2	3:C:741:HOH:O	2.43	0.46
1:C:170[B]:GLN:NE2	3:C:610:HOH:O	2.49	0.45
1:D:148[A]:ARG:CZ	1:D:317:ARG:HB2	2.46	0.45
1:B:261[B]:THR:HG22	1:B:286:ASP:O	2.16	0.45
1:D:224[B]:ARG:NH2	1:D:224[B]:ARG:CG	2.79	0.45
1:A:196:GLU:HB3	1:A:226:TYR:CE2	2.51	0.44
1:C:140:VAL:HG11	1:C:252:LEU:HB3	1.98	0.44
1:C:57:VAL:HG22	1:C:124:ASP:HB2	1.99	0.44
1:D:107:ALA:HB1	1:D:138:MET:HB3	2.00	0.44
1:C:49:VAL:HG21	1:C:67:TRP:CE2	2.52	0.44
1:C:153:GLU:O	1:C:154:ALA:HB2	2.17	0.44
1:B:254:LYS:NZ	3:B:726:HOH:O	2.50	0.44
1:A:125:LEU:HD21	1:A:135:THR:HB	1.99	0.44
1:B:220:ASP:HB3	1:B:224:ARG:NH2	2.32	0.44
1:D:106:VAL:HG21	1:D:238:TYR:HE1	1.83	0.44
1:C:28:PHE:HB3	1:C:68:TYR:CD1	2.53	0.43
1:C:176:TRP:CD1	1:D:179:SER:HB3	2.53	0.43
1:D:121:ARG:HD2	3:D:711:HOH:O	2.19	0.43
1:A:57:VAL:CG1	1:A:83:VAL:HG22	2.49	0.43
1:D:50:LYS:HE3	1:D:117:PHE:CD1	2.53	0.43
1:D:140:VAL:HG11	1:D:252:LEU:HB3	2.00	0.43
1:B:129:SER:OG	1:B:130:ILE:N	2.52	0.43
1:C:121[B]:ARG:NH2	1:C:319:ARG:NH1	2.66	0.43
1:A:39:ARG:CZ	1:A:116:GLN:NE2	2.82	0.43
1:A:112:LYS:O	1:A:116:GLN:HG3	2.18	0.43
1:D:28:PHE:HB3	1:D:68:TYR:CD1	2.53	0.43
1:A:39:ARG:HG2	1:A:116:GLN:NE2	2.34	0.42
1:C:158:ASP:HA	1:C:246:VAL:HG13	2.00	0.42
1:D:213:VAL:HG21	1:D:302:GLU:HA	2.00	0.42
1:A:217:ARG:HD2	3:A:732:HOH:O	2.18	0.42
1:A:149:LEU:HD11	1:A:151:TYR:CE1	2.55	0.42
1:C:107:ALA:HB1	1:C:138:MET:HB3	2.01	0.42
1:D:292:LEU:HD12	1:D:292:LEU:N	2.35	0.42
1:B:74:MET:HB2	1:B:75:PRO:HD3	2.02	0.42
1:B:261[B]:THR:HG23	1:B:287:VAL:HB	2.02	0.42
1:A:39:ARG:NE	1:A:116:GLN:NE2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163[B]:ARG:HA	1:C:163[B]:ARG:HD2	1.78	0.42
1:B:261[B]:THR:HG23	1:B:287:VAL:CB	2.49	0.41
1:D:115:ARG:HA	1:D:115:ARG:HD2	1.75	0.41
1:D:186[B]:ARG:HD3	1:D:186[B]:ARG:HA	1.42	0.41
1:C:149:LEU:HB3	1:C:261:THR:HG22	2.02	0.41
1:D:125:LEU:HD21	1:D:135:THR:HB	2.02	0.41
1:A:39:ARG:CZ	1:A:116:GLN:HE22	2.34	0.41
1:A:120:ASP:O	1:A:121:ARG:HG3	2.20	0.41
1:B:135:THR:O	1:B:138:MET:HG3	2.21	0.41
1:B:280:MET:CE	3:B:637:HOH:O	2.70	0.40
1:C:135:THR:O	1:C:138:MET:HG3	2.20	0.40
1:B:208:ALA:O	1:B:269:HIS:HD2	2.04	0.40
1:D:61:HIS:HB2	1:D:69:GLU:OE1	2.22	0.40
1:D:129:SER:OG	1:D:130:ILE:N	2.52	0.40
1:D:135:THR:O	1:D:138:MET:HG3	2.21	0.40
1:C:149:LEU:HD11	1:C:151:TYR:CE1	2.56	0.40
1:D:74:MET:HB2	1:D:75:PRO:HD3	2.03	0.40

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	301/301 (100%)	294 (98%)	7 (2%)	0	100	100
1	B	297/301 (99%)	289 (97%)	7 (2%)	1 (0%)	37	25
1	C	303/301 (101%)	296 (98%)	7 (2%)	0	100	100
1	D	306/301 (102%)	299 (98%)	6 (2%)	1 (0%)	37	25
All	All	1207/1204 (100%)	1178 (98%)	27 (2%)	2 (0%)	44	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	320	HIS
1	D	154	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/248 (101%)	245 (98%)	5 (2%)	50	37
1	B	246/248 (99%)	241 (98%)	5 (2%)	50	37
1	C	252/248 (102%)	249 (99%)	3 (1%)	67	59
1	D	255/248 (103%)	253 (99%)	2 (1%)	79	74
All	All	1003/992 (101%)	988 (98%)	15 (2%)	62	50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	MET
1	A	212[A]	GLU
1	A	212[B]	GLU
1	A	226	TYR
1	A	301	GLU
1	B	138	MET
1	B	226	TYR
1	B	256	ARG
1	B	301	GLU
1	B	319	ARG
1	C	138	MET
1	C	226	TYR
1	C	321	HIS
1	D	138	MET
1	D	226	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	170	GLN
1	A	230	HIS
1	A	308	ASN
1	B	71	HIS
1	B	269	HIS
1	B	321	HIS
1	C	320	HIS
1	D	170	GLN
1	D	243	ASN
1	D	320	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands 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	0PZ	C	401	-	7,7,7	0.40	0	6,8,8	0.68	0
2	0PZ	A	401	-	7,7,7	0.47	0	6,8,8	0.38	0
2	0PZ	D	401	-	7,7,7	0.46	0	6,8,8	0.53	0
2	0PZ	B	401	-	7,7,7	0.41	0	6,8,8	0.54	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
2	0PZ	C	401	-	-	3/4/6/6	0/1/1/1
2	0PZ	A	401	-	-	2/4/6/6	0/1/1/1
2	0PZ	D	401	-	-	3/4/6/6	0/1/1/1
2	0PZ	B	401	-	-	2/4/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	0PZ	C3-C4-C5-O
2	A	401	0PZ	C3-C4-C5-C6
2	B	401	0PZ	C3-C4-C5-O
2	C	401	0PZ	C3-C4-C5-C6
2	D	401	0PZ	C3-C4-C5-O
2	C	401	0PZ	C3-C4-C5-O
2	B	401	0PZ	C1-C2-C3-C4
2	D	401	0PZ	C2-C3-C4-C5
2	C	401	0PZ	C2-C3-C4-C5
2	D	401	0PZ	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	0PZ	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

### 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	295/301 (98%)	-0.47	2 (0%) 84 86	7, 14, 30, 84	9 (3%)
1	B	297/301 (98%)	-0.22	7 (2%) 59 62	7, 15, 38, 126	3 (1%)
1	C	297/301 (98%)	-0.36	7 (2%) 59 62	7, 14, 31, 78	11 (3%)
1	D	297/301 (98%)	-0.35	6 (2%) 64 68	4, 14, 31, 85	12 (4%)
All	All	1186/1204 (98%)	-0.35	22 (1%) 66 69	4, 14, 33, 126	35 (2%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	GLY	5.7
1	B	319	ARG	5.3
1	B	321	HIS	5.1
1	B	25	ALA	4.5
1	C	320	HIS	4.3
1	A	319	ARG	4.1
1	C	319	ARG	4.0
1	D	318	GLY	4.0
1	B	320	HIS	3.9
1	C	25	ALA	3.8
1	C	321	HIS	3.8
1	D	321	HIS	3.7
1	D	319	ARG	3.7
1	A	318	GLY	3.5
1	B	317	ARG	3.1
1	D	25	ALA	3.0
1	D	212	GLU	2.7
1	B	212	GLU	2.6
1	C	318	GLY	2.6
1	C	170[A]	GLN	2.4
1	C	120	ASP	2.1
1	D	224[A]	ARG	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( $\text{\AA}^2$ )	Q<0.9
2	0PZ	C	401	7/7	0.73	0.21	17,34,36,37	0
2	0PZ	D	401	7/7	0.73	0.22	31,35,43,44	0
2	0PZ	A	401	7/7	0.81	0.19	20,30,38,38	0
2	0PZ	B	401	7/7	0.81	0.18	16,30,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.