



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:30 PM UTC

PDB ID : 8A2E / pdb_00008a2e
Title : Crystal Structure of Human Parechovirus 3 2A protein
Authors : von Castelmur, E.; Zhu, L.; wang, X.; Fry, E.; Ren, J.; Perrakis, A.; Stuart, D.I.
Deposited on : 2022-06-03
Resolution : 2.29 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

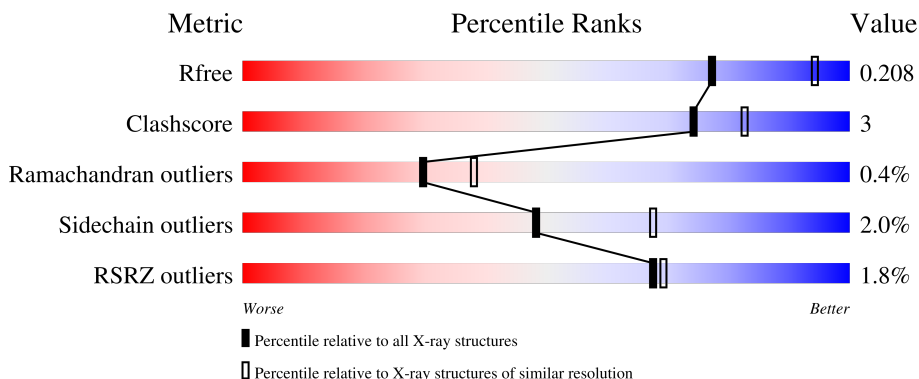
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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.



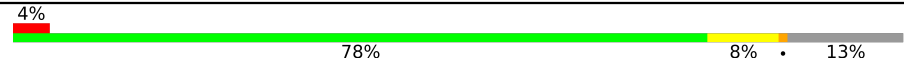

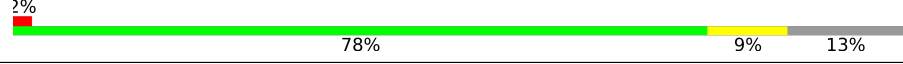
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	AAA	157	 86% 8% • 6%
1	BBB	157	 81% 6% 13%
1	CCC	157	 3% 82% 12% 6%
1	DDD	157	 80% 6% • 13%
1	EEE	157	 83% 10% • 6%

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Mol	Chain	Length	Quality of chain
1	FFF	157	 4% 78% 8% • 13%
1	GGG	157	 % 85% 8% • 6%
1	HHH	157	 2% 78% 9% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9145 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 2A protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	148	1175	750	194	225	6	0	0	0
1	BBB	136	1092	700	181	206	5	0	1	0
1	CCC	148	1175	750	194	225	6	0	0	0
1	DDD	137	1088	697	179	207	5	0	0	0
1	EEE	148	1175	750	194	225	6	0	0	0
1	FFF	136	1084	695	178	206	5	0	0	0
1	GGG	148	1175	750	194	225	6	0	0	0
1	HHH	136	1074	688	176	205	5	0	0	0

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	0	MET	-	initiating methionine	UNP U3KRG6
AAA	1	SER	-	expression tag	UNP U3KRG6
AAA	11	MET	LYS	variant	UNP U3KRG6
AAA	31	GLU	ASP	variant	UNP U3KRG6
AAA	66	GLY	GLU	variant	UNP U3KRG6
AAA	149	LEU	-	expression tag	UNP U3KRG6
AAA	150	GLU	-	expression tag	UNP U3KRG6
AAA	151	HIS	-	expression tag	UNP U3KRG6
AAA	152	HIS	-	expression tag	UNP U3KRG6
AAA	153	HIS	-	expression tag	UNP U3KRG6
AAA	154	HIS	-	expression tag	UNP U3KRG6
AAA	155	HIS	-	expression tag	UNP U3KRG6
AAA	156	HIS	-	expression tag	UNP U3KRG6

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	MET	-	initiating methionine	UNP U3KRG6
BBB	1	SER	-	expression tag	UNP U3KRG6
BBB	11	MET	LYS	variant	UNP U3KRG6
BBB	31	GLU	ASP	variant	UNP U3KRG6
BBB	66	GLY	GLU	variant	UNP U3KRG6
BBB	149	LEU	-	expression tag	UNP U3KRG6
BBB	150	GLU	-	expression tag	UNP U3KRG6
BBB	151	HIS	-	expression tag	UNP U3KRG6
BBB	152	HIS	-	expression tag	UNP U3KRG6
BBB	153	HIS	-	expression tag	UNP U3KRG6
BBB	154	HIS	-	expression tag	UNP U3KRG6
BBB	155	HIS	-	expression tag	UNP U3KRG6
BBB	156	HIS	-	expression tag	UNP U3KRG6
CCC	0	MET	-	initiating methionine	UNP U3KRG6
CCC	1	SER	-	expression tag	UNP U3KRG6
CCC	11	MET	LYS	variant	UNP U3KRG6
CCC	31	GLU	ASP	variant	UNP U3KRG6
CCC	66	GLY	GLU	variant	UNP U3KRG6
CCC	149	LEU	-	expression tag	UNP U3KRG6
CCC	150	GLU	-	expression tag	UNP U3KRG6
CCC	151	HIS	-	expression tag	UNP U3KRG6
CCC	152	HIS	-	expression tag	UNP U3KRG6
CCC	153	HIS	-	expression tag	UNP U3KRG6
CCC	154	HIS	-	expression tag	UNP U3KRG6
CCC	155	HIS	-	expression tag	UNP U3KRG6
CCC	156	HIS	-	expression tag	UNP U3KRG6
DDD	0	MET	-	initiating methionine	UNP U3KRG6
DDD	1	SER	-	expression tag	UNP U3KRG6
DDD	11	MET	LYS	variant	UNP U3KRG6
DDD	31	GLU	ASP	variant	UNP U3KRG6
DDD	66	GLY	GLU	variant	UNP U3KRG6
DDD	149	LEU	-	expression tag	UNP U3KRG6
DDD	150	GLU	-	expression tag	UNP U3KRG6
DDD	151	HIS	-	expression tag	UNP U3KRG6
DDD	152	HIS	-	expression tag	UNP U3KRG6
DDD	153	HIS	-	expression tag	UNP U3KRG6
DDD	154	HIS	-	expression tag	UNP U3KRG6
DDD	155	HIS	-	expression tag	UNP U3KRG6
DDD	156	HIS	-	expression tag	UNP U3KRG6
EEE	0	MET	-	initiating methionine	UNP U3KRG6
EEE	1	SER	-	expression tag	UNP U3KRG6
EEE	11	MET	LYS	variant	UNP U3KRG6

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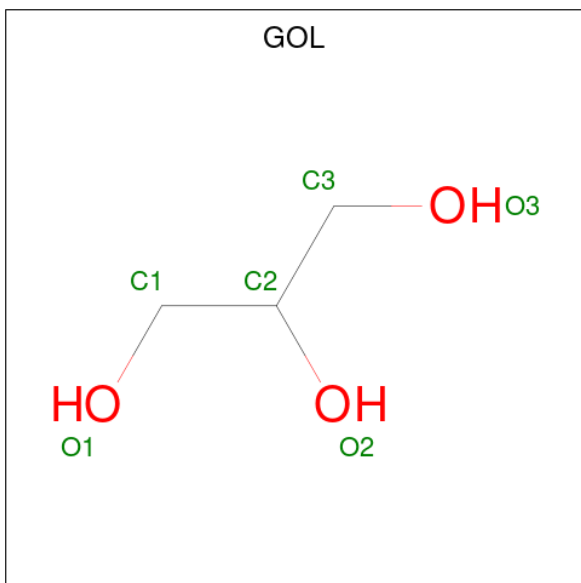
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	31	GLU	ASP	variant	UNP U3KRG6
EEE	66	GLY	GLU	variant	UNP U3KRG6
EEE	149	LEU	-	expression tag	UNP U3KRG6
EEE	150	GLU	-	expression tag	UNP U3KRG6
EEE	151	HIS	-	expression tag	UNP U3KRG6
EEE	152	HIS	-	expression tag	UNP U3KRG6
EEE	153	HIS	-	expression tag	UNP U3KRG6
EEE	154	HIS	-	expression tag	UNP U3KRG6
EEE	155	HIS	-	expression tag	UNP U3KRG6
EEE	156	HIS	-	expression tag	UNP U3KRG6
FFF	0	MET	-	initiating methionine	UNP U3KRG6
FFF	1	SER	-	expression tag	UNP U3KRG6
FFF	11	MET	LYS	variant	UNP U3KRG6
FFF	31	GLU	ASP	variant	UNP U3KRG6
FFF	66	GLY	GLU	variant	UNP U3KRG6
FFF	149	LEU	-	expression tag	UNP U3KRG6
FFF	150	GLU	-	expression tag	UNP U3KRG6
FFF	151	HIS	-	expression tag	UNP U3KRG6
FFF	152	HIS	-	expression tag	UNP U3KRG6
FFF	153	HIS	-	expression tag	UNP U3KRG6
FFF	154	HIS	-	expression tag	UNP U3KRG6
FFF	155	HIS	-	expression tag	UNP U3KRG6
FFF	156	HIS	-	expression tag	UNP U3KRG6
GGG	0	MET	-	initiating methionine	UNP U3KRG6
GGG	1	SER	-	expression tag	UNP U3KRG6
GGG	11	MET	LYS	variant	UNP U3KRG6
GGG	31	GLU	ASP	variant	UNP U3KRG6
GGG	66	GLY	GLU	variant	UNP U3KRG6
GGG	149	LEU	-	expression tag	UNP U3KRG6
GGG	150	GLU	-	expression tag	UNP U3KRG6
GGG	151	HIS	-	expression tag	UNP U3KRG6
GGG	152	HIS	-	expression tag	UNP U3KRG6
GGG	153	HIS	-	expression tag	UNP U3KRG6
GGG	154	HIS	-	expression tag	UNP U3KRG6
GGG	155	HIS	-	expression tag	UNP U3KRG6
GGG	156	HIS	-	expression tag	UNP U3KRG6
HHH	0	MET	-	initiating methionine	UNP U3KRG6
HHH	1	SER	-	expression tag	UNP U3KRG6
HHH	11	MET	LYS	variant	UNP U3KRG6
HHH	31	GLU	ASP	variant	UNP U3KRG6
HHH	66	GLY	GLU	variant	UNP U3KRG6
HHH	149	LEU	-	expression tag	UNP U3KRG6

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Chain	Residue	Modelled	Actual	Comment	Reference
HHH	150	GLU	-	expression tag	UNP U3KRG6
HHH	151	HIS	-	expression tag	UNP U3KRG6
HHH	152	HIS	-	expression tag	UNP U3KRG6
HHH	153	HIS	-	expression tag	UNP U3KRG6
HHH	154	HIS	-	expression tag	UNP U3KRG6
HHH	155	HIS	-	expression tag	UNP U3KRG6
HHH	156	HIS	-	expression tag	UNP U3KRG6

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 6 3 3	0	0
2	BBB	1	Total C O 6 3 3	0	0
2	DDD	1	Total C O 6 3 3	0	0
2	FFF	1	Total C O 6 3 3	0	0
2	HHH	1	Total C O 6 3 3	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	CCC	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	EEE	1	Total	O	S	0	0
			5	4	1		
3	GGG	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	4	Total	O	0	0
			4	4		
4	BBB	9	Total	O	0	0
			9	9		
4	CCC	10	Total	O	0	0
			10	10		
4	DDD	5	Total	O	0	0
			5	5		

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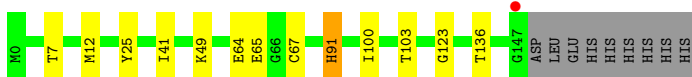
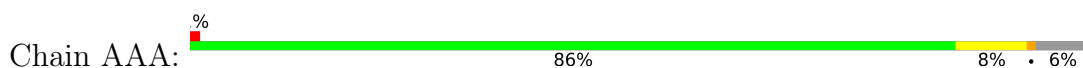
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	EEE	2	Total O 2 2	0	0
4	FFF	1	Total O 1 1	0	0
4	GGG	2	Total O 2 2	0	0
4	HHH	4	Total O 4 4	0	0

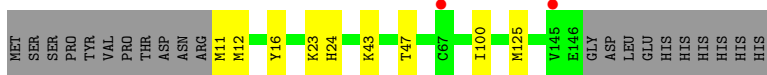
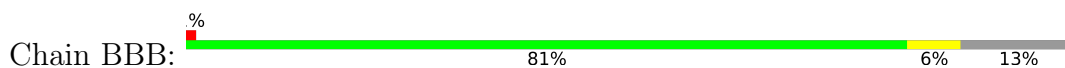
3 Residue-property plots [i](#)

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.

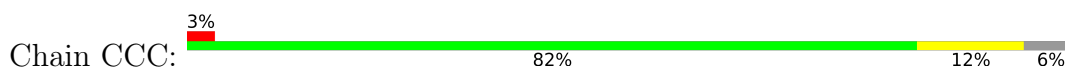
- Molecule 1: 2A protein



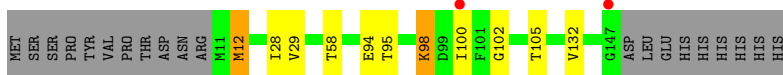
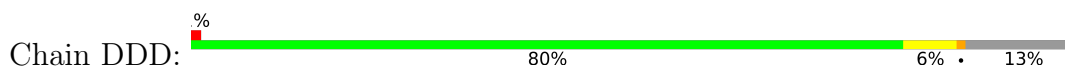
- Molecule 1: 2A protein



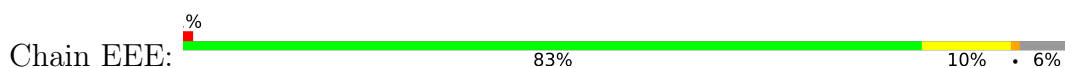
- Molecule 1: 2A protein



- Molecule 1: 2A protein



- Molecule 1: 2A protein



- Molecule 1: 2A protein

4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	141.68Å 141.68Å 183.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.58 – 2.29 73.58 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.58-2.29) 100.0 (73.58-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.178 , 0.214 0.180 , 0.208	Depositor DCC
R_{free} test set	3220 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtrriage
Anisotropy	0.014	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9145	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	AAA	0.94	0/1201	1.29	0/1628
1	BBB	0.96	0/1118	1.33	0/1513
1	CCC	0.92	0/1201	1.30	0/1628
1	DDD	0.99	1/1111 (0.1%)	1.39	0/1504
1	EEE	0.94	0/1201	1.34	0/1628
1	FFF	0.96	1/1107 (0.1%)	1.38	0/1499
1	GGG	0.97	0/1201	1.34	0/1628
1	HHH	1.00	0/1096	1.43	0/1484
All	All	0.96	2/9236 (0.0%)	1.35	0/12512

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	58	THR	N-CA	5.26	1.49	1.46
1	DDD	58	THR	N-CA	5.20	1.49	1.46

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	AAA	1175	0	1153	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	1092	0	1079	6	0
1	CCC	1175	0	1153	10	0
1	DDD	1088	0	1069	5	0
1	EEE	1175	0	1153	11	0
1	FFF	1084	0	1066	9	0
1	GGG	1175	0	1153	11	0
1	HHH	1074	0	1047	8	0
2	AAA	6	0	8	1	0
2	BBB	6	0	8	0	0
2	DDD	6	0	8	0	0
2	FFF	6	0	8	1	0
2	HHH	6	0	8	0	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	0	0
3	CCC	10	0	0	0	0
3	EEE	15	0	0	0	0
3	GGG	5	0	0	0	0
4	AAA	4	0	0	0	0
4	BBB	9	0	0	0	0
4	CCC	10	0	0	0	0
4	DDD	5	0	0	0	0
4	EEE	2	0	0	0	0
4	FFF	1	0	0	0	0
4	GGG	2	0	0	0	0
4	HHH	4	0	0	0	0
All	All	9145	0	8913	56	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 3.

All (56) 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:EEE:136:THR:HB	1:FFF:125:MET:HE1	1.67	0.77
1:AAA:67:CYS:HB3	1:DDD:132:VAL:HG12	1.80	0.64
1:DDD:98:LYS:HA	1:DDD:102:GLY:O	1.99	0.62
1:HHH:54:ARG:NH1	1:HHH:92:ASN:O	2.34	0.60
1:CCC:41:ILE:HD13	1:CCC:123:GLY:HA3	1.85	0.58
1:AAA:41:ILE:HD13	1:AAA:123:GLY:HA3	1.83	0.58
1:EEE:65:GLU:HA	1:EEE:65:GLU:OE1	2.04	0.57
1:GGG:65:GLU:HA	1:GGG:65:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:132:VAL:HG21	1:FFF:126:SER:HA	1.87	0.56
1:HHH:43:LYS:O	1:HHH:47:THR:HG23	2.08	0.54
1:HHH:76:TYR:CG	1:HHH:114:LEU:HD23	2.44	0.53
1:CCC:104:HIS:CD2	1:CCC:106:LEU:O	2.62	0.52
1:BBB:43:LYS:O	1:BBB:47:THR:HG23	2.10	0.52
1:GGG:25:TYR:OH	1:GGG:64:GLU:OE2	2.19	0.52
1:HHH:76:TYR:CB	1:HHH:114:LEU:HD23	2.40	0.52
1:DDD:95:THR:HB	1:DDD:98:LYS:HD2	1.91	0.51
1:EEE:136:THR:CB	1:FFF:125:MET:HE1	2.38	0.51
1:GGG:7:THR:HA	1:GGG:103:THR:OG1	2.10	0.51
1:CCC:7:THR:HA	1:CCC:103:THR:OG1	2.10	0.51
1:EEE:41:ILE:HD13	1:EEE:123:GLY:HA3	1.93	0.50
1:GGG:46:LEU:HD13	1:GGG:144:ALA:HB2	1.94	0.50
1:CCC:65:GLU:HA	1:CCC:65:GLU:OE1	2.12	0.49
1:DDD:12:MET:HG2	1:DDD:100:ILE:O	2.13	0.48
1:AAA:65:GLU:HA	1:AAA:65:GLU:OE1	2.13	0.47
1:FFF:12:MET:N	1:FFF:12:MET:SD	2.87	0.47
1:AAA:7:THR:HA	1:AAA:103:THR:OG1	2.14	0.47
1:AAA:136:THR:HB	1:BBB:125:MET:HE1	1.98	0.46
1:BBB:12:MET:HG2	1:BBB:100:ILE:HA	1.96	0.46
1:EEE:101:PHE:CE2	1:EEE:111:ALA:HB1	2.51	0.46
1:EEE:145:VAL:HB	1:FFF:79:SER:HB2	1.98	0.45
1:FFF:140:PHE:CZ	1:GGG:74:VAL:HG13	2.51	0.45
1:CCC:92:ASN:ND2	1:EEE:3:PRO:HB3	2.31	0.45
1:CCC:69:LEU:HD11	1:CCC:118:ILE:HG23	1.98	0.45
1:GGG:16:TYR:HA	1:GGG:24:HIS:O	2.16	0.45
1:GGG:31:GLU:H	1:GGG:31:GLU:CD	2.25	0.44
1:EEE:83:SER:O	1:EEE:109:HIS:ND1	2.50	0.44
1:DDD:94:GLU:HG3	1:DDD:95:THR:HG23	1.99	0.44
1:AAA:12:MET:HE1	1:AAA:100:ILE:HA	1.99	0.43
1:GGG:132:VAL:HG21	1:HHH:126:SER:HA	2.00	0.43
1:EEE:12:MET:HE1	1:EEE:100:ILE:HA	2.00	0.43
1:CCC:41:ILE:CD1	1:CCC:123:GLY:HA3	2.47	0.43
1:FFF:140:PHE:CE1	1:GGG:74:VAL:CG1	3.01	0.43
1:CCC:12:MET:HA	1:CCC:28:ILE:O	2.19	0.42
2:FFF:201:GOL:H32	1:GGG:70:ASP:HB2	2.00	0.42
1:HHH:71:TYR:CD1	1:HHH:71:TYR:C	2.97	0.42
1:AAA:91:HIS:CE1	2:AAA:201:GOL:HO2	2.38	0.41
1:GGG:145:VAL:HB	1:HHH:79:SER:HB2	2.02	0.41
1:AAA:25:TYR:OH	1:AAA:64:GLU:OE1	2.27	0.41
1:BBB:16:TYR:CD1	1:BBB:23:LYS:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:16:TYR:HA	1:BBB:24:HIS:O	2.21	0.41
1:CCC:77:LEU:HD22	1:CCC:117:THR:HG22	2.02	0.41
1:FFF:43:LYS:O	1:FFF:47:THR:HG23	2.21	0.41
1:EEE:74:VAL:CG1	1:HHH:140:PHE:CE1	3.04	0.41
1:CCC:16:TYR:HA	1:CCC:24:HIS:O	2.21	0.40
1:BBB:11:MET:HE3	1:BBB:12:MET:HE1	2.03	0.40
1:FFF:29:VAL:HG21	1:FFF:34:TYR:CE2	2.57	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	AAA	146/157 (93%)	142 (97%)	4 (3%)	0	100	100
1	BBB	135/157 (86%)	131 (97%)	4 (3%)	0	100	100
1	CCC	146/157 (93%)	142 (97%)	3 (2%)	1 (1%)	18	23
1	DDD	135/157 (86%)	128 (95%)	6 (4%)	1 (1%)	18	23
1	EEE	146/157 (93%)	140 (96%)	6 (4%)	0	100	100
1	FFF	134/157 (85%)	128 (96%)	6 (4%)	0	100	100
1	GGG	146/157 (93%)	139 (95%)	7 (5%)	0	100	100
1	HHH	134/157 (85%)	122 (91%)	10 (8%)	2 (2%)	8	8
All	All	1122/1256 (89%)	1072 (96%)	46 (4%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	HHH	102	GLY
1	HHH	104	HIS
1	DDD	105	THR

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Mol	Chain	Res	Type
1	CCC	66	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	AAA	130/139 (94%)	128 (98%)	2 (2%)	57	75
1	BBB	120/139 (86%)	120 (100%)	0	100	100
1	CCC	130/139 (94%)	128 (98%)	2 (2%)	57	75
1	DDD	119/139 (86%)	115 (97%)	4 (3%)	32	49
1	EEE	130/139 (94%)	125 (96%)	5 (4%)	29	44
1	FFF	119/139 (86%)	115 (97%)	4 (3%)	32	49
1	GGG	130/139 (94%)	129 (99%)	1 (1%)	73	86
1	HHH	116/139 (84%)	114 (98%)	2 (2%)	53	72
All	All	994/1112 (89%)	974 (98%)	20 (2%)	48	67

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

Mol	Chain	Res	Type
1	AAA	49	LYS
1	AAA	91	HIS
1	CCC	67	CYS
1	CCC	91	HIS
1	DDD	12	MET
1	DDD	28	ILE
1	DDD	29	VAL
1	DDD	98	LYS
1	EEE	83	SER
1	EEE	91	HIS
1	EEE	109	HIS
1	EEE	135	THR
1	EEE	139	GLU
1	FFF	11	MET

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Mol	Chain	Res	Type
1	FFF	12	MET
1	FFF	68	GLU
1	FFF	88	SER
1	GGG	31	GLU
1	HHH	67	CYS
1	HHH	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
2	GOL	FFF	201	-	5,5,5	0.07	0	5,5,5	0.28	0
2	GOL	HHH	201	-	5,5,5	0.09	0	5,5,5	0.31	0
3	SO4	EEE	203	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	GGG	201	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	AAA	202	-	4,4,4	0.33	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	BBB	201	-	5,5,5	0.09	0	5,5,5	0.29	0
3	SO4	EEE	202	-	4,4,4	0.33	0	6,6,6	0.08	0
2	GOL	DDD	201	-	5,5,5	0.06	0	5,5,5	0.28	0
3	SO4	EEE	201	-	4,4,4	0.33	0	6,6,6	0.07	0
3	SO4	CCC	201	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	BBB	202	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	CCC	202	-	4,4,4	0.32	0	6,6,6	0.09	0
2	GOL	AAA	201	-	5,5,5	0.10	0	5,5,5	0.32	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	FFF	201	-	-	0/4/4/4	-
2	GOL	HHH	201	-	-	2/4/4/4	-
2	GOL	BBB	201	-	-	0/4/4/4	-
2	GOL	DDD	201	-	-	4/4/4/4	-
2	GOL	AAA	201	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	201	GOL	O1-C1-C2-O2
2	DDD	201	GOL	O1-C1-C2-C3
2	AAA	201	GOL	O1-C1-C2-C3
2	HHH	201	GOL	O1-C1-C2-C3
2	AAA	201	GOL	O1-C1-C2-O2
2	AAA	201	GOL	O2-C2-C3-O3
2	HHH	201	GOL	O1-C1-C2-O2
2	DDD	201	GOL	C1-C2-C3-O3
2	DDD	201	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	FFF	201	GOL	1	0
2	AAA	201	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

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	AAA	148/157 (94%)	0.10	1 (0%) 84 85	54, 69, 98, 111	0
1	BBB	136/157 (86%)	0.01	2 (1%) 72 73	34, 66, 100, 131	1 (0%)
1	CCC	148/157 (94%)	0.04	5 (3%) 48 50	48, 65, 92, 108	0
1	DDD	137/157 (87%)	0.27	2 (1%) 72 73	56, 83, 143, 183	0
1	EEE	148/157 (94%)	0.06	1 (0%) 84 85	56, 70, 105, 114	0
1	FFF	136/157 (86%)	0.31	6 (4%) 39 41	60, 88, 137, 172	0
1	GGG	148/157 (94%)	0.08	1 (0%) 84 85	55, 73, 107, 133	0
1	HHH	136/157 (86%)	0.33	3 (2%) 62 64	57, 92, 167, 221	0
All	All	1137/1256 (90%)	0.15	21 (1%) 67 69	34, 74, 133, 221	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	147	GLY	4.4
1	CCC	147	GLY	3.7
1	FFF	72	PHE	3.1
1	GGG	147	GLY	3.0
1	CCC	67	CYS	2.8
1	DDD	147	GLY	2.7
1	BBB	145	VAL	2.7
1	FFF	76	TYR	2.6
1	FFF	105	THR	2.5
1	DDD	100	ILE	2.5
1	HHH	103	THR	2.4
1	CCC	81	VAL	2.3
1	HHH	93	CYS	2.2
1	EEE	147	GLY	2.2
1	FFF	11	MET	2.2
1	HHH	105	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	FFF	145	VAL	2.2
1	FFF	103	THR	2.2
1	BBB	67	CYS	2.1
1	CCC	105	THR	2.1
1	CCC	91	HIS	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(Å ²)	Q<0.9
3	SO4	EEE	203	5/5	0.53	0.10	136,138,145,147	0
3	SO4	CCC	202	5/5	0.68	0.12	127,133,140,143	0
3	SO4	CCC	201	5/5	0.69	0.08	140,143,148,149	0
3	SO4	EEE	202	5/5	0.70	0.08	120,133,137,137	0
2	GOL	AAA	201	6/6	0.73	0.12	113,117,118,120	0
3	SO4	BBB	202	5/5	0.73	0.07	134,145,146,149	0
3	SO4	AAA	202	5/5	0.78	0.08	121,125,129,133	0
3	SO4	GGG	201	5/5	0.78	0.09	123,141,143,147	0
3	SO4	EEE	201	5/5	0.80	0.10	126,128,136,138	0
2	GOL	FFF	201	6/6	0.88	0.20	91,99,112,127	0
2	GOL	DDD	201	6/6	0.90	0.15	77,85,88,92	0
2	GOL	BBB	201	6/6	0.93	0.12	75,84,90,90	0
2	GOL	HHH	201	6/6	0.93	0.12	90,98,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.