Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 07:16 AM EST

PDB ID	:	3NW3
Title	:	Crystal structure of the complex of peptidoglycan recognition protein (PGRP-S) with the PGN Fragment at 2.5 A resolution
Authors	:	Sharma, P.; Dube, D.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2010-07-09
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

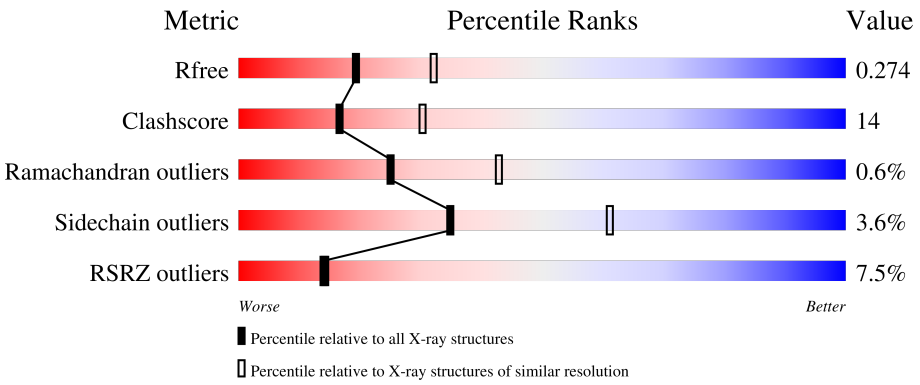
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	10% 84% 16%
1	B	171	13% 60% 36%
1	C	171	3% 80% 18%
1	D	171	4% 69% 29%

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
5	DGN	D	203	-	-	-	X
6	ALA	D	204	-	-	-	X
7	LAC	D	205	-	-	-	X

2 Entry composition (i)

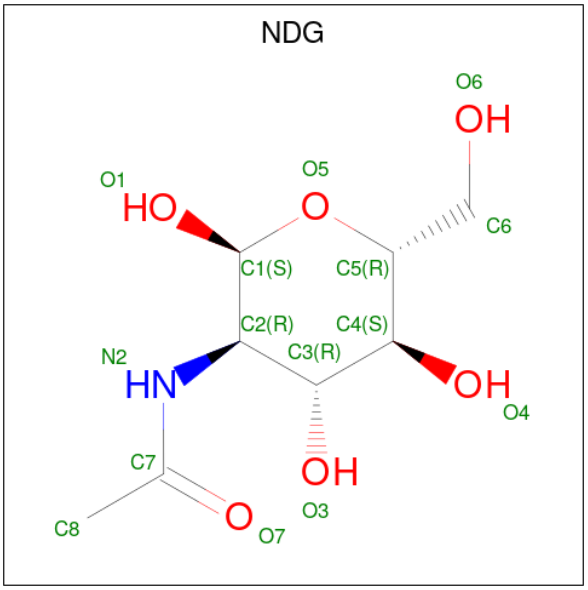
There are 8 unique types of molecules in this entry. The entry contains 5791 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

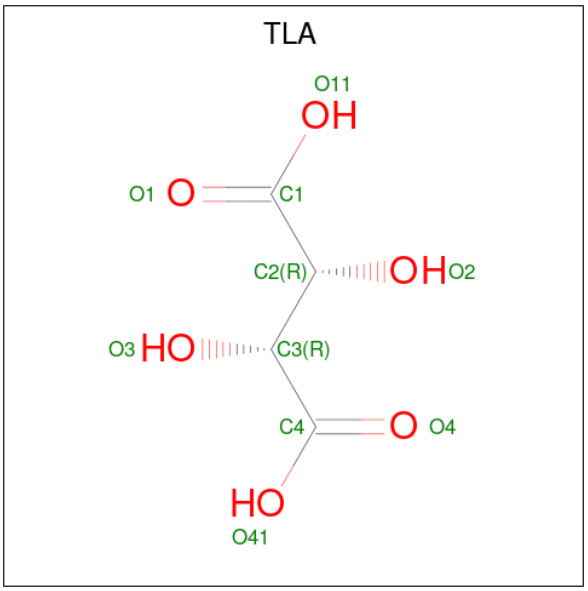
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	171	1337	834	254	241	8	0	0	0
1	B	171	1337	834	254	241	8	0	0	0
1	C	171	1337	834	254	241	8	0	0	0
1	D	171	1337	834	254	241	8	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



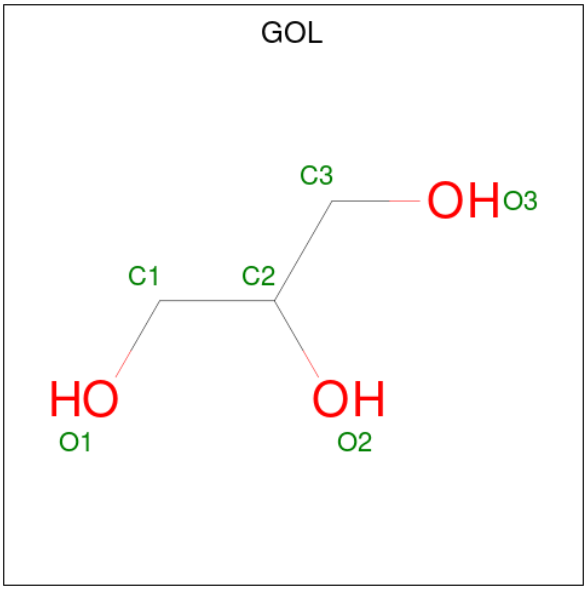
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	15	8	1	6	0	0

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



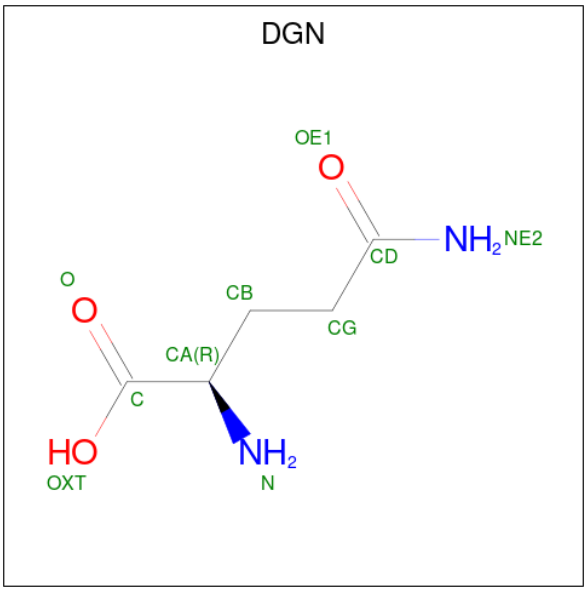
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	D	1	10	4	6	0	0

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



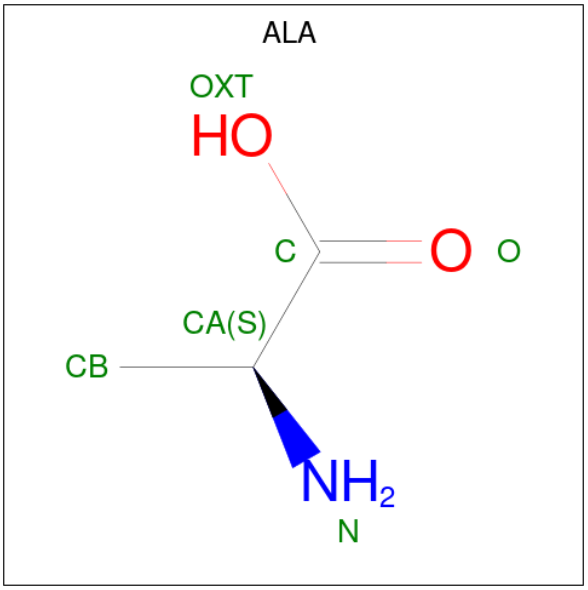
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	D	1	6	3	3	0	0

- Molecule 5 is D-GLUTAMINE (three-letter code: DGN) (formula: $C_5H_{10}N_2O_3$).



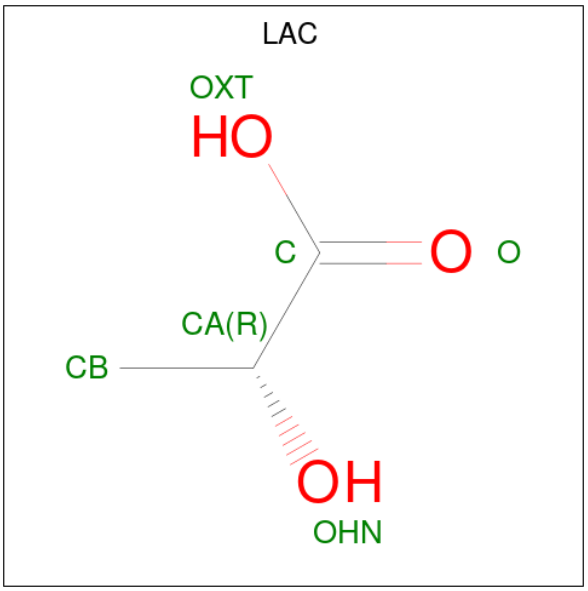
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	D	1	10	5	2	3	0	0

- Molecule 6 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	D	1	5	3	1	1	0	0

- Molecule 7 is LACTIC ACID (three-letter code: LAC) (formula: $C_3H_6O_3$).



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

- Molecule 8 is water.

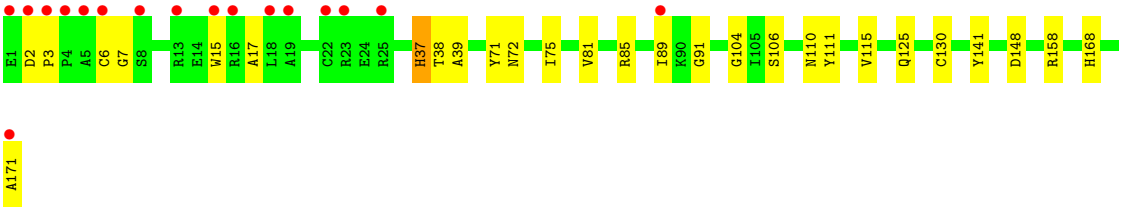
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	102	102	102	0	0
			Total	O		
8	B	92	92	92	0	0
			Total	O		
8	C	107	107	107	0	0
			Total	O		
8	D	92	92	92	0	0

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.

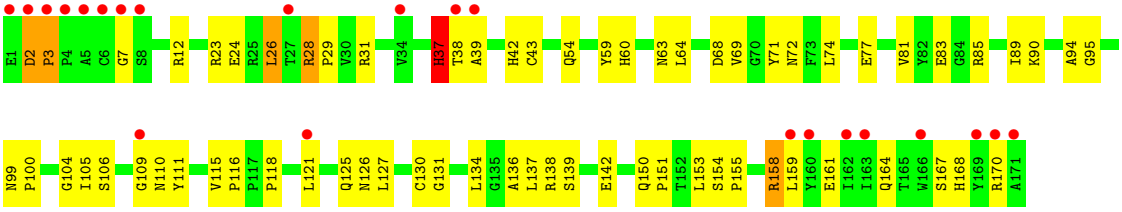
• Molecule 1: Peptidoglycan recognition protein 1

Chain A:



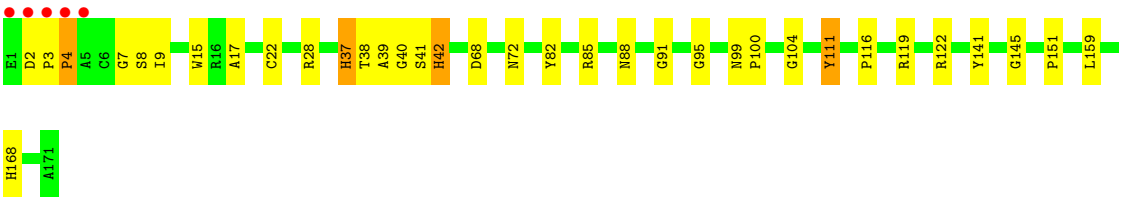
• Molecule 1: Peptidoglycan recognition protein 1

Chain B:



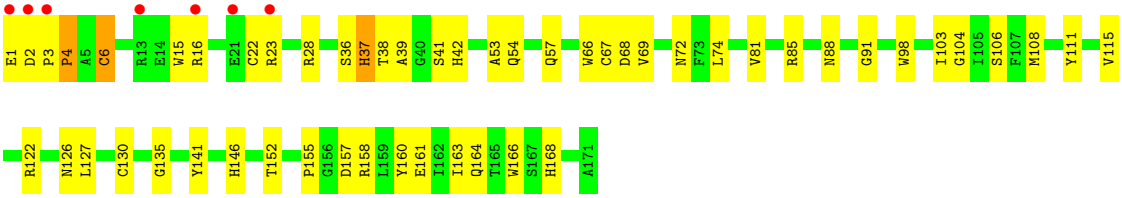
• Molecule 1: Peptidoglycan recognition protein 1

Chain C:



• Molecule 1: Peptidoglycan recognition protein 1

Chain D:


E1
D2
P3
P4
A5
C6
R13
E14
W15
R16
E21
C22
R23
R28
S36
H37
T38
A39
G40
S41
H42
A53
Q54
Q57
W66
C67
D68
V69
N72
F73
L74
V81
R85
N88
G91
W98
I103
G104
I105
S106
F107
M108
Y111
V115
R122
N126
L127
C130
G135
Y141
H146
T152
P155
G156
D157
R158
L159
Y160
E161
I162
I163
Q164
T165
W166
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	87.17Å 102.00Å 161.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 2.50 47.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.63-2.50) 97.7 (47.63-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.236 , 0.249 0.224 , 0.274	Depositor DCC
R_{free} test set	1273 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.680	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 64.2	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	0.94	EDS
Total number of atoms	5791	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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: NDG, LAC, GOL, DGN, TLA

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	0.76	1/1871 (0.1%)
1	B	0.43	0/1374	0.80	3/1871 (0.2%)
1	C	0.64	3/1374 (0.2%)	0.76	1/1871 (0.1%)
1	D	0.38	0/1374	0.72	0/1871
All	All	0.49	3/5496 (0.1%)	0.76	5/7484 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	TYR	CD1-CE1	-5.91	1.30	1.39
1	C	111	TYR	CD1-CE1	-5.62	1.30	1.39
1	C	82	TYR	CD2-CE2	-5.61	1.30	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	26	LEU	N-CA-C	-5.90	95.08	111.00
1	B	26	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	6	CYS	N-CA-C	5.43	125.66	111.00
1	B	37	HIS	N-CA-C	-5.35	96.56	111.00
1	C	145	GLY	N-CA-C	-5.06	100.46	113.10

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	1337	0	1288	19	0
1	B	1337	0	1288	62	0
1	C	1337	0	1288	28	0
1	D	1337	0	1288	42	0
2	C	15	0	11	0	0
3	D	10	0	4	0	0
4	D	6	0	8	0	0
5	D	10	0	7	2	0
6	D	5	0	4	0	0
7	D	4	0	0	0	0
8	A	102	0	0	1	0
8	B	92	0	0	2	0
8	C	107	0	0	0	0
8	D	92	0	0	1	0
All	All	5791	0	5186	150	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 14.

All (150) 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:B:158:ARG:CG	1:B:158:ARG:HH11	1.57	1.16
1:B:158:ARG:HH11	1:B:158:ARG:HG3	1.00	1.16
1:B:72:ASN:ND2	1:B:104:GLY:H	1.45	1.14
1:B:72:ASN:HD22	1:B:104:GLY:N	1.59	1.01
1:D:72:ASN:ND2	1:D:104:GLY:H	1.59	1.01
1:D:3:PRO:HB2	1:D:4:PRO:HD3	1.43	0.99
1:D:72:ASN:HD22	1:D:104:GLY:H	1.05	0.98
1:A:72:ASN:HD22	1:A:104:GLY:H	0.96	0.95
1:B:158:ARG:HG3	1:B:158:ARG:NH1	1.74	0.95
1:C:72:ASN:HD22	1:C:104:GLY:H	1.16	0.92
1:C:72:ASN:ND2	1:C:104:GLY:H	1.68	0.91
1:C:28:ARG:HH21	1:C:88:ASN:HD21	1.20	0.89
1:B:115:VAL:HG12	1:B:158:ARG:HB3	1.54	0.89
1:B:111:TYR:CD1	1:B:116:PRO:HG3	2.08	0.88
1:B:72:ASN:HD22	1:B:104:GLY:H	0.87	0.87
1:D:1:GLU:O	8:D:301:HOH:O	1.93	0.86
1:B:111:TYR:CE1	1:B:116:PRO:HG3	2.11	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ARG:HH11	1:D:23:ARG:HB3	1.40	0.85
1:A:72:ASN:ND2	1:A:104:GLY:H	1.76	0.83
1:D:23:ARG:HB3	1:D:23:ARG:NH1	1.98	0.79
1:B:158:ARG:O	1:B:161:GLU:HG2	1.84	0.77
1:D:85:ARG:HD2	1:D:91:GLY:HA2	1.66	0.77
1:D:72:ASN:HD22	1:D:104:GLY:N	1.83	0.76
1:B:59:TYR:HD1	1:B:63:ASN:HD22	1.37	0.72
1:B:28:ARG:CB	1:B:136:ALA:HA	2.20	0.72
1:D:2:ASP:HB3	1:D:3:PRO:HA	1.70	0.72
1:B:158:ARG:CG	1:B:158:ARG:NH1	2.30	0.71
1:D:98:TRP:HZ2	5:D:203:DGN:HB3	1.57	0.69
1:B:37:HIS:HD2	1:B:111:TYR:H	1.42	0.68
1:B:37:HIS:CD2	1:B:110:ASN:HA	2.29	0.67
1:B:28:ARG:HB2	1:B:136:ALA:HA	1.75	0.67
1:A:141:TYR:O	1:A:168:HIS:HD2	1.79	0.66
1:C:28:ARG:HH21	1:C:88:ASN:ND2	1.91	0.66
1:D:42:HIS:CD2	1:D:42:HIS:H	2.16	0.64
1:D:28:ARG:HH21	1:D:88:ASN:HD21	1.44	0.64
1:D:3:PRO:CB	1:D:4:PRO:HD3	2.24	0.64
1:C:72:ASN:HD22	1:C:104:GLY:N	1.92	0.64
1:D:37:HIS:HD2	1:D:111:TYR:H	1.45	0.64
1:D:74:LEU:HD22	1:D:108:MET:HE2	1.80	0.64
1:C:37:HIS:HD2	1:C:111:TYR:H	1.45	0.63
1:B:158:ARG:HH11	1:B:158:ARG:HG2	1.59	0.63
1:D:6:CYS:HB2	1:D:130:CYS:HA	1.81	0.63
1:B:121:LEU:O	1:B:125:GLN:HG2	1.99	0.62
1:C:42:HIS:H	1:C:42:HIS:CD2	2.17	0.62
1:B:72:ASN:ND2	1:B:104:GLY:N	2.28	0.61
1:D:115:VAL:HG12	1:D:158:ARG:HB3	1.84	0.60
1:C:85:ARG:HD2	1:C:91:GLY:HA2	1.84	0.59
1:B:115:VAL:CG1	1:B:158:ARG:HB3	2.30	0.59
1:D:57:GLN:HG3	1:D:69:VAL:HB	1.85	0.58
1:B:167:SER:OG	1:B:168:HIS:N	2.36	0.58
1:B:77:GLU:HG3	8:B:201:HOH:O	2.03	0.58
1:B:60:HIS:HA	1:B:64:LEU:HD12	1.85	0.57
1:B:12:ARG:HG3	1:B:83:GLU:OE1	2.05	0.57
1:B:105:ILE:HG13	1:B:105:ILE:O	2.05	0.57
1:B:118:PRO:HD2	8:B:206:HOH:O	2.05	0.56
1:C:7:GLY:C	1:C:9:ILE:H	2.09	0.56
1:B:7:GLY:HA2	1:B:126:ASN:HD21	1.71	0.56
1:B:2:ASP:H	1:B:3:PRO:CD	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:PRO:HB2	1:D:4:PRO:CD	2.27	0.55
1:C:37:HIS:CD2	1:C:111:TYR:H	2.24	0.55
1:B:85:ARG:HB3	1:B:89:ILE:HB	1.88	0.54
1:D:22:CYS:SG	1:D:68:ASP:HB3	2.48	0.54
1:D:74:LEU:HD22	1:D:108:MET:CE	2.36	0.54
1:A:72:ASN:HD22	1:A:104:GLY:N	1.82	0.54
1:B:43:CYS:O	1:B:77:GLU:HB2	2.07	0.54
1:B:81:VAL:HG11	1:B:127:LEU:HD13	1.90	0.54
1:C:15:TRP:CH2	1:C:17:ALA:HB2	2.43	0.54
1:B:74:LEU:N	1:B:74:LEU:HD12	2.23	0.54
1:D:141:TYR:O	1:D:168:HIS:HD2	1.91	0.53
1:D:53:ALA:HA	1:D:108:MET:HE1	1.89	0.53
1:B:29:PRO:HB2	1:B:138:ARG:HB3	1.90	0.53
1:B:94:ALA:C	1:B:150:GLN:HE22	2.12	0.53
1:B:158:ARG:N	1:B:158:ARG:HD3	2.24	0.52
1:B:68:ASP:OD1	1:B:69:VAL:N	2.40	0.52
1:B:150:GLN:CG	1:B:151:PRO:HD2	2.40	0.52
1:D:28:ARG:HH21	1:D:88:ASN:ND2	2.07	0.52
1:D:22:CYS:N	1:D:67:CYS:HB2	2.25	0.51
1:B:37:HIS:CD2	1:B:111:TYR:H	2.25	0.51
1:A:148:ASP:HB3	1:A:171:ALA:OXT	2.11	0.50
1:C:141:TYR:O	1:C:168:HIS:HD2	1.94	0.50
1:B:28:ARG:HB3	1:B:136:ALA:HA	1.94	0.50
1:B:95:GLY:N	1:B:150:GLN:HE22	2.09	0.50
1:C:38:THR:O	1:C:39:ALA:HB3	2.11	0.50
1:D:160:TYR:O	1:D:164:GLN:HG3	2.11	0.50
1:B:31:ARG:HG2	1:B:138:ARG:HD3	1.93	0.50
1:C:151:PRO:HD3	1:D:66:TRP:CH2	2.47	0.50
1:B:42:HIS:HB3	1:B:109:GLY:HA3	1.94	0.50
1:B:37:HIS:HD2	1:B:110:ASN:HA	1.76	0.49
1:B:2:ASP:H	1:B:3:PRO:HD3	1.78	0.49
1:D:81:VAL:HG11	1:D:127:LEU:HD13	1.95	0.48
1:D:122:ARG:O	1:D:126:ASN:HB2	2.13	0.48
1:C:15:TRP:CZ3	1:C:17:ALA:HB2	2.48	0.48
1:B:38:THR:O	1:B:39:ALA:HB3	2.14	0.48
1:B:131:GLY:HA3	1:B:137:LEU:HD12	1.95	0.48
1:A:37:HIS:HD2	1:A:110:ASN:HA	1.79	0.48
1:A:141:TYR:O	1:A:168:HIS:CD2	2.64	0.48
1:D:37:HIS:CD2	1:D:111:TYR:H	2.29	0.47
1:B:150:GLN:HG3	1:B:151:PRO:HD2	1.97	0.47
1:B:71:TYR:CD1	1:B:106:SER:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HE	1:B:31:ARG:HB3	1.43	0.46
1:D:28:ARG:HD3	1:D:135:GLY:O	2.16	0.46
1:A:37:HIS:CD2	1:A:110:ASN:HA	2.51	0.45
1:C:111:TYR:CE1	1:C:116:PRO:HG3	2.51	0.45
1:D:157:ASP:O	1:D:161:GLU:HB2	2.16	0.45
1:B:142:GLU:OE1	1:B:170:ARG:HG2	2.16	0.45
1:A:38:THR:O	1:A:39:ALA:HB3	2.16	0.45
1:C:28:ARG:NH2	1:C:88:ASN:HD21	2.01	0.45
1:C:159:LEU:HD12	1:C:159:LEU:O	2.16	0.45
1:D:36:SER:OG	1:D:106:SER:HB2	2.17	0.45
1:B:59:TYR:O	1:B:63:ASN:HB2	2.17	0.44
1:D:146:HIS:H	1:D:155:PRO:HD3	1.81	0.44
1:A:125:GLN:HG2	8:A:287:HOH:O	2.17	0.44
1:B:26:LEU:HG	1:B:90:LYS:HA	2.00	0.44
1:C:99:ASN:N	1:C:100:PRO:HD2	2.33	0.44
1:C:119:ARG:HB3	1:C:122:ARG:NH1	2.33	0.44
1:D:68:ASP:OD1	1:D:69:VAL:N	2.47	0.44
1:B:125:GLN:HG2	1:B:125:GLN:H	1.54	0.43
1:A:37:HIS:HD2	1:A:111:TYR:H	1.66	0.43
1:A:71:TYR:CD1	1:A:106:SER:HB2	2.53	0.43
1:A:7:GLY:N	1:A:130:CYS:SG	2.91	0.43
1:B:24:GLU:OE1	1:B:90:LYS:HE2	2.19	0.43
1:A:2:ASP:HA	1:A:3:PRO:HD2	1.81	0.43
1:C:42:HIS:CD2	1:C:42:HIS:N	2.85	0.43
1:D:103:ILE:HD13	1:D:103:ILE:HA	1.92	0.42
1:A:85:ARG:HB3	1:A:89:ILE:HB	2.01	0.42
1:B:37:HIS:HD2	1:B:111:TYR:N	2.14	0.42
1:A:75:ILE:HD13	1:A:81:VAL:HG22	2.00	0.42
1:A:115:VAL:HG12	1:A:158:ARG:HB3	2.01	0.42
1:D:163:ILE:HG22	1:D:166:TRP:CZ2	2.55	0.42
1:C:95:GLY:O	1:C:99:ASN:CG	2.58	0.42
1:A:15:TRP:CZ2	1:A:17:ALA:HB2	2.55	0.42
1:B:155:PRO:HB2	1:B:159:LEU:HG	2.01	0.42
1:B:111:TYR:CD1	1:B:116:PRO:CG	2.93	0.41
1:B:158:ARG:N	1:B:158:ARG:CD	2.83	0.41
1:D:98:TRP:CZ2	5:D:203:DGN:HB3	2.46	0.41
1:B:99:ASN:N	1:B:100:PRO:CD	2.83	0.41
1:C:2:ASP:HA	1:C:3:PRO:HD3	1.86	0.41
1:C:141:TYR:O	1:C:168:HIS:CD2	2.73	0.41
1:D:53:ALA:CA	1:D:108:MET:HE1	2.48	0.41
1:B:118:PRO:HA	1:B:121:LEU:HG	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:THR:C	1:C:40:GLY:H	2.23	0.41
1:D:42:HIS:CD2	1:D:42:HIS:N	2.86	0.41
1:B:155:PRO:O	1:B:159:LEU:HD23	2.21	0.41
1:D:15:TRP:O	1:D:16:ARG:HB2	2.21	0.41
1:C:2:ASP:O	1:C:4:PRO:HD3	2.21	0.41
1:C:7:GLY:C	1:C:9:ILE:N	2.75	0.40
1:C:22:CYS:SG	1:C:68:ASP:HB3	2.62	0.40
1:B:153:LEU:HD23	1:B:153:LEU:HA	1.97	0.40
1:A:85:ARG:HD2	1:A:91:GLY:HA2	2.03	0.40
1:D:38:THR:O	1:D:39:ALA: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	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
1	B	169/171 (99%)	158 (94%)	9 (5%)	2 (1%)	13	24
1	C	169/171 (99%)	160 (95%)	8 (5%)	1 (1%)	25	43
1	D	169/171 (99%)	162 (96%)	6 (4%)	1 (1%)	25	43
All	All	676/684 (99%)	636 (94%)	36 (5%)	4 (1%)	25	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASP
1	C	4	PRO
1	D	4	PRO
1	B	3	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	139/139 (100%)	138 (99%)	1 (1%)	84	94
1	B	139/139 (100%)	129 (93%)	10 (7%)	14	28
1	C	139/139 (100%)	135 (97%)	4 (3%)	42	69
1	D	139/139 (100%)	134 (96%)	5 (4%)	35	61
All	All	556/556 (100%)	536 (96%)	20 (4%)	35	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	B	23	ARG
1	B	28	ARG
1	B	37	HIS
1	B	54	GLN
1	B	130	CYS
1	B	134	LEU
1	B	139	SER
1	B	154	SER
1	B	158	ARG
1	B	164	GLN
1	C	8	SER
1	C	37	HIS
1	C	41	SER
1	C	42	HIS
1	D	6	CYS
1	D	37	HIS
1	D	41	SER
1	D	54	GLN
1	D	152	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	72	ASN
1	A	168	HIS
1	B	37	HIS
1	B	72	ASN
1	B	126	ASN
1	B	150	GLN
1	C	37	HIS
1	C	42	HIS
1	C	72	ASN
1	C	88	ASN
1	C	168	HIS
1	D	37	HIS
1	D	42	HIS
1	D	63	ASN
1	D	72	ASN
1	D	88	ASN
1	D	150	GLN
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)

6 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	D	201	-	9,9,9	1.22	0	12,12,12	0.91	0
4	GOL	D	202	-	5,5,5	0.32	0	5,5,5	0.23	0
6	ALA	D	204	7,5	3,4,5	0.45	0	2,4,6	1.00	0
5	DGN	D	203	6	8,9,9	0.78	0	10,11,11	1.25	1 (10%)
7	LAC	D	205	2,6	3,3,5	0.52	0	2,2,6	0.94	0
2	NDG	C	201	7	15,15,15	0.75	0	21,21,21	2.07	7 (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
3	TLA	D	201	-	-	0/12/12/12	-
4	GOL	D	202	-	-	2/4/4/4	-
6	ALA	D	204	7,5	-	0/0/2/4	-
5	DGN	D	203	6	-	1/9/9/9	-
7	LAC	D	205	2,6	-	0/0/1/4	-
2	NDG	C	201	7	-	3/6/26/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201	NDG	O5-C1-C2	5.06	114.60	109.52
2	C	201	NDG	C3-C2-N2	-4.33	102.44	110.62
5	D	203	DGN	CB-CA-N	-3.37	101.34	110.17
2	C	201	NDG	C1-C2-N2	-3.17	107.06	110.73
2	C	201	NDG	O3-C3-C4	2.74	116.68	110.35
2	C	201	NDG	C3-C4-C5	-2.35	106.05	110.24
2	C	201	NDG	C1-C2-C3	2.22	113.57	110.54
2	C	201	NDG	O1-C1-O5	2.20	116.97	110.38

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	202	GOL	C1-C2-C3-O3
5	D	203	DGN	CA-CB-CG-CD
2	C	201	NDG	O5-C5-C6-O6
4	D	202	GOL	O2-C2-C3-O3
2	C	201	NDG	C4-C5-C6-O6
2	C	201	NDG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	203	DGN	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%)	0.52	17 (9%)	7	7	30, 48, 70, 98	0
1	B	171/171 (100%)	0.84	22 (12%)	3	3	40, 63, 94, 98	0
1	C	171/171 (100%)	-0.03	5 (2%)	51	55	18, 32, 55, 98	0
1	D	171/171 (100%)	0.18	7 (4%)	37	40	25, 45, 65, 98	0
All	All	684/684 (100%)	0.38	51 (7%)	14	14	18, 47, 85, 98	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	PRO	14.0
1	B	4	PRO	10.9
1	A	4	PRO	8.4
1	A	2	ASP	8.2
1	B	2	ASP	7.4
1	B	7	GLY	6.5
1	D	2	ASP	6.3
1	D	3	PRO	6.1
1	B	5	ALA	5.8
1	B	1	GLU	5.6
1	C	1	GLU	5.0
1	B	159	LEU	5.0
1	A	13	ARG	4.8
1	A	1	GLU	4.7
1	C	2	ASP	4.5
1	C	3	PRO	4.3
1	C	5	ALA	4.3
1	D	1	GLU	4.2
1	B	3	PRO	4.0
1	A	19	ALA	3.8
1	B	170	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	23	ARG	3.2
1	B	171	ALA	3.2
1	A	15	TRP	3.0
1	A	5	ALA	2.9
1	B	6	CYS	2.8
1	A	16	ARG	2.8
1	B	166	TRP	2.7
1	C	4	PRO	2.6
1	B	160	TYR	2.6
1	D	23	ARG	2.6
1	B	34	VAL	2.6
1	B	27	THR	2.5
1	B	121	LEU	2.5
1	B	169	TYR	2.5
1	A	6	CYS	2.4
1	B	163	ILE	2.4
1	D	21	GLU	2.2
1	A	22	CYS	2.2
1	B	162	ILE	2.2
1	A	25	ARG	2.2
1	A	18	LEU	2.2
1	B	109	GLY	2.2
1	D	16	ARG	2.2
1	A	171	ALA	2.1
1	D	13	ARG	2.1
1	A	8	SER	2.1
1	B	38	THR	2.1
1	B	8	SER	2.0
1	B	39	ALA	2.0
1	A	89	ILE	2.0

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
7	LAC	D	205	4/6	0.51	0.51	69,69,70,71	0
6	ALA	D	204	5/6	0.56	0.56	74,76,78,80	0
2	NDG	C	201	15/15	0.63	0.38	60,65,67,68	0
5	DGN	D	203	10/10	0.72	0.50	42,46,77,78	0
3	TLA	D	201	10/10	0.87	0.20	23,25,26,27	2
4	GOL	D	202	6/6	0.91	0.24	47,47,47,50	0

6.5 Other polymers (i)

There are no such residues in this entry.