Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 06:47 pm GMT

PDB ID	:	5G1O
Title	:	Aspartate transcarbamoylase domain of human CAD in apo form
Authors	:	Ruiz-Ramos, A.; Grande-Garcia, A.; Moreno-Morcillo, M.D.; Ramon-Maiques, S.
Deposited on	:	2016-03-29
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 ⓘ 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 ⓘ) were used in the production of this report:

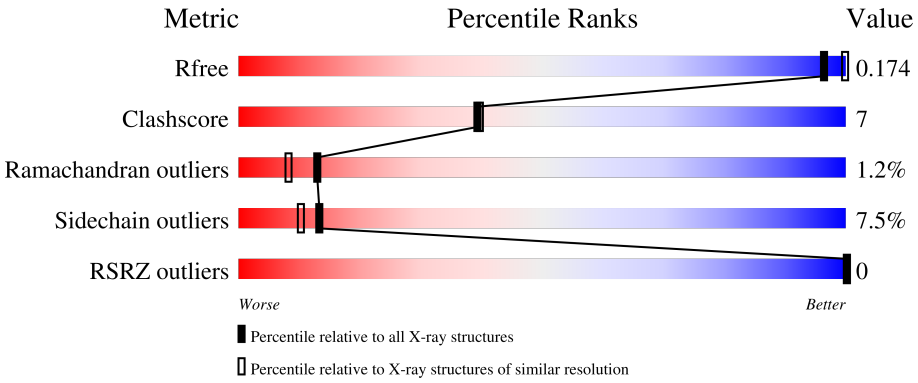
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	314	70% 21% • 6%
1	B	314	71% 21% • 6%
1	C	314	72% 18% • 8%
1	D	314	74% 17% • 7%
1	E	314	77% 17% •• •

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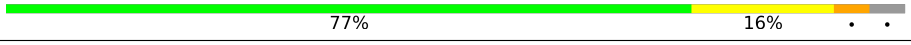
Mol	Chain	Length	Quality of chain
1	F	314	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14089 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 CAD protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2260	1423	406	411	20			
1	B	296	Total	C	N	O	S	0	0	0
			2246	1416	403	406	21			
1	C	290	Total	C	N	O	S	0	0	0
			2236	1410	398	408	20			
1	D	291	Total	C	N	O	S	0	0	0
			2220	1399	398	403	20			
1	E	300	Total	C	N	O	S	0	0	0
			2305	1456	416	412	21			
1	F	301	Total	C	N	O	S	0	0	0
			2305	1449	415	420	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1912	GLY	-	expression tag	UNP P27708
A	1913	PRO	-	expression tag	UNP P27708
A	1914	MET	-	expression tag	UNP P27708
B	1912	GLY	-	expression tag	UNP P27708
B	1913	PRO	-	expression tag	UNP P27708
B	1914	MET	-	expression tag	UNP P27708
C	1912	GLY	-	expression tag	UNP P27708
C	1913	PRO	-	expression tag	UNP P27708
C	1914	MET	-	expression tag	UNP P27708
D	1912	GLY	-	expression tag	UNP P27708
D	1913	PRO	-	expression tag	UNP P27708
D	1914	MET	-	expression tag	UNP P27708
E	1912	GLY	-	expression tag	UNP P27708
E	1913	PRO	-	expression tag	UNP P27708
E	1914	MET	-	expression tag	UNP P27708
F	1912	GLY	-	expression tag	UNP P27708
F	1913	PRO	-	expression tag	UNP P27708

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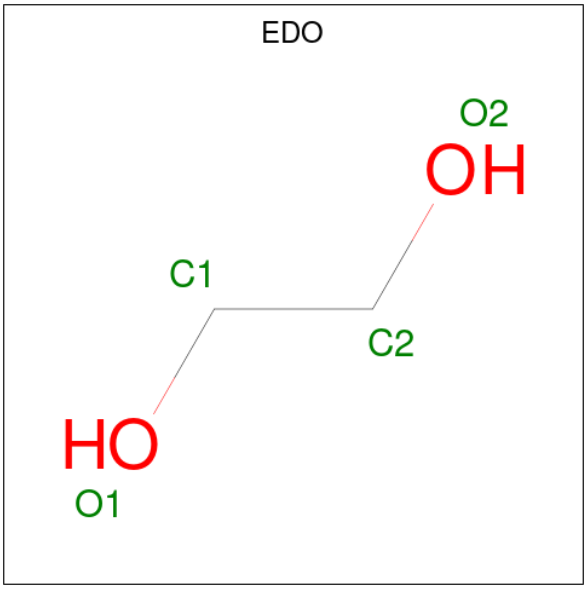
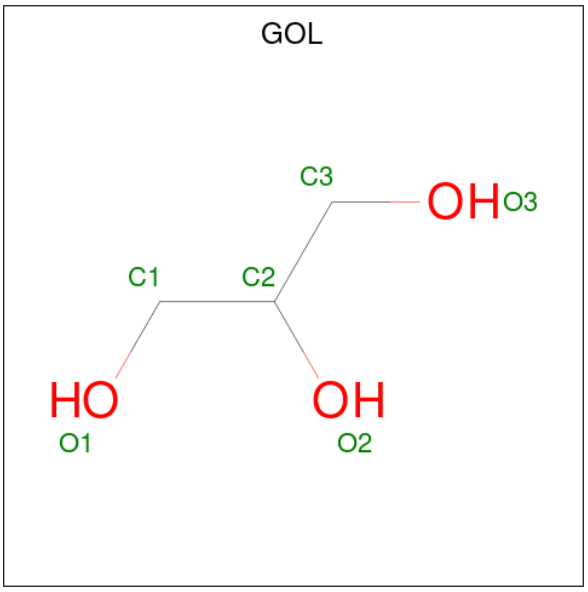
Chain	Residue	Modelled	Actual	Comment	Reference
F	1914	MET	-	expression tag	UNP P27708

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

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



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

- Molecule 4 is water.

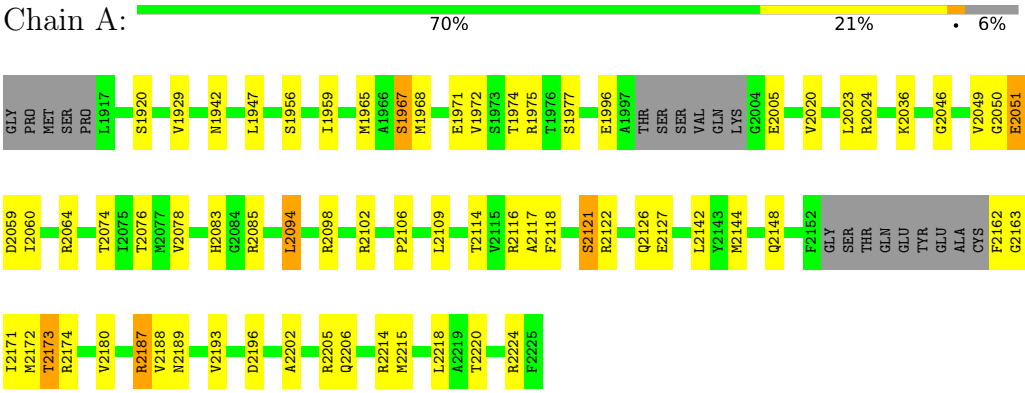
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	95	Total O 95 95	0	0
4	B	75	Total O 75 75	0	0
4	C	55	Total O 55 55	0	0
4	D	94	Total O 94 94	0	0
4	E	72	Total O 72 72	0	0
4	F	94	Total O 94 94	0	0

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.

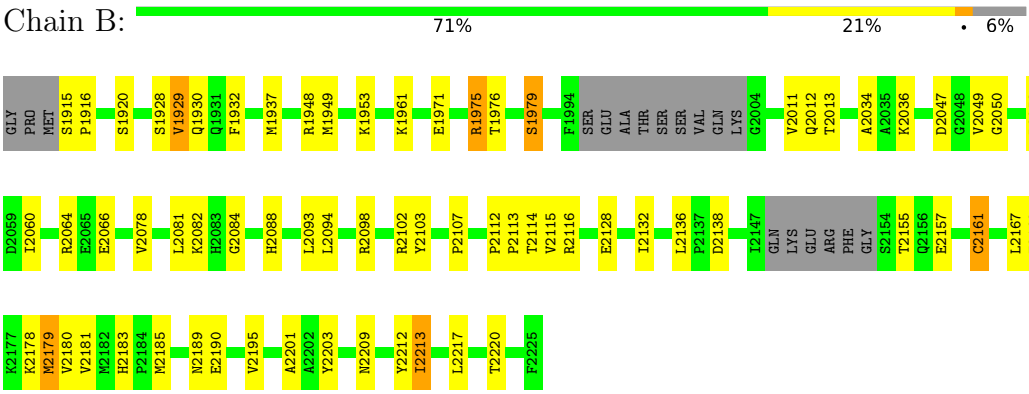
• Molecule 1: CAD protein

Chain A:



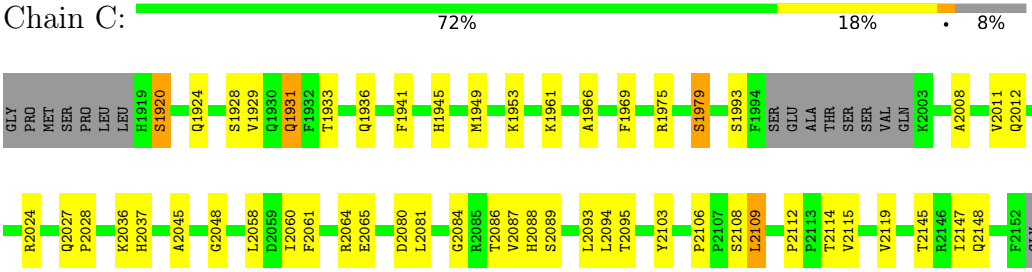
• Molecule 1: CAD protein

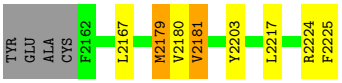
Chain B:



• Molecule 1: CAD protein

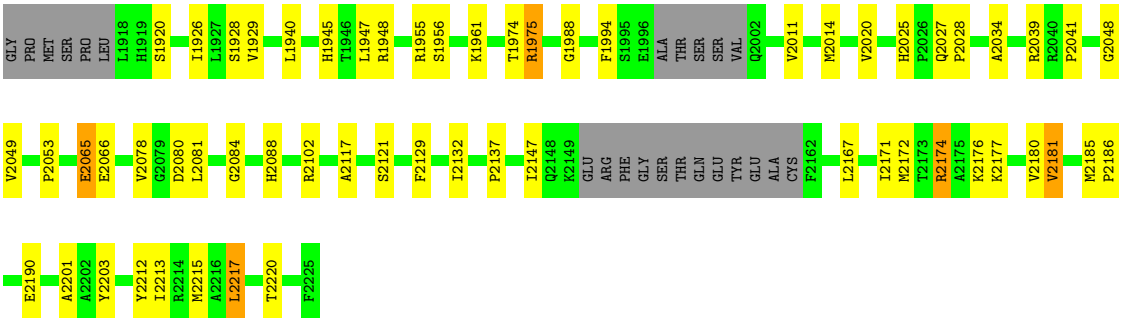
Chain C:





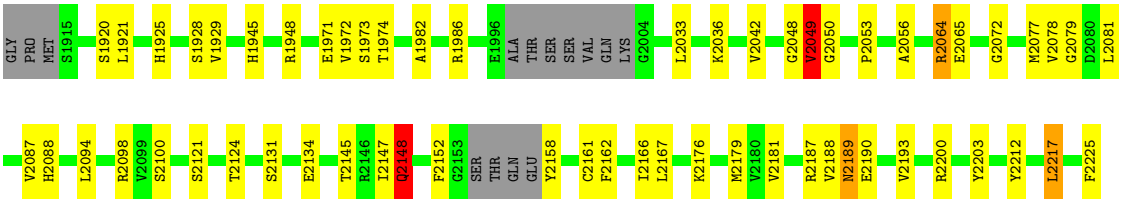
• Molecule 1: CAD protein

Chain D:



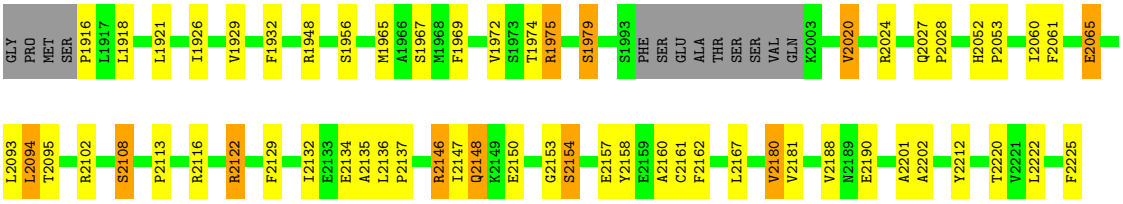
• Molecule 1: CAD protein

Chain E:



• Molecule 1: CAD protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.79Å 157.89Å 82.72Å 90.00° 120.00° 90.00°	Depositor
Resolution (Å)	42.43 – 2.10 42.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (42.43-2.10) 94.2 (42.43-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.150 , 0.172 0.153 , 0.174	Depositor DCC
R_{free} test set	5050 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 19.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.450 for -h-l,k,h 0.450 for l,k,-h-l 0.329 for -h-l,-k,l 0.328 for l,-k,h 0.328 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.095 for H, K, L 0.245 for H+L, -K, -L 0.251 for H, -K, -H-L 0.071 for L, K, -H-L 0.096 for -H-L, K, H 0.242 for L, -K, H	Depositor
Outliers	1 of 100993 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14089	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.40	0/2299	0.66	0/3104
1	B	0.41	0/2286	0.67	0/3094
1	C	0.41	0/2275	0.68	0/3073
1	D	0.41	0/2259	0.64	0/3055
1	E	0.43	0/2348	0.66	0/3173
1	F	0.40	0/2344	0.66	1/3168 (0.0%)
All	All	0.41	0/13811	0.66	1/18667 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1916	PRO	N-CA-CB	6.04	110.55	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1915	SER	Peptide

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Mol	Chain	Res	Type	Group
1	F	2160	ALA	Peptide

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	2260	0	2282	44	0
1	B	2246	0	2236	37	0
1	C	2236	0	2252	31	0
1	D	2220	0	2221	32	0
1	E	2305	0	2310	32	0
1	F	2305	0	2320	31	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	E	4	0	6	0	0
2	F	8	0	12	0	0
3	C	6	0	8	0	0
3	E	6	0	8	0	0
4	A	95	0	0	1	0
4	B	75	0	0	1	0
4	C	55	0	0	1	0
4	D	94	0	0	0	0
4	E	72	0	0	0	0
4	F	94	0	0	1	0
All	All	14089	0	13667	201	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 (201) 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:2065:GLU:OE1	1:E:1945:HIS:HE1	1.23	1.20
1:C:2065:GLU:OE1	1:E:1945:HIS:CE1	2.09	1.05
1:B:2082:LYS:HA	1:B:2112:PRO:HD3	1.55	0.86
1:D:2137:PRO:HG3	1:D:2174:ARG:HD2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1975:ARG:O	1:C:1979:SER:HB3	1.81	0.80
1:A:1929:VAL:HG21	1:A:2056:ALA:HB3	1.64	0.79
1:E:2049:VAL:H	1:E:2050:GLY:HA2	1.49	0.76
1:B:2078:VAL:HG11	1:B:2132:ILE:HD11	1.69	0.75
1:F:2157:GLU:O	1:F:2161:CYS:HB2	1.89	0.71
1:A:2117:ALA:O	1:A:2121:SER:OG	2.08	0.70
1:C:2147:ILE:O	1:C:2148:GLN:HG3	1.92	0.69
1:E:2033:LEU:HA	1:E:2036:LYS:HD2	1.73	0.69
1:C:2080:ASP:HB2	1:C:2147:ILE:HA	1.75	0.68
1:B:2047:ASP:OD1	1:B:2050:GLY:HA2	1.94	0.68
1:F:2132:ILE:O	1:F:2136:LEU:HB2	1.95	0.67
1:F:1921:LEU:HD11	1:F:1932:PHE:CE1	2.30	0.67
1:C:2081:LEU:O	1:C:2088:HIS:NE2	2.28	0.67
1:D:2081:LEU:O	1:D:2088:HIS:NE2	2.28	0.65
1:C:2011:VAL:O	1:C:2015:SER:OG	2.14	0.65
1:E:1929:VAL:HG21	1:E:2056:ALA:HB3	1.79	0.64
1:D:2137:PRO:CG	1:D:2174:ARG:HD2	2.29	0.63
1:E:1929:VAL:CG2	1:E:2053:PRO:HA	2.29	0.62
1:A:1929:VAL:HG22	1:A:2053:PRO:HA	1.81	0.62
1:A:2188:VAL:HG12	1:A:2189:ASN:N	2.15	0.62
1:E:2072:GLY:N	1:E:2098:ARG:O	2.32	0.61
1:F:2095:THR:HG23	1:F:2122:ARG:HG2	1.82	0.61
1:A:2170:HIS:O	1:A:2173:THR:OG1	2.18	0.61
1:B:2157:GLU:O	1:B:2161:CYS:HB2	2.00	0.60
1:D:2137:PRO:HG3	1:D:2174:ARG:CD	2.29	0.60
1:A:2171:ILE:HA	1:A:2174:ARG:HH11	1.66	0.60
1:F:2020:VAL:HG13	1:F:2222:LEU:HD21	1.84	0.59
1:D:2181:VAL:HG13	1:D:2201:ALA:HA	1.84	0.59
1:D:1920:SER:HB2	1:D:2220:THR:HG23	1.83	0.58
1:B:2012:GLN:NE2	4:B:4033:HOH:O	2.36	0.58
1:B:2011:VAL:HG21	1:B:2034:ALA:HB1	1.85	0.58
1:B:2209:ASN:O	1:B:2213:ILE:HG23	2.04	0.57
1:B:2167:LEU:HD23	1:B:2168:THR:N	2.19	0.57
1:B:2167:LEU:HD21	1:B:2172:MET:HG2	1.86	0.57
1:E:1925:HIS:HD2	1:E:2042:VAL:H	1.53	0.57
1:A:2005:GLU:OE2	1:C:1975:ARG:NH2	2.39	0.56
1:C:1933:THR:N	1:C:1936:GLN:OE1	2.38	0.56
1:E:1948:ARG:HA	1:E:2212:TYR:CE1	2.41	0.55
1:E:2152:PHE:CE2	1:E:2158:TYR:HD1	2.24	0.55
1:B:2084:GLY:O	1:B:2088:HIS:CD2	2.60	0.55
1:C:2060:ILE:HD11	1:C:2093:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2158:TYR:O	1:F:2162:PHE:HD1	1.91	0.54
1:B:2181:VAL:HG13	1:B:2201:ALA:HA	1.89	0.54
1:E:2189:ASN:HD22	1:E:2190:GLU:N	2.07	0.53
1:F:1921:LEU:HD13	1:F:1926:ILE:HD12	1.91	0.53
1:B:2179:MET:HG2	1:B:2180:VAL:N	2.23	0.53
1:F:2153:GLY:O	1:F:2154:SER:HB3	2.09	0.53
1:D:2137:PRO:HD3	1:D:2174:ARG:HD2	1.91	0.52
1:C:1949:MET:HB3	1:C:1953:LYS:HE3	1.91	0.52
1:F:2146:ARG:HB3	1:F:2190:GLU:CD	2.30	0.52
1:D:1926:ILE:HG21	1:D:2217:LEU:HD11	1.90	0.52
1:D:2020:VAL:HG23	1:D:2041:PRO:O	2.10	0.52
1:F:1929:VAL:HG13	1:F:2053:PRO:HA	1.92	0.52
1:B:1975:ARG:O	1:B:1979:SER:HB2	2.10	0.52
1:A:2162:PHE:O	1:A:2164:GLN:N	2.34	0.52
1:B:1929:VAL:HG11	1:B:2056:ALA:HB3	1.92	0.52
1:A:2180:VAL:CG2	1:A:2202:ALA:HB3	2.40	0.51
1:A:2187:ARG:NH2	1:A:2196:ASP:OD2	2.37	0.51
1:D:1945:HIS:CE1	1:D:1948:ARG:HH21	2.28	0.51
1:D:2190:GLU:OE1	1:D:2190:GLU:N	2.34	0.51
1:A:2118:PHE:CZ	1:A:2122:ARG:HG3	2.46	0.51
1:A:1929:VAL:CG2	1:A:2053:PRO:HA	2.41	0.50
1:A:1920:SER:HB3	1:A:2220:THR:HG23	1.93	0.50
1:A:2050:GLY:O	1:A:2051:GLU:C	2.48	0.50
1:C:2087:VAL:HG21	1:C:2145:THR:HG21	1.94	0.50
1:E:2048:GLY:O	1:E:2049:VAL:HG13	2.11	0.50
1:D:1947:LEU:HD13	1:D:2215:MET:HB3	1.94	0.50
1:C:2008:ALA:O	1:C:2012:GLN:HB2	2.12	0.50
1:C:2060:ILE:HD11	1:C:2093:LEU:HD21	1.93	0.50
1:C:2036:LYS:HD3	1:C:2037:HIS:CE1	2.47	0.50
1:D:1928:SER:HA	1:D:2053:PRO:HG3	1.93	0.50
1:D:2137:PRO:CD	1:D:2174:ARG:HD2	2.42	0.50
1:C:1928:SER:O	1:C:1931:GLN:HG2	2.12	0.49
1:F:2113:PRO:HA	1:F:2116:ARG:HB2	1.94	0.49
1:F:2181:VAL:HG13	1:F:2201:ALA:HA	1.94	0.49
1:F:2153:GLY:O	1:F:2154:SER:CB	2.60	0.49
1:E:1929:VAL:HG22	1:E:2053:PRO:HA	1.94	0.49
1:D:1994:PHE:HD1	1:D:2014:MET:CE	2.26	0.49
1:B:2066:GLU:HB3	1:B:2180:VAL:HG21	1.95	0.49
1:C:2106:PRO:HG2	1:C:2109:LEU:HG	1.94	0.49
1:D:2011:VAL:HG21	1:D:2034:ALA:HB1	1.94	0.49
1:E:2049:VAL:N	1:E:2050:GLY:HA2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2183:HIS:HE2	1:B:2190:GLU:HG3	1.78	0.49
1:C:1945:HIS:CE1	1:E:2065:GLU:HG3	2.48	0.49
1:E:2131:SER:OG	1:E:2134:GLU:HB2	2.13	0.49
1:E:2176:LYS:O	1:E:2200:ARG:NH1	2.44	0.49
1:B:1975:ARG:CG	1:B:1975:ARG:HH11	2.25	0.48
1:D:2080:ASP:HB2	1:D:2147:ILE:HA	1.94	0.48
1:E:2081:LEU:O	1:E:2088:HIS:NE2	2.45	0.48
1:F:2061:PHE:CE1	1:F:2065:GLU:HG3	2.49	0.48
1:C:2028:PRO:HA	1:C:2048:GLY:HA3	1.96	0.48
1:A:1965:MET:HE1	1:A:1967:SER:HB2	1.95	0.48
1:E:2166:ILE:HG12	1:E:2190:GLU:HA	1.94	0.48
1:E:2147:ILE:O	1:E:2148:GLN:HG2	2.14	0.47
1:B:2167:LEU:HD22	1:B:2195:VAL:HG21	1.96	0.47
1:D:2066:GLU:HB3	1:D:2180:VAL:HG21	1.96	0.47
1:F:2129:PHE:CD2	1:F:2134:GLU:HB3	2.50	0.47
1:A:1959:ILE:HG22	1:A:2224:ARG:HG3	1.96	0.47
1:A:2187:ARG:HH22	1:A:2196:ASP:CG	2.19	0.47
1:A:2202:ALA:HB2	1:A:2205:ARG:HH21	1.79	0.47
1:F:1965:MET:HE1	1:F:1967:SER:HB2	1.96	0.47
1:A:2214:ARG:O	1:A:2218:LEU:HG	2.15	0.47
1:E:1920:SER:OG	1:E:2225:PHE:O	2.29	0.46
1:F:2095:THR:CG2	1:F:2122:ARG:HG2	2.45	0.46
1:C:1920:SER:O	1:C:1924:GLN:NE2	2.48	0.46
1:B:1932:PHE:HB3	1:B:1937:MET:HG3	1.97	0.46
1:A:1965:MET:CE	1:A:1967:SER:HB2	2.46	0.46
1:C:2179:MET:CE	1:C:2181:VAL:HG12	2.46	0.46
1:F:1921:LEU:HD13	1:F:1926:ILE:CD1	2.46	0.46
1:F:1975:ARG:HG3	4:F:4018:HOH:O	2.15	0.46
1:A:1929:VAL:HG21	1:A:2056:ALA:CB	2.41	0.46
1:D:1945:HIS:CE1	1:D:2065:GLU:OE2	2.69	0.46
1:A:2078:VAL:HG21	1:A:2144:MET:HE2	1.97	0.45
1:B:1929:VAL:HG13	1:B:2053:PRO:HA	1.98	0.45
1:F:1948:ARG:HG3	1:F:2212:TYR:CE2	2.51	0.45
1:F:2136:LEU:N	1:F:2137:PRO:CD	2.80	0.45
1:A:2167:LEU:HD22	1:A:2172:MET:HG2	1.98	0.45
1:B:1949:MET:HB3	1:B:1953:LYS:HE3	1.97	0.45
1:B:2190:GLU:OE1	1:B:2190:GLU:N	2.41	0.45
1:D:2025:HIS:CE1	1:D:2027:GLN:HB3	2.52	0.45
1:D:1994:PHE:HD1	1:D:2014:MET:HE3	1.79	0.45
1:F:1965:MET:CE	1:F:1967:SER:HB2	2.47	0.45
1:E:2176:LYS:HB2	1:E:2179:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2167:LEU:HD21	1:B:2172:MET:CG	2.46	0.45
1:D:2088:HIS:N	1:D:2088:HIS:CD2	2.85	0.44
1:E:1971:GLU:O	1:E:1973:SER:N	2.51	0.44
1:C:2024:ARG:HB2	1:C:2045:ALA:HB3	1.99	0.44
1:C:2081:LEU:CD1	1:C:2103:TYR:HB3	2.48	0.44
1:A:1942:ASN:ND2	4:A:4013:HOH:O	2.41	0.44
1:A:1947:LEU:HD13	1:A:2215:MET:HB3	2.00	0.44
1:C:1966:ALA:HB3	1:C:2021:VAL:HG22	1.99	0.44
1:E:2077:MET:SD	1:E:2087:VAL:HG13	2.57	0.44
1:A:2076:THR:HG23	1:A:2102:ARG:HB2	1.99	0.44
1:B:1928:SER:OG	1:B:1930:GLN:HB2	2.18	0.44
1:B:2081:LEU:CD1	1:B:2103:TYR:HB3	2.48	0.44
1:D:1975:ARG:NH2	1:D:2186:PRO:HB3	2.33	0.44
1:F:2129:PHE:HD2	1:F:2134:GLU:HB3	1.83	0.43
1:A:1974:THR:HA	1:A:1977:SER:OG	2.18	0.43
1:F:2108:SER:OG	1:F:2157:GLU:OE2	2.24	0.43
1:F:2060:ILE:HD13	1:F:2093:LEU:HD23	2.00	0.43
1:D:2172:MET:C	1:D:2174:ARG:H	2.20	0.43
1:E:2147:ILE:HG21	1:E:2152:PHE:CZ	2.53	0.43
1:B:2049:VAL:N	1:B:2050:GLY:HA2	2.33	0.43
1:A:2059:ASP:OD1	1:A:2206:GLN:NE2	2.49	0.43
1:E:1982:ALA:O	1:E:1986:ARG:HG3	2.19	0.43
1:D:2078:VAL:HG11	1:D:2132:ILE:HD11	2.00	0.43
1:B:2113:PRO:HA	1:B:2116:ARG:HE	1.84	0.43
1:B:2060:ILE:CD1	1:B:2093:LEU:HD23	2.49	0.43
1:D:1948:ARG:HA	1:D:2212:TYR:CE1	2.53	0.43
1:D:1961:LYS:HA	1:D:1988:GLY:O	2.18	0.43
1:E:2078:VAL:HG12	1:E:2079:GLY:N	2.34	0.43
1:A:2180:VAL:HG21	1:A:2202:ALA:HB3	2.01	0.42
4:C:4034:HOH:O	1:E:2064:ARG:NH2	2.30	0.42
1:D:2185:MET:HA	1:D:2185:MET:HE2	2.00	0.42
1:F:2147:ILE:O	1:F:2148:GLN:CB	2.67	0.42
1:A:2106:PRO:HG2	1:A:2109:LEU:HD12	2.01	0.42
1:A:2060:ILE:HD11	1:A:2094:LEU:HD13	2.01	0.42
1:C:2086:THR:O	1:C:2089:SER:HB3	2.19	0.42
1:D:2028:PRO:HA	1:D:2048:GLY:HA3	2.00	0.42
1:F:1969:PHE:HD2	1:F:2024:ARG:HD3	1.84	0.42
1:A:2188:VAL:CG1	1:A:2189:ASN:N	2.81	0.42
1:A:2049:VAL:C	1:A:2085:ARG:HD3	2.39	0.42
1:A:2202:ALA:O	1:A:2206:GLN:HB2	2.20	0.42
1:B:1948:ARG:HA	1:B:2212:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2136:LEU:HD11	1:B:2179:MET:HE3	2.02	0.42
1:A:2116:ARG:HA	1:A:2126:GLN:HE22	1.85	0.42
1:D:2102:ARG:HD3	1:D:2129:PHE:CE1	2.55	0.42
1:E:1921:LEU:HD23	1:E:1921:LEU:N	2.35	0.42
1:C:2179:MET:C	1:C:2179:MET:SD	2.98	0.42
1:E:2217:LEU:HD23	1:E:2217:LEU:HA	1.82	0.42
1:A:2187:ARG:HD2	1:A:2187:ARG:C	2.40	0.42
1:B:2178:LYS:HG2	1:B:2178:LYS:O	2.19	0.42
1:E:2147:ILE:HG21	1:E:2152:PHE:CE2	2.55	0.41
1:F:2180:VAL:HG22	1:F:2202:ALA:HB2	2.01	0.41
1:A:1968:MET:O	1:A:2023:LEU:HD12	2.20	0.41
1:B:2102:ARG:NH1	1:B:2138:ASP:HB2	2.35	0.41
1:A:1975:ARG:HH12	1:B:2013:THR:HG21	1.84	0.41
1:B:1975:ARG:CG	1:B:1975:ARG:NH1	2.82	0.41
1:A:2024:ARG:NH1	1:A:2046:GLY:HA3	2.35	0.41
1:A:1956:SER:HB2	1:B:1961:LYS:HE3	2.03	0.41
1:A:2102:ARG:HA	1:A:2127:GLU:O	2.20	0.41
1:A:2202:ALA:HB2	1:A:2205:ARG:NH2	2.36	0.41
1:B:1920:SER:HB2	1:B:2220:THR:HB	2.03	0.41
1:B:2112:PRO:HB2	1:B:2115:VAL:HG23	2.03	0.41
1:C:1969:PHE:CD2	1:C:2024:ARG:HD3	2.56	0.41
1:D:1955:ARG:HG3	1:D:1956:SER:N	2.36	0.41
1:E:2147:ILE:CG2	1:E:2152:PHE:CE2	3.03	0.41
1:F:1975:ARG:O	1:F:1979:SER:HB2	2.20	0.41
1:C:2112:PRO:HG2	1:C:2115:VAL:CG2	2.51	0.41
1:F:2027:GLN:HA	1:F:2028:PRO:HD2	1.96	0.41
1:C:1941:PHE:CE1	1:C:2061:PHE:HB2	2.56	0.40
1:A:2078:VAL:HG21	1:A:2144:MET:CE	2.51	0.40
1:A:2142:LEU:HG	1:A:2144:MET:HE2	2.02	0.40
1:C:2087:VAL:CG2	1:C:2145:THR:HG21	2.51	0.40
1:F:2102:ARG:NH1	1:F:2135:ALA:O	2.54	0.40
1:C:2115:VAL:O	1:C:2119:VAL:HG23	2.21	0.40
1:D:2117:ALA:O	1:D:2121:SER:HB3	2.21	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	288/314 (92%)	262 (91%)	21 (7%)	5 (2%)	9 4
1	B	290/314 (92%)	274 (94%)	12 (4%)	4 (1%)	11 6
1	C	284/314 (90%)	268 (94%)	14 (5%)	2 (1%)	22 18
1	D	285/314 (91%)	267 (94%)	16 (6%)	2 (1%)	22 18
1	E	294/314 (94%)	275 (94%)	15 (5%)	4 (1%)	11 6
1	F	297/314 (95%)	270 (91%)	23 (8%)	4 (1%)	12 7
All	All	1738/1884 (92%)	1616 (93%)	101 (6%)	21 (1%)	13 8

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	2154	SER
1	A	2148	GLN
1	A	2163	GLY
1	B	2189	ASN
1	C	2084	GLY
1	C	2095	THR
1	D	2084	GLY
1	E	2049	VAL
1	A	2051	GLU
1	D	2176	LYS
1	F	2094	LEU
1	A	2036	LYS
1	B	2155	THR
1	E	1972	VAL
1	E	2148	GLN
1	A	1972	VAL
1	B	1916	PRO
1	F	2148	GLN
1	E	2188	VAL
1	F	2188	VAL

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Mol	Chain	Res	Type
1	B	2107	PRO

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	244/268 (91%)	229 (94%)	15 (6%)	18 16
1	B	237/268 (88%)	218 (92%)	19 (8%)	12 8
1	C	242/268 (90%)	219 (90%)	23 (10%)	8 5
1	D	237/268 (88%)	222 (94%)	15 (6%)	18 15
1	E	245/268 (91%)	226 (92%)	19 (8%)	12 9
1	F	247/268 (92%)	229 (93%)	18 (7%)	14 11
All	All	1452/1608 (90%)	1343 (92%)	109 (8%)	13 10

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1967	SER
1	A	1971	GLU
1	A	1996	GLU
1	A	2020	VAL
1	A	2064	ARG
1	A	2074	THR
1	A	2083	HIS
1	A	2094	LEU
1	A	2098	ARG
1	A	2114	THR
1	A	2121	SER
1	A	2167	LEU
1	A	2173	THR
1	A	2187	ARG
1	A	2193	VAL
1	B	1929	VAL
1	B	1971	GLU

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Mol	Chain	Res	Type
1	B	1975	ARG
1	B	1976	THR
1	B	1979	SER
1	B	2036	LYS
1	B	2058	LEU
1	B	2064	ARG
1	B	2094	LEU
1	B	2098	ARG
1	B	2114	THR
1	B	2128	GLU
1	B	2161	CYS
1	B	2176	LYS
1	B	2179	MET
1	B	2185	MET
1	B	2203	TYR
1	B	2213	ILE
1	B	2217	LEU
1	C	1920	SER
1	C	1929	VAL
1	C	1931	GLN
1	C	1961	LYS
1	C	1979	SER
1	C	1993	SER
1	C	2015	SER
1	C	2020	VAL
1	C	2027	GLN
1	C	2058	LEU
1	C	2064	ARG
1	C	2094	LEU
1	C	2108	SER
1	C	2109	LEU
1	C	2114	THR
1	C	2167	LEU
1	C	2179	MET
1	C	2180	VAL
1	C	2181	VAL
1	C	2203	TYR
1	C	2217	LEU
1	C	2224	ARG
1	C	2225	PHE
1	D	1929	VAL
1	D	1940	LEU

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Mol	Chain	Res	Type
1	D	1974	THR
1	D	1975	ARG
1	D	2039	ARG
1	D	2049	VAL
1	D	2065	GLU
1	D	2167	LEU
1	D	2171	ILE
1	D	2174	ARG
1	D	2177	LYS
1	D	2181	VAL
1	D	2203	TYR
1	D	2213	ILE
1	D	2217	LEU
1	E	1928	SER
1	E	1974	THR
1	E	2049	VAL
1	E	2064	ARG
1	E	2094	LEU
1	E	2100	SER
1	E	2121	SER
1	E	2124	THR
1	E	2145	THR
1	E	2148	GLN
1	E	2161	CYS
1	E	2162	PHE
1	E	2167	LEU
1	E	2181	VAL
1	E	2187	ARG
1	E	2189	ASN
1	E	2193	VAL
1	E	2203	TYR
1	E	2217	LEU
1	F	1918	LEU
1	F	1956	SER
1	F	1972	VAL
1	F	1974	THR
1	F	1975	ARG
1	F	1979	SER
1	F	2020	VAL
1	F	2052	HIS
1	F	2065	GLU
1	F	2094	LEU

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Mol	Chain	Res	Type
1	F	2108	SER
1	F	2122	ARG
1	F	2146	ARG
1	F	2150	GLU
1	F	2167	LEU
1	F	2180	VAL
1	F	2220	THR
1	F	2225	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2126	GLN
1	D	1945	HIS
1	D	2027	GLN
1	D	2052	HIS
1	D	2126	GLN
1	E	1925	HIS
1	E	1945	HIS
1	E	2189	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	GOL	C	3226	-	5,5,5	0.34	0	5,5,5	0.23	0
2	EDO	F	3226	-	3,3,3	0.49	0	2,2,2	0.36	0
3	GOL	E	3227	-	5,5,5	0.38	0	5,5,5	0.18	0
2	EDO	A	3226	-	3,3,3	0.37	0	2,2,2	0.60	0
2	EDO	F	3227	-	3,3,3	0.50	0	2,2,2	0.20	0
2	EDO	B	3226	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	E	3226	-	3,3,3	0.54	0	2,2,2	0.12	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	C	3226	-	-	0/4/4/4	-
2	EDO	F	3226	-	-	0/1/1/1	-
3	GOL	E	3227	-	-	4/4/4/4	-
2	EDO	A	3226	-	-	1/1/1/1	-
2	EDO	F	3227	-	-	1/1/1/1	-
2	EDO	B	3226	-	-	1/1/1/1	-
2	EDO	E	3226	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	3227	GOL	C1-C2-C3-O3
3	E	3227	GOL	O2-C2-C3-O3
2	E	3226	EDO	O1-C1-C2-O2
2	A	3226	EDO	O1-C1-C2-O2
2	F	3227	EDO	O1-C1-C2-O2
3	E	3227	GOL	O1-C1-C2-C3
2	B	3226	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	E	3227	GOL	O1-C1-C2-O2

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

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	294/314 (93%)	-0.73	0	100	100	22, 35, 50, 58	0
1	B	296/314 (94%)	-0.72	0	100	100	21, 35, 46, 51	0
1	C	290/314 (92%)	-0.75	0	100	100	20, 33, 49, 58	0
1	D	291/314 (92%)	-0.78	0	100	100	20, 32, 46, 54	0
1	E	300/314 (95%)	-0.75	0	100	100	21, 32, 49, 54	0
1	F	301/314 (95%)	-0.72	0	100	100	22, 34, 50, 62	0
All	All	1772/1884 (94%)	-0.74	0	100	100	20, 34, 48, 62	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
3	GOL	E	3227	6/6	0.85	0.21	55,56,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	E	3226	4/4	0.93	0.08	50,50,50,51	0
3	GOL	C	3226	6/6	0.94	0.13	42,42,43,44	0
2	EDO	A	3226	4/4	0.96	0.11	22,23,25,28	0
2	EDO	F	3226	4/4	0.96	0.12	41,42,43,47	0
2	EDO	F	3227	4/4	0.97	0.07	39,39,41,41	0
2	EDO	B	3226	4/4	0.98	0.07	26,26,26,28	0

6.5 Other polymers (i)

There are no such residues in this entry.