W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:22 PM GMT

PDB ID : 3QYG
Title : Crystal Structure of Co-type Nitrile Hydratase beta-E56Q from Pseudomonas putida.
Authors : Brodkin, H.R.; Novak, W.R.P.; Ringe, D.; Petsko, G.A.
Deposited on : 2011-03-03
Resolution : 2.30 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.
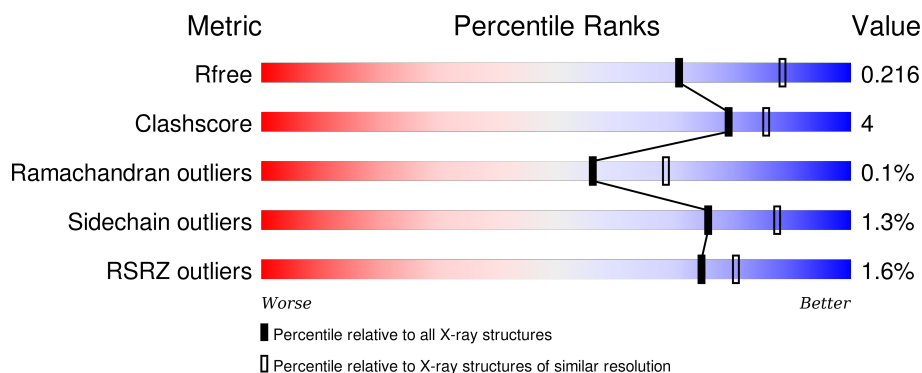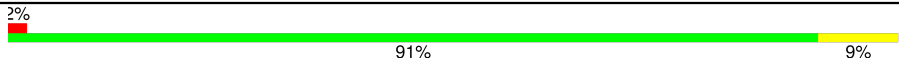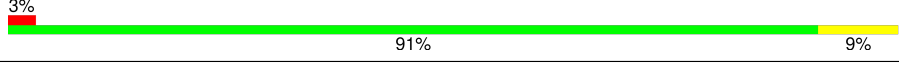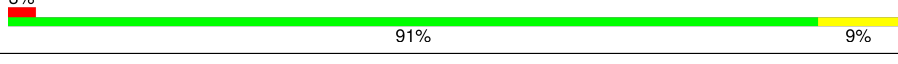

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 >=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 <=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	226	
1	C	226	
1	E	226	
1	G	226	
2	B	219	

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Mol	Chain	Length	Quality of chain
2	D	219	2% ▮ 91% 9%
2	F	219	3% ▮ 91% 9%
2	H	219	3% ▮ 91% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14164 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
			1542	982	262	290	8			
1	C	201	Total	C	N	O	S	0	0	0
			1543	983	264	288	8			
1	E	200	Total	C	N	O	S	0	2	0
			1550	989	264	289	8			
1	G	200	Total	C	N	O	S	0	1	0
			1541	982	265	286	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	3	0
			1731	1093	312	322	4			
2	D	219	Total	C	N	O	S	0	3	0
			1727	1092	309	322	4			
2	F	219	Total	C	N	O	S	0	3	0
			1729	1093	311	321	4			
2	H	219	Total	C	N	O	S	0	3	0
			1721	1089	307	321	4			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total 147	O 147	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	146	Total 146	O 146	0	0
5	C	105	Total 105	O 105	0	0
5	D	146	Total 146	O 146	0	0
5	E	114	Total 114	O 114	0	0
5	F	138	Total 138	O 138	0	0
5	G	120	Total 120	O 120	0	0
5	H	136	Total 136	O 136	0	0

3 Residue-property plots ⓘ

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
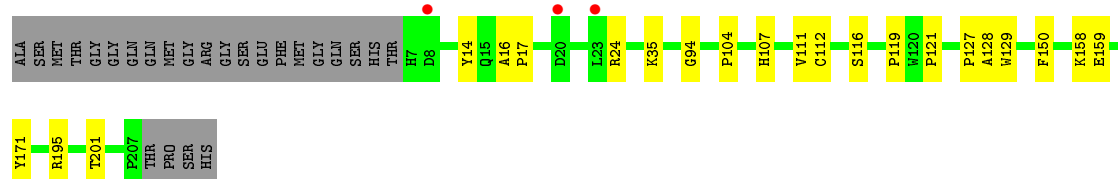
• Molecule 1: Co-type Nitrile Hydratase alpha subunit
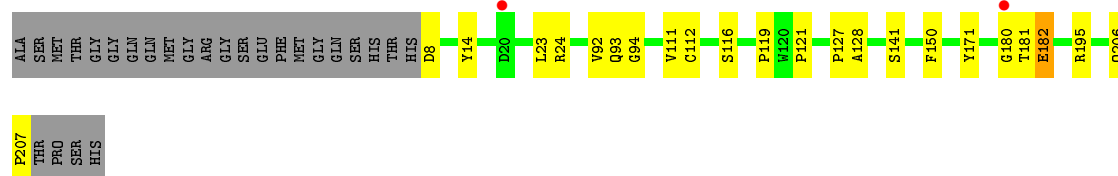
• Molecule 1: Co-type Nitrile Hydratase alpha subunit
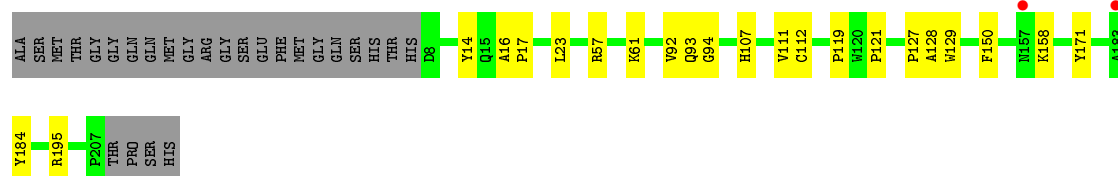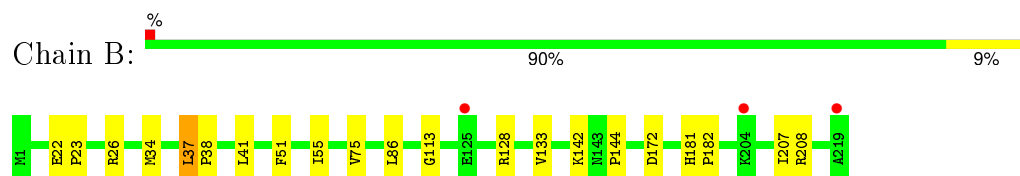
• Molecule 1: Co-type Nitrile Hydratase alpha subunit

• Molecule 2: Co-type Nitrile Hydratase beta subunit

Chain B:

90% 9%

M1 E22 P23 R26 M34 L37 P38 L41 F51 I55 V75 L86 G113 E125 R128 V133 K142 N143 P144 D172 H181 P182 K204 I207 R208 A219

• Molecule 2: Co-type Nitrile Hydratase beta subunit

Chain D:

2% 91% 9%

M1 R18 R26 M34 L37 P38 L41 F51 I55 V75 T87 E90 E124 R128 V145 D172 H181 P182 S202 P203 K204 I207 A219

• Molecule 2: Co-type Nitrile Hydratase beta subunit

Chain F:

3% 91% 9%

M1 R18 E19 R26 M34 L37 P38 F51 V75 G94 K95 K100 T101 A102 I110 E124 R128 V133 P144 D172 E180 H181 W196 A200 S201 S202 P203 K204 I207 A219

• Molecule 2: Co-type Nitrile Hydratase beta subunit

Chain H:

3% 91% 9%

M1 R18 E19 P20 N21 E22 P23 M34 L37 P38 F51 V75 K95 R128 V133 D172 H181 V193 Q198 D199 A200 S201 S202 P203 K204 I207 A219

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.96Å 137.55Å 85.42Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	45.37 – 2.30 45.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (45.37-2.30) 96.1 (45.37-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.31 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.196 , 0.224 0.188 , 0.216	Depositor DCC
R_{free} test set	4037 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.1	EDS
Estimated twinning fraction	0.010 for l,k,-h 0.031 for h,-k,-l 0.107 for l,-k,h	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 80843 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14164	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 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	0.32	0/1566	0.49	0/2142
1	C	0.32	0/1568	0.69	3/2145 (0.1%)
1	E	0.32	0/1574	0.49	1/2151 (0.0%)
1	G	0.36	0/1565	0.50	0/2140
2	B	0.35	0/1779	0.79	5/2422 (0.2%)
2	D	0.35	0/1775	0.73	5/2418 (0.2%)
2	F	0.36	0/1778	0.59	4/2424 (0.2%)
2	H	0.36	0/1770	0.54	2/2413 (0.1%)
All	All	0.34	0/13375	0.62	20/18255 (0.1%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	128	ARG	NE-CZ-NH1	-19.16	110.72	120.30
2	B	128	ARG	NE-CZ-NH2	18.25	129.43	120.30
2	D	26	ARG	NE-CZ-NH1	-17.30	111.65	120.30
2	D	26	ARG	NE-CZ-NH2	16.17	128.38	120.30
1	C	24	ARG	NE-CZ-NH2	-16.11	112.24	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	1542	0	1518	10	0
1	C	1543	0	1519	14	0
1	E	1550	0	1531	16	0
1	G	1541	0	1522	15	0
2	B	1731	0	1674	13	0
2	D	1727	0	1670	15	0
2	F	1729	0	1669	13	0
2	H	1721	0	1654	12	0
3	A	6	0	8	0	0
3	C	6	0	8	0	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	147	0	0	1	0
5	B	146	0	0	2	0
5	C	105	0	0	0	0
5	D	146	0	0	1	0
5	E	114	0	0	1	0
5	F	138	0	0	1	0
5	G	120	0	0	3	0
5	H	136	0	0	1	0
All	All	14164	0	12789	91	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 4.

The worst 5 of 91 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:H:204:LYS:HB2	5:H:726:HOH:O	1.84	0.76
2:F:100:LYS:HE3	2:F:102:ALA:O	1.86	0.75
2:B:113:GLY:HA3	2:F:110:ILE:HG22	1.74	0.70
1:G:150:PHE:CE2	2:H:18:ARG:HD3	2.28	0.69
1:C:119:PRO:HG3	1:C:171:TYR:O	1.94	0.67

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	197/226 (87%)	193 (98%)	4 (2%)	0	100	100
1	C	197/226 (87%)	191 (97%)	5 (2%)	1 (0%)	34	41
1	E	198/226 (88%)	192 (97%)	5 (2%)	1 (0%)	34	41
1	G	197/226 (87%)	190 (96%)	7 (4%)	0	100	100
2	B	220/219 (100%)	218 (99%)	2 (1%)	0	100	100
2	D	220/219 (100%)	220 (100%)	0	0	100	100
2	F	220/219 (100%)	219 (100%)	1 (0%)	0	100	100
2	H	220/219 (100%)	217 (99%)	3 (1%)	0	100	100
All	All	1669/1780 (94%)	1640 (98%)	27 (2%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	SER
1	E	116	SER

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	159/180 (88%)	159 (100%)	0	100	100
1	C	159/180 (88%)	159 (100%)	0	100	100
1	E	159/180 (88%)	157 (99%)	2 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	158/180 (88%)	157 (99%)	1 (1%)	90	96
2	B	180/177 (102%)	176 (98%)	4 (2%)	60	77
2	D	180/177 (102%)	177 (98%)	3 (2%)	68	83
2	F	180/177 (102%)	177 (98%)	3 (2%)	68	83
2	H	178/177 (101%)	174 (98%)	4 (2%)	60	77
All	All	1353/1428 (95%)	1336 (99%)	17 (1%)	76	87

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	23	LEU
1	E	182	GLU
2	H	34	MET
2	D	172	ASP
2	H	95	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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	0.97	0	3,8,10	1.94	1 (33%)
1	CSD	A	117	1,4	3,7,8	1.00	0	3,8,10	1.52	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	CSD	C	115	1,4	3,7,8	0.96	0	3,8,10	2.13	2 (66%)
1	CSD	C	117	1,4	3,7,8	0.90	0	3,8,10	1.81	2 (66%)
1	CSD	E	115	1,4	3,7,8	1.20	0	3,8,10	1.60	1 (33%)
1	CSD	E	117	1,4	3,7,8	1.02	0	3,8,10	1.84	1 (33%)
1	CSD	G	115	1,4	3,7,8	0.99	0	3,8,10	2.49	2 (66%)
1	CSD	G	117	1,4	3,7,8	1.01	0	3,8,10	1.35	1 (33%)

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	-	1/2/6/8	0/0/0/0
1	CSD	G	117	1,4	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	115	CSD	OD1-SG-CB	-3.19	100.09	105.40
1	A	115	CSD	O-C-CA	-3.00	117.67	125.49
1	E	115	CSD	O-C-CA	-2.75	118.33	125.49
1	G	115	CSD	O-C-CA	-2.72	118.41	125.49
1	C	115	CSD	O-C-CA	-2.62	118.67	125.49

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
1	C	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	0.37	0	5,5,5	0.22	0
3	GOL	C	212	-	5,5,5	0.33	0	5,5,5	0.46	0
3	GOL	E	212	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	G	212	-	5,5,5	0.41	0	5,5,5	0.69	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.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	199/226 (88%)	-0.07	0	100	100	18, 24, 32, 37	0
1	C	199/226 (88%)	-0.06	3 (1%)	76	81	18, 24, 33, 39	0
1	E	198/226 (87%)	-0.20	2 (1%)	84	88	18, 24, 32, 37	1 (0%)
1	G	198/226 (87%)	-0.14	2 (1%)	84	88	18, 24, 33, 38	0
2	B	219/219 (100%)	-0.02	3 (1%)	78	83	19, 23, 33, 47	1 (0%)
2	D	219/219 (100%)	-0.06	4 (1%)	71	78	19, 23, 31, 47	0
2	F	219/219 (100%)	-0.05	7 (3%)	51	60	19, 23, 35, 47	0
2	H	219/219 (100%)	-0.10	6 (2%)	58	67	19, 23, 34, 47	0
All	All	1670/1780 (93%)	-0.09	27 (1%)	74	80	18, 23, 33, 47	2 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	219	ALA	3.1
2	F	200	ALA	3.1
2	D	219	ALA	2.8
2	H	219	ALA	2.7
2	F	94	GLY	2.7

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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
1	CSD	A	115	8/9	0.99	0.15	-	17,17,18,18	0
1	CSD	C	115	8/9	0.99	0.16	-	18,18,18,19	0
1	CSD	E	115	8/9	0.98	0.11	-	17,18,18,18	0
1	CSD	E	117	8/9	0.98	0.11	-	18,18,18,19	0
1	CSD	C	117	8/9	0.98	0.14	-	18,18,18,19	0
1	CSD	A	117	8/9	0.99	0.13	-	18,18,18,19	0
1	CSD	G	117	8/9	0.98	0.13	-	18,18,18,19	0
1	CSD	G	115	8/9	0.98	0.12	-	18,18,18,18	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
3	GOL	G	212	6/6	0.90	0.15	1.36	20,21,21,22	0
3	GOL	A	212	6/6	0.91	0.15	0.20	20,20,21,21	0
3	GOL	C	212	6/6	0.91	0.14	0.06	20,21,21,22	0
3	GOL	E	212	6/6	0.96	0.11	-0.61	20,20,21,21	0
4	3CO	G	213	1/1	0.99	0.14	-	18,18,18,18	0
4	3CO	E	213	1/1	0.99	0.12	-	18,18,18,18	0
4	3CO	C	213	1/1	1.00	0.13	-	18,18,18,18	0
4	3CO	A	213	1/1	1.00	0.14	-	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.