Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 04:12 PM EDT

PDB ID	:	3QJ1
Title	:	Crystal structure of camel peptidoglycan recognition protein, PGRP-S with a trapped diethylene glycol in the ligand diffusion channel at 3.2 A resolution
Authors	:	Sharma, P.; Yamini, S.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2011-01-28
Resolution	:	3.20 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 (i)) were used in the production of this report:

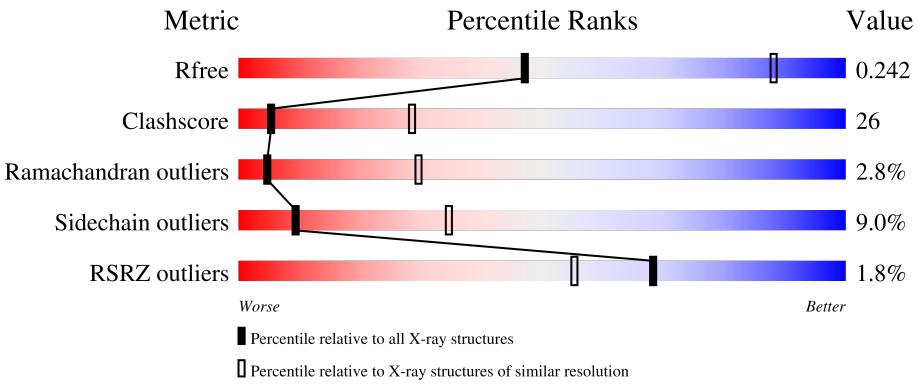
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	171	3%, 62%, 29%, 9%
1	B	171	%, 50%, 43%, 7% •
1	C	171	2%, 58%, 35%, 5% •
1	D	171	%, 60%, 33%, 6% •

2 Entry composition (i)

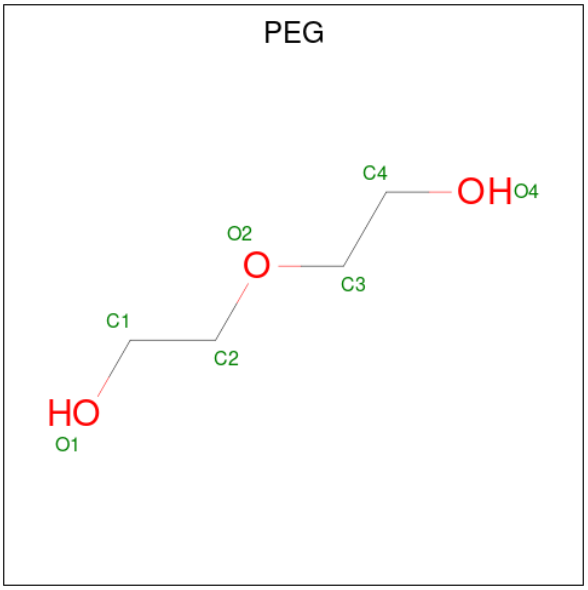
There are 5 unique types of molecules in this entry. The entry contains 5452 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan recognition protein 1.

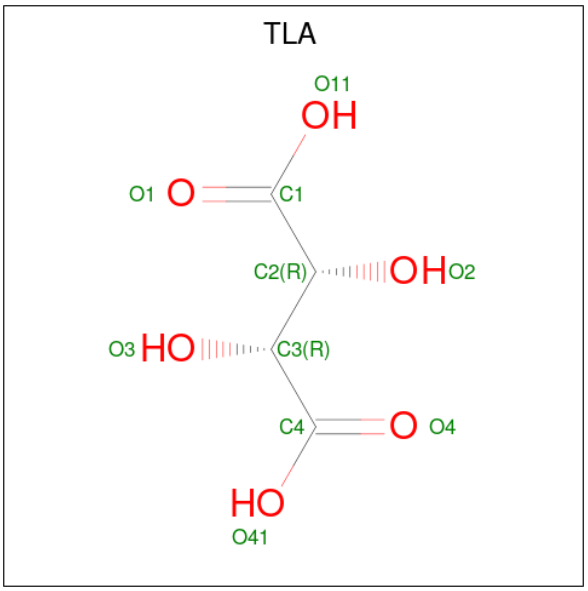
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1337	834	254	241	8	0	0	0
1	B	171	1337	834	254	241	8	0	0	0
1	C	171	1337	834	254	241	8	0	0	0
1	D	171	1337	834	254	241	8	0	0	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



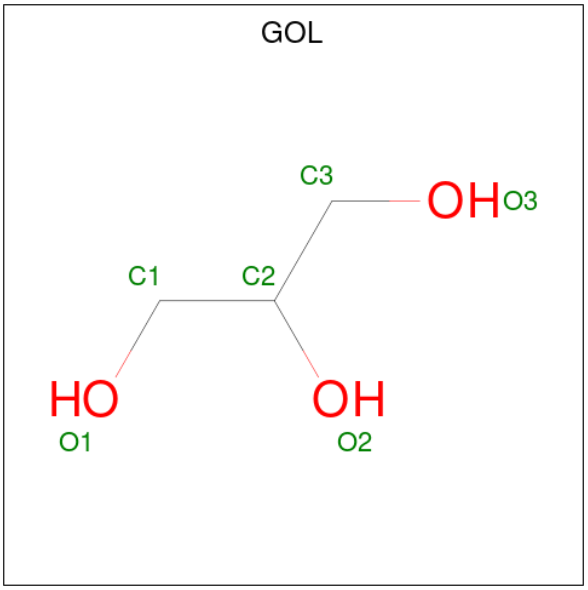
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	7	4	3	0	0

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	10	4	6	0	0

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



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

- Molecule 5 is water.

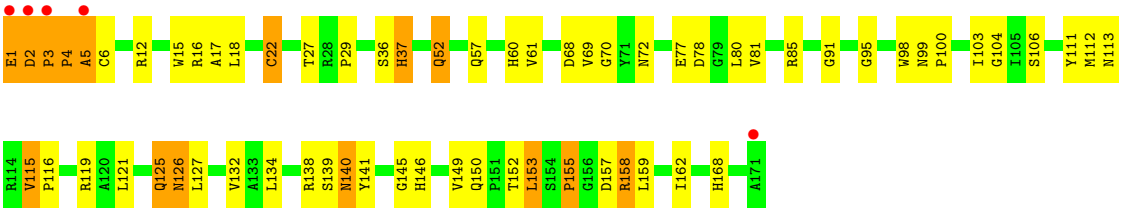
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	21	21	21	0	0
			Total	O		
5	B	24	24	24	0	0
			Total	O		
5	C	19	19	19	0	0
			Total	O		
5	D	17	17	17	0	0

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.

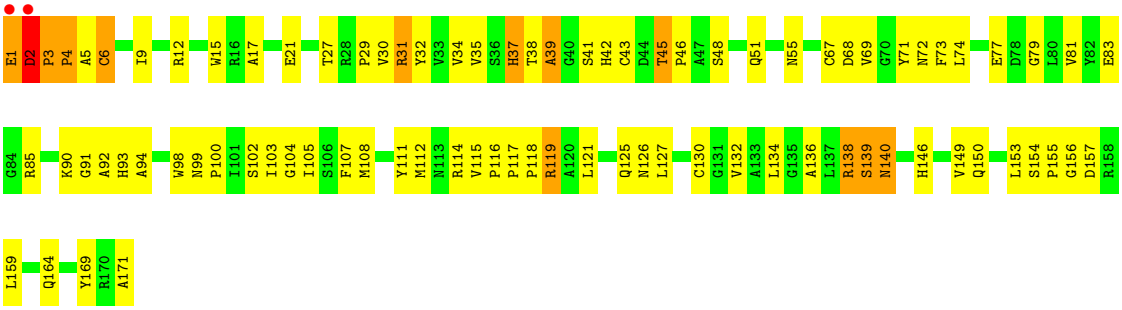
• Molecule 1: Peptidoglycan recognition protein 1

Chain A:



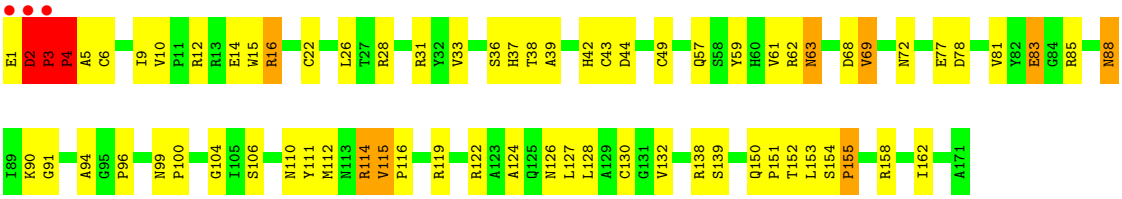
• Molecule 1: Peptidoglycan recognition protein 1

Chain B:



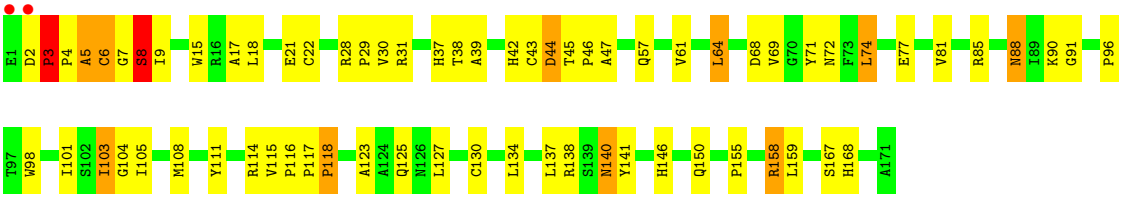
• Molecule 1: Peptidoglycan recognition protein 1

Chain C:



• Molecule 1: Peptidoglycan recognition protein 1

Chain D:


E1
D2
P3
P4
A5
C6
G7
S8
I9
W15
R16
A17
L18
E21
C22
R28
P29
V30
R31
H37
T38
A39
H42
C43
D44
T45
P46
A47
Q57
V61
L64
D68
V69
G70
Y71
N72
F73
L74
E77
V81
R85
N88
I89
K90
G91
P96
T97
W98
I101
S102
I103
G104
I105
M108
Y111
R114
V115
P116
P117
P118
A123
A124
Q125
N126
L127
C130
L134
L137
R138
S139
N140
Y141
H146
Q150
P155
R158
L159
S167
H168
A171

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	89.54Å 100.60Å 163.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.35 – 3.20 42.35 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.35-3.20) 96.1 (42.35-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.248 0.190 , 0.242	Depositor DCC
R_{free} test set	585 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 31.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5452	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: GOL, TLA, PEG

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	0.46	0/1374	0.82	2/1871 (0.1%)
1	B	0.50	0/1374	0.78	0/1871
1	C	0.46	0/1374	0.75	1/1871 (0.1%)
1	D	0.59	2/1374 (0.1%)	0.82	4/1871 (0.2%)
All	All	0.50	2/5496 (0.0%)	0.79	7/7484 (0.1%)

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	2
1	C	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3	PRO	C-N	9.45	1.52	1.34
1	D	6	CYS	C-N	-5.18	1.23	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	CYS	CB-CA-C	-9.16	92.08	110.40
1	D	3	PRO	C-N-CD	6.44	141.93	128.40
1	D	140	ASN	CB-CA-C	-5.82	98.75	110.40
1	D	3	PRO	O-C-N	5.81	132.15	121.10
1	D	8	SER	N-CA-C	-5.09	97.25	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2	ASP	C-N-CD	-5.07	109.45	120.60
1	A	22	CYS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	ASP	Peptide
1	B	3	PRO	Peptide
1	C	2	ASP	Peptide
1	C	3	PRO	Peptide
1	C	4	PRO	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	1337	0	1288	56	0
1	B	1337	0	1288	81	0
1	C	1337	0	1288	72	0
1	D	1337	0	1288	75	0
2	B	7	0	10	1	0
3	C	10	0	4	1	0
4	D	6	0	8	2	0
5	A	21	0	0	3	0
5	B	24	0	0	2	0
5	C	19	0	0	0	0
5	D	17	0	0	2	0
All	All	5452	0	5174	277	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 26.

All (277) 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:D:3:PRO:HG2	1:D:4:PRO:CD	1.63	1.29
1:D:3:PRO:CG	1:D:4:PRO:HD3	1.80	1.11
1:C:112:MET:HE3	1:C:153:LEU:HB3	1.31	1.08
1:B:72:ASN:ND2	1:B:104:GLY:H	1.53	1.06
1:D:72:ASN:ND2	1:D:104:GLY:H	1.53	1.06
1:C:96:PRO:HG3	1:D:96:PRO:HG3	1.42	1.01
1:D:72:ASN:HD22	1:D:104:GLY:H	1.01	1.00
1:D:3:PRO:HG2	1:D:4:PRO:HD3	1.03	0.99
1:B:94:ALA:H	1:B:99:ASN:HD21	1.07	0.98
1:C:2:ASP:HB3	1:C:4:PRO:HD3	1.51	0.93
1:C:94:ALA:H	1:C:99:ASN:HD21	1.18	0.92
1:B:72:ASN:HD22	1:B:104:GLY:H	1.15	0.91
1:A:72:ASN:HD22	1:A:104:GLY:H	1.17	0.90
1:D:57:GLN:O	1:D:61:VAL:HG23	1.72	0.90
1:D:115:VAL:HG12	1:D:158:ARG:HB3	1.54	0.90
1:B:112:MET:HE3	1:B:153:LEU:HB3	1.55	0.89
1:D:8:SER:HA	5:D:184:HOH:O	1.73	0.87
1:A:72:ASN:ND2	1:A:104:GLY:H	1.76	0.84
1:A:121:LEU:O	1:A:125:GLN:HG3	1.79	0.82
1:C:112:MET:CE	1:C:153:LEU:HB3	2.11	0.81
1:C:115:VAL:HG12	1:C:162:ILE:HD11	1.62	0.81
1:A:72:ASN:HD22	1:A:104:GLY:N	1.80	0.80
1:D:72:ASN:HD22	1:D:104:GLY:N	1.79	0.80
1:C:96:PRO:HG3	1:D:96:PRO:CG	2.12	0.80
1:C:59:TYR:HD1	1:C:63:ASN:HD22	1.29	0.78
1:C:1:GLU:CG	1:C:1:GLU:O	2.30	0.77
1:D:3:PRO:CG	1:D:4:PRO:CD	2.48	0.77
1:B:94:ALA:H	1:B:99:ASN:ND2	1.81	0.77
1:C:4:PRO:O	1:C:4:PRO:HG2	1.85	0.76
1:C:62:ARG:HG3	1:C:62:ARG:HH11	1.50	0.76
1:B:112:MET:CE	1:B:153:LEU:HB3	2.18	0.74
1:C:111:TYR:CE1	1:C:116:PRO:HG3	2.22	0.74
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.54	0.73
1:B:72:ASN:HD22	1:B:104:GLY:N	1.87	0.71
1:B:35:VAL:HG22	1:B:105:ILE:HD11	1.73	0.71
1:C:1:GLU:O	1:C:1:GLU:HG2	1.90	0.70
1:B:31:ARG:HG2	1:B:32:TYR:CE2	2.26	0.69
1:A:155:PRO:HB2	1:A:159:LEU:HD23	1.74	0.69
1:B:138:ARG:HE	1:B:140:ASN:HD21	1.41	0.69
1:D:2:ASP:O	1:D:3:PRO:C	2.29	0.69
1:C:28:ARG:HH21	1:C:88:ASN:ND2	1.91	0.68
1:B:111:TYR:CD1	1:B:116:PRO:HD3	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PRO:HG2	1:A:159:LEU:HD13	1.74	0.68
1:D:105:ILE:O	1:D:105:ILE:HG13	1.93	0.68
5:A:174:HOH:O	1:B:118:PRO:HD2	1.94	0.67
1:B:72:ASN:ND2	1:B:104:GLY:N	2.37	0.67
1:D:4:PRO:O	1:D:6:CYS:N	2.29	0.66
1:B:37:HIS:HD2	1:B:111:TYR:H	1.42	0.66
1:B:9:ILE:HG21	1:B:83:GLU:HB2	1.76	0.66
1:C:37:HIS:CE1	1:C:154:SER:HA	2.31	0.65
1:D:74:LEU:HD22	1:D:108:MET:HE3	1.78	0.65
1:B:32:TYR:HB2	1:B:102:SER:HB3	1.78	0.65
1:A:36:SER:OG	1:A:106:SER:HB3	1.97	0.64
1:D:155:PRO:HB2	1:D:159:LEU:HD23	1.79	0.64
1:A:85:ARG:HD2	1:A:91:GLY:HA2	1.80	0.64
1:B:12:ARG:HD2	5:B:189:HOH:O	1.98	0.64
1:A:115:VAL:HG12	1:A:162:ILE:HD11	1.81	0.63
1:C:72:ASN:HD22	1:C:104:GLY:H	1.46	0.63
1:D:2:ASP:O	1:D:5:ALA:N	2.32	0.63
1:A:2:ASP:OD2	1:A:2:ASP:N	2.32	0.62
1:A:15:TRP:CZ2	1:A:17:ALA:HB2	2.35	0.62
1:C:132:VAL:CG1	1:C:139:SER:HA	2.29	0.62
1:C:38:THR:O	1:C:39:ALA:HB3	2.00	0.62
1:A:37:HIS:HD2	1:A:111:TYR:H	1.47	0.62
1:D:3:PRO:O	1:D:4:PRO:C	2.38	0.61
1:D:81:VAL:HG11	1:D:127:LEU:HD13	1.81	0.61
1:D:3:PRO:HG2	1:D:4:PRO:HD2	1.72	0.61
1:B:2:ASP:N	1:B:2:ASP:OD1	2.30	0.61
1:B:38:THR:O	1:B:39:ALA:HB3	2.00	0.61
1:D:3:PRO:CB	1:D:4:PRO:HD3	2.30	0.60
1:A:132:VAL:HG13	1:A:139:SER:HA	1.83	0.60
1:B:45:THR:HG22	1:B:48:SER:H	1.67	0.60
1:B:31:ARG:HG2	1:B:32:TYR:CD2	2.37	0.60
1:D:140:ASN:C	1:D:140:ASN:OD1	2.38	0.60
1:C:42:HIS:CG	1:C:114:ARG:HH22	2.20	0.59
1:C:94:ALA:H	1:C:99:ASN:ND2	1.95	0.59
1:B:81:VAL:HG11	1:B:127:LEU:HD13	1.84	0.59
1:D:37:HIS:ND1	1:D:155:PRO:HA	2.18	0.59
1:C:12:ARG:HG3	1:C:83:GLU:CG	2.33	0.59
1:C:111:TYR:CD1	1:C:116:PRO:HG3	2.37	0.59
1:C:150:GLN:HB2	1:C:151:PRO:HD2	1.85	0.59
1:B:90:LYS:HG3	1:B:99:ASN:O	2.02	0.58
1:C:37:HIS:HD2	1:C:110:ASN:HA	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:HIS:ND1	1:C:154:SER:HA	2.18	0.58
1:C:115:VAL:CG1	1:C:162:ILE:HD11	2.31	0.58
1:B:132:VAL:HG11	1:B:139:SER:HB3	1.84	0.58
1:D:74:LEU:HD22	1:D:108:MET:CE	2.34	0.58
1:A:15:TRP:CH2	1:A:17:ALA:HB2	2.39	0.57
1:A:138:ARG:HE	1:A:140:ASN:HD21	1.53	0.57
1:B:30:VAL:HG23	1:B:136:ALA:O	2.05	0.57
5:A:174:HOH:O	1:B:119:ARG:HB3	2.04	0.57
1:C:132:VAL:HG11	1:C:139:SER:HA	1.85	0.57
1:C:72:ASN:ND2	1:C:104:GLY:H	2.02	0.57
1:D:38:THR:O	1:D:39:ALA:HB3	2.04	0.57
1:A:99:ASN:N	1:A:100:PRO:HD2	2.20	0.56
1:B:171:ALA:HB1	5:B:185:HOH:O	2.03	0.56
1:D:146:HIS:CE1	4:D:172:GOL:H32	2.40	0.56
1:C:94:ALA:N	1:C:99:ASN:HD21	1.96	0.56
1:C:150:GLN:HA	1:D:64:LEU:HD13	1.87	0.56
1:D:141:TYR:O	1:D:168:HIS:HD2	1.88	0.56
1:B:38:THR:O	1:B:39:ALA:CB	2.53	0.56
1:C:59:TYR:HD1	1:C:63:ASN:ND2	2.00	0.56
1:A:4:PRO:O	1:A:5:ALA:C	2.43	0.56
1:B:45:THR:HG23	1:B:46:PRO:HD2	1.88	0.56
1:B:155:PRO:HB2	1:B:159:LEU:HD23	1.88	0.56
1:B:164:GLN:HA	1:B:169:TYR:CG	2.41	0.56
1:C:150:GLN:O	1:C:152:THR:HG22	2.07	0.55
1:D:115:VAL:HG12	1:D:158:ARG:CB	2.33	0.55
1:B:5:ALA:O	1:B:6:CYS:C	2.42	0.55
1:D:28:ARG:HH21	1:D:88:ASN:HD21	1.55	0.55
1:A:4:PRO:O	1:A:6:CYS:N	2.39	0.55
1:A:158:ARG:HG2	1:A:158:ARG:NH1	2.20	0.55
1:D:42:HIS:CG	1:D:114:ARG:HH11	2.24	0.55
1:C:62:ARG:HG3	1:C:62:ARG:NH1	2.20	0.55
1:C:22:CYS:SG	1:C:68:ASP:HB3	2.46	0.54
1:D:3:PRO:CB	1:D:4:PRO:CD	2.85	0.54
1:D:77:GLU:HG2	1:D:117:PRO:HD2	1.88	0.54
1:A:37:HIS:CD2	1:A:111:TYR:H	2.25	0.54
1:A:152:THR:OG1	1:A:153:LEU:N	2.41	0.54
1:B:132:VAL:CG1	1:B:139:SER:HB3	2.37	0.54
1:D:3:PRO:O	1:D:5:ALA:N	2.41	0.54
1:B:146:HIS:HD1	1:B:154:SER:CB	2.21	0.54
1:C:128:LEU:O	1:C:132:VAL:HG23	2.07	0.54
1:A:36:SER:HA	1:A:155:PRO:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG11	1:A:127:LEU:HD13	1.89	0.53
1:C:39:ALA:HA	1:C:110:ASN:ND2	2.23	0.53
1:D:22:CYS:SG	1:D:68:ASP:HB3	2.48	0.53
1:D:15:TRP:CH2	1:D:17:ALA:HB2	2.43	0.53
1:D:37:HIS:CD2	1:D:111:TYR:H	2.26	0.53
1:B:94:ALA:O	1:B:98:TRP:HB2	2.08	0.53
1:A:149:VAL:O	1:A:150:GLN:HG2	2.08	0.53
1:D:111:TYR:CD1	1:D:116:PRO:HD3	2.43	0.53
1:C:2:ASP:HB3	1:C:4:PRO:CD	2.33	0.53
1:B:9:ILE:CG2	1:B:83:GLU:HB2	2.39	0.53
1:B:29:PRO:HB2	1:B:138:ARG:HB3	1.89	0.53
1:C:10:VAL:HG12	1:C:14:GLU:HB3	1.91	0.53
1:D:28:ARG:HH21	1:D:88:ASN:ND2	2.06	0.53
1:B:1:GLU:OE2	1:B:2:ASP:OD1	2.27	0.52
1:B:146:HIS:HD1	1:B:154:SER:HB3	1.74	0.52
1:A:125:GLN:HB2	1:B:4:PRO:HG2	1.90	0.52
1:D:43:CYS:O	1:D:44:ASP:HB3	2.10	0.52
1:B:79:GLY:HA3	1:B:119:ARG:HG3	1.91	0.52
1:B:43:CYS:O	1:B:77:GLU:HB2	2.09	0.52
1:C:2:ASP:OD1	1:C:3:PRO:N	2.42	0.52
1:C:85:ARG:HD2	1:C:91:GLY:HA2	1.91	0.51
1:A:112:MET:SD	1:A:157:ASP:OD1	2.69	0.51
1:A:125:GLN:HB2	1:B:4:PRO:CG	2.40	0.51
1:B:79:GLY:CA	1:B:119:ARG:HG3	2.41	0.51
1:C:43:CYS:O	1:C:77:GLU:HB2	2.11	0.51
1:A:22:CYS:SG	1:A:68:ASP:HB2	2.51	0.51
1:A:60:HIS:ND1	1:A:70:GLY:N	2.57	0.51
1:B:164:GLN:HA	1:B:169:TYR:CD2	2.46	0.51
1:A:126:ASN:HD21	1:B:5:ALA:C	2.14	0.50
1:C:83:GLU:O	1:C:83:GLU:HG3	2.11	0.50
1:D:141:TYR:O	1:D:168:HIS:CD2	2.64	0.50
1:D:4:PRO:O	1:D:6:CYS:SG	2.69	0.50
1:A:1:GLU:OE1	1:A:2:ASP:OD2	2.30	0.50
1:B:93:HIS:CG	1:B:104:GLY:HA3	2.47	0.50
1:C:31:ARG:HD2	1:C:138:ARG:HH12	1.76	0.50
1:B:3:PRO:O	1:B:4:PRO:O	2.30	0.50
1:C:26:LEU:HG	1:C:90:LYS:HA	1.94	0.50
1:C:36:SER:O	1:C:106:SER:HA	2.12	0.50
1:D:4:PRO:C	1:D:6:CYS:N	2.65	0.50
1:A:12:ARG:HB3	1:A:17:ALA:HB3	1.93	0.50
1:C:12:ARG:HA	1:C:15:TRP:NE1	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:C	1:A:140:ASN:HD22	2.15	0.49
1:A:98:TRP:CD1	1:A:149:VAL:HB	2.48	0.49
1:A:72:ASN:ND2	1:A:103:ILE:HA	2.27	0.49
1:C:42:HIS:CB	1:C:114:ARG:HH22	2.25	0.49
1:C:42:HIS:CG	1:C:114:ARG:NH2	2.81	0.49
1:D:4:PRO:C	1:D:6:CYS:H	2.17	0.49
1:A:15:TRP:CE2	1:A:17:ALA:HB2	2.47	0.48
1:C:114:ARG:O	1:C:158:ARG:HB2	2.13	0.48
1:D:38:THR:OG1	1:D:108:MET:HA	2.14	0.48
1:D:45:THR:O	1:D:47:ALA:N	2.47	0.48
1:A:111:TYR:CD1	1:A:116:PRO:HG3	2.49	0.48
1:B:146:HIS:ND1	1:B:154:SER:HB3	2.29	0.48
1:B:105:ILE:O	1:B:105:ILE:HG13	2.12	0.48
1:B:15:TRP:CZ3	1:B:17:ALA:HB2	2.49	0.47
1:B:85:ARG:HH12	1:B:92:ALA:HB2	1.80	0.47
1:C:4:PRO:O	1:C:4:PRO:CG	2.46	0.47
1:A:52:GLN:OE1	1:A:52:GLN:HA	2.10	0.47
1:A:68:ASP:OD2	1:A:69:VAL:N	2.37	0.47
1:B:73:PHE:O	1:B:105:ILE:HA	2.15	0.47
1:C:153:LEU:H	3:C:172:TLA:HB	1.61	0.47
1:D:42:HIS:CG	1:D:114:ARG:NH1	2.82	0.47
1:D:45:THR:C	1:D:47:ALA:N	2.68	0.47
1:A:99:ASN:N	1:A:100:PRO:CD	2.78	0.47
1:C:9:ILE:HG23	1:C:81:VAL:HG12	1.96	0.47
1:D:146:HIS:H	1:D:155:PRO:HD3	1.79	0.47
1:D:146:HIS:HE2	1:D:150:GLN:HG3	1.79	0.47
1:B:67:CYS:O	1:B:68:ASP:HB2	2.15	0.47
1:B:77:GLU:HG2	1:B:117:PRO:HD2	1.97	0.47
1:C:112:MET:HE3	1:C:153:LEU:CB	2.22	0.47
1:C:37:HIS:ND1	1:C:155:PRO:HA	2.30	0.47
1:D:155:PRO:O	1:D:159:LEU:HB3	2.15	0.47
1:D:46:PRO:HD3	5:D:177:HOH:O	2.14	0.46
1:B:121:LEU:O	1:B:125:GLN:HG2	2.15	0.46
1:A:2:ASP:HA	1:A:3:PRO:HD3	1.30	0.46
1:A:141:TYR:O	1:A:168:HIS:HD2	1.99	0.46
1:A:22:CYS:SG	1:A:68:ASP:CB	3.04	0.46
1:C:124:ALA:O	1:C:127:LEU:HB3	2.16	0.46
1:D:98:TRP:CE3	1:D:101:ILE:HD11	2.50	0.46
1:C:99:ASN:N	1:C:100:PRO:HD2	2.31	0.46
1:A:29:PRO:HB2	1:A:138:ARG:HG2	1.97	0.46
1:D:31:ARG:CZ	1:D:138:ARG:HH11	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLY:O	1:A:99:ASN:ND2	2.49	0.45
1:C:39:ALA:C	1:C:110:ASN:HD22	2.18	0.45
1:D:15:TRP:CZ3	1:D:17:ALA:HB2	2.51	0.45
1:B:37:HIS:CD2	1:B:111:TYR:H	2.29	0.45
1:C:26:LEU:HG	1:C:90:LYS:CA	2.46	0.45
1:C:96:PRO:CG	1:D:96:PRO:HG3	2.30	0.45
1:D:158:ARG:HA	1:D:158:ARG:HD2	1.89	0.45
1:B:107:PHE:HB3	1:B:111:TYR:CE2	2.52	0.45
1:D:3:PRO:C	1:D:5:ALA:N	2.71	0.44
1:A:77:GLU:O	1:A:119:ARG:NE	2.48	0.44
1:B:116:PRO:HA	1:B:117:PRO:HD3	1.87	0.44
1:D:37:HIS:HD2	1:D:111:TYR:H	1.64	0.44
1:C:2:ASP:OD1	1:C:3:PRO:CD	2.66	0.44
1:D:68:ASP:OD1	1:D:69:VAL:N	2.51	0.44
1:D:111:TYR:CD2	1:D:111:TYR:N	2.85	0.44
1:A:132:VAL:CG1	1:A:139:SER:HA	2.48	0.44
1:A:145:GLY:O	1:A:146:HIS:C	2.56	0.44
1:B:103:ILE:HG22	1:B:105:ILE:HG23	1.99	0.44
1:B:69:VAL:O	1:B:85:ARG:NE	2.50	0.44
5:A:181:HOH:O	1:B:3:PRO:HG3	2.17	0.44
1:B:15:TRP:CE3	1:B:17:ALA:HB2	2.52	0.44
1:A:98:TRP:C	1:A:100:PRO:HD2	2.38	0.43
1:A:68:ASP:CG	1:A:69:VAL:H	2.22	0.43
1:B:21:GLU:C	1:B:67:CYS:HB2	2.38	0.43
1:B:68:ASP:OD1	1:B:69:VAL:HG12	2.18	0.43
1:B:93:HIS:H	1:B:99:ASN:HD21	1.66	0.43
1:B:126:ASN:O	1:B:127:LEU:C	2.56	0.43
1:C:31:ARG:HD2	1:C:138:ARG:NH1	2.33	0.43
1:B:37:HIS:CE1	1:B:154:SER:HA	2.53	0.43
1:C:68:ASP:O	1:C:69:VAL:C	2.57	0.43
1:A:121:LEU:O	1:A:125:GLN:CG	2.59	0.43
1:A:140:ASN:H	1:A:140:ASN:ND2	2.16	0.43
1:C:127:LEU:O	1:C:130:CYS:HB3	2.19	0.43
1:C:14:GLU:C	1:C:16:ARG:H	2.21	0.43
1:C:28:ARG:HH21	1:C:88:ASN:HD21	1.63	0.42
1:C:62:ARG:NH1	1:C:62:ARG:CG	2.80	0.42
1:D:68:ASP:O	1:D:69:VAL:C	2.55	0.42
1:B:73:PHE:HB2	1:B:105:ILE:HG22	2.01	0.42
1:B:115:VAL:HG23	1:B:116:PRO:O	2.19	0.42
1:C:119:ARG:HB3	1:C:122:ARG:NH1	2.35	0.42
1:B:6:CYS:HB3	2:B:172:PEG:O4	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:TRP:NE1	1:B:149:VAL:HB	2.35	0.42
1:B:156:GLY:O	1:B:157:ASP:C	2.59	0.42
1:D:85:ARG:HH11	1:D:91:GLY:HA2	1.85	0.42
1:D:130:CYS:O	1:D:134:LEU:HG	2.20	0.42
1:D:30:VAL:HB	1:D:137:LEU:HD23	2.01	0.41
1:B:74:LEU:HD23	1:B:108:MET:SD	2.60	0.41
1:B:51:GLN:NE2	1:B:55:ASN:OD1	2.53	0.41
1:B:91:GLY:HA3	1:B:93:HIS:CD2	2.55	0.41
1:C:44:ASP:N	1:C:44:ASP:OD1	2.51	0.41
1:A:78:ASP:OD2	1:A:80:LEU:HD12	2.21	0.41
1:D:9:ILE:HD11	1:D:127:LEU:CD1	2.50	0.41
1:D:103:ILE:O	1:D:103:ILE:HG22	2.20	0.41
1:D:138:ARG:O	1:D:141:TYR:HB3	2.20	0.41
1:A:57:GLN:O	1:A:61:VAL:HG23	2.20	0.41
1:B:34:VAL:HG23	1:B:102:SER:HB2	2.03	0.41
1:A:81:VAL:HG21	1:A:127:LEU:HB2	2.03	0.41
1:D:71:TYR:OH	4:D:172:GOL:H31	2.20	0.41
1:B:149:VAL:HG23	1:B:150:GLN:HG2	2.02	0.41
1:C:33:VAL:HG11	1:C:128:LEU:HD21	2.03	0.41
1:B:90:LYS:HD2	1:B:100:PRO:HB3	2.01	0.41
1:D:90:LYS:HE2	1:D:90:LYS:HB3	1.90	0.41
1:B:155:PRO:O	1:B:159:LEU:HB3	2.20	0.40
1:C:49:CYS:SG	1:C:78:ASP:HB3	2.61	0.40
1:D:81:VAL:HG23	1:D:123:ALA:HB1	2.02	0.40
1:B:91:GLY:HA3	1:B:93:HIS:HD2	1.86	0.40
1:C:39:ALA:CA	1:C:110:ASN:HD22	2.34	0.40
1:D:37:HIS:ND1	1:D:37:HIS:O	2.54	0.40
1:D:117:PRO:O	1:D:118:PRO:C	2.60	0.40
1:C:57:GLN:O	1:C:61:VAL:HG23	2.21	0.40
1:D:29:PRO:HG2	1:D:138:ARG:NH2	2.36	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	169/171 (99%)	145 (86%)	21 (12%)	3 (2%)	8	41
1	B	169/171 (99%)	145 (86%)	19 (11%)	5 (3%)	4	28
1	C	169/171 (99%)	149 (88%)	13 (8%)	7 (4%)	3	21
1	D	169/171 (99%)	144 (85%)	21 (12%)	4 (2%)	6	34
All	All	676/684 (99%)	583 (86%)	74 (11%)	19 (3%)	5	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	B	2	ASP
1	B	4	PRO
1	C	3	PRO
1	C	5	ALA
1	D	3	PRO
1	D	5	ALA
1	D	44	ASP
1	A	4	PRO
1	A	5	ALA
1	B	139	SER
1	D	7	GLY
1	B	6	CYS
1	C	16	ARG
1	C	4	PRO
1	C	6	CYS
1	B	39	ALA
1	C	2	ASP
1	C	69	VAL

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	139/139 (100%)	123 (88%)	16 (12%)	5 24
1	B	139/139 (100%)	124 (89%)	15 (11%)	6 27
1	C	139/139 (100%)	131 (94%)	8 (6%)	20 55
1	D	139/139 (100%)	128 (92%)	11 (8%)	12 43
All	All	556/556 (100%)	506 (91%)	50 (9%)	9 34

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	2	ASP
1	A	16	ARG
1	A	18	LEU
1	A	27	THR
1	A	37	HIS
1	A	52	GLN
1	A	113	ASN
1	A	115	VAL
1	A	125	GLN
1	A	126	ASN
1	A	134	LEU
1	A	140	ASN
1	A	153	LEU
1	A	155	PRO
1	A	158	ARG
1	B	1	GLU
1	B	2	ASP
1	B	27	THR
1	B	31	ARG
1	B	37	HIS
1	B	41	SER
1	B	42	HIS
1	B	45	THR
1	B	71	TYR
1	B	114	ARG
1	B	119	ARG
1	B	130	CYS
1	B	134	LEU
1	B	138	ARG
1	B	140	ASN
1	C	4	PRO
1	C	63	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	83	GLU
1	C	88	ASN
1	C	114	ARG
1	C	115	VAL
1	C	126	ASN
1	C	155	PRO
1	D	8	SER
1	D	18	LEU
1	D	21	GLU
1	D	64	LEU
1	D	74	LEU
1	D	88	ASN
1	D	103	ILE
1	D	118	PRO
1	D	125	GLN
1	D	158	ARG
1	D	167	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	140	ASN
1	A	150	GLN
1	A	164	GLN
1	B	37	HIS
1	B	51	GLN
1	B	72	ASN
1	B	99	ASN
1	B	140	ASN
1	B	150	GLN
1	C	72	ASN
1	C	88	ASN
1	C	99	ASN
1	C	110	ASN
1	C	168	HIS
1	D	72	ASN
1	D	88	ASN
1	D	168	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	TLA	C	172	-	9,9,9	1.13	1 (11%)	12,12,12	1.59	4 (33%)
2	PEG	B	172	-	6,6,6	1.44	1 (16%)	5,5,5	0.83	0
4	GOL	D	172	-	5,5,5	0.24	0	5,5,5	0.64	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	TLA	C	172	-	-	0/12/12/12	-
2	PEG	B	172	-	-	3/4/4/4	-
4	GOL	D	172	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	172	TLA	O3-C3	2.33	1.46	1.42
2	B	172	PEG	O4-C4	2.30	1.53	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	172	TLA	O41-C4-C3	2.68	120.52	113.27
3	C	172	TLA	O11-C1-C2	2.34	119.59	113.27
3	C	172	TLA	O41-C4-O4	-2.16	119.18	124.09
3	C	172	TLA	O11-C1-O1	-2.15	119.20	124.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	172	PEG	O1-C1-C2-O2
2	B	172	PEG	C1-C2-O2-C3
2	B	172	PEG	O2-C3-C4-O4
4	D	172	GOL	C1-C2-C3-O3
4	D	172	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	172	TLA	1	0
2	B	172	PEG	1	0
4	D	172	GOL	2	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 (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(Å^2)	Q<0.9
1	A	171/171 (100%)	-0.42	5 (2%)	51	36	13, 28, 48, 69	0
1	B	171/171 (100%)	-0.40	2 (1%)	79	67	17, 37, 56, 72	0
1	C	171/171 (100%)	-0.50	3 (1%)	68	55	10, 25, 46, 73	0
1	D	171/171 (100%)	-0.50	2 (1%)	79	67	8, 28, 46, 87	0
All	All	684/684 (100%)	-0.46	12 (1%)	68	55	8, 29, 51, 87	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASP	5.9
1	A	3	PRO	5.8
1	A	1	GLU	4.5
1	C	2	ASP	4.1
1	C	1	GLU	3.5
1	B	2	ASP	3.1
1	A	171	ALA	3.0
1	C	3	PRO	3.0
1	B	1	GLU	2.8
1	A	5	ALA	2.1
1	D	2	ASP	2.1
1	D	1	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	PEG	B	172	7/7	0.78	0.26	52,55,57,57	0
3	TLA	C	172	10/10	0.83	0.35	47,51,56,59	0
4	GOL	D	172	6/6	0.88	0.21	38,44,45,48	0

6.5 Other polymers (i)

There are no such residues in this entry.