Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:10 PM GMT

PDB ID	:	4NZ0
Title	:	The EMCV 3Dpol structure at 2.8A resolution
Authors	:	Vives-adrian, L.; Ferrer-orta, C.; Verdaguer, N.
Deposited on	:	2013-12-11
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

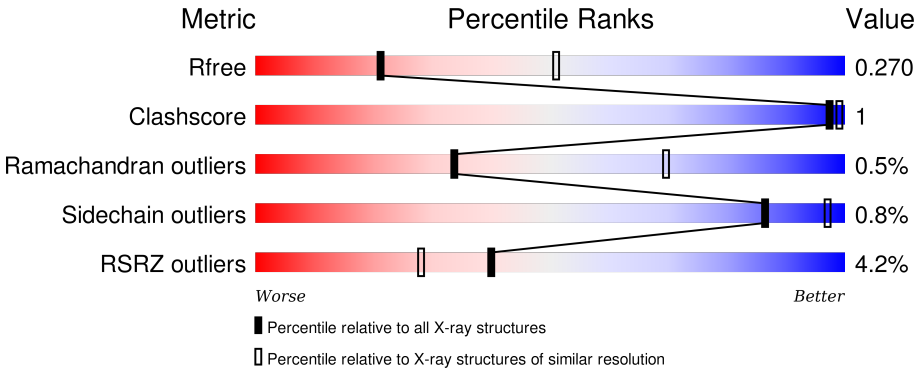
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	460	96%
1	B	460	16%, 94%, 5%
1	C	460	4%, 95%, 5%
1	D	460	3%, 96%
1	E	460	95%

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Mol	Chain	Length	Quality of chain
1	F	460	95% 5%

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
2	GOL	D	503	-	-	-	X
2	GOL	E	503	-	-	-	X
2	GOL	F	501	-	-	-	X
2	GOL	F	502	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22240 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.

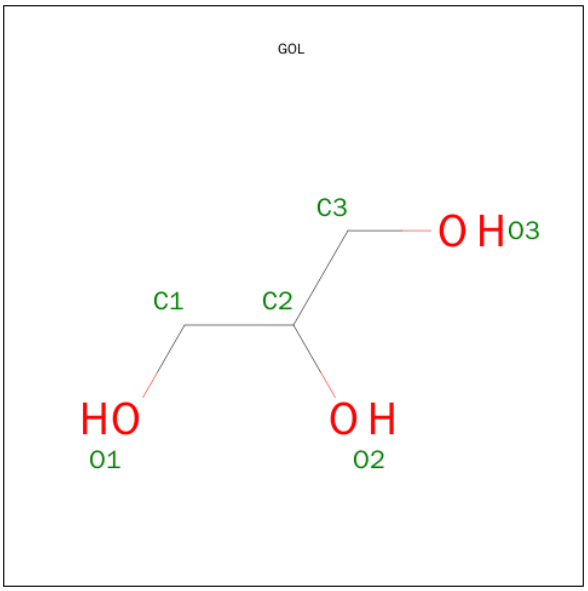
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	1	0
			3689	2362	628	684	15			
1	B	460	Total	C	N	O	S	0	0	0
			3681	2357	625	684	15			
1	C	460	Total	C	N	O	S	0	0	0
			3681	2357	625	684	15			
1	D	460	Total	C	N	O	S	0	0	0
			3681	2357	625	684	15			
1	E	460	Total	C	N	O	S	0	1	0
			3692	2363	629	685	15			
1	F	460	Total	C	N	O	S	0	0	0
			3681	2357	625	684	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	MET	VAL	SEE REMARK 999	UNP P12296
B	247	MET	VAL	SEE REMARK 999	UNP P12296
C	247	MET	VAL	SEE REMARK 999	UNP P12296
D	247	MET	VAL	SEE REMARK 999	UNP P12296
E	247	MET	VAL	SEE REMARK 999	UNP P12296
F	247	MET	VAL	SEE REMARK 999	UNP P12296

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



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is water.

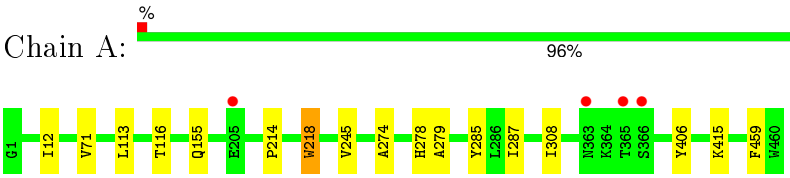
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	6	Total O 6 6	0	0
4	C	4	Total O 4 4	0	0
4	D	8	Total O 8 8	0	0
4	E	25	Total O 25 25	0	0
4	F	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

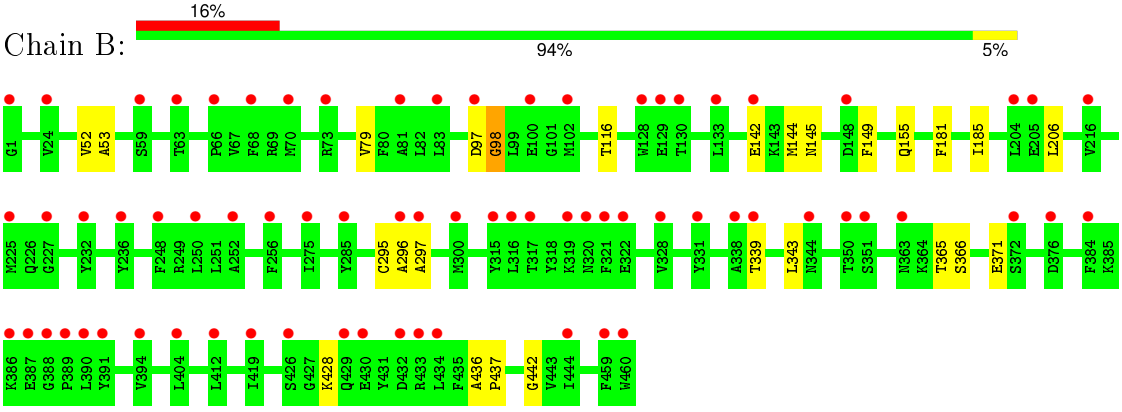
- Molecule 1: Genome polyprotein

Chain A:



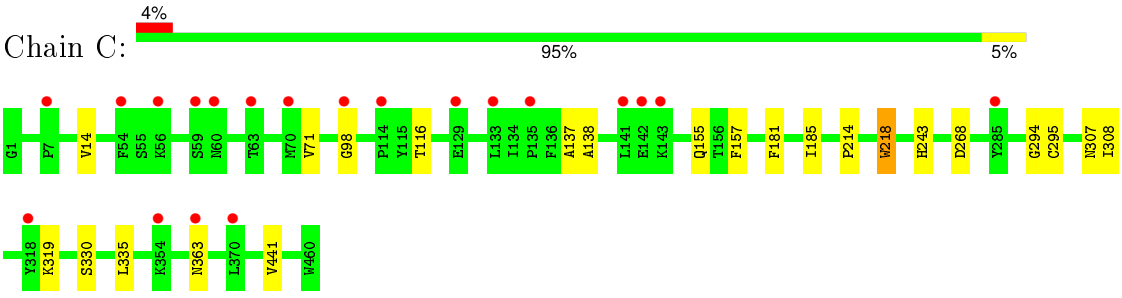
- Molecule 1: Genome polyprotein

Chain B:



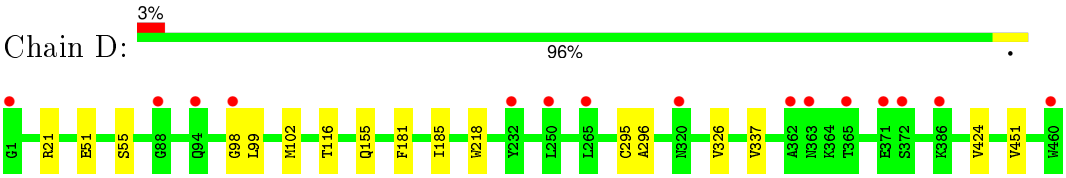
- Molecule 1: Genome polyprotein

Chain C:



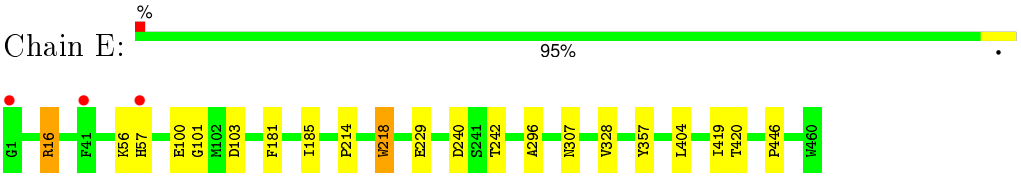
- Molecule 1: Genome polyprotein

Chain D:



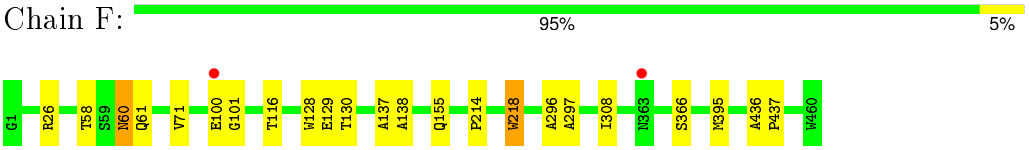
• Molecule 1: Genome polyprotein

Chain E:



• Molecule 1: Genome polyprotein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	230.40Å 140.79Å 170.58Å 90.00° 125.86° 90.00°	Depositor
Resolution (Å)	138.20 – 2.80 49.32 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.8 (138.20-2.80) 97.9 (49.32-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.246 , 0.268 0.244 , 0.270	Depositor DCC
R_{free} test set	5368 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 119535 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	22240	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL

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	0.26	0/3780	0.44	0/5121
1	B	0.28	0/3769	0.44	0/5107
1	C	0.27	0/3769	0.43	0/5107
1	D	0.27	0/3769	0.44	0/5107
1	E	0.27	0/3780	0.45	0/5121
1	F	0.27	0/3769	0.45	0/5107
All	All	0.27	0/22636	0.44	0/30670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3689	0	3671	11	0
1	B	3681	0	3658	9	0
1	C	3681	0	3658	10	0
1	D	3681	0	3660	7	0
1	E	3692	0	3670	10	0
1	F	3681	0	3658	9	0
2	D	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	18	0	24	0	0
2	F	12	0	16	0	0
3	D	1	0	0	0	0
4	A	29	0	0	0	0
4	B	6	0	0	0	0
4	C	4	0	0	0	0
4	D	8	0	0	0	0
4	E	25	0	0	0	0
4	F	14	0	0	0	0
All	All	22240	0	22039	55	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 1.

All (55) 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:E:16[B]:ARG:HG2	1:E:16[B]:ARG:O	1.99	0.63
1:A:285:TYR:CE2	1:A:287:ILE:HD11	2.35	0.62
1:F:71:VAL:HG13	1:F:308:ILE:HG23	1.82	0.62
1:C:181:PHE:CE2	1:C:185:ILE:HD11	2.40	0.56
1:A:214:PRO:O	1:A:218:TRP:HB2	2.06	0.56
1:A:116:THR:HG21	1:A:155:GLN:HE22	1.72	0.55
1:A:71:VAL:HG13	1:A:308:ILE:HG23	1.91	0.53
1:B:52:VAL:O	1:B:53:ALA:HB3	2.09	0.52
1:E:214:PRO:O	1:E:218:TRP:HB2	2.11	0.51
1:C:71:VAL:HG13	1:C:308:ILE:HG23	1.92	0.51
1:B:181:PHE:CE2	1:B:185:ILE:HD11	2.46	0.51
1:D:326:VAL:HG13	1:D:337:VAL:HG13	1.93	0.51
1:D:116:THR:HG21	1:D:155:GLN:HE22	1.77	0.49
1:F:60:ASN:HD22	1:F:61:GLN:N	2.10	0.49
1:D:99:LEU:O	1:D:102:MET:N	2.45	0.49
1:F:214:PRO:O	1:F:218:TRP:HB2	2.14	0.48
1:A:459:PHE:HB3	1:B:365:THR:HB	1.96	0.47
1:B:295:CYS:O	1:B:297:ALA:N	2.47	0.47
1:F:137:ALA:O	1:F:138:ALA:HB3	2.15	0.47
1:C:14:VAL:HG13	1:C:157:PHE:HB2	1.97	0.46
1:E:420:THR:HG21	1:E:446:PRO:HD2	1.98	0.46
1:A:285:TYR:CD2	1:A:287:ILE:HD11	2.52	0.46
1:D:51:GLU:O	1:D:55:SER:N	2.49	0.45
1:A:12:ILE:HD12	1:A:279:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:PHE:CE2	1:D:185:ILE:HD11	2.51	0.45
1:B:116:THR:OG1	1:B:155:GLN:NE2	2.47	0.45
1:E:16[B]:ARG:CG	1:E:16[B]:ARG:O	2.65	0.44
1:E:56:LYS:HB2	1:E:57:HIS:HA	1.99	0.44
1:C:137:ALA:O	1:C:138:ALA:HB3	2.18	0.44
1:B:339:THR:HG21	1:B:343:LEU:HD21	2.00	0.44
1:A:245:VAL:HG23	1:A:274:ALA:HB1	2.00	0.44
1:B:79:VAL:HG12	1:B:206:LEU:HD12	1.99	0.43
1:A:406:TYR:O	1:A:415:LYS:NZ	2.51	0.43
1:F:129:GLU:O	1:F:130:THR:OG1	2.34	0.43
1:E:404:LEU:HD21	1:E:419:ILE:HG21	2.00	0.43
1:A:12:ILE:HD13	1:A:113:LEU:HD11	2.01	0.43
1:F:100:GLU:HA	1:F:101:GLY:HA2	1.78	0.43
1:C:441:VAL:HG12	1:C:441:VAL:O	2.17	0.43
1:A:278:HIS:CD2	1:A:287:ILE:HD13	2.54	0.43
1:C:330:SER:HB3	1:C:335:LEU:HD22	2.01	0.42
1:F:116:THR:HG21	1:F:155:GLN:HE22	1.85	0.42
1:E:181:PHE:CE2	1:E:185:ILE:HD11	2.54	0.42
1:E:307:ASN:HB3	1:E:328:VAL:HG11	2.01	0.42
1:D:424:VAL:CG2	1:D:451:VAL:HG13	2.50	0.42
1:D:295:CYS:HA	1:D:296:ALA:HA	1.76	0.42
1:E:242:THR:HG21	1:E:357:TYR:HA	2.01	0.41
1:E:100:GLU:HB3	1:E:101:GLY:HA3	2.02	0.41
1:C:214:PRO:O	1:C:218:TRP:HB2	2.20	0.41
1:C:294:GLY:HA2	1:C:295:CYS:HA	1.89	0.41
1:B:97:ASP:N	1:B:98:GLY:HA3	2.36	0.41
1:F:436:ALA:N	1:F:437:PRO:CD	2.85	0.40
1:C:363:ASN:HD22	1:C:363:ASN:N	2.19	0.40
1:B:436:ALA:N	1:B:437:PRO:CD	2.84	0.40
1:F:296:ALA:O	1:F:297:ALA:HB3	2.22	0.40
1:C:116:THR:HG21	1:C:155:GLN:HE22	1.87	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	459/460 (100%)	439 (96%)	20 (4%)	0	100	100
1	B	458/460 (100%)	414 (90%)	37 (8%)	7 (2%)	13	40
1	C	458/460 (100%)	427 (93%)	29 (6%)	2 (0%)	39	74
1	D	458/460 (100%)	437 (95%)	20 (4%)	1 (0%)	52	84
1	E	459/460 (100%)	435 (95%)	22 (5%)	2 (0%)	39	74
1	F	458/460 (100%)	431 (94%)	26 (6%)	1 (0%)	52	84
All	All	2750/2760 (100%)	2583 (94%)	154 (6%)	13 (0%)	34	69

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	ALA
1	B	442	GLY
1	B	144	MET
1	B	366	SER
1	F	366	SER
1	C	243	HIS
1	E	296	ALA
1	E	229	GLU
1	B	371	GLU
1	B	428	LYS
1	B	98	GLY
1	C	98	GLY
1	D	98	GLY

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	400/399 (100%)	399 (100%)	1 (0%)	94	99
1	B	399/399 (100%)	396 (99%)	3 (1%)	86	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	399/399 (100%)	395 (99%)	4 (1%)	82 96
1	D	399/399 (100%)	397 (100%)	2 (0%)	92 98
1	E	400/399 (100%)	395 (99%)	5 (1%)	76 94
1	F	399/399 (100%)	393 (98%)	6 (2%)	72 93
All	All	2396/2394 (100%)	2375 (99%)	21 (1%)	86 96

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	TRP
1	B	142	GLU
1	B	145	ASN
1	B	149	PHE
1	C	218	TRP
1	C	268	ASP
1	C	307	ASN
1	C	319	LYS
1	D	21	ARG
1	D	218	TRP
1	E	16[A]	ARG
1	E	16[B]	ARG
1	E	103	ASP
1	E	218	TRP
1	E	240	ASP
1	F	26	ARG
1	F	58	THR
1	F	60	ASN
1	F	128	TRP
1	F	218	TRP
1	F	395	MET

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

Mol	Chain	Res	Type
1	A	146	ASN
1	A	155	GLN
1	A	307	ASN
1	B	155	GLN
1	B	169	GLN
1	B	342	GLN

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Mol	Chain	Res	Type
1	C	61	GLN
1	C	155	GLN
1	C	226	GLN
1	C	238	ASN
1	C	363	ASN
1	D	145	ASN
1	D	155	GLN
1	D	226	GLN
1	E	155	GLN
1	F	60	ASN
1	F	155	GLN
1	F	278	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	D	501	-	5,5,5	0.24	0	5,5,5	0.16	0
2	GOL	D	502	-	5,5,5	0.21	0	5,5,5	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	D	503	-	5,5,5	0.24	0	5,5,5	0.22	0
2	GOL	E	501	-	5,5,5	0.21	0	5,5,5	0.28	0
2	GOL	E	502	-	5,5,5	0.23	0	5,5,5	0.17	0
2	GOL	E	503	-	5,5,5	0.26	0	5,5,5	0.15	0
2	GOL	F	501	-	5,5,5	0.24	0	5,5,5	0.16	0
2	GOL	F	502	-	5,5,5	0.23	0	5,5,5	0.22	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	D	501	-	-	0/4/4/4	0/0/0/0
2	GOL	D	502	-	-	0/4/4/4	0/0/0/0
2	GOL	D	503	-	-	0/4/4/4	0/0/0/0
2	GOL	E	501	-	-	0/4/4/4	0/0/0/0
2	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	GOL	E	503	-	-	0/4/4/4	0/0/0/0
2	GOL	F	501	-	-	0/4/4/4	0/0/0/0
2	GOL	F	502	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	460/460 (100%)	0.12	4 (0%) 85 79	57, 73, 103, 121	0
1	B	460/460 (100%)	0.84	72 (15%) 3 1	78, 126, 151, 162	0
1	C	460/460 (100%)	0.43	20 (4%) 39 27	75, 107, 134, 146	0
1	D	460/460 (100%)	0.28	15 (3%) 50 38	59, 92, 120, 136	0
1	E	460/460 (100%)	0.13	3 (0%) 89 84	56, 78, 102, 139	0
1	F	460/460 (100%)	0.15	2 (0%) 93 90	59, 76, 103, 113	0
All	All	2760/2760 (100%)	0.33	116 (4%) 40 28	56, 89, 137, 162	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	TYR	8.2
1	B	460	TRP	7.1
1	D	363	ASN	6.6
1	B	459	PHE	5.5
1	B	316	LEU	5.4
1	B	384	PHE	5.0
1	C	135	PRO	4.6
1	B	315	TYR	4.6
1	B	70	MET	4.5
1	B	363	ASN	4.4
1	D	362	ALA	4.4
1	B	148	ASP	4.3
1	B	227	GLY	4.3
1	E	1	GLY	4.1
1	D	365	THR	3.9
1	B	391	TYR	3.8
1	B	389	PRO	3.8
1	A	363	ASN	3.8
1	C	141	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	296	ALA	3.7
1	B	100	GLU	3.7
1	B	319	LYS	3.6
1	B	1	GLY	3.6
1	D	1	GLY	3.6
1	B	102	MET	3.5
1	B	388	GLY	3.5
1	B	419	ILE	3.4
1	B	250	LEU	3.3
1	C	142	GLU	3.3
1	C	370	LEU	3.3
1	B	426	SER	3.2
1	A	365	THR	3.2
1	C	133	LEU	3.1
1	B	322	GLU	3.1
1	B	225	MET	3.1
1	C	354	LYS	3.1
1	B	252	ALA	3.1
1	E	57	HIS	3.1
1	F	363	ASN	3.0
1	B	128	TRP	3.0
1	B	142	GLU	3.0
1	B	386	LYS	3.0
1	B	338	ALA	3.0
1	B	81	ALA	3.0
1	C	363	ASN	3.0
1	C	60	ASN	2.9
1	E	41	PHE	2.9
1	B	297	ALA	2.9
1	B	344	ASN	2.9
1	C	114	PRO	2.9
1	B	429	GLN	2.9
1	D	265	LEU	2.9
1	B	351	SER	2.9
1	B	256	PHE	2.9
1	B	66	PRO	2.9
1	B	133	LEU	2.8
1	B	394	VAL	2.8
1	D	371	GLU	2.8
1	B	248	PHE	2.7
1	B	97	ASP	2.7
1	B	63	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	387	GLU	2.7
1	C	285	TYR	2.7
1	B	83	LEU	2.6
1	C	129	GLU	2.6
1	B	285	TYR	2.6
1	B	317	THR	2.6
1	B	321	PHE	2.5
1	B	390	LEU	2.5
1	D	372	SER	2.5
1	B	275	ILE	2.5
1	B	339	THR	2.5
1	B	24	VAL	2.5
1	B	331	TYR	2.5
1	C	318	TYR	2.5
1	C	54	PHE	2.5
1	D	386	LYS	2.5
1	C	56	LYS	2.4
1	C	143	LYS	2.4
1	B	216	VAL	2.4
1	A	205	GLU	2.4
1	C	7	PRO	2.4
1	B	404	LEU	2.3
1	C	98	GLY	2.3
1	B	372	SER	2.3
1	B	320	ASN	2.3
1	D	98	GLY	2.3
1	B	205	GLU	2.3
1	B	376	ASP	2.3
1	B	432	ASP	2.3
1	B	68	PHE	2.3
1	F	100	GLU	2.3
1	B	129	GLU	2.2
1	C	59	SER	2.2
1	D	232	TYR	2.2
1	D	460	TRP	2.2
1	B	434	LEU	2.2
1	D	250	LEU	2.2
1	C	63	THR	2.2
1	B	412	LEU	2.2
1	D	94	GLN	2.1
1	B	300	MET	2.1
1	B	430	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	130	THR	2.1
1	B	328	VAL	2.1
1	C	70	MET	2.1
1	B	444	ILE	2.1
1	D	88	GLY	2.1
1	A	366	SER	2.1
1	B	204	LEU	2.1
1	B	236	TYR	2.1
1	B	350	THR	2.0
1	D	320	ASN	2.0
1	B	59	SER	2.0
1	B	433	ARG	2.0
1	B	73	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	E	503	6/6	0.90	0.39	6.07	102,103,104,104	0
2	GOL	F	501	6/6	0.81	0.34	5.32	106,107,108,108	0
2	GOL	F	502	6/6	0.82	0.33	5.27	82,82,82,82	0
2	GOL	D	503	6/6	0.80	0.26	2.93	91,92,93,93	0
2	GOL	E	501	6/6	0.82	0.30	1.78	92,94,95,96	0
2	GOL	D	502	6/6	0.91	0.30	1.28	88,89,89,90	0
2	GOL	D	501	6/6	0.85	0.21	0.25	89,90,90,90	0
3	CL	D	504	1/1	0.94	0.17	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	E	502	6/6	0.82	0.29	-	126,127,127,128	0

6.5 Other polymers (i)

There are no such residues in this entry.