Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 11:44 AM EDT

PDB ID	:	3QXE
Title	:	Crystal Structure of Co-type Nitrile Hydratase from Pseudomonas putida.
Authors	:	Brodkin, H.R.; Novak, W.R.P.; Ringe, D.; Petsko, G.A.
Deposited on	:	2011-03-01
Resolution	:	2.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

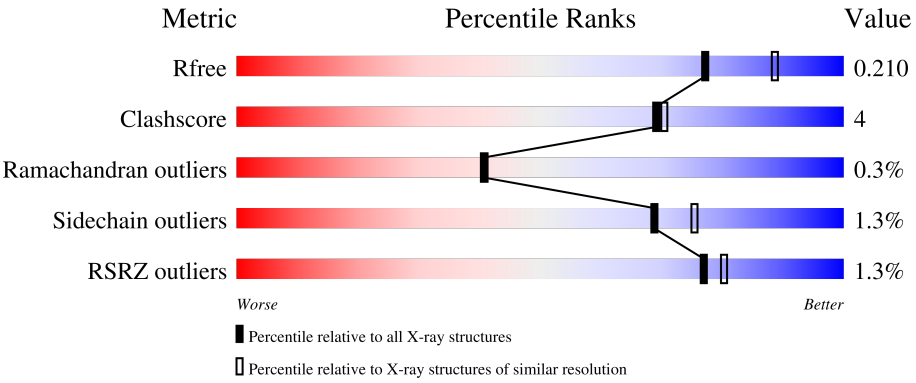
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 >=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 <=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	83% 6% 11%
1	C	226	78% 10% 11%
1	E	226	81% 6% 12%
1	G	226	81% 8% 12%
2	B	219	91% 9%

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Mol	Chain	Length	Quality of chain
2	D	219	2% 89% 11%
2	F	219	2% 90% 10%
2	H	219	2% 88% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	H	220	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14259 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
			1551	987	264	292	8			
1	C	201	Total	C	N	O	S	0	0	0
			1551	987	264	292	8			
1	E	200	Total	C	N	O	S	0	0	0
			1538	980	261	289	8			
1	G	200	Total	C	N	O	S	0	0	0
			1538	980	261	289	8			

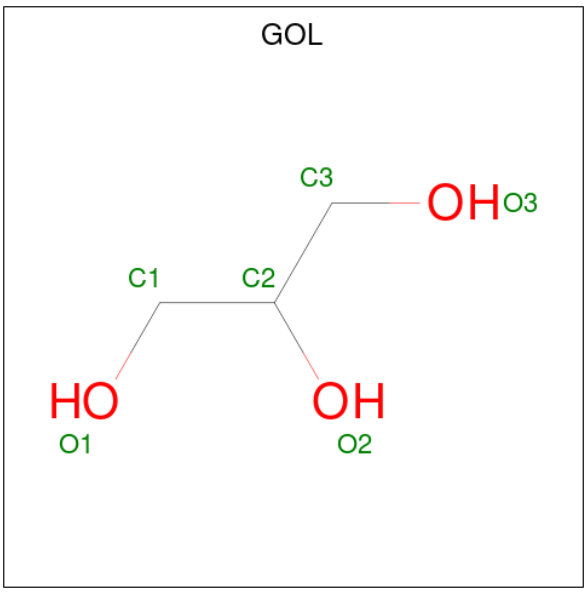
- Molecule 2 is a protein called Co-type Nitrile Hydratase beta subunit.

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
			1720	1087	307	322	4			

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	143	Total O 143 143	0	0
5	B	174	Total O 174 174	0	0
5	C	115	Total O 115 115	0	0

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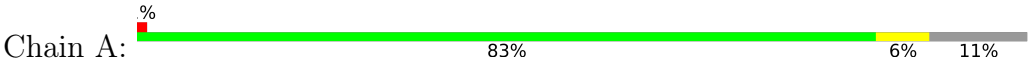
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	167	Total O 167 167	0	0
5	E	129	Total O 129 129	0	0
5	F	153	Total O 153 153	0	0
5	G	121	Total O 121 121	0	0
5	H	141	Total O 141 141	0	0

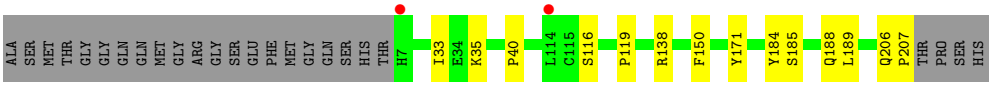
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Co-type Nitrile Hydratase alpha subunit

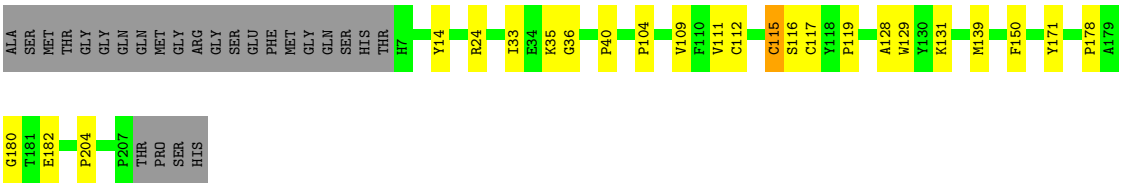
Chain A:





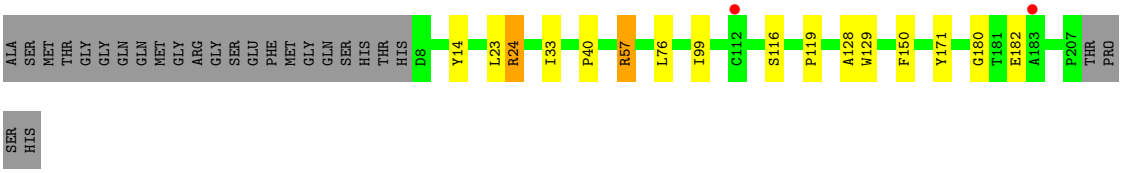
• Molecule 1: Co-type Nitrile Hydratase alpha subunit

Chain C:



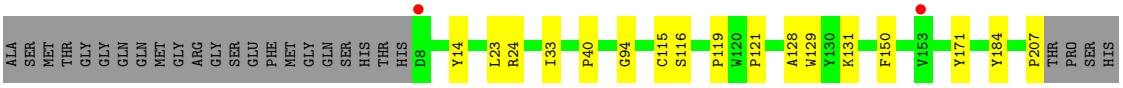
• Molecule 1: Co-type Nitrile Hydratase alpha subunit

Chain E:



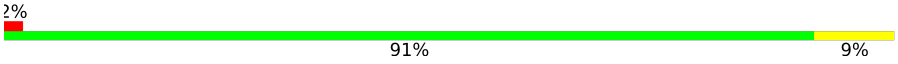
• Molecule 1: Co-type Nitrile Hydratase alpha subunit

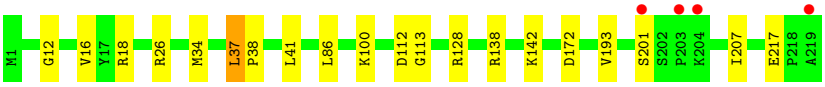
Chain G:



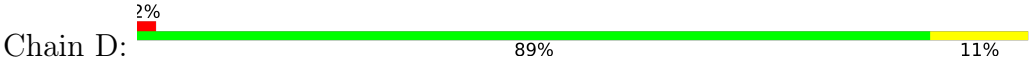
• Molecule 2: Co-type Nitrile Hydratase beta subunit

Chain B:

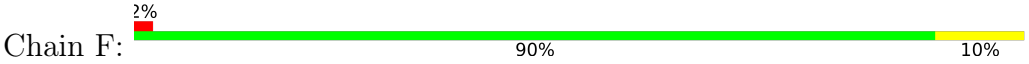




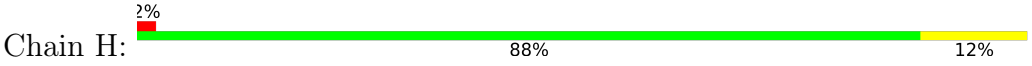
• Molecule 2: Co-type Nitrile Hydratase beta subunit



• Molecule 2: Co-type Nitrile Hydratase beta subunit



• Molecule 2: Co-type Nitrile Hydratase beta subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.20Å 137.43Å 85.38Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	37.60 – 2.10 37.60 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (37.60-2.10) 98.6 (37.60-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.176 , 0.217 0.170 , 0.210	Depositor DCC
R_{free} test set	5392 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,k,-h 0.029 for h,-k,-l 0.098 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14259	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3CO, CSD, GOL

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	0.52	0/1576	0.61	0/2155
1	C	0.50	0/1576	0.78	3/2155 (0.1%)
1	E	0.55	0/1562	0.62	1/2136 (0.0%)
1	G	0.54	0/1562	0.62	2/2136 (0.1%)
2	B	0.55	0/1768	0.87	4/2408 (0.2%)
2	D	0.55	0/1775	0.87	6/2418 (0.2%)
2	F	0.53	0/1767	0.65	3/2408 (0.1%)
2	H	0.53	0/1768	0.66	3/2408 (0.1%)
All	All	0.53	0/13354	0.72	22/18224 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	26	ARG	NE-CZ-NH1	-19.95	110.32	120.30
2	D	26	ARG	NE-CZ-NH2	19.13	129.86	120.30
2	B	128	ARG	NE-CZ-NH1	-18.79	110.90	120.30
2	B	128	ARG	NE-CZ-NH2	18.20	129.40	120.30
1	C	24	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	C	24	ARG	NE-CZ-NH1	15.50	128.05	120.30
2	B	128	ARG	CD-NE-CZ	9.27	136.58	123.60
2	D	26	ARG	CD-NE-CZ	9.15	136.42	123.60
1	C	24	ARG	CD-NE-CZ	7.08	133.51	123.60
2	F	128	ARG	NE-CZ-NH2	-6.89	116.86	120.30
2	D	128	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	H	128	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	F	128	ARG	NE-CZ-NH1	6.35	123.47	120.30
2	H	128	ARG	NE-CZ-NH1	6.33	123.46	120.30
2	F	26	ARG	NE-CZ-NH2	-6.01	117.30	120.30
2	D	128	ARG	NE-CZ-NH1	5.85	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	26	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	B	26	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	G	24	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	G	24	ARG	NE-CZ-NH2	5.26	122.93	120.30
2	D	37	LEU	CB-CG-CD2	5.26	119.94	111.00
1	E	24	ARG	NE-CZ-NH1	-5.21	117.70	120.30

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	1551	0	1527	9	0
1	C	1551	0	1527	18	0
1	E	1538	0	1518	11	0
1	G	1538	0	1518	11	0
2	B	1720	0	1660	13	0
2	D	1727	0	1668	18	0
2	F	1719	0	1660	16	0
2	H	1720	0	1660	19	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	3	0
4	C	6	0	8	1	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	3	0
4	H	6	0	8	4	0
5	A	143	0	0	0	0
5	B	174	0	0	1	0
5	C	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	167	0	0	0	0
5	E	129	0	0	1	0
5	F	153	0	0	4	0
5	G	121	0	0	3	0
5	H	141	0	0	1	0
All	All	14259	0	12802	95	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.

All (95) 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)
4:C:213:GOL:H32	2:D:66:GLY:O	1.85	0.75
1:E:150:PHE:CE2	2:F:18:ARG:HD2	2.26	0.70
1:C:182:GLU:H	1:C:182:GLU:CD	1.99	0.65
1:A:185:SER:OG	1:A:188:GLN:HG3	1.97	0.65
2:H:17:TYR:OH	2:H:19:GLU:HG2	1.97	0.65
1:E:57:ARG:N	1:E:57:ARG:HD2	2.11	0.64
2:B:113:GLY:HA3	2:F:110:ILE:HG22	1.79	0.63
2:F:144:PRO:HD2	5:F:229:HOH:O	1.99	0.60
4:G:213:GOL:H11	2:H:66:GLY:O	2.03	0.59
2:B:193:VAL:HG22	2:B:201:SER:OG	2.02	0.59
1:C:104:PRO:HG2	1:G:184:TYR:CZ	2.37	0.59
1:C:35:LYS:NZ	2:D:90:GLU:OE2	2.30	0.58
2:B:113:GLY:HA3	2:F:110:ILE:CG2	2.35	0.57
1:G:129:TRP:CD1	2:H:18:ARG:HG2	2.40	0.56
2:H:193:VAL:HG22	2:H:201:SER:OG	2.05	0.56
1:E:182:GLU:CD	1:E:182:GLU:H	2.09	0.56
1:C:178:PRO:HG3	1:C:204:PRO:HB2	1.86	0.56
2:D:37:LEU:HB3	2:D:38:PRO:HD3	1.90	0.54
2:F:193:VAL:HG22	2:F:201:SER:OG	2.07	0.54
2:H:144:PRO:HD2	5:H:247:HOH:O	2.09	0.53
2:H:37:LEU:HB3	2:H:38:PRO:HD3	1.90	0.53
2:B:112:ASP:HB2	5:B:1078:HOH:O	2.07	0.53
1:E:129:TRP:CD1	2:F:18:ARG:HG2	2.44	0.53
2:B:37:LEU:HB3	2:B:38:PRO:HD3	1.92	0.52
1:G:150:PHE:CZ	2:H:18:ARG:HD3	2.46	0.51
1:E:180:GLY:HA2	1:E:182:GLU:OE2	2.12	0.50
1:E:119:PRO:HG3	1:E:171:TYR:O	2.12	0.50
1:G:150:PHE:CE2	2:H:18:ARG:HD3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:62[B]:HIS:ND1	5:F:983:HOH:O	2.14	0.49
2:H:17:TYR:CE2	2:H:19:GLU:HG3	2.47	0.49
2:F:37:LEU:HB3	2:F:38:PRO:HD3	1.95	0.49
2:F:193:VAL:HG23	5:F:882:HOH:O	2.13	0.49
2:H:12:GLY:H	4:H:220:GOL:C1	2.26	0.48
1:G:129:TRP:CG	2:H:18:ARG:HG2	2.48	0.48
2:H:14:GLY:H	4:H:220:GOL:H12	1.79	0.48
1:C:119:PRO:HG3	1:C:171:TYR:O	2.13	0.48
1:C:180:GLY:HA2	1:C:182:GLU:OE1	2.13	0.48
2:B:12:GLY:N	4:B:220:GOL:O3	2.47	0.47
1:C:111:VAL:HG22	1:C:112:CYS:N	2.29	0.47
2:H:12:GLY:H	4:H:220:GOL:H11	1.79	0.47
1:A:184:TYR:HB3	1:A:189:LEU:HG	1.97	0.47
2:B:138[B]:ARG:HD2	2:B:217:GLU:OE2	2.14	0.47
1:G:119:PRO:HG3	1:G:171:TYR:O	2.14	0.47
1:C:129:TRP:CE2	2:D:18:ARG:HD2	2.50	0.47
1:A:138:ARG:HD2	4:B:220:GOL:H2	1.97	0.46
1:E:150:PHE:CZ	2:F:18:ARG:HD2	2.49	0.46
2:D:51:PHE:CD2	2:D:75:VAL:HG11	2.50	0.46
1:E:24:ARG:NH1	5:E:1187:HOH:O	2.45	0.45
2:H:138[B]:ARG:HD2	2:H:217:GLU:OE2	2.17	0.45
2:H:204:LYS:HD3	2:H:204:LYS:HA	1.81	0.44
1:C:150:PHE:HZ	2:D:16:VAL:HG11	1.82	0.44
2:H:11:HIS:HA	4:H:220:GOL:O3	2.18	0.44
1:C:36:GLY:CA	2:D:100:LYS:HG3	2.48	0.44
1:G:33:ILE:CD1	1:G:40:PRO:HG3	2.48	0.43
1:A:206:GLN:HA	1:A:207:PRO:HD3	1.90	0.43
2:D:138[B]:ARG:HD2	2:D:217:GLU:OE2	2.18	0.43
2:F:207:ILE:HD12	2:F:207:ILE:N	2.34	0.43
1:G:14:TYR:CZ	1:G:128:ALA:HB3	2.54	0.43
1:G:131:LYS:HD2	2:H:68:TYR:CD1	2.54	0.43
2:F:204:LYS:HD3	2:F:204:LYS:HA	1.79	0.42
1:G:207:PRO:HD2	5:G:1017:HOH:O	2.19	0.42
1:A:150:PHE:HZ	2:B:16:VAL:HG11	1.83	0.42
1:A:119:PRO:HG3	1:A:171:TYR:O	2.19	0.42
1:C:33:ILE:HD13	1:C:40:PRO:HG3	2.01	0.42
1:C:36:GLY:HA3	2:D:100:LYS:HG3	2.00	0.42
1:A:33:ILE:CD1	1:A:40:PRO:HG3	2.50	0.42
2:H:195:LEU:HD12	2:H:207:ILE:HD13	2.02	0.42
1:C:131:LYS:HD2	2:D:68:TYR:CD1	2.55	0.42
1:C:14:TYR:CZ	1:C:128:ALA:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:ILE:CD1	1:E:40:PRO:HG3	2.50	0.41
4:G:213:GOL:H12	5:G:1005:HOH:O	2.19	0.41
1:A:35:LYS:HD3	2:B:86:LEU:CD2	2.50	0.41
2:D:37:LEU:HD22	2:D:41:LEU:HG	2.01	0.41
1:E:14:TYR:CZ	1:E:128:ALA:HB3	2.55	0.41
2:B:37:LEU:HD22	2:B:41:LEU:HG	2.01	0.41
2:F:138[B]:ARG:HD2	2:F:217:GLU:OE2	2.20	0.41
2:F:195:LEU:HD12	2:F:207:ILE:HD13	2.02	0.41
1:C:33:ILE:CD1	1:C:40:PRO:HG3	2.50	0.41
2:F:100:LYS:HE3	2:F:102:ALA:O	2.21	0.41
2:F:19:GLU:HG3	5:F:757:HOH:O	2.21	0.41
4:G:213:GOL:C1	5:G:1005:HOH:O	2.68	0.41
1:A:150:PHE:CE2	2:B:18:ARG:HD3	2.56	0.41
2:B:12:GLY:CA	4:B:220:GOL:O3	2.69	0.41
1:C:131:LYS:HD2	2:D:68:TYR:CE1	2.56	0.41
1:G:94:GLY:HA3	1:G:121:PRO:HG2	2.01	0.41
2:D:55:ILE:HG13	2:D:75:VAL:CG2	2.51	0.41
2:B:207:ILE:HD12	2:B:207:ILE:N	2.36	0.40
2:D:207:ILE:N	2:D:207:ILE:HD12	2.36	0.40
1:C:115:CSD:OD1	2:D:52:ARG:NE	2.50	0.40
1:E:76:LEU:HG	1:E:99:ILE:HG13	2.04	0.40
1:C:109:VAL:HG11	1:C:139:MET:HE2	2.02	0.40
2:D:14:GLY:N	4:D:220:GOL:O1	2.39	0.40
2:D:204:LYS:HD3	2:D:204:LYS:HA	1.79	0.40
2:H:180:GLU:O	2:H:181:HIS:C	2.60	0.40
2:D:195:LEU:HD12	2:D:207:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/226 (87%)	190 (96%)	6 (3%)	1 (0%)	29	26
1	C	197/226 (87%)	193 (98%)	3 (2%)	1 (0%)	29	26
1	E	196/226 (87%)	191 (97%)	4 (2%)	1 (0%)	29	26
1	G	196/226 (87%)	190 (97%)	5 (3%)	1 (0%)	29	26
2	B	219/219 (100%)	215 (98%)	3 (1%)	1 (0%)	29	26
2	D	220/219 (100%)	217 (99%)	3 (1%)	0	100	100
2	F	219/219 (100%)	216 (99%)	3 (1%)	0	100	100
2	H	219/219 (100%)	217 (99%)	2 (1%)	0	100	100
All	All	1663/1780 (93%)	1629 (98%)	29 (2%)	5 (0%)	41	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	SER
1	A	116	SER
1	G	116	SER
2	B	100	LYS
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	161/180 (89%)	161 (100%)	0	100	100
1	C	161/180 (89%)	161 (100%)	0	100	100
1	E	159/180 (88%)	157 (99%)	2 (1%)	69	75
1	G	159/180 (88%)	158 (99%)	1 (1%)	86	90
2	B	179/177 (101%)	175 (98%)	4 (2%)	52	57
2	D	180/177 (102%)	176 (98%)	4 (2%)	52	57
2	F	179/177 (101%)	176 (98%)	3 (2%)	60	67
2	H	179/177 (101%)	175 (98%)	4 (2%)	52	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1357/1428 (95%)	1339 (99%)	18 (1%)	69 75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	34	MET
2	B	37	LEU
2	B	142	LYS
2	B	172	ASP
2	D	34	MET
2	D	37	LEU
2	D	152	ARG
2	D	172	ASP
1	E	23	LEU
1	E	57	ARG
2	F	23	PRO
2	F	34	MET
2	F	172	ASP
1	G	23	LEU
2	H	34	MET
2	H	95	LYS
2	H	152	ARG
2	H	172	ASP

Sometimes 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	E	117	1,3	3,7,8	0.98	0	1,8,10	1.31	0
1	CSD	G	115	1,3	3,7,8	1.06	0	1,8,10	2.05	1 (100%)
1	CSD	A	115	1,3	3,7,8	1.07	0	1,8,10	1.11	0
1	CSD	C	117	1,3	3,7,8	1.24	0	1,8,10	2.50	1 (100%)
1	CSD	G	117	1,3	3,7,8	1.06	0	1,8,10	1.17	0
1	CSD	E	115	1,3	3,7,8	1.15	0	1,8,10	1.21	0
1	CSD	A	117	1,3	3,7,8	0.90	0	1,8,10	0.68	0
1	CSD	C	115	1,3	3,7,8	1.05	0	1,8,10	2.27	1 (100%)

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	E	117	1,3	-	1/2/6/8	-
1	CSD	G	115	1,3	-	1/2/6/8	-
1	CSD	A	115	1,3	-	1/2/6/8	-
1	CSD	C	117	1,3	-	1/2/6/8	-
1	CSD	G	117	1,3	-	1/2/6/8	-
1	CSD	E	115	1,3	-	1/2/6/8	-
1	CSD	A	117	1,3	-	1/2/6/8	-
1	CSD	C	115	1,3	-	1/2/6/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	117	CSD	OD1-SG-CB	-2.50	100.77	105.54
1	C	115	CSD	OD1-SG-CB	-2.27	101.22	105.54
1	G	115	CSD	OD1-SG-CB	-2.05	101.63	105.54

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	115	CSD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	GOL	F	220	-	5,5,5	0.44	0	5,5,5	0.53	0
4	GOL	E	213	-	5,5,5	0.49	0	5,5,5	0.45	0
4	GOL	A	213	-	5,5,5	0.48	0	5,5,5	0.72	0
4	GOL	H	220	-	5,5,5	0.29	0	5,5,5	0.54	0
4	GOL	D	220	-	5,5,5	0.40	0	5,5,5	1.07	0
4	GOL	G	213	-	5,5,5	0.36	0	5,5,5	0.76	0
4	GOL	C	213	-	5,5,5	0.52	0	5,5,5	0.33	0
4	GOL	B	220	-	5,5,5	0.42	0	5,5,5	0.96	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
4	GOL	F	220	-	-	0/4/4/4	-
4	GOL	E	213	-	-	2/4/4/4	-
4	GOL	A	213	-	-	4/4/4/4	-
4	GOL	H	220	-	-	2/4/4/4	-
4	GOL	D	220	-	-	4/4/4/4	-
4	GOL	G	213	-	-	4/4/4/4	-
4	GOL	C	213	-	-	2/4/4/4	-
4	GOL	B	220	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	213	GOL	O1-C1-C2-C3
4	B	220	GOL	O1-C1-C2-O2
4	B	220	GOL	O1-C1-C2-C3
4	D	220	GOL	O1-C1-C2-C3
4	D	220	GOL	O2-C2-C3-O3
4	G	213	GOL	O1-C1-C2-C3
4	G	213	GOL	C1-C2-C3-O3
4	H	220	GOL	O1-C1-C2-C3
4	A	213	GOL	O1-C1-C2-O2
4	G	213	GOL	O2-C2-C3-O3
4	A	213	GOL	C1-C2-C3-O3
4	C	213	GOL	O1-C1-C2-C3
4	D	220	GOL	C1-C2-C3-O3
4	E	213	GOL	O1-C1-C2-C3
4	D	220	GOL	O1-C1-C2-O2
4	G	213	GOL	O1-C1-C2-O2
4	H	220	GOL	O1-C1-C2-O2
4	C	213	GOL	O1-C1-C2-O2
4	E	213	GOL	O1-C1-C2-O2
4	A	213	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	220	GOL	4	0
4	D	220	GOL	1	0
4	G	213	GOL	3	0
4	C	213	GOL	1	0
4	B	220	GOL	3	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^{th} 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^2)	Q<0.9
1	A	199/226 (88%)	-0.27	2 (1%) 82 85	11, 21, 35, 56	2 (1%)
1	C	199/226 (88%)	-0.22	0 100 100	13, 22, 38, 58	3 (1%)
1	E	198/226 (87%)	-0.24	2 (1%) 82 85	12, 21, 36, 47	3 (1%)
1	G	198/226 (87%)	-0.25	2 (1%) 82 85	13, 22, 37, 52	2 (1%)
2	B	219/219 (100%)	-0.26	4 (1%) 68 72	13, 20, 43, 60	4 (1%)
2	D	219/219 (100%)	-0.33	4 (1%) 68 72	14, 21, 37, 58	3 (1%)
2	F	219/219 (100%)	-0.30	4 (1%) 68 72	13, 20, 39, 59	2 (0%)
2	H	219/219 (100%)	-0.35	4 (1%) 68 72	15, 21, 45, 59	3 (1%)
All	All	1670/1780 (93%)	-0.28	22 (1%) 77 80	11, 21, 38, 60	22 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	183	ALA	3.0
1	A	7	HIS	2.7
2	F	201	SER	2.6
1	E	112	CYS	2.5
2	D	203	PRO	2.5
2	B	203	PRO	2.4
2	F	200	ALA	2.4
2	D	199	ASP	2.4
1	A	114	LEU	2.3
2	D	219	ALA	2.3
2	F	204	LYS	2.3
2	B	201	SER	2.2
2	H	21	ASN	2.2
2	D	128	ARG	2.2
2	B	219	ALA	2.1
2	H	202	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	219	ALA	2.1
2	F	203	PRO	2.1
1	G	8	ASP	2.0
2	H	203	PRO	2.0
1	G	153	VAL	2.0
2	B	204	LYS	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^{th} 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^2)	Q<0.9
1	CSD	E	117	8/9	0.98	0.15	12,14,16,17	0
1	CSD	G	117	8/9	0.98	0.14	12,14,17,17	0
1	CSD	C	115	8/9	0.99	0.14	11,13,14,17	0
1	CSD	C	117	8/9	0.99	0.16	13,15,16,20	0
1	CSD	E	115	8/9	0.99	0.16	9,12,16,16	0
1	CSD	A	115	8/9	0.99	0.16	8,12,14,18	0
1	CSD	G	115	8/9	0.99	0.13	11,14,16,18	0
1	CSD	A	117	8/9	0.99	0.17	12,13,15,18	0

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^{th} 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^2)	Q<0.9
4	GOL	H	220	6/6	0.87	0.15	24,39,52,56	0
4	GOL	B	220	6/6	0.91	0.17	17,24,36,45	0
4	GOL	D	220	6/6	0.92	0.20	21,33,42,44	0
4	GOL	G	213	6/6	0.94	0.15	22,25,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	F	220	6/6	0.94	0.20	23,29,31,77	0
4	GOL	A	213	6/6	0.96	0.10	13,17,22,35	0
4	GOL	C	213	6/6	0.96	0.09	16,19,31,32	0
4	GOL	E	213	6/6	0.98	0.17	18,20,21,39	0
3	3CO	E	212	1/1	0.99	0.12	13,13,13,13	0
3	3CO	G	212	1/1	1.00	0.10	13,13,13,13	0
3	3CO	C	212	1/1	1.00	0.10	14,14,14,14	0
3	3CO	A	212	1/1	1.00	0.11	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.