



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3QZ5  
Title : Crystal Structure of Co-type Nitrile Hydratase alpha-E168Q from *Pseudomonas putida*.  
Authors : Brodtkin, H.R.; Novak, W.R.P.; Ringe, D.; Petsko, G.A.  
Deposited on : 2011-03-04  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

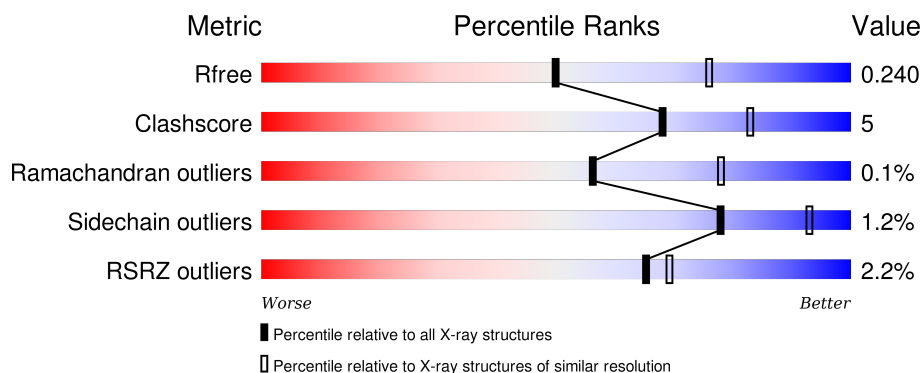
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	211	<div> <div></div> <div>85%10%5%</div> </div>
1	C	211	<div> <div>5%</div> <div>82%12%5%</div> </div>
1	E	211	<div> <div></div> <div>86%9%5%</div> </div>
1	G	211	<div> <div>3%</div> <div>82%13%5%</div> </div>
2	B	219	<div> <div>2%</div> <div>86%13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	219	 5% 85% 14%
2	F	219	 % 89% 11%
2	H	219	 % 87% 13%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13490 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 Co-type Nitrile Hydratase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1547	985	265	289	8			
1	C	201	Total	C	N	O	S	0	0	0
			1543	983	265	287	8			
1	E	200	Total	C	N	O	S	0	0	0
			1523	973	258	284	8			
1	G	200	Total	C	N	O	S	0	0	0
			1526	973	261	284	8			

- Molecule 2 is a protein called Co-type Nitrile Hydratase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	2	0
			1720	1087	307	322	4			
2	D	219	Total	C	N	O	S	0	3	0
			1727	1092	308	323	4			
2	F	219	Total	C	N	O	S	0	2	0
			1719	1087	307	321	4			
2	H	219	Total	C	N	O	S	0	2	0
			1711	1083	303	321	4			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Co	0	0
			1	1		
4	A	1	Total	Co	0	0
			1	1		
4	C	1	Total	Co	0	0
			1	1		
4	E	1	Total	Co	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		

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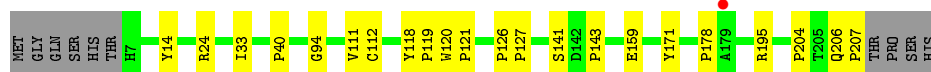
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	60	Total 60	O 60	0	0
5	C	31	Total 31	O 31	0	0
5	D	61	Total 61	O 61	0	0
5	E	52	Total 52	O 52	0	0
5	F	64	Total 64	O 64	0	0
5	G	49	Total 49	O 49	0	0
5	H	64	Total 64	O 64	0	0

### 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 errors 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.

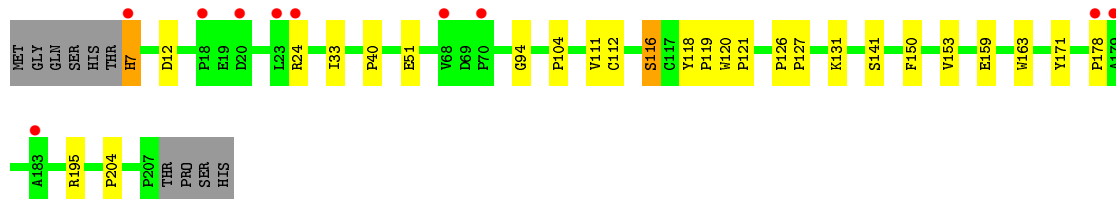
- Molecule 1: Co-type Nitrile Hydratase alpha subunit

Chain A:



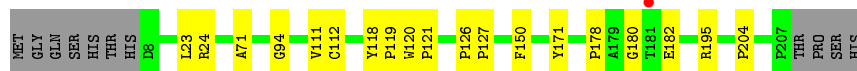
- Molecule 1: Co-type Nitrile Hydratase alpha subunit

Chain C:



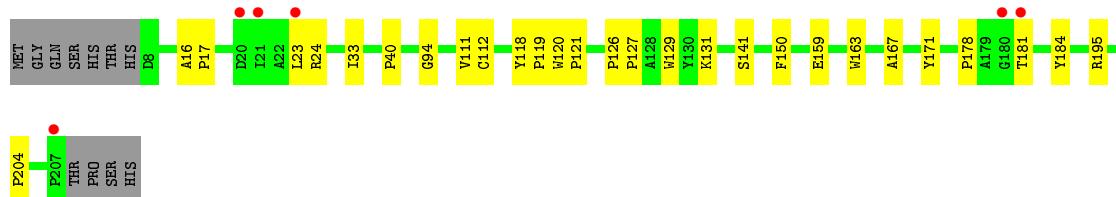
- Molecule 1: Co-type Nitrile Hydratase alpha subunit

Chain E:



- Molecule 1: Co-type Nitrile Hydratase alpha subunit

Chain G:

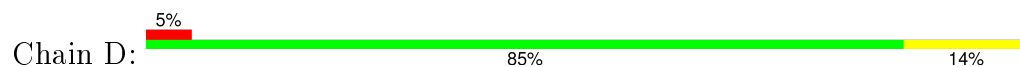


- Molecule 2: Co-type Nitrile Hydratase beta subunit

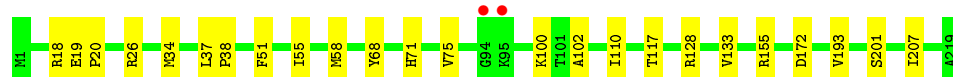
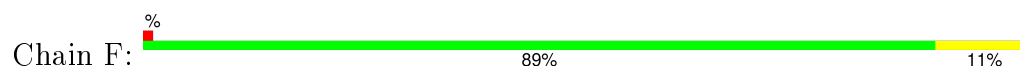
Chain B:



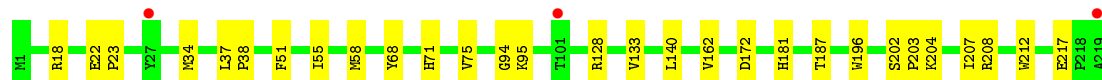
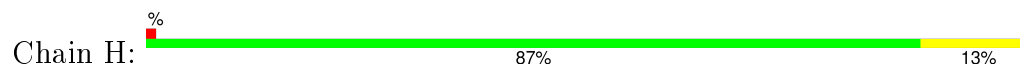
- Molecule 2: Co-type Nitrile Hydratase beta subunit



- Molecule 2: Co-type Nitrile Hydratase beta subunit



- Molecule 2: Co-type Nitrile Hydratase beta subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.53Å 137.97Å 85.32Å 90.00° 91.97° 90.00°	Depositor
Resolution (Å)	45.40 – 2.50 45.41 – 2.47	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.40-2.50) 96.8 (45.41-2.47)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.208 , 0.249 0.197 , 0.240	Depositor DCC
$R_{free}$ test set	3316 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.8	EDS
Estimated twinning fraction	0.016 for l,k,-h 0.036 for h,-k,-l 0.100 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 65897 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, 3CO, CSD

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	0.21	0/1572	0.45	2/2150 (0.1%)
1	C	0.24	0/1568	0.66	3/2145 (0.1%)
1	E	0.25	0/1547	0.45	1/2118 (0.0%)
1	G	0.21	0/1550	0.45	1/2122 (0.0%)
2	B	0.27	0/1768	0.75	5/2408 (0.2%)
2	D	0.27	0/1775	0.68	5/2418 (0.2%)
2	F	0.26	0/1767	0.53	4/2408 (0.2%)
2	H	0.26	0/1759	0.47	2/2397 (0.1%)
All	All	0.25	0/13306	0.57	23/18166 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	ARG	NE-CZ-NH1	-18.77	110.92	120.30
2	B	128	ARG	NE-CZ-NH2	18.32	129.46	120.30
1	C	24	ARG	NE-CZ-NH2	-16.15	112.23	120.30
1	C	24	ARG	NE-CZ-NH1	15.50	128.05	120.30
2	D	26	ARG	NE-CZ-NH1	-15.35	112.63	120.30
2	D	26	ARG	NE-CZ-NH2	14.88	127.74	120.30
2	B	128	ARG	CD-NE-CZ	9.14	136.40	123.60
2	F	26	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	B	26	ARG	NE-CZ-NH2	-7.85	116.37	120.30
2	F	26	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	B	26	ARG	NE-CZ-NH1	7.26	123.93	120.30
2	D	26	ARG	CD-NE-CZ	7.26	133.76	123.60
1	C	24	ARG	CD-NE-CZ	7.25	133.76	123.60
2	F	128	ARG	NE-CZ-NH2	-6.49	117.05	120.30
2	D	128	ARG	NE-CZ-NH2	-6.48	117.06	120.30
2	H	128	ARG	NE-CZ-NH2	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	128	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	H	128	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	D	128	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	24	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	G	24	ARG	NE-CZ-NH1	-5.49	117.55	120.30
1	E	24	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	24	ARG	NE-CZ-NH2	5.03	122.82	120.30

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	1547	0	1525	14	0
1	C	1543	0	1522	22	0
1	E	1523	0	1496	12	0
1	G	1526	0	1501	21	0
2	B	1720	0	1660	19	0
2	D	1727	0	1668	23	0
2	F	1719	0	1660	14	0
2	H	1711	0	1645	22	0
3	A	6	0	8	0	0
3	C	6	0	8	1	0
3	E	6	0	8	0	0
3	G	6	0	8	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	65	0	0	2	0
5	B	60	0	0	1	0
5	C	31	0	0	1	0
5	D	61	0	0	2	0
5	E	52	0	0	0	0
5	F	64	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	49	0	0	0	0
5	H	64	0	0	2	0
All	All	13490	0	12709	121	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 5.

All (121) 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)
2:B:113:GLY:HA3	2:F:110:ILE:HG22	1.68	0.76
2:F:100:LYS:HE3	2:F:102:ALA:O	1.89	0.72
2:H:37:LEU:HB3	2:H:38:PRO:HD3	1.83	0.60
2:F:37:LEU:HB3	2:F:38:PRO:HD3	1.83	0.59
3:C:212:GOL:H32	2:D:66:GLY:O	2.01	0.59
1:C:159:GLU:HG3	2:D:204:LYS:O	2.03	0.58
1:E:180:GLY:HA2	1:E:182:GLU:OE2	2.04	0.58
2:B:37:LEU:HB3	2:B:38:PRO:HD3	1.85	0.57
1:E:150:PHE:CZ	2:F:18:ARG:HD2	2.39	0.57
2:D:37:LEU:HB3	2:D:38:PRO:HD3	1.85	0.57
1:G:129:TRP:CD1	2:H:18:ARG:HG2	2.41	0.56
1:A:119:PRO:HG3	1:A:171:TYR:O	2.06	0.56
1:E:127:PRO:HG3	1:E:195:ARG:CZ	2.36	0.56
1:C:116:SER:HB2	1:C:131:LYS:HG2	1.88	0.56
1:C:119:PRO:HG3	1:C:171:TYR:O	2.06	0.55
1:A:127:PRO:HG3	1:A:195:ARG:CZ	2.36	0.55
1:G:94:GLY:HA3	1:G:121:PRO:HG2	1.89	0.55
2:D:89:THR:O	2:D:93:THR:HG23	2.06	0.55
1:C:127:PRO:HG3	1:C:195:ARG:CZ	2.37	0.55
1:C:94:GLY:HA3	1:C:121:PRO:HG2	1.89	0.54
1:A:94:GLY:HA3	1:A:121:PRO:HG2	1.88	0.54
1:G:127:PRO:HG3	1:G:195:ARG:CZ	2.36	0.54
1:G:119:PRO:HG3	1:G:171:TYR:O	2.06	0.54
1:E:94:GLY:HA3	1:E:121:PRO:HG2	1.88	0.54
1:E:119:PRO:HG3	1:E:171:TYR:O	2.07	0.54
1:G:159:GLU:HG3	2:H:204:LYS:O	2.09	0.53
1:C:178:PRO:HG3	1:C:204:PRO:HB2	1.92	0.52
1:E:178:PRO:HG3	1:E:204:PRO:HB2	1.92	0.52
2:H:94:GLY:O	2:H:95:LYS:HD2	2.10	0.52
2:D:98:SER:O	2:D:101:THR:HG23	2.10	0.51
1:A:111:VAL:HG22	1:A:112:CYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HD2	2:D:68:TYR:CD1	2.46	0.50
2:D:52:ARG:HD2	5:D:359:HOH:O	2.11	0.50
2:H:181:HIS:HB3	5:H:228:HOH:O	2.12	0.50
1:G:131:LYS:HD2	2:H:68:TYR:CD1	2.46	0.50
1:C:111:VAL:HG22	1:C:112:CYS:N	2.27	0.50
1:A:178:PRO:HG3	1:A:204:PRO:HB2	1.92	0.50
1:G:178:PRO:HG3	1:G:204:PRO:HB2	1.93	0.50
1:G:129:TRP:CG	2:H:18:ARG:HG2	2.46	0.50
2:F:55:ILE:O	2:F:58:MET:HG2	2.12	0.50
1:G:111:VAL:HG22	1:G:112:CYS:N	2.27	0.50
2:D:55:ILE:O	2:D:58:MET:HG2	2.12	0.49
2:B:55:ILE:O	2:B:58:MET:HG2	2.13	0.49
1:A:159:GLU:HG3	2:B:204:LYS:O	2.13	0.49
1:C:104:PRO:HG2	1:G:184:TYR:CE1	2.47	0.48
2:H:55:ILE:O	2:H:58:MET:HG2	2.13	0.48
1:E:111:VAL:HG22	1:E:112:CYS:N	2.27	0.48
2:D:68:TYR:O	2:D:71:HIS:HB2	2.14	0.48
1:E:120:TRP:HB2	1:E:121:PRO:HD3	1.96	0.47
2:B:68:TYR:O	2:B:71:HIS:HB2	2.14	0.47
1:C:120:TRP:HB2	1:C:121:PRO:HD3	1.96	0.47
1:A:120:TRP:HB2	1:A:121:PRO:HD3	1.96	0.47
2:B:98:SER:HB2	5:B:300:HOH:O	2.14	0.47
2:F:68:TYR:O	2:F:71:HIS:HB2	2.14	0.47
1:C:118:TYR:CG	1:C:126:PRO:HG3	2.50	0.47
1:A:141:SER:HA	2:B:196:TRP:NE1	2.30	0.47
1:G:163:TRP:CZ2	2:H:208:ARG:HD3	2.50	0.46
1:G:118:TYR:CG	1:G:126:PRO:HG3	2.50	0.46
2:H:68:TYR:O	2:H:71:HIS:HB2	2.15	0.46
2:D:51:PHE:CD2	2:D:75:VAL:HG11	2.50	0.46
1:G:167:ALA:HA	2:H:212:TRP:HH2	1.79	0.46
2:H:51:PHE:CD2	2:H:75:VAL:HG11	2.50	0.46
2:B:51:PHE:CD2	2:B:75:VAL:HG11	2.50	0.46
1:A:118:TYR:CG	1:A:126:PRO:HG3	2.50	0.46
1:E:118:TYR:CG	1:E:126:PRO:HG3	2.51	0.46
2:B:22:GLU:HA	2:B:23:PRO:HD3	1.84	0.45
1:G:120:TRP:HB2	1:G:121:PRO:HD3	1.97	0.45
2:F:51:PHE:CD2	2:F:75:VAL:HG11	2.50	0.45
1:G:181:THR:HA	1:G:184:TYR:CD1	2.52	0.45
1:A:206:GLN:HA	1:A:207:PRO:HD3	1.84	0.45
2:D:207:ILE:HD12	2:D:207:ILE:N	2.32	0.45
2:H:207:ILE:HD12	2:H:207:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ALA:HA	1:G:17:PRO:HD3	1.91	0.44
1:G:150:PHE:CE2	2:H:18:ARG:HD3	2.53	0.44
2:B:55:ILE:HG13	2:B:75:VAL:CG2	2.48	0.44
1:A:14:TYR:CE2	2:B:19:GLU:HB2	2.52	0.44
2:F:19:GLU:HA	2:F:20:PRO:HD3	1.82	0.43
2:B:207:ILE:HD12	2:B:207:ILE:N	2.33	0.43
2:F:207:ILE:N	2:F:207:ILE:HD12	2.34	0.43
2:H:55:ILE:HG13	2:H:75:VAL:CG2	2.49	0.43
2:H:22:GLU:HA	2:H:23:PRO:HD3	1.85	0.43
2:D:55:ILE:HG13	2:D:75:VAL:CG2	2.49	0.43
1:C:118:TYR:CD2	1:C:126:PRO:HG3	2.54	0.43
2:H:202:SER:HA	2:H:203:PRO:HD3	1.89	0.43
1:C:7:HIS:NE2	1:E:71:ALA:HA	2.34	0.43
2:F:55:ILE:HG13	2:F:75:VAL:CG2	2.49	0.42
1:A:118:TYR:CD2	1:A:126:PRO:HG3	2.54	0.42
2:F:155:ARG:NH2	5:F:233:HOH:O	2.52	0.42
1:C:163:TRP:CZ2	2:D:208:ARG:HD3	2.54	0.42
1:G:118:TYR:CD2	1:G:126:PRO:HG3	2.54	0.42
1:E:118:TYR:CD2	1:E:126:PRO:HG3	2.54	0.42
5:A:251:HOH:O	2:B:26:ARG:NH1	2.52	0.42
2:B:109:ALA:HB2	2:F:117:THR:HG21	2.02	0.42
2:H:58:MET:HB2	5:H:246:HOH:O	2.19	0.41
1:C:141:SER:HA	2:D:196:TRP:NE1	2.35	0.41
2:D:37:LEU:HD12	2:D:72:TRP:CH2	2.56	0.41
1:G:131:LYS:HD2	2:H:68:TYR:CG	2.56	0.41
1:A:33:ILE:CD1	1:A:40:PRO:HG3	2.51	0.41
1:C:12:ASP:HB2	5:D:225:HOH:O	2.20	0.41
1:C:33:ILE:CD1	1:C:40:PRO:HG3	2.51	0.41
1:G:33:ILE:CD1	1:G:40:PRO:HG3	2.51	0.41
2:B:37:LEU:HD22	2:B:41:LEU:HG	2.03	0.41
2:B:37:LEU:HD12	2:B:72:TRP:CH2	2.56	0.41
1:C:131:LYS:HD2	2:D:68:TYR:CE1	2.56	0.41
1:C:131:LYS:HD2	2:D:68:TYR:CG	2.55	0.41
1:G:141:SER:HA	2:H:196:TRP:NE1	2.35	0.41
2:B:193:VAL:HG22	2:B:201:SER:OG	2.21	0.41
2:F:193:VAL:HG22	2:F:201:SER:OG	2.21	0.41
1:E:150:PHE:CE2	2:F:18:ARG:HD2	2.56	0.41
2:D:19:GLU:HA	2:D:20:PRO:HD3	1.83	0.41
1:C:51:GLU:OE2	2:D:31:LYS:HE2	2.21	0.41
2:H:140:LEU:HD21	2:H:217:GLU:HB3	2.03	0.40
2:B:140:LEU:HD21	2:B:217:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:VAL:HG23	2:B:163:ILE:HG13	2.04	0.40
1:C:153:VAL:HA	5:C:222:HOH:O	2.20	0.40
1:C:150:PHE:HZ	2:D:16:VAL:HG11	1.85	0.40
2:D:162:VAL:HG22	2:D:187:THR:O	2.21	0.40
1:A:143:PRO:HD2	5:A:224:HOH:O	2.20	0.40
2:D:140:LEU:HD21	2:D:217:GLU:HB3	2.03	0.40
2:D:37:LEU:HD22	2:D:41:LEU:HG	2.03	0.40
2:H:162:VAL:HG22	2:H:187:THR:O	2.22	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	197/211 (93%)	189 (96%)	8 (4%)	0	100	100
1	C	197/211 (93%)	190 (96%)	6 (3%)	1 (0%)	34	55
1	E	196/211 (93%)	188 (96%)	8 (4%)	0	100	100
1	G	196/211 (93%)	187 (95%)	9 (5%)	0	100	100
2	B	219/219 (100%)	214 (98%)	5 (2%)	0	100	100
2	D	220/219 (100%)	214 (97%)	6 (3%)	0	100	100
2	F	219/219 (100%)	217 (99%)	2 (1%)	0	100	100
2	H	219/219 (100%)	215 (98%)	4 (2%)	0	100	100
All	All	1663/1720 (97%)	1614 (97%)	48 (3%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	SER

### 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	160/170 (94%)	160 (100%)	0	100	100
1	C	159/170 (94%)	158 (99%)	1 (1%)	90	97
1	E	155/170 (91%)	154 (99%)	1 (1%)	90	97
1	G	156/170 (92%)	155 (99%)	1 (1%)	90	97
2	B	179/177 (101%)	175 (98%)	4 (2%)	60	84
2	D	180/177 (102%)	177 (98%)	3 (2%)	68	89
2	F	179/177 (101%)	176 (98%)	3 (2%)	68	89
2	H	177/177 (100%)	174 (98%)	3 (2%)	68	89
All	All	1345/1388 (97%)	1329 (99%)	16 (1%)	78	93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	34	MET
2	B	37	LEU
2	B	133	VAL
2	B	172	ASP
1	C	7	HIS
2	D	34	MET
2	D	37	LEU
2	D	172	ASP
1	E	23	LEU
2	F	34	MET
2	F	133	VAL
2	F	172	ASP
1	G	23	LEU
2	H	34	MET
2	H	133	VAL
2	H	172	ASP

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



Mol	Chain	Res	Type
2	B	21	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z  > 2$
1	CSD	A	115	1,4	3,7,8	1.04	0	3,8,10	1.74	1 (33%)
1	CSD	A	117	1,4	3,7,8	0.99	0	3,8,10	1.50	0
1	CSD	C	115	1,4	3,7,8	0.98	0	3,8,10	1.75	1 (33%)
1	CSD	C	117	1,4	3,7,8	0.99	0	3,8,10	1.33	0
1	CSD	E	115	1,4	3,7,8	1.02	0	3,8,10	1.61	1 (33%)
1	CSD	E	117	1,4	3,7,8	1.04	0	3,8,10	1.24	0
1	CSD	G	115	1,4	3,7,8	1.01	0	3,8,10	1.80	1 (33%)
1	CSD	G	117	1,4	3,7,8	0.97	0	3,8,10	1.24	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
1	CSD	A	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	A	117	1,4	-	1/2/6/8	0/0/0/0
1	CSD	C	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	C	117	1,4	-	1/2/6/8	0/0/0/0
1	CSD	E	115	1,4	-	1/2/6/8	0/0/0/0
1	CSD	E	117	1,4	-	1/2/6/8	0/0/0/0
1	CSD	G	115	1,4	-	0/2/6/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	G	117	1,4	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	CSD	O-C-CA	-2.52	118.92	125.49
1	G	115	CSD	O-C-CA	-2.47	119.05	125.49
1	A	115	CSD	O-C-CA	-2.47	119.05	125.49
1	C	115	CSD	O-C-CA	-2.43	119.15	125.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	115	CSD	CA-CB-SG-OD1
1	E	115	CSD	CA-CB-SG-OD1
1	A	117	CSD	CA-CB-SG-OD1
1	A	115	CSD	CA-CB-SG-OD1
1	E	117	CSD	CA-CB-SG-OD1
1	C	117	CSD	CA-CB-SG-OD1
1	G	117	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	GOL	A	212	-	5,5,5	0.34	0	5,5,5	0.25	0
3	GOL	C	212	-	5,5,5	0.34	0	5,5,5	0.27	0
3	GOL	E	212	-	5,5,5	0.37	0	5,5,5	0.43	0
3	GOL	G	212	-	5,5,5	0.41	0	5,5,5	0.14	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	GOL	A	212	-	-	0/4/4/4	0/0/0/0
3	GOL	C	212	-	-	0/4/4/4	0/0/0/0
3	GOL	E	212	-	-	0/4/4/4	0/0/0/0
3	GOL	G	212	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	212	GOL	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	199/211 (94%)	0.05	1 (0%) 91 92	9, 23, 44, 66	0
1	C	199/211 (94%)	0.26	10 (5%) 32 37	13, 27, 52, 71	0
1	E	198/211 (93%)	-0.03	1 (0%) 91 92	10, 23, 41, 60	1 (0%)
1	G	198/211 (93%)	0.12	6 (3%) 54 59	14, 26, 47, 64	0
2	B	219/219 (100%)	0.11	4 (1%) 71 75	11, 23, 53, 70	1 (0%)
2	D	219/219 (100%)	0.15	10 (4%) 36 41	14, 26, 57, 72	0
2	F	219/219 (100%)	0.09	2 (0%) 85 88	10, 23, 49, 71	0
2	H	219/219 (100%)	0.14	3 (1%) 78 80	13, 26, 53, 70	0
All	All	1670/1720 (97%)	0.11	37 (2%) 65 69	9, 25, 50, 72	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	4.3
2	D	98	SER	3.9
1	C	183	ALA	3.2
1	G	181	THR	3.2
1	C	24	ARG	3.1
1	G	180	GLY	3.1
2	D	92	ALA	3.0
1	C	7	HIS	3.0
2	D	124	GLU	2.9
2	D	129	ALA	2.8
2	D	93	THR	2.8
2	B	203	PRO	2.8
2	F	95	LYS	2.7
1	A	179	ALA	2.6
2	H	219	ALA	2.6
2	F	94	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	27	TYR	2.6
1	C	23	LEU	2.5
1	C	68	VAL	2.4
1	G	21	ILE	2.4
2	D	204	LYS	2.3
1	G	23	LEU	2.3
1	C	18	PRO	2.3
2	B	128	ARG	2.3
1	E	181	THR	2.2
2	D	97	ALA	2.2
2	D	219	ALA	2.2
2	D	128	ARG	2.2
1	C	178	PRO	2.1
2	H	101	THR	2.1
1	C	179	ALA	2.1
1	G	20	ASP	2.1
2	B	204	LYS	2.1
1	C	70	PRO	2.0
1	C	20	ASP	2.0
1	G	207	PRO	2.0
2	D	203	PRO	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	A	117	8/9	0.97	0.17	-	3,10,37,40	0
1	CSD	C	117	8/9	0.97	0.17	-	7,13,27,49	0
1	CSD	E	117	8/9	0.96	0.16	-	11,13,27,48	0
1	CSD	G	117	8/9	0.95	0.15	-	2,14,20,22	0
1	CSD	C	115	8/9	0.99	0.13	-	8,12,21,50	0
1	CSD	A	115	8/9	0.98	0.14	-	2,9,17,22	0
1	CSD	G	115	8/9	0.98	0.16	-	6,23,37,38	0
1	CSD	E	115	8/9	0.97	0.16	-	10,21,26,34	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	E	212	6/6	0.92	0.18	1.09	10,19,23,34	0
3	GOL	C	212	6/6	0.92	0.15	0.76	15,23,35,36	0
3	GOL	G	212	6/6	0.94	0.15	-0.02	18,27,29,45	0
3	GOL	A	212	6/6	0.96	0.15	-0.43	9,24,26,32	0
4	3CO	C	213	1/1	0.96	0.17	-	12,12,12,12	0
4	3CO	E	213	1/1	0.99	0.15	-	14,14,14,14	0
4	3CO	A	213	1/1	0.97	0.17	-	19,19,19,19	0
4	3CO	G	213	1/1	0.99	0.14	-	14,14,14,14	0

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

There are no such residues in this entry.