



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:04 AM UTC

PDB ID : 2GNN / pdb_00002gnn
Title : Crystal Structure of the Orf Virus NZ2 Variant of VEGF-E
Authors : Prota, A.E.; Pieren, M.; Wagner, A.; Kostrewa, D.; Winkler, F.K.; Ballmer-Hofer, K.
Deposited on : 2006-04-10
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

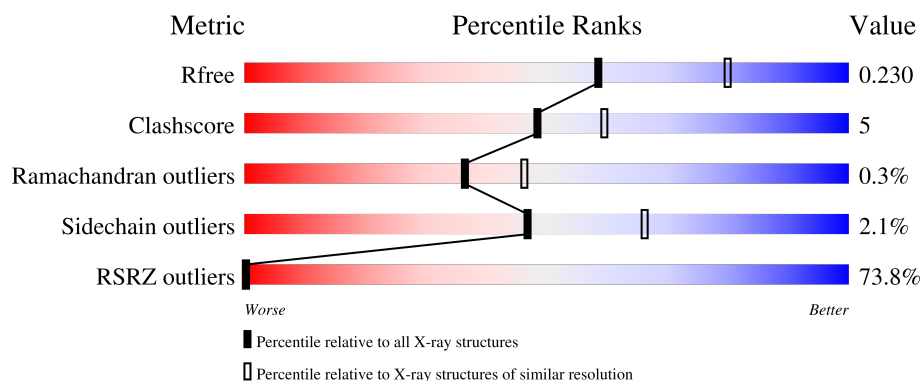
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	127	55% 63% 9% 28%
1	B	127	38% 64% 11% 25%
1	C	127	61% 61% 10% 29%
1	D	127	61% 61% 11% 27%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3144 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 Vascular endothelial growth factor homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	1	0
			716	439	126	140	11			
1	B	95	Total	C	N	O	S	0	0	0
			719	437	130	141	11			
1	C	90	Total	C	N	O	S	0	0	0
			700	429	124	136	11			
1	D	93	Total	C	N	O	S	0	0	0
			700	427	124	138	11			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLU	-	cloning artifact	UNP P52584
A	6	ALA	-	cloning artifact	UNP P52584
A	7	GLU	-	cloning artifact	UNP P52584
A	8	ALA	-	cloning artifact	UNP P52584
A	9	GLU	-	cloning artifact	UNP P52584
A	10	PHE	-	cloning artifact	UNP P52584
A	77	THR	SER	SEE REMARK 999	UNP P52584
A	124	VAL	-	cloning artifact	UNP P52584
A	125	ASP	-	cloning artifact	UNP P52584
A	126	HIS	-	expression tag	UNP P52584
A	127	HIS	-	expression tag	UNP P52584
A	128	HIS	-	expression tag	UNP P52584
A	129	HIS	-	expression tag	UNP P52584
A	130	HIS	-	expression tag	UNP P52584
A	131	HIS	-	expression tag	UNP P52584
B	5	GLU	-	cloning artifact	UNP P52584
B	6	ALA	-	cloning artifact	UNP P52584
B	7	GLU	-	cloning artifact	UNP P52584
B	8	ALA	-	cloning artifact	UNP P52584
B	9	GLU	-	cloning artifact	UNP P52584
B	10	PHE	-	cloning artifact	UNP P52584

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	THR	SER	SEE REMARK 999	UNP P52584
B	124	VAL	-	cloning artifact	UNP P52584
B	125	ASP	-	cloning artifact	UNP P52584
B	126	HIS	-	expression tag	UNP P52584
B	127	HIS	-	expression tag	UNP P52584
B	128	HIS	-	expression tag	UNP P52584
B	129	HIS	-	expression tag	UNP P52584
B	130	HIS	-	expression tag	UNP P52584
B	131	HIS	-	expression tag	UNP P52584
C	5	GLU	-	cloning artifact	UNP P52584
C	6	ALA	-	cloning artifact	UNP P52584
C	7	GLU	-	cloning artifact	UNP P52584
C	8	ALA	-	cloning artifact	UNP P52584
C	9	GLU	-	cloning artifact	UNP P52584
C	10	PHE	-	cloning artifact	UNP P52584
C	77	THR	SER	SEE REMARK 999	UNP P52584
C	124	VAL	-	cloning artifact	UNP P52584
C	125	ASP	-	cloning artifact	UNP P52584
C	126	HIS	-	expression tag	UNP P52584
C	127	HIS	-	expression tag	UNP P52584
C	128	HIS	-	expression tag	UNP P52584
C	129	HIS	-	expression tag	UNP P52584
C	130	HIS	-	expression tag	UNP P52584
C	131	HIS	-	expression tag	UNP P52584
D	5	GLU	-	cloning artifact	UNP P52584
D	6	ALA	-	cloning artifact	UNP P52584
D	7	GLU	-	cloning artifact	UNP P52584
D	8	ALA	-	cloning artifact	UNP P52584
D	9	GLU	-	cloning artifact	UNP P52584
D	10	PHE	-	cloning artifact	UNP P52584
D	77	THR	SER	SEE REMARK 999	UNP P52584
D	124	VAL	-	cloning artifact	UNP P52584
D	125	ASP	-	cloning artifact	UNP P52584
D	126	HIS	-	expression tag	UNP P52584
D	127	HIS	-	expression tag	UNP P52584
D	128	HIS	-	expression tag	UNP P52584
D	129	HIS	-	expression tag	UNP P52584
D	130	HIS	-	expression tag	UNP P52584
D	131	HIS	-	expression tag	UNP P52584

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

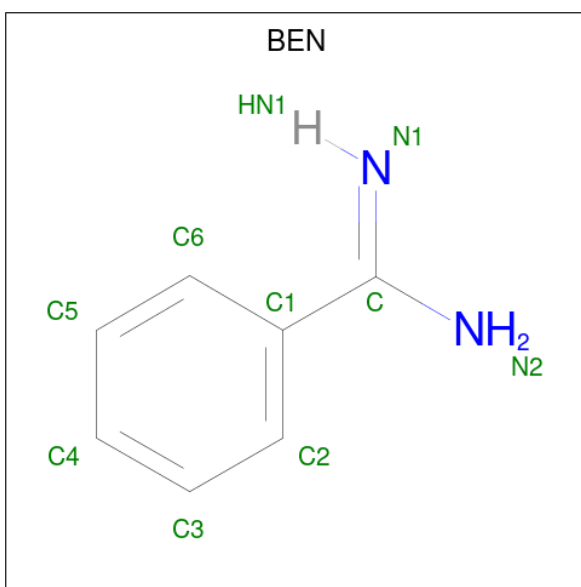
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



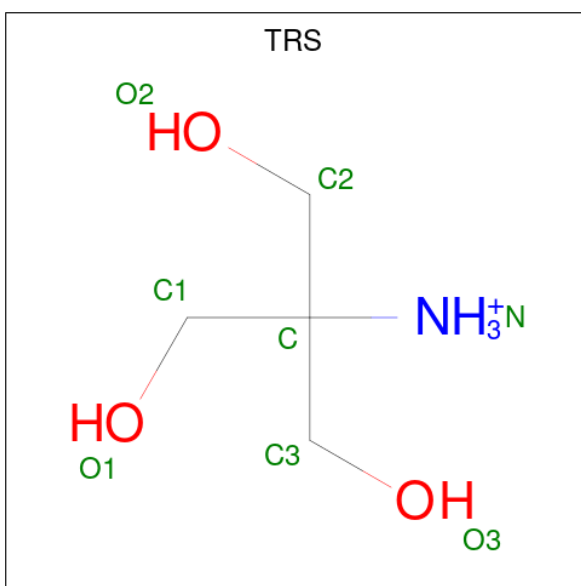
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	B	1	Total	C	N	0	0
			9	7	2		
4	D	1	Total	C	N	0	0
			9	7	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

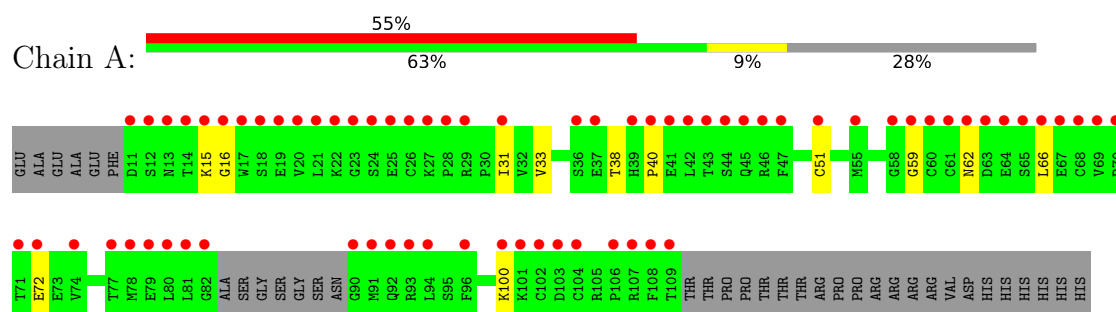
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	40	Total	O	0	0
			40	40		
8	B	47	Total	O	0	0
			47	47		
8	C	44	Total	O	0	0
			44	44		
8	D	46	Total	O	0	0
			46	46		

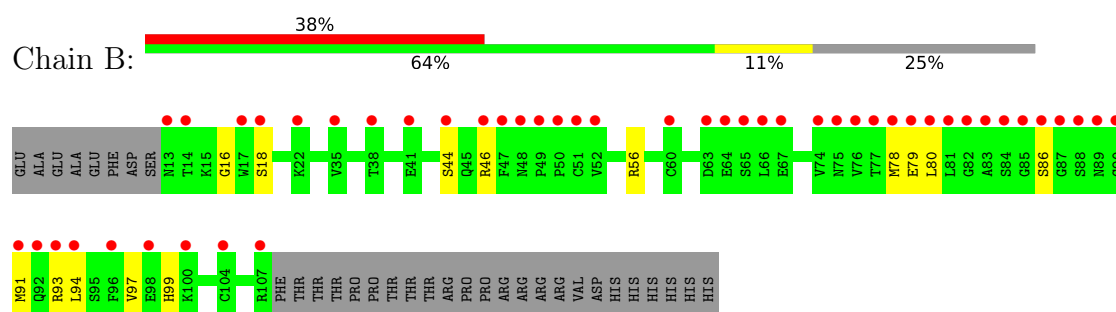
3 Residue-property plots [i](#)

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.

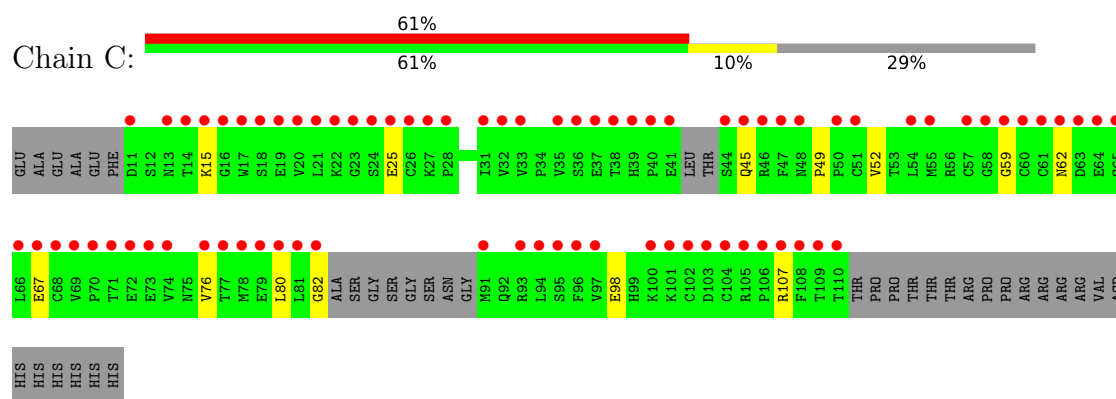
- Molecule 1: Vascular endothelial growth factor homolog



- Molecule 1: Vascular endothelial growth factor homolog

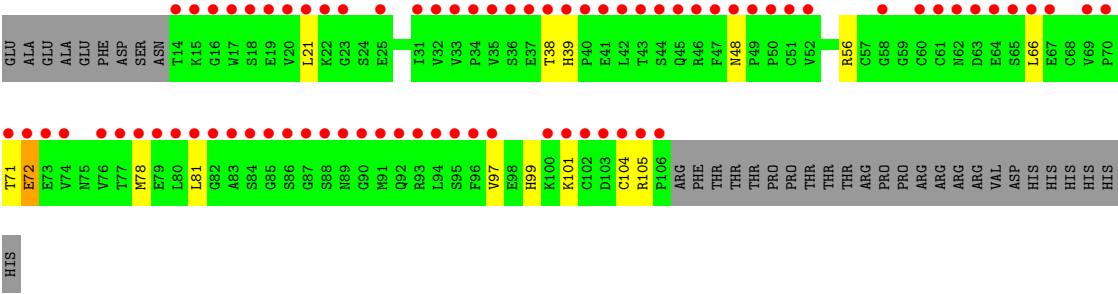


- Molecule 1: Vascular endothelial growth factor homolog



- Molecule 1: Vascular endothelial growth factor homolog





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.60Å 98.60Å 240.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.30 48.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.48-2.30) 98.7 (48.48-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.247 0.211 , 0.230	Depositor DCC
R_{free} test set	2687 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3144	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, SO4, BEN, NAG, 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	0.61	0/734	0.77	1/991 (0.1%)
1	B	0.62	0/732	0.79	0/989
1	C	0.69	1/712 (0.1%)	0.78	1/960 (0.1%)
1	D	0.62	0/713	0.77	0/964
All	All	0.64	1/2891 (0.0%)	0.78	2/3904 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	GLY	C-O	10.06	1.43	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	GLY	N-CA-C	-7.05	102.29	111.52
1	A	59	GLY	N-CA-C	-5.70	103.60	111.76

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	716	0	692	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	719	0	697	14	0
1	C	700	0	675	6	0
1	D	700	0	678	9	0
2	A	1	0	0	0	0
2	C	2	0	0	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	9	0	7	0	0
4	B	9	0	7	2	0
4	D	9	0	7	0	0
5	A	8	0	12	0	0
5	C	8	0	12	0	0
6	A	24	0	32	2	0
6	B	18	0	24	4	0
6	C	6	0	8	0	0
7	B	14	0	13	0	0
7	D	14	0	13	0	0
8	A	40	0	0	0	0
8	B	47	0	0	1	0
8	C	44	0	0	0	0
8	D	46	0	0	1	0
All	All	3144	0	2877	32	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 5.

All (32) 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:A:66:LEU:HD12	8:D:1031:HOH:O	1.62	0.97
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.53	0.74
1:B:16:GLY:HA3	6:B:604:GOL:H12	1.80	0.62
1:A:72:GLU:HG2	1:A:100:LYS:HB2	1.82	0.62
1:A:15:LYS:HB2	1:B:78:MET:HG2	1.83	0.60
1:B:56:ARG:NH1	1:B:97:VAL:O	2.33	0.57
1:B:56:ARG:HD3	1:B:99:HIS:CE1	2.40	0.55
1:B:56:ARG:HD2	8:B:1033:HOH:O	2.05	0.55
1:B:56:ARG:HG2	1:B:56:ARG:NH1	2.17	0.54
1:B:44:SER:HB2	4:B:1002:BEN:H4	1.90	0.54
1:D:66:LEU:HD13	1:D:104:CYS:HB3	1.91	0.53
1:A:38:THR:O	1:A:40:PRO:HD3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:608:GOL:H12	1:C:25:GLU:HG2	1.93	0.51
1:B:44:SER:CB	4:B:1002:BEN:H4	2.41	0.50
1:A:16:GLY:HA3	6:A:602:GOL:H12	1.93	0.50
1:B:18:SER:H	6:B:604:GOL:H31	1.77	0.50
1:C:49:PRO:HD2	1:C:80:LEU:HD22	1.95	0.49
1:D:56:ARG:NH2	1:D:97:VAL:O	2.36	0.49
1:B:86:SER:OG	6:B:608:GOL:H11	2.14	0.47
1:D:48:ASN:HB2	1:D:81:LEU:HB3	1.96	0.47
1:D:38:THR:OG1	1:D:39:HIS:HD2	1.99	0.46
1:C:15:LYS:HD2	1:D:78:MET:HE2	1.98	0.46
6:A:606:GOL:H11	1:B:46:ARG:HH22	1.80	0.45
1:D:72:GLU:HB3	1:D:101:LYS:HB2	1.98	0.45
1:A:33:VAL:O	1:A:51:CYS:HB2	2.16	0.44
1:D:56:ARG:HD3	1:D:99:HIS:CE1	2.53	0.43
1:D:71:THR:O	1:D:72:GLU:HB2	2.17	0.43
1:C:76:VAL:HG21	1:C:98:GLU:CD	2.44	0.43
1:B:79:GLU:HG2	1:B:91:MET:HE3	2.01	0.42
1:B:80:LEU:HD12	1:B:94:LEU:HD12	2.00	0.42
1:C:67:GLU:HG3	1:C:107:ARG:NH1	2.35	0.42
1:C:49:PRO:HG3	1:D:21:LEU:HD12	2.02	0.41

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	89/127 (70%)	86 (97%)	3 (3%)	0	100	100
1	B	93/127 (73%)	92 (99%)	1 (1%)	0	100	100
1	C	84/127 (66%)	81 (96%)	3 (4%)	0	100	100
1	D	91/127 (72%)	89 (98%)	1 (1%)	1 (1%)	11	13
All	All	357/508 (70%)	348 (98%)	8 (2%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	72	GLU

5.3.2 Protein sidechains ⓘ

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	87/116 (75%)	85 (98%)	2 (2%)	44	63
1	B	86/116 (74%)	85 (99%)	1 (1%)	63	79
1	C	85/116 (73%)	82 (96%)	3 (4%)	32	48
1	D	84/116 (72%)	83 (99%)	1 (1%)	63	79
All	All	342/464 (74%)	335 (98%)	7 (2%)	47	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	62	ASN
1	B	93	ARG
1	C	45	GLN
1	C	52	VAL
1	C	62	ASN
1	D	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	92	GLN
1	C	45	GLN
1	C	48	ASN
1	D	39	HIS
1	D	62	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	$\# Z > 2$
3	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.42	0
6	GOL	A	601	-	5,5,5	0.39	0	5,5,5	0.36	0
6	GOL	A	610	-	5,5,5	0.33	0	5,5,5	0.37	0
5	TRS	C	901	-	7,7,7	0.34	0	9,9,9	0.60	0
6	GOL	B	609	-	5,5,5	0.39	0	5,5,5	0.18	0
4	BEN	B	1002	-	9,9,9	0.47	0	7,11,11	1.63	1 (14%)
6	GOL	C	603	-	5,5,5	0.39	0	5,5,5	0.24	0
6	GOL	A	606	-	5,5,5	0.36	0	5,5,5	0.32	0
5	TRS	A	900	-	7,7,7	0.37	0	9,9,9	0.59	0
3	SO4	C	500	-	4,4,4	0.20	0	6,6,6	0.37	0
7	NAG	B	1001	1	14,14,15	0.55	0	17,19,21	1.29	2 (11%)
6	GOL	B	604	-	5,5,5	0.41	0	5,5,5	0.19	0
4	BEN	A	1001	-	9,9,9	0.38	0	7,11,11	1.80	1 (14%)
7	NAG	D	1002	1	14,14,15	0.45	0	17,19,21	1.35	2 (11%)
4	BEN	D	1003	-	9,9,9	1.22	1 (11%)	7,11,11	0.83	1 (14%)
6	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.22	0
6	GOL	B	608	-	5,5,5	0.42	0	5,5,5	0.26	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
6	GOL	A	601	-	-	2/4/4/4	-
6	GOL	A	610	-	-	4/4/4/4	-
5	TRS	C	901	-	-	6/9/9/9	-
6	GOL	B	609	-	-	0/4/4/4	-
4	BEN	B	1002	-	-	0/4/4/4	0/1/1/1
6	GOL	C	603	-	-	0/4/4/4	-
6	GOL	A	606	-	-	0/4/4/4	-
5	TRS	A	900	-	-	2/9/9/9	-
7	NAG	B	1001	1	-	4/6/23/26	0/1/1/1
6	GOL	B	604	-	-	2/4/4/4	-
4	BEN	A	1001	-	-	0/4/4/4	0/1/1/1
7	NAG	D	1002	1	-	4/6/23/26	0/1/1/1
4	BEN	D	1003	-	-	0/4/4/4	0/1/1/1
6	GOL	A	602	-	-	2/4/4/4	-
6	GOL	B	608	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1003	BEN	C1-C	2.71	1.52	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1002	NAG	O5-C1-C2	-3.46	105.94	111.29
7	B	1001	NAG	O5-C1-C2	-3.22	106.31	111.29
4	A	1001	BEN	C6-C1-C2	3.17	122.61	118.57
4	B	1002	BEN	C6-C1-C2	2.84	122.18	118.57
7	D	1002	NAG	C1-O5-C5	2.65	115.73	112.19
7	B	1001	NAG	C1-O5-C5	2.45	115.47	112.19
4	D	1003	BEN	C1-C-N2	2.09	121.19	118.01

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	901	TRS	C1-C-C2-O2
5	C	901	TRS	C3-C-C2-O2
5	C	901	TRS	N-C-C2-O2
6	A	601	GOL	O1-C1-C2-C3
6	B	604	GOL	O1-C1-C2-C3
6	B	608	GOL	O1-C1-C2-C3
7	B	1001	NAG	C8-C7-N2-C2
7	B	1001	NAG	O7-C7-N2-C2
7	D	1002	NAG	C8-C7-N2-C2
7	D	1002	NAG	O7-C7-N2-C2
7	B	1001	NAG	O5-C5-C6-O6
7	B	1001	NAG	C4-C5-C6-O6
7	D	1002	NAG	C4-C5-C6-O6
7	D	1002	NAG	O5-C5-C6-O6
6	A	601	GOL	O1-C1-C2-O2
6	A	602	GOL	O1-C1-C2-C3
6	A	610	GOL	O1-C1-C2-C3
6	A	610	GOL	C1-C2-C3-O3
6	A	602	GOL	O1-C1-C2-O2
6	B	604	GOL	O1-C1-C2-O2
6	B	608	GOL	O1-C1-C2-O2
6	A	610	GOL	O2-C2-C3-O3
5	A	900	TRS	N-C-C1-O1
6	A	610	GOL	O1-C1-C2-O2
5	A	900	TRS	C3-C-C1-O1
5	C	901	TRS	C3-C-C1-O1
5	C	901	TRS	C2-C-C3-O3
5	C	901	TRS	N-C-C1-O1

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1002	BEN	2	0
6	A	606	GOL	1	0
6	B	604	GOL	2	0
6	A	602	GOL	1	0
6	B	608	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	92/127 (72%)	3.38	70 (76%)  	51, 61, 97, 103	1 (1%)
1	B	95/127 (74%)	2.05	48 (50%)  	51, 61, 75, 86	0
1	C	90/127 (70%)	4.09	78 (86%)  	50, 62, 91, 97	0
1	D	93/127 (73%)	4.02	77 (82%)  	54, 62, 79, 84	0
All	All	370/508 (72%)	3.37	273 (73%)  	50, 62, 87, 103	1 (0%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	THR	13.6
1	C	109	THR	9.5
1	D	44	SER	9.5
1	A	109	THR	9.2
1	D	89	ASN	9.1
1	D	85	GLY	9.1
1	D	88	SER	9.0
1	D	82	GLY	8.6
1	D	90	GLY	8.6
1	C	108	PHE	8.4
1	A	11	ASP	8.2
1	D	80	LEU	8.2
1	D	86	SER	8.1
1	D	83	ALA	7.9
1	A	14	THR	7.9
1	A	42	LEU	7.6
1	C	62	ASN	7.4
1	D	84	SER	7.3
1	D	45	GLN	7.3
1	D	42	LEU	7.2
1	C	17	TRP	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	15	LYS	6.9
1	D	81	LEU	6.8
1	A	17	TRP	6.6
1	C	66	LEU	6.6
1	D	92	GLN	6.6
1	C	61	CYS	6.6
1	C	103	ASP	6.6
1	C	21	LEU	6.4
1	C	106	PRO	6.4
1	A	90	GLY	6.4
1	D	43	THR	6.3
1	C	18	SER	6.2
1	D	46	ARG	6.1
1	B	13	ASN	6.1
1	A	44	SER	6.0
1	D	48	ASN	6.0
1	A	13	ASN	6.0
1	D	87	GLY	6.0
1	D	47	PHE	5.9
1	C	59	GLY	5.9
1	C	11	ASP	5.9
1	C	65	SER	5.8
1	C	41	GLU	5.7
1	A	18	SER	5.7
1	C	14	THR	5.7
1	C	64	GLU	5.7
1	C	80	LEU	5.7
1	C	78	MET	5.7
1	D	62	ASN	5.6
1	C	104	CYS	5.6
1	C	107	ARG	5.6
1	C	47	PHE	5.6
1	D	17	TRP	5.5
1	D	36	SER	5.4
1	C	94	LEU	5.4
1	C	63	ASP	5.4
1	C	46	ARG	5.4
1	D	40	PRO	5.4
1	D	94	LEU	5.4
1	D	49	PRO	5.3
1	C	93	ARG	5.3
1	C	67	GLU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	12	SER	5.2
1	C	105	ARG	5.2
1	C	60	CYS	5.2
1	A	43	THR	5.2
1	C	79	GLU	5.1
1	D	79	GLU	5.1
1	D	91	MET	5.0
1	A	108	PHE	5.0
1	A	15	LYS	5.0
1	A	23	GLY	4.9
1	A	37[A]	GLU	4.9
1	C	96	PHE	4.9
1	D	50	PRO	4.9
1	D	52	VAL	4.8
1	A	47	PHE	4.8
1	D	22	LYS	4.8
1	A	81	LEU	4.7
1	A	21	LEU	4.7
1	A	62	ASN	4.7
1	A	40	PRO	4.7
1	D	93	ARG	4.6
1	C	69	VAL	4.6
1	A	22	LYS	4.6
1	D	41	GLU	4.5
1	A	36	SER	4.5
1	C	50	PRO	4.5
1	B	80	LEU	4.5
1	C	82	GLY	4.5
1	D	60	CYS	4.5
1	B	88	SER	4.4
1	B	81	LEU	4.4
1	D	39	HIS	4.4
1	D	21	LEU	4.4
1	A	51	CYS	4.3
1	A	46	ARG	4.3
1	A	96	PHE	4.3
1	A	20	VAL	4.2
1	C	13	ASN	4.2
1	D	51	CYS	4.2
1	A	101	LYS	4.2
1	B	107	ARG	4.2
1	A	92	GLN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	16	GLY	4.1
1	A	78	MET	4.1
1	B	85	GLY	4.1
1	D	78	MET	4.1
1	C	68	CYS	4.1
1	C	81	LEU	4.0
1	C	24	SER	4.0
1	A	61	CYS	4.0
1	B	89	ASN	4.0
1	D	65	SER	4.0
1	A	66	LEU	4.0
1	D	35	VAL	3.9
1	B	83	ALA	3.9
1	A	25	GLU	3.9
1	C	91	MET	3.9
1	C	71	THR	3.9
1	A	103	ASP	3.9
1	D	15	LYS	3.9
1	D	71	THR	3.9
1	A	60	CYS	3.8
1	C	102	CYS	3.8
1	D	25	GLU	3.8
1	D	103	ASP	3.8
1	A	24	SER	3.8
1	D	14	THR	3.8
1	D	97	VAL	3.8
1	D	16	GLY	3.8
1	C	77	THR	3.7
1	A	45	GLN	3.7
1	A	72	GLU	3.7
1	C	26	CYS	3.7
1	C	22	LYS	3.7
1	A	63	ASP	3.7
1	D	18	SER	3.7
1	B	100	LYS	3.7
1	C	25	GLU	3.6
1	B	90	GLY	3.6
1	A	100	LYS	3.6
1	C	36	SER	3.6
1	D	96	PHE	3.6
1	C	16	GLY	3.6
1	D	105	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	72	GLU	3.6
1	A	82	GLY	3.6
1	D	19	GLU	3.5
1	A	26	CYS	3.5
1	C	23	GLY	3.4
1	B	48	ASN	3.4
1	C	70	PRO	3.4
1	C	45	GLN	3.4
1	A	93	ARG	3.3
1	B	79	GLU	3.3
1	D	58	GLY	3.2
1	A	41	GLU	3.2
1	A	59	GLY	3.2
1	C	100	LYS	3.2
1	A	94	LEU	3.2
1	C	39	HIS	3.2
1	D	77	THR	3.2
1	D	76	VAL	3.2
1	D	106	PRO	3.2
1	A	71	THR	3.2
1	C	31	ILE	3.1
1	A	80	LEU	3.1
1	A	64	GLU	3.1
1	C	101	LYS	3.1
1	B	86	SER	3.0
1	C	51	CYS	3.0
1	A	91	MET	3.0
1	A	79	GLU	3.0
1	D	66	LEU	3.0
1	D	38	THR	3.0
1	A	107	ARG	3.0
1	B	93	ARG	3.0
1	A	19	GLU	3.0
1	C	19	GLU	3.0
1	D	61	CYS	3.0
1	D	67	GLU	3.0
1	A	106	PRO	3.0
1	C	35	VAL	2.9
1	C	27	LYS	2.9
1	B	35	VAL	2.9
1	A	58	GLY	2.9
1	B	63	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	95	SER	2.9
1	C	58	GLY	2.9
1	D	100	LYS	2.9
1	C	20	VAL	2.9
1	D	20	VAL	2.9
1	C	38	THR	2.9
1	B	82	GLY	2.9
1	C	44	SER	2.8
1	D	33	VAL	2.8
1	C	76	VAL	2.8
1	A	77	THR	2.8
1	A	104	CYS	2.8
1	A	39	HIS	2.8
1	B	44	SER	2.8
1	B	64	GLU	2.8
1	B	76	VAL	2.8
1	C	33	VAL	2.8
1	C	48	ASN	2.7
1	B	60	CYS	2.7
1	C	40	PRO	2.7
1	D	101	LYS	2.7
1	B	74	VAL	2.7
1	A	27	LYS	2.7
1	B	14	THR	2.7
1	D	23	GLY	2.7
1	D	95	SER	2.7
1	C	32	VAL	2.6
1	D	63	ASP	2.6
1	C	55	MET	2.6
1	B	75	ASN	2.6
1	B	77	THR	2.6
1	A	65	SER	2.6
1	D	64	GLU	2.6
1	B	94	LEU	2.6
1	C	37	GLU	2.6
1	A	102	CYS	2.5
1	C	57	CYS	2.5
1	B	92	GLN	2.5
1	D	37	GLU	2.5
1	B	49	PRO	2.5
1	B	41	GLU	2.5
1	B	65	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	84	SER	2.5
1	C	74	VAL	2.4
1	D	69	VAL	2.4
1	B	22	LYS	2.4
1	B	78	MET	2.4
1	B	67	GLU	2.4
1	D	72	GLU	2.4
1	D	34	PRO	2.4
1	B	104	CYS	2.4
1	D	32	VAL	2.4
1	D	70	PRO	2.3
1	A	74	VAL	2.3
1	D	104	CYS	2.3
1	B	91	MET	2.3
1	B	46	ARG	2.3
1	B	47	PHE	2.3
1	A	28	PRO	2.3
1	B	50	PRO	2.3
1	C	73	GLU	2.3
1	D	102	CYS	2.2
1	A	55	MET	2.2
1	A	31	ILE	2.2
1	A	69	VAL	2.2
1	C	54	LEU	2.2
1	B	52	VAL	2.2
1	A	70	PRO	2.2
1	B	87	GLY	2.2
1	D	73	GLU	2.2
1	A	67	GLU	2.2
1	A	68	CYS	2.2
1	B	17	TRP	2.1
1	D	74	VAL	2.1
1	C	28	PRO	2.1
1	B	18	SER	2.1
1	C	97	VAL	2.1
1	B	96	PHE	2.1
1	B	38	THR	2.1
1	B	98	GLU	2.0
1	B	51	CYS	2.0
1	B	66	LEU	2.0
1	A	29	ARG	2.0
1	D	31	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	BEN	D	1003	9/9	0.50	0.34	89,90,91,91	0
6	GOL	A	602	6/6	0.61	0.25	92,96,101,104	0
5	TRS	A	900	8/8	0.63	0.25	103,104,105,105	0
6	GOL	B	604	6/6	0.66	0.31	107,109,110,112	0
5	TRS	C	901	8/8	0.67	0.32	109,113,116,116	0
7	NAG	B	1001	14/15	0.69	0.25	100,108,117,121	0
6	GOL	A	606	6/6	0.71	0.29	104,118,120,120	0
3	SO4	A	501	5/5	0.73	0.17	61,76,77,84	0
6	GOL	B	608	6/6	0.74	0.32	109,113,114,115	0
6	GOL	A	601	6/6	0.74	0.25	97,107,109,110	0
7	NAG	D	1002	14/15	0.74	0.26	69,101,107,112	0
3	SO4	C	500	5/5	0.75	0.18	73,81,85,87	0
6	GOL	C	603	6/6	0.80	0.28	100,111,114,114	0
6	GOL	B	609	6/6	0.82	0.26	108,115,118,119	0
2	CL	C	705	1/1	0.84	0.17	84,84,84,84	0
6	GOL	A	610	6/6	0.87	0.25	119,124,124,125	0
4	BEN	B	1002	9/9	0.91	0.15	32,38,47,50	0
2	CL	A	702	1/1	0.91	0.13	87,87,87,87	0
2	CL	C	704	1/1	0.93	0.14	80,80,80,80	0
4	BEN	A	1001	9/9	0.93	0.33	28,34,40,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.