Full wwPDB X-ray Structure Validation Report (i)

Jan 25, 2023 – 09:56 AM EST

PDB ID	:	4LR4
Title	:	Crystal structure of a putative secreted protein (EUBREC_3654) from Eubacterium rectale at 2.43 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2013-07-19
Resolution	:	2.43 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:

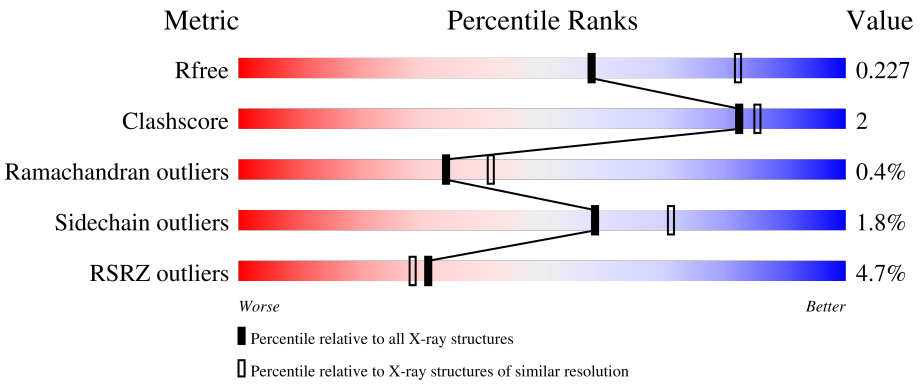
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	370	5% 87% 6% 7%
1	B	370	5% 86% 7% 7%
1	C	370	3% 87% 6% 6%
1	D	370	5% 83% 10% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11652 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.

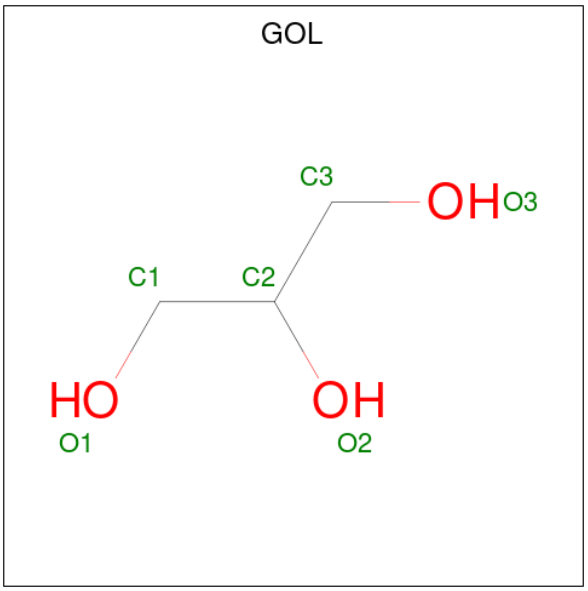
- Molecule 1 is a protein called hypothetical protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	345	2699	1700	426	562	5	6	0	1	0
1	B	345	2699	1700	426	562	5	6	0	1	0
1	C	346	2699	1702	424	562	5	6	0	1	0
1	D	345	2696	1700	426	559	5	6	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP C4ZEB7
B	0	GLY	-	expression tag	UNP C4ZEB7
C	0	GLY	-	expression tag	UNP C4ZEB7
D	0	GLY	-	expression tag	UNP C4ZEB7

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	A	1	6	3	3	0	0
			Total	C	O		
2	B	1	6	3	3	0	0
			Total	C	O		
2	B	1	6	3	3	0	0
			Total	C	O		
2	B	1	6	3	3	0	0
			Total	C	O		
2	B	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0
			Total	C	O		
2	C	1	6	3	3	0	0

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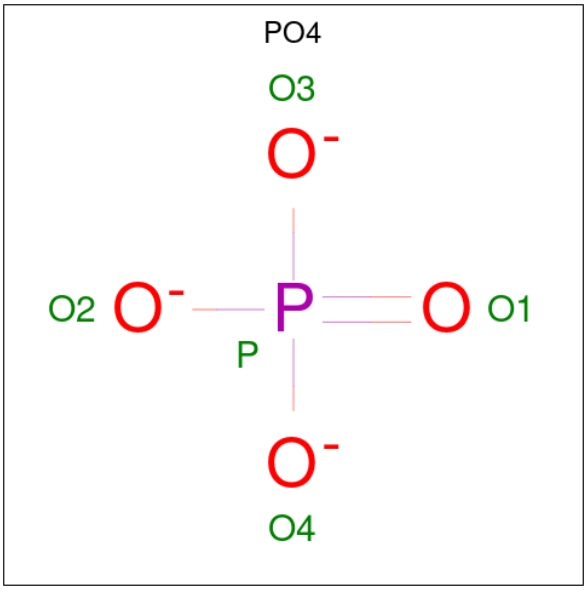
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	D	1	6	3	3	0	0
			Total	C	O		
2	D	1	6	3	3	0	0
			Total	C	O		
2	D	1	6	3	3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	A	1	10	8	2	0	1
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	C	1	5	4	1	0	0
			Total	O	P		
3	C	1	10	8	2	0	1
			Total	O	P		
3	C	1	10	8	2	0	1
			Total	O	P		
3	D	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	D	1	5	4	1	0	0
			Total	O	P		
3	D	1	5	4	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	B	1	1	1	0	0
			Total	Cl		
4	C	3	3	3	0	0
			Total	Cl		
4	D	4	4	4	0	0

- Molecule 5 is water.

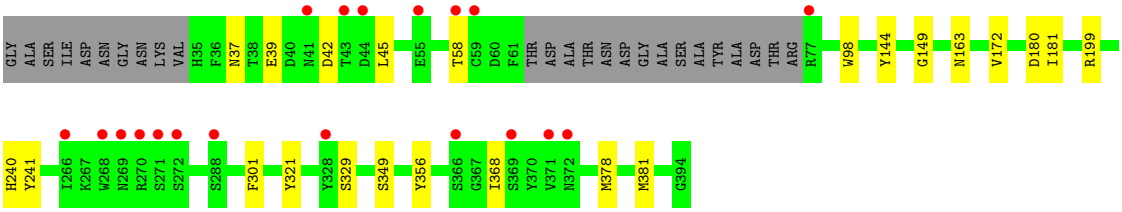
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	187	187	187	0	0
			Total	O		
5	B	136	136	136	0	0
			Total	O		
5	C	202	202	202	0	0
			Total	O		
5	D	158	158	158	0	0

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.

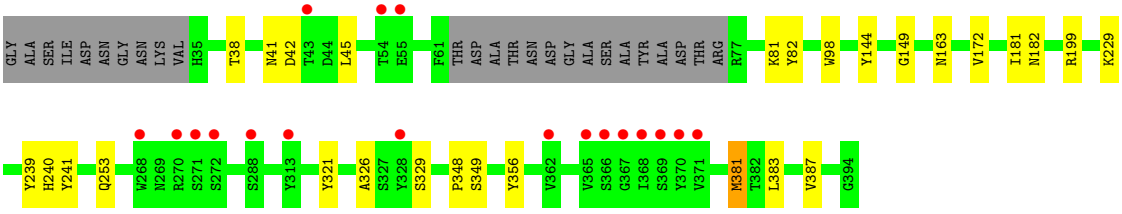
• Molecule 1: hypothetical protein

Chain A:



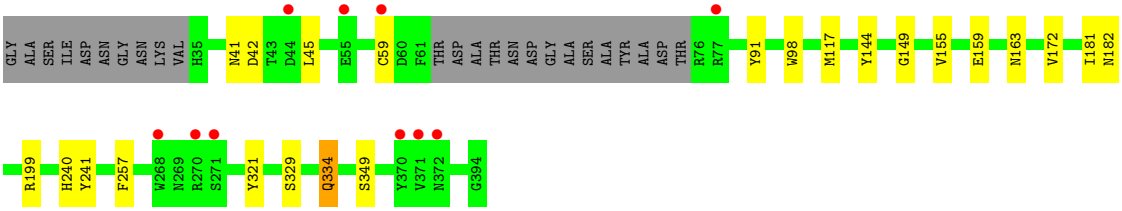
• Molecule 1: hypothetical protein

Chain B:



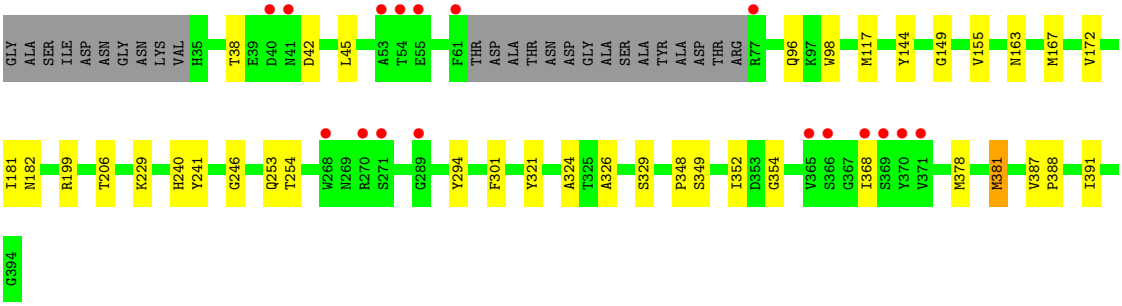
• Molecule 1: hypothetical protein

Chain C:



• Molecule 1: hypothetical protein

Chain D:


GLY ALA SER ILE ASP ASN GLY ASN LYS VAL H35 T38 E39 D40 N41 D42 L45 A53 T54 E55 F61 THR ASP ALA THR ASN ASP GLY ALA SER ALA TYR ALA ASP THR ARG R77 Q96 K97 W98 M117 Y144 G149 V155 N163 M167 V172
I181 N182 R199 T206 K229 H240 Y241 G246 Q253 T254 W268 M269 R270 S271 G289 Y294 F301 Y321 A324 T325 A326 S329 P348 S349 I352 D353 G354 V365 S366 G367 I368 S369 Y370 V371 M378 M381 V387 P388 I391
G394

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.02Å 106.73Å 115.08Å 90.00° 92.45° 90.00°	Depositor
Resolution (Å)	48.96 – 2.43 48.96 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.96-2.43) 98.2 (48.96-2.43)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.42Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.186 , 0.216 0.200 , 0.227	Depositor DCC
R_{free} test set	4383 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5882e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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, CL, PO4

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	0.53	0/2760	0.67	0/3752
1	B	0.51	1/2760 (0.0%)	0.65	0/3752
1	C	0.51	0/2760	0.67	0/3754
1	D	0.52	1/2757 (0.0%)	0.66	0/3749
All	All	0.52	2/11037 (0.0%)	0.66	0/15007

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	381	MSE	SE-CE	-5.48	1.63	1.95
1	B	381	MSE	SE-CE	-5.34	1.64	1.95

There are no bond angle outliers.

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	2699	0	2506	9	0
1	B	2699	0	2506	15	0
1	C	2699	0	2501	10	0
1	D	2696	0	2506	18	0
2	A	24	0	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	32	1	0
2	C	36	0	48	2	0
2	D	18	0	24	2	0
3	A	20	0	0	0	0
3	B	5	0	0	1	0
3	C	25	0	0	1	0
3	D	15	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
5	A	187	0	0	0	0
5	B	136	0	0	0	0
5	C	202	0	0	0	0
5	D	158	0	0	0	0
All	All	11652	0	10155	52	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 2.

All (52) 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:206:THR:H	2:D:401:GOL:H32	1.28	0.98
1:D:301:PHE:CZ	1:D:381:MSE:HE3	2.03	0.92
1:A:301:PHE:CZ	1:A:381:MSE:HE3	2.14	0.82
1:B:381:MSE:HE2	1:B:383:LEU:HD21	1.74	0.69
1:B:356:TYR:CD2	1:B:381:MSE:HE1	2.28	0.68
1:D:301:PHE:HZ	1:D:381:MSE:HE3	1.55	0.67
1:B:42:ASP:HB2	1:B:45:LEU:HG	1.78	0.66
1:B:239:TYR:H	2:B:401:GOL:H11	1.65	0.61
1:A:301:PHE:HZ	1:A:381:MSE:HE3	1.65	0.58
1:C:42:ASP:HB2	1:C:45:LEU:HG	1.87	0.56
1:C:182:ASN:ND2	3:C:408[A]:PO4:O2	2.37	0.56
1:D:42:ASP:HB2	1:D:45:LEU:HG	1.87	0.56
1:A:42:ASP:HB2	1:A:45:LEU:HG	1.86	0.55
1:C:117:MSE:HE1	1:C:155[B]:VAL:HG22	1.88	0.55
1:D:117:MSE:HE1	1:D:155[A]:VAL:HG22	1.87	0.55
1:B:381:MSE:HE2	1:B:383:LEU:CD2	2.36	0.55
1:B:253:GLN:HG3	1:B:387:VAL:HG22	1.90	0.54
1:B:182:ASN:ND2	3:B:405:PO4:O1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:CD2	1:A:240:HIS:CE1	3.00	0.49
1:D:253:GLN:HG3	1:D:387:VAL:HG22	1.95	0.48
1:D:326:ALA:HB2	1:D:348:PRO:HG2	1.94	0.48
1:D:294:TYR:HB3	1:D:352:ILE:HG12	1.96	0.48
1:A:37:ASN:ND2	1:A:39:GLU:HG2	2.28	0.48
1:D:324:ALA:HB1	1:D:354:GLY:HA3	1.95	0.48
1:C:91:TYR:CD1	2:C:402:GOL:H11	2.49	0.47
1:B:326:ALA:HB2	1:B:348:PRO:HG2	1.96	0.46
1:C:172:VAL:HG11	1:C:241:TYR:HB3	1.97	0.46
1:A:356:TYR:CD2	1:A:381:MSE:HE1	2.51	0.46
1:C:163:ASN:OD1	1:C:199:ARG:NH2	2.49	0.46
1:D:96:GLN:HA	2:D:402:GOL:H31	1.97	0.45
1:D:172:VAL:HG11	1:D:241:TYR:HB3	1.97	0.45
1:B:172:VAL:HG11	1:B:241:TYR:HB3	1.99	0.45
1:B:163:ASN:OD1	1:B:199:ARG:NH2	2.50	0.45
1:A:172:VAL:HG11	1:A:241:TYR:HB3	1.99	0.44
1:B:98:TRP:CD2	1:B:240:HIS:CE1	3.05	0.44
1:D:98:TRP:CD2	1:D:240:HIS:CE1	3.06	0.44
1:D:182:ASN:ND2	3:D:405:PO4:O4	2.42	0.44
1:D:163:ASN:OD1	1:D:199:ARG:NH2	2.50	0.44
1:C:144:TYR:CE1	1:C:149:GLY:HA2	2.53	0.44
1:D:38:THR:HG21	1:D:229:LYS:HD2	2.00	0.43
1:D:144:TYR:CE1	1:D:149:GLY:HA2	2.53	0.43
1:B:144:TYR:CE1	1:B:149:GLY:HA2	2.53	0.43
1:B:381:MSE:CE	1:B:383:LEU:HD21	2.47	0.43
1:C:59:CYS:HB2	1:C:257:PHE:CD1	2.54	0.43
1:A:144:TYR:CE1	1:A:149:GLY:HA2	2.55	0.42
1:C:98:TRP:CD2	1:C:240:HIS:CE1	3.07	0.42
1:D:388:PRO:HG2	1:D:391:ILE:HB	2.02	0.42
1:B:38:THR:HG21	1:B:229:LYS:HD2	2.01	0.42
1:A:163:ASN:OD1	1:A:199:ARG:NH2	2.52	0.41
1:B:81:LYS:HE2	1:B:82:TYR:CZ	2.55	0.41
1:C:334:GLN:HE22	2:C:403:GOL:H11	1.85	0.41
1:D:163:ASN:HB3	1:D:246:GLY:O	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	342/370 (92%)	334 (98%)	6 (2%)	2 (1%)	25	29
1	B	342/370 (92%)	335 (98%)	6 (2%)	1 (0%)	41	49
1	C	343/370 (93%)	335 (98%)	7 (2%)	1 (0%)	41	49
1	D	342/370 (92%)	334 (98%)	6 (2%)	2 (1%)	25	29
All	All	1369/1480 (92%)	1338 (98%)	25 (2%)	6 (0%)	34	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	378	MSE
1	A	378	MSE
1	B	181	ILE
1	A	181	ILE
1	C	181	ILE
1	D	181	ILE

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	300/314 (96%)	294 (98%)	6 (2%)	55	67
1	B	300/314 (96%)	296 (99%)	4 (1%)	69	80
1	C	299/314 (95%)	293 (98%)	6 (2%)	55	67
1	D	299/314 (95%)	293 (98%)	6 (2%)	55	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1198/1256 (95%)	1176 (98%)	22 (2%)	59 71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	180	ASP
1	A	321	TYR
1	A	329	SER
1	A	349	SER
1	A	368	ILE
1	B	41	ASN
1	B	321	TYR
1	B	329	SER
1	B	349	SER
1	C	41	ASN
1	C	159	GLU
1	C	321	TYR
1	C	329	SER
1	C	334	GLN
1	C	349	SER
1	D	167	MSE
1	D	254	THR
1	D	321	TYR
1	D	329	SER
1	D	349	SER
1	D	368	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	334	GLN

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)

Of 39 ligands modelled in this entry, 9 are monoatomic - leaving 30 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	$\#\|Z\| > 2$
2	GOL	B	404	-	5,5,5	0.14	0	5,5,5	0.17	0
2	GOL	A	403	-	5,5,5	0.09	0	5,5,5	0.18	0
2	GOL	C	403	-	5,5,5	0.07	0	5,5,5	0.50	0
2	GOL	D	401	-	5,5,5	0.08	0	5,5,5	0.40	0
2	GOL	D	403	-	5,5,5	0.08	0	5,5,5	0.31	0
2	GOL	D	402	-	5,5,5	0.13	0	5,5,5	0.45	0
2	GOL	A	402	-	5,5,5	0.08	0	5,5,5	0.09	0
2	GOL	C	401	-	5,5,5	0.12	0	5,5,5	0.22	0
3	PO4	A	405	-	4,4,4	1.45	1 (25%)	6,6,6	0.83	0
3	PO4	B	405	-	4,4,4	1.23	0	6,6,6	0.84	0
3	PO4	D	405	-	4,4,4	1.17	0	6,6,6	0.57	0
3	PO4	C	408[B]	-	4,4,4	1.31	1 (25%)	6,6,6	0.60	0
3	PO4	C	408[A]	-	4,4,4	1.08	1 (25%)	6,6,6	0.53	0
2	GOL	B	403	-	5,5,5	0.13	0	5,5,5	0.34	0
3	PO4	C	409[B]	-	4,4,4	1.58	1 (25%)	6,6,6	0.43	0
3	PO4	C	409[A]	-	4,4,4	1.54	1 (25%)	6,6,6	0.42	0
3	PO4	D	406	-	4,4,4	1.10	0	6,6,6	0.77	0
2	GOL	B	401	-	5,5,5	0.16	0	5,5,5	0.28	0
2	GOL	C	405	-	5,5,5	0.07	0	5,5,5	0.25	0
2	GOL	C	406	-	5,5,5	0.14	0	5,5,5	0.27	0
2	GOL	A	401	-	5,5,5	0.16	0	5,5,5	0.20	0
3	PO4	D	404	-	4,4,4	1.29	1 (25%)	6,6,6	0.58	0
3	PO4	A	406	-	4,4,4	0.95	0	6,6,6	0.70	0
2	GOL	C	402	-	5,5,5	0.07	0	5,5,5	0.29	0
2	GOL	A	404	-	5,5,5	0.17	0	5,5,5	0.28	0
2	GOL	C	404	-	5,5,5	0.13	0	5,5,5	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	A	407[B]	-	4,4,4	1.20	1 (25%)	6,6,6	0.54	0
3	PO4	A	407[A]	-	4,4,4	0.99	0	6,6,6	0.50	0
2	GOL	B	402	-	5,5,5	0.09	0	5,5,5	0.38	0
3	PO4	C	407	-	4,4,4	1.03	0	6,6,6	0.92	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
2	GOL	C	406	-	-	0/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	A	403	-	-	2/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	B	404	-	-	2/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	C	402	-	-	0/4/4/4	-
2	GOL	C	403	-	-	0/4/4/4	-
2	GOL	D	401	-	-	1/4/4/4	-
2	GOL	D	403	-	-	0/4/4/4	-
2	GOL	A	404	-	-	0/4/4/4	-
2	GOL	B	402	-	-	0/4/4/4	-
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	C	404	-	-	2/4/4/4	-
2	GOL	B	401	-	-	0/4/4/4	-
2	GOL	C	405	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	409[B]	PO4	P-O1	2.88	1.57	1.50
3	C	409[A]	PO4	P-O1	2.83	1.57	1.50
3	A	405	PO4	P-O1	2.55	1.56	1.50
3	D	404	PO4	P-O1	2.38	1.56	1.50
3	C	408[B]	PO4	P-O1	2.25	1.56	1.50
3	A	407[B]	PO4	P-O1	2.22	1.56	1.50
3	C	408[A]	PO4	P-O1	2.11	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	403	GOL	O1-C1-C2-O2
2	A	403	GOL	O1-C1-C2-C3
2	B	404	GOL	O1-C1-C2-C3
2	B	404	GOL	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-C3
2	C	404	GOL	O1-C1-C2-C3
2	D	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	C	404	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	GOL	1	0
2	D	401	GOL	1	0
2	D	402	GOL	1	0
3	B	405	PO4	1	0
3	D	405	PO4	1	0
3	C	408[A]	PO4	1	0
2	B	401	GOL	1	0
2	C	402	GOL	1	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	339/370 (91%)	0.27	19 (5%)	24	20	25, 48, 99, 123	0
1	B	339/370 (91%)	0.24	18 (5%)	26	23	29, 54, 99, 137	0
1	C	340/370 (91%)	0.16	10 (2%)	51	47	29, 45, 81, 110	0
1	D	339/370 (91%)	0.17	17 (5%)	28	26	29, 50, 98, 121	0
All	All	1357/1480 (91%)	0.21	64 (4%)	31	29	25, 49, 97, 137	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ARG	5.3
1	A	268	TRP	5.0
1	A	271	SER	4.8
1	B	268	TRP	4.8
1	B	368	ILE	4.7
1	B	366	SER	4.6
1	A	371	VAL	4.4
1	B	270	ARG	4.2
1	D	366	SER	4.1
1	D	368	ILE	3.9
1	B	371	VAL	3.9
1	D	40	ASP	3.8
1	C	55	GLU	3.7
1	B	313	TYR	3.6
1	B	55	GLU	3.6
1	D	55	GLU	3.6
1	D	268	TRP	3.6
1	D	365	VAL	3.5
1	A	269	ASN	3.5
1	C	270	ARG	3.4
1	D	270	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	272	SER	3.3
1	D	77	ARG	3.2
1	D	369	SER	3.2
1	B	370	TYR	3.1
1	D	371	VAL	3.0
1	A	372	ASN	3.0
1	A	59	CYS	3.0
1	B	369	SER	3.0
1	A	77	ARG	2.9
1	C	371	VAL	2.9
1	B	272	SER	2.9
1	A	55	GLU	2.9
1	A	266	ILE	2.8
1	B	271	SER	2.8
1	C	59	CYS	2.7
1	D	289	GLY	2.7
1	D	53	ALA	2.7
1	A	43	THR	2.7
1	D	41	ASN	2.6
1	A	44	ASP	2.6
1	B	367	GLY	2.5
1	A	328	TYR	2.5
1	D	54	THR	2.5
1	C	268	TRP	2.5
1	C	44	ASP	2.4
1	A	366	SER	2.4
1	A	369	SER	2.4
1	A	41	ASN	2.3
1	B	288	SER	2.3
1	C	372	ASN	2.3
1	C	271	SER	2.3
1	A	288	SER	2.3
1	D	61	PHE	2.3
1	B	365	VAL	2.2
1	C	370	TYR	2.2
1	D	271	SER	2.2
1	B	362	VAL	2.2
1	A	58	THR	2.1
1	B	54	THR	2.1
1	D	370	TYR	2.1
1	C	77	ARG	2.1
1	B	43	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	328	TYR	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
2	GOL	C	406	6/6	0.65	0.30	85,88,91,93	0
2	GOL	D	403	6/6	0.70	0.22	87,89,90,91	0
4	CL	D	408	1/1	0.70	0.18	86,86,86,86	0
2	GOL	C	404	6/6	0.73	0.20	76,81,82,82	0
4	CL	A	408	1/1	0.80	0.19	97,97,97,97	0
4	CL	C	412	1/1	0.84	0.16	107,107,107,107	0
2	GOL	A	404	6/6	0.85	0.19	71,74,76,76	0
2	GOL	B	401	6/6	0.85	0.18	69,71,71,72	0
2	GOL	C	403	6/6	0.85	0.24	59,64,64,65	0
2	GOL	A	401	6/6	0.85	0.19	67,69,70,72	0
2	GOL	C	405	6/6	0.85	0.24	98,98,99,99	0
4	CL	D	410	1/1	0.86	0.15	81,81,81,81	0
4	CL	B	406	1/1	0.88	0.14	85,85,85,85	0
3	PO4	D	406	5/5	0.89	0.21	105,106,108,109	0
3	PO4	B	405	5/5	0.89	0.26	95,95,96,96	0
3	PO4	C	409[B]	5/5	0.90	0.21	41,43,44,46	5
2	GOL	A	402	6/6	0.90	0.18	45,49,53,55	0
2	GOL	B	402	6/6	0.90	0.23	78,78,79,80	0
3	PO4	A	407[A]	5/5	0.90	0.27	66,67,68,69	5
3	PO4	A	407[B]	5/5	0.90	0.27	57,60,62,62	5
2	GOL	C	401	6/6	0.90	0.20	62,68,72,73	0
3	PO4	C	409[A]	5/5	0.90	0.21	48,51,53,54	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	404	6/6	0.91	0.18	60,66,68,69	0
2	GOL	A	403	6/6	0.91	0.22	77,77,79,80	0
3	PO4	D	405	5/5	0.91	0.27	85,85,85,86	0
2	GOL	D	401	6/6	0.92	0.13	59,60,61,62	0
3	PO4	D	404	5/5	0.92	0.17	111,111,111,112	0
3	PO4	A	406	5/5	0.92	0.33	48,50,51,54	5
3	PO4	C	408[A]	5/5	0.93	0.26	41,42,45,45	5
4	CL	D	407	1/1	0.93	0.12	82,82,82,82	0
3	PO4	C	408[B]	5/5	0.93	0.26	47,51,52,54	5
4	CL	D	409	1/1	0.93	0.10	85,85,85,85	0
2	GOL	B	403	6/6	0.93	0.19	58,58,60,63	0
4	CL	C	410	1/1	0.94	0.14	64,64,64,64	0
3	PO4	C	407	5/5	0.95	0.15	95,96,97,97	0
2	GOL	D	402	6/6	0.95	0.19	48,48,52,57	0
2	GOL	C	402	6/6	0.96	0.19	47,50,52,57	0
4	CL	C	411	1/1	0.97	0.15	77,77,77,77	0
3	PO4	A	405	5/5	0.97	0.17	70,73,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.