



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 PM GMT

PDB ID : 4POS
Title : Structure of Human Polyomavirus 9 VP1 pentamer in complex with 3'-sialyllactosamine
Authors : Khan, Z.M.; Stehle, T.
Deposited on : 2014-02-26
Resolution : 2.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

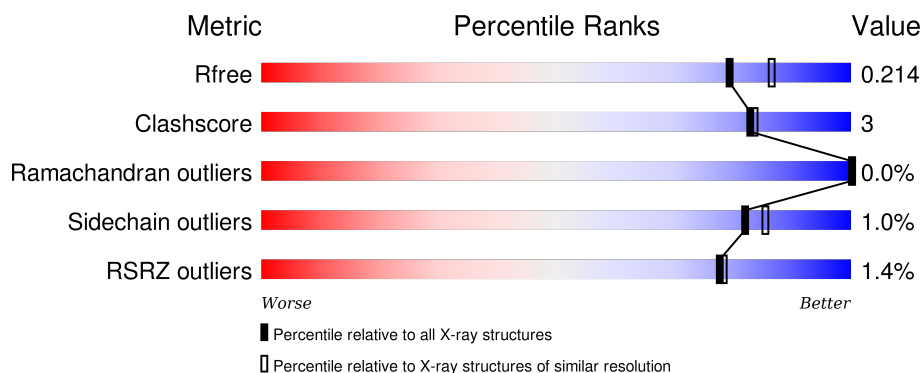
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 $\leq 5\%$. 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	278	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	278	<div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	C	278	<div> <div>2%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	D	278	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	E	278	<div> <div>%</div> <div>89%</div> <div>7%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	278	
1	G	278	
1	H	278	
1	I	278	
1	J	278	

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
3	EDO	A	402	-	-	-	X
3	EDO	A	403	-	-	-	X
3	EDO	A	405	-	-	-	X
3	EDO	A	406	-	-	X	X
3	EDO	B	403	-	-	-	X
3	EDO	B	404	-	-	-	X
3	EDO	C	402	-	-	-	X
3	EDO	D	402	-	-	-	X
3	EDO	E	402	-	-	-	X
3	EDO	F	402	-	-	-	X
3	EDO	F	404	-	-	-	X
3	EDO	G	402	-	-	-	X
3	EDO	G	403	-	-	-	X
3	EDO	H	402	-	-	-	X
3	EDO	H	404	-	-	-	X
3	EDO	H	405	-	-	-	X
3	EDO	I	402	-	-	-	X
3	EDO	I	404	-	-	-	X
3	EDO	I	405	-	-	-	X
3	EDO	J	402	-	-	-	X
4	IPA	A	408	-	-	-	X
4	IPA	B	406	-	-	-	X
4	IPA	C	403	-	-	-	X
4	IPA	E	404	-	-	-	X
4	IPA	F	406	-	-	-	X
4	IPA	G	404	-	-	-	X
4	IPA	H	406	-	-	-	X
4	IPA	I	406	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IPA	J	403	-	-	-	X
5	GAL	A	411	-	-	-	X
5	GAL	B	409	-	-	-	X
5	GAL	D	407	-	-	-	X
5	GAL	G	407	-	-	-	X
5	GAL	J	406	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23830 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	2	1	0
			2068	1302	342	413	11			
1	B	270	Total	C	N	O	S	3	1	0
			2065	1301	341	412	11			
1	C	269	Total	C	N	O	S	0	1	0
			2059	1298	343	407	11			
1	D	271	Total	C	N	O	S	0	2	0
			2080	1308	344	417	11			
1	E	270	Total	C	N	O	S	1	0	0
			2059	1297	341	410	11			
1	F	272	Total	C	N	O	S	2	1	0
			2087	1315	344	417	11			
1	G	270	Total	C	N	O	S	6	2	0
			2072	1305	343	413	11			
1	H	271	Total	C	N	O	S	0	1	0
			2071	1303	343	414	11			
1	I	272	Total	C	N	O	S	0	0	0
			2067	1301	343	412	11			
1	J	274	Total	C	N	O	S	0	1	0
			2095	1319	346	419	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
A	28	SER	-	EXPRESSION TAG	UNP E9NQ90
A	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
A	30	MET	-	EXPRESSION TAG	UNP E9NQ90
B	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
B	28	SER	-	EXPRESSION TAG	UNP E9NQ90
B	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
B	30	MET	-	EXPRESSION TAG	UNP E9NQ90
C	27	GLY	-	EXPRESSION TAG	UNP E9NQ90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	SER	-	EXPRESSION TAG	UNP E9NQ90
C	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
C	30	MET	-	EXPRESSION TAG	UNP E9NQ90
D	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
D	28	SER	-	EXPRESSION TAG	UNP E9NQ90
D	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
D	30	MET	-	EXPRESSION TAG	UNP E9NQ90
E	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
E	28	SER	-	EXPRESSION TAG	UNP E9NQ90
E	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
E	30	MET	-	EXPRESSION TAG	UNP E9NQ90
F	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
F	28	SER	-	EXPRESSION TAG	UNP E9NQ90
F	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
F	30	MET	-	EXPRESSION TAG	UNP E9NQ90
G	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
G	28	SER	-	EXPRESSION TAG	UNP E9NQ90
G	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
G	30	MET	-	EXPRESSION TAG	UNP E9NQ90
H	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
H	28	SER	-	EXPRESSION TAG	UNP E9NQ90
H	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
H	30	MET	-	EXPRESSION TAG	UNP E9NQ90
I	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
I	28	SER	-	EXPRESSION TAG	UNP E9NQ90
I	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
I	30	MET	-	EXPRESSION TAG	UNP E9NQ90
J	27	GLY	-	EXPRESSION TAG	UNP E9NQ90
J	28	SER	-	EXPRESSION TAG	UNP E9NQ90
J	29	HIS	-	EXPRESSION TAG	UNP E9NQ90
J	30	MET	-	EXPRESSION TAG	UNP E9NQ90

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

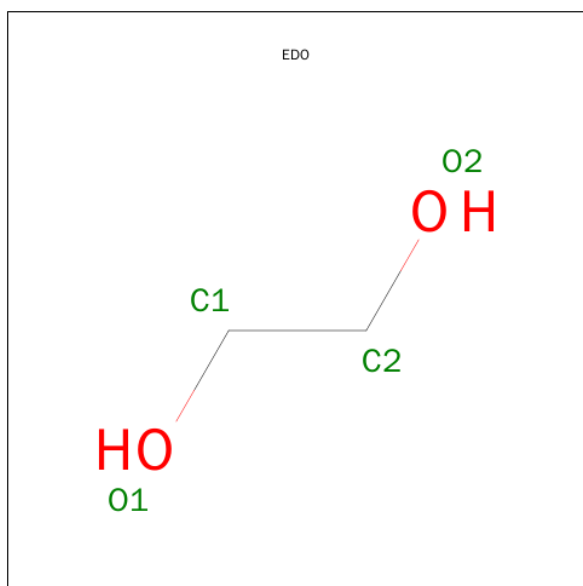
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	I	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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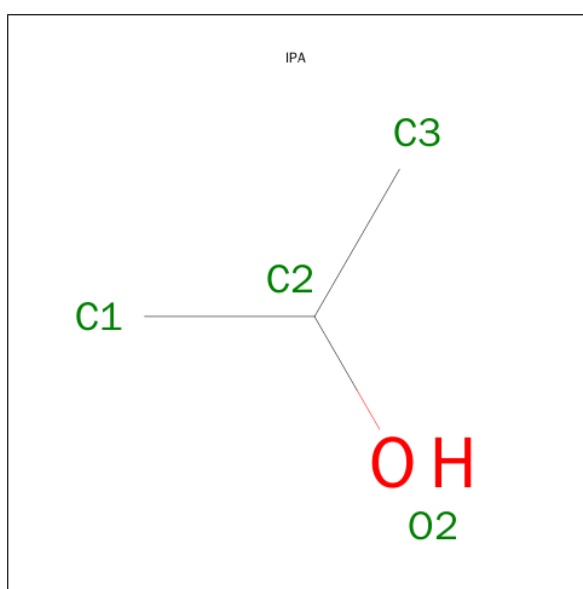
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	B	1	Total	C	O	0	0
			4	3	1		
4	C	1	Total	C	O	0	0
			4	3	1		
4	D	1	Total	C	O	0	0
			4	3	1		
4	E	1	Total	C	O	0	0
			4	3	1		
4	F	1	Total	C	O	0	0
			4	3	1		
4	G	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	3	1		
4	I	1	Total	C	O	0	0
			4	3	1		
4	J	1	Total	C	O	0	0
			4	3	1		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			46	25	2	19		
5	B	3	Total	C	N	O	0	0
			46	25	2	19		
5	D	3	Total	C	N	O	0	0
			46	25	2	19		
5	E	3	Total	C	N	O	0	0
			46	25	2	19		
5	F	3	Total	C	N	O	0	0
			46	25	2	19		
5	G	3	Total	C	N	O	0	0
			46	25	2	19		
5	H	3	Total	C	N	O	0	0
			46	25	2	19		
5	I	3	Total	C	N	O	0	0
			46	25	2	19		
5	J	3	Total	C	N	O	0	0
			46	25	2	19		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	232	Total	O	0	0
			232	232		
6	B	269	Total	O	0	0
			269	269		
6	C	214	Total	O	0	0
			214	214		
6	D	237	Total	O	0	0
			237	237		
6	E	255	Total	O	0	0
			255	255		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	280	Total 280	O 280	0	0
6	G	248	Total 248	O 248	0	0
6	H	267	Total 267	O 267	0	0
6	I	259	Total 259	O 259	0	0
6	J	262	Total 262	O 262	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.

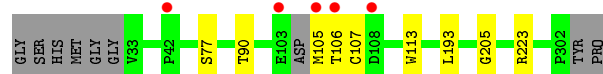
- Molecule 1: VP1



- Molecule 1: VP1



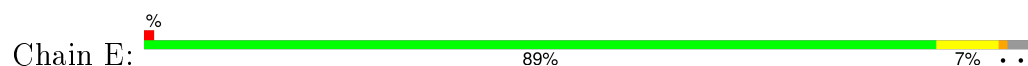
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1

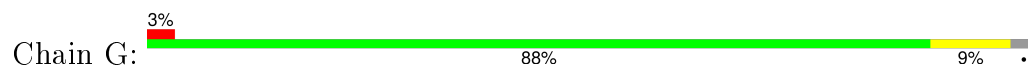


- Molecule 1: VP1

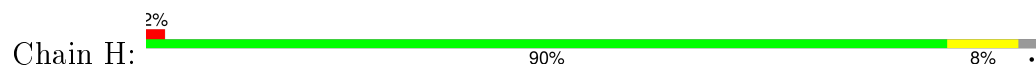




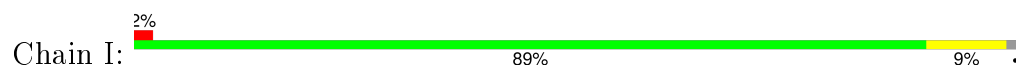
- Molecule 1: VP1



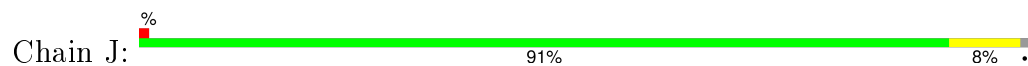
- Molecule 1: VP1



- Molecule 1: VP1



- Molecule 1: VP1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.91Å 180.63Å 199.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	133.88 – 2.00 48.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (133.88-2.00) 98.0 (48.06-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0025	Depositor
R, R_{free}	0.179 , 0.213 0.181 , 0.214	Depositor DCC
R_{free} test set	11549 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 230735 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23830	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IPA, NAG, CA, EDO, SIA, GAL

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	1/2112 (0.0%)	0.61	0/2884
1	B	0.51	0/2112	0.60	0/2884
1	C	0.48	1/2105 (0.0%)	0.57	0/2872
1	D	0.49	1/2124 (0.0%)	0.59	0/2900
1	E	0.51	3/2103 (0.1%)	0.59	1/2872 (0.0%)
1	F	0.50	2/2133 (0.1%)	0.58	0/2913
1	G	0.50	1/2116 (0.0%)	0.60	0/2890
1	H	0.51	0/2115	0.62	0/2888
1	I	0.50	2/2111 (0.1%)	0.60	0/2882
1	J	0.50	1/2141 (0.0%)	0.60	0/2923
All	All	0.50	12/21172 (0.1%)	0.60	1/28908 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	113	TRP	CD2-CE2	5.74	1.48	1.41
1	A	51	TYR	C-N	-5.71	1.21	1.34
1	E	212	TRP	CD2-CE2	5.57	1.48	1.41
1	C	113	TRP	CD2-CE2	5.31	1.47	1.41
1	F	212	TRP	CD2-CE2	5.30	1.47	1.41
1	G	212	TRP	CD2-CE2	5.28	1.47	1.41
1	E	283	TRP	CD2-CE2	5.19	1.47	1.41
1	F	113	TRP	CD2-CE2	5.12	1.47	1.41
1	D	113	TRP	CD2-CE2	5.08	1.47	1.41
1	J	212	TRP	CD2-CE2	5.04	1.47	1.41
1	E	113	TRP	CD2-CE2	5.02	1.47	1.41
1	I	212	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	107	CYS	CA-CB-SG	-5.04	104.92	114.00

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	2068	0	2041	14	0
1	B	2065	0	2044	11	0
1	C	2059	0	2046	5	0
1	D	2080	0	2048	13	0
1	E	2059	0	2038	15	0
1	F	2087	0	2056	13	0
1	G	2072	0	2050	23	0
1	H	2071	0	2044	16	2
1	I	2067	0	2043	13	0
1	J	2095	0	2063	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	24	0	36	10	0
3	B	16	0	24	3	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
3	E	8	0	12	2	0
3	F	16	0	24	6	0
3	G	8	0	12	1	0
3	H	16	0	24	4	0
3	I	16	0	24	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	4	0	6	0	0
4	A	4	0	8	0	0
4	B	4	0	8	0	0
4	C	4	0	8	0	0
4	D	4	0	8	0	0
4	E	4	0	8	0	0
4	F	4	0	8	0	0
4	G	4	0	8	1	0
4	H	4	0	8	1	0
4	I	4	0	8	0	0
4	J	4	0	8	0	0
5	A	46	0	40	1	0
5	B	46	0	40	2	0
5	D	46	0	40	1	0
5	E	46	0	40	0	0
5	F	46	0	40	0	0
5	G	46	0	40	1	0
5	H	46	0	40	0	0
5	I	46	0	40	1	0
5	J	46	0	40	2	2
6	A	232	0	0	3	0
6	B	269	0	0	1	0
6	C	214	0	0	1	0
6	D	237	0	0	1	0
6	E	255	0	0	2	0
6	F	280	0	0	3	0
6	G	248	0	0	2	0
6	H	267	0	0	2	0
6	I	259	0	0	2	0
6	J	262	0	0	3	0
All	All	23830	0	21093	125	2

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 (125) 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:G:104:ASP:HB3	1:G:107:CYS:SG	1.90	1.10
1:C:107:CYS:SG	1:G:107:CYS:HB3	1.96	1.04
3:I:404:EDO:H21	1:J:223:ARG:HD2	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:CYS:SG	1:G:107:CYS:CB	2.45	1.03
3:F:405:EDO:H22	1:G:223:ARG:HD2	1.52	0.91
1:G:104:ASP:CB	1:G:107:CYS:SG	2.66	0.84
1:A:223:ARG:CD	3:A:406:EDO:H12	2.08	0.83
1:F:274:HIS:HD2	6:F:774:HOH:O	1.64	0.79
1:I:250:ASP:HA	3:I:405:EDO:H22	1.63	0.78
3:I:404:EDO:H21	1:J:223:ARG:CD	2.14	0.78
1:A:223:ARG:HD2	3:A:406:EDO:H12	1.66	0.76
1:E:107:CYS:HG	1:J:107:CYS:HG	0.78	0.76
1:G:274:HIS:HD2	6:G:745:HOH:O	1.70	0.74
1:B:274:HIS:HD2	6:B:763:HOH:O	1.71	0.74
1:G:105:MET:HG2	1:G:105:MET:O	1.87	0.73
1:J:274:HIS:HD2	6:J:757:HOH:O	1.71	0.73
1:H:106:THR:HB	6:H:744:HOH:O	1.90	0.71
1:H:63:ASP:OD2	3:H:405:EDO:H11	1.91	0.70
1:I:274:HIS:HD2	6:I:645:HOH:O	1.74	0.68
1:J:274:HIS:CD2	6:J:757:HOH:O	2.44	0.68
3:F:405:EDO:H22	1:G:223:ARG:CD	2.24	0.68
1:G:217:SER:HB3	3:G:402:EDO:H22	1.75	0.67
1:H:63:ASP:OD2	3:H:405:EDO:C1	2.45	0.64
1:E:274:HIS:HD2	6:E:684:HOH:O	1.81	0.64
1:A:243:SER:HA	3:B:404:EDO:H11	1.79	0.64
1:G:104:ASP:CG	1:G:107:CYS:SG	2.77	0.64
1:F:273:ILE:CD1	6:F:776:HOH:O	2.46	0.63
1:E:104:ASP:OD1	1:E:106:THR:OG1	2.14	0.62
1:G:104:ASP:OD2	1:G:107:CYS:SG	2.59	0.61
1:D:276:ASN:HB3	5:D:405:SIA:O1B	2.03	0.59
1:H:104:ASP:OD1	1:H:106:THR:OG1	2.18	0.58
1:F:223:ARG:HG2	3:F:404:EDO:H11	1.88	0.56
1:H:274:HIS:HD2	6:H:664:HOH:O	1.88	0.56
1:G:34:GLU:HB3	1:G:300:LYS:HB3	1.88	0.55
1:B:37:GLU:HG3	1:H:37:GLU:HG3	1.89	0.55
1:C:90:THR:OG1	1:C:205:GLY:HA2	2.07	0.54
1:F:84:ASN:HB2	1:F:87:THR:HG23	1.88	0.54
5:G:407:GAL:H2	1:H:77:SER:HB2	1.91	0.53
1:G:104:ASP:OD1	1:G:106:THR:OG1	2.26	0.52
1:E:209:VAL:HG11	1:E:268:VAL:HG21	1.92	0.51
1:G:209:VAL:HG11	1:G:268:VAL:HG21	1.93	0.51
1:I:131:LEU:HG	1:J:283:TRP:CZ2	2.45	0.51
1:J:101:LEU:HD21	1:J:113:TRP:CZ2	2.46	0.50
1:D:84:ASN:HB2	1:D:87:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:227:SER:HB2	4:G:404:IPA:H31	1.92	0.50
1:D:131:LEU:HD11	1:E:273:ILE:HD13	1.93	0.50
5:J:405:NAG:H1	5:J:405:NAG:H82	1.94	0.49
1:B:107:CYS:HG	1:H:107:CYS:HG	0.54	0.49
1:D:34:GLU:HB3	1:D:300:LYS:HB3	1.94	0.49
1:F:121:GLU:HG2	1:G:216:PRO:HG3	1.94	0.49
1:J:104:ASP:OD1	1:J:106:THR:OG1	2.26	0.49
1:F:273:ILE:HD11	6:F:776:HOH:O	2.08	0.49
3:A:406:EDO:H11	1:E:242:ASN:O	2.13	0.49
5:A:411:GAL:H2	1:B:77:SER:HB2	1.94	0.48
1:E:278:SER:O	1:E:279:GLU:HB2	2.13	0.48
1:H:209:VAL:HG11	1:H:268:VAL:HG21	1.95	0.48
1:G:51:TYR:CD2	3:H:402:EDO:H21	2.49	0.48
1:I:48:ILE:HD12	1:I:48:ILE:C	2.34	0.48
1:C:223[B]:ARG:HD2	6:C:679:HOH:O	2.13	0.47
1:A:250:ASP:HA	3:A:406:EDO:H21	1.96	0.47
1:A:223:ARG:HD3	3:A:406:EDO:H12	1.92	0.47
1:F:209:VAL:HG11	1:F:268:VAL:HG21	1.97	0.47
1:I:31:GLY:C	1:I:33:VAL:H	2.18	0.47
3:A:407:EDO:H21	6:A:652:HOH:O	2.14	0.47
1:D:259:LYS:NZ	6:D:732:HOH:O	2.37	0.46
1:F:242:ASN:O	3:F:405:EDO:H21	2.16	0.46
1:I:223:ARG:HD2	3:I:405:EDO:O2	2.16	0.46
1:G:278:SER:O	1:G:279:GLU:HB2	2.16	0.46
1:D:131:LEU:HG	1:E:283:TRP:CZ2	2.50	0.46
1:A:239:GLN:NE2	6:A:693:HOH:O	2.48	0.46
1:D:90:THR:OG1	1:D:205:GLY:HA2	2.15	0.46
1:J:128:LEU:HD22	1:J:148:VAL:HB	1.98	0.46
1:F:273:ILE:HD13	1:J:131:LEU:HD21	1.98	0.46
1:E:157:SER:OG	1:E:266:SER:HB2	2.16	0.45
1:H:90:THR:OG1	1:H:205:GLY:HA2	2.16	0.45
1:E:193:LEU:HD11	3:E:402:EDO:H22	1.97	0.45
1:F:90:THR:OG1	1:F:205:GLY:HA2	2.16	0.45
1:J:84:ASN:HB2	1:J:87:THR:HG23	1.99	0.45
1:D:64:GLU:HG2	1:E:78:LYS:HE2	1.99	0.45
1:D:37:GLU:HG3	1:F:37:GLU:HG3	1.99	0.45
1:E:84:ASN:HB2	1:E:87:THR:HG23	1.98	0.45
1:E:198:LYS:HZ1	3:E:402:EDO:C2	2.30	0.45
1:F:223:ARG:CG	3:F:404:EDO:H11	2.47	0.44
1:H:156:PHE:HE2	4:H:406:IPA:H12	1.82	0.44
1:A:217:SER:HB3	3:A:402:EDO:H21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:276:ASN:HB3	5:J:404:SIA:O1B	2.18	0.44
1:I:209:VAL:HG11	1:I:268:VAL:HG21	2.00	0.44
3:F:402:EDO:H11	1:J:51:TYR:CD2	2.52	0.44
1:H:157:SER:OG	1:H:266:SER:HB2	2.18	0.44
1:B:276:ASN:HB3	5:B:407:SIA:O1A	2.17	0.44
1:A:33:VAL:HG12	1:A:302:PRO:HG3	2.00	0.44
1:G:157:SER:OG	1:G:266:SER:HB2	2.18	0.43
5:B:409:GAL:H2	1:C:77:SER:HB2	1.99	0.43
1:G:33:VAL:HG12	1:G:302:PRO:HG3	2.00	0.43
1:I:157:SER:OG	1:I:266:SER:HB2	2.18	0.43
1:A:131:LEU:HD11	1:B:273:ILE:CD1	2.48	0.43
1:B:217:SER:HB3	3:B:402:EDO:H21	2.00	0.43
1:I:276:ASN:HB3	5:I:407:SIA:O1A	2.19	0.43
3:A:402:EDO:H22	1:E:51:TYR:CD2	2.54	0.43
1:B:51:TYR:CD2	3:B:403:EDO:H22	2.54	0.43
1:F:278:SER:O	1:F:279:GLU:HB2	2.19	0.43
1:I:278:SER:O	1:I:279:GLU:HB2	2.19	0.43
1:G:149:GLN:HA	6:G:642:HOH:O	2.19	0.42
1:H:278:SER:O	1:H:279:GLU:HB2	2.18	0.42
1:D:75:ALA:HB2	1:D:81:ASP:OD1	2.18	0.42
1:H:131:LEU:HG	1:I:283:TRP:CZ2	2.54	0.42
6:I:710:HOH:O	1:J:220:GLU:HG3	2.19	0.42
3:I:404:EDO:H12	1:J:250:ASP:HA	2.01	0.42
1:I:255:GLY:O	3:I:403:EDO:H11	2.20	0.42
1:A:90:THR:OG1	1:A:205:GLY:HA2	2.19	0.42
1:A:221:ASN:OD1	3:A:404:EDO:H22	2.19	0.42
1:G:90:THR:OG1	1:G:205:GLY:HA2	2.20	0.42
1:D:64:GLU:OE1	1:E:78:LYS:HD3	2.20	0.41
3:H:403:EDO:H12	1:I:217:SER:HB3	2.02	0.41
3:A:406:EDO:H22	6:A:724:HOH:O	2.20	0.41
1:A:209:VAL:HG11	1:A:268:VAL:HG21	2.02	0.41
1:A:131:LEU:HD11	1:B:273:ILE:HD13	2.03	0.41
1:H:243:SER:HB2	3:I:405:EDO:H11	2.02	0.41
1:J:149:GLN:HA	6:J:758:HOH:O	2.21	0.41
1:B:273:ILE:CG2	1:B:281:GLN:HB3	2.50	0.40
1:D:128:LEU:HD22	1:D:148:VAL:HB	2.02	0.40
1:G:240:PHE:O	1:H:226:GLY:N	2.54	0.40
1:B:90:THR:OG1	1:B:205:GLY:HA2	2.21	0.40
1:A:223:ARG:NH2	1:A:254:VAL:O	2.55	0.40
1:D:64:GLU:HG3	6:E:612:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:ASP:OD1	5:J:405:NAG:O7[2_554]	2.07	0.13
1:H:108:ASP:OD2	5:J:405:NAG:O7[2_554]	2.08	0.12

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	269/278 (97%)	256 (95%)	13 (5%)	0	100	100
1	B	269/278 (97%)	258 (96%)	11 (4%)	0	100	100
1	C	266/278 (96%)	255 (96%)	11 (4%)	0	100	100
1	D	271/278 (98%)	260 (96%)	11 (4%)	0	100	100
1	E	268/278 (96%)	256 (96%)	12 (4%)	0	100	100
1	F	271/278 (98%)	262 (97%)	9 (3%)	0	100	100
1	G	270/278 (97%)	257 (95%)	13 (5%)	0	100	100
1	H	270/278 (97%)	257 (95%)	13 (5%)	0	100	100
1	I	270/278 (97%)	257 (95%)	12 (4%)	1 (0%)	39	33
1	J	273/278 (98%)	261 (96%)	12 (4%)	0	100	100
All	All	2697/2780 (97%)	2579 (96%)	117 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	32	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	236/240 (98%)	234 (99%)	2 (1%)	86	89
1	B	236/240 (98%)	234 (99%)	2 (1%)	86	89
1	C	235/240 (98%)	232 (99%)	3 (1%)	76	79
1	D	237/240 (99%)	235 (99%)	2 (1%)	86	89
1	E	235/240 (98%)	232 (99%)	3 (1%)	76	79
1	F	238/240 (99%)	237 (100%)	1 (0%)	93	95
1	G	237/240 (99%)	236 (100%)	1 (0%)	93	95
1	H	236/240 (98%)	234 (99%)	2 (1%)	86	89
1	I	235/240 (98%)	231 (98%)	4 (2%)	68	71
1	J	238/240 (99%)	234 (98%)	4 (2%)	68	71
All	All	2363/2400 (98%)	2339 (99%)	24 (1%)	82	85

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	THR
1	A	193	LEU
1	B	121	GLU
1	B	193	LEU
1	C	105	MET
1	C	106	THR
1	C	193	LEU
1	D	131	LEU
1	D	193	LEU
1	E	103	GLU
1	E	131	LEU
1	E	193	LEU
1	F	193	LEU
1	G	193	LEU
1	H	121	GLU
1	H	193	LEU
1	I	106	THR
1	I	121	GLU
1	I	193	LEU
1	I	227	SER

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Mol	Chain	Res	Type
1	J	100	MET
1	J	108	ASP
1	J	131	LEU
1	J	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	B	274	HIS
1	C	58	ASN
1	E	196	ASN
1	E	274	HIS
1	F	274	HIS
1	G	274	HIS
1	H	274	HIS
1	I	196	ASN
1	I	274	HIS
1	J	47	GLN
1	J	274	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 ⓘ

27 carbohydrates 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
5	SIA	A	409	5	16,20,21	0.64	0	18,28,31	0.93	1 (5%)
5	NAG	A	410	5	15,15,15	0.54	0	17,21,21	1.61	2 (11%)
5	GAL	A	411	5	11,11,12	0.55	0	14,15,17	0.82	0
5	SIA	B	407	5	16,20,21	0.55	0	18,28,31	0.67	0
5	NAG	B	408	5	15,15,15	0.39	0	17,21,21	0.73	0
5	GAL	B	409	5	11,11,12	0.46	0	14,15,17	1.40	1 (7%)
5	SIA	D	405	5	16,20,21	0.42	0	18,28,31	0.80	0
5	NAG	D	406	5	15,15,15	0.49	0	17,21,21	0.98	0
5	GAL	D	407	5	11,11,12	0.50	0	14,15,17	1.29	1 (7%)
5	SIA	E	405	5	16,20,21	0.47	0	18,28,31	0.85	0
5	NAG	E	406	5	15,15,15	0.54	0	17,21,21	1.07	2 (11%)
5	GAL	E	407	5	11,11,12	0.70	0	14,15,17	1.16	2 (14%)
5	SIA	F	407	5	16,20,21	0.55	0	18,28,31	0.76	0
5	NAG	F	408	5	15,15,15	0.51	0	17,21,21	0.97	1 (5%)
5	GAL	F	409	5	11,11,12	0.78	1 (9%)	14,15,17	0.91	1 (7%)
5	SIA	G	405	5	16,20,21	0.45	0	18,28,31	0.67	0
5	NAG	G	406	5	15,15,15	0.47	0	17,21,21	1.12	2 (11%)
5	GAL	G	407	5	11,11,12	0.57	0	14,15,17	1.07	1 (7%)
5	SIA	H	407	5	16,20,21	0.52	0	18,28,31	0.52	0
5	NAG	H	408	5	15,15,15	0.49	0	17,21,21	0.99	1 (5%)
5	GAL	H	409	5	11,11,12	0.74	0	14,15,17	1.43	2 (14%)
5	SIA	I	407	5	16,20,21	0.74	0	18,28,31	0.88	0
5	NAG	I	408	5	15,15,15	0.51	0	17,21,21	0.96	1 (5%)
5	GAL	I	409	5	11,11,12	0.58	0	14,15,17	0.98	1 (7%)
5	SIA	J	404	5	16,20,21	0.49	0	18,28,31	0.57	0
5	NAG	J	405	5	15,15,15	0.42	0	17,21,21	2.00	4 (23%)
5	GAL	J	406	5	11,11,12	0.51	0	14,15,17	0.99	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
5	SIA	A	409	5	-	0/14/34/38	0/1/1/1
5	NAG	A	410	5	-	0/6/26/26	0/1/1/1
5	GAL	A	411	5	-	0/2/19/22	0/1/1/1
5	SIA	B	407	5	-	0/14/34/38	0/1/1/1
5	NAG	B	408	5	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	B	409	5	-	0/2/19/22	0/1/1/1
5	SIA	D	405	5	-	0/14/34/38	0/1/1/1
5	NAG	D	406	5	-	0/6/26/26	0/1/1/1
5	GAL	D	407	5	-	0/2/19/22	0/1/1/1
5	SIA	E	405	5	-	0/14/34/38	0/1/1/1
5	NAG	E	406	5	-	0/6/26/26	0/1/1/1
5	GAL	E	407	5	-	0/2/19/22	0/1/1/1
5	SIA	F	407	5	-	0/14/34/38	0/1/1/1
5	NAG	F	408	5	-	0/6/26/26	0/1/1/1
5	GAL	F	409	5	-	0/2/19/22	0/1/1/1
5	SIA	G	405	5	-	0/14/34/38	0/1/1/1
5	NAG	G	406	5	-	0/6/26/26	0/1/1/1
5	GAL	G	407	5	-	0/2/19/22	0/1/1/1
5	SIA	H	407	5	-	0/14/34/38	0/1/1/1
5	NAG	H	408	5	-	0/6/26/26	0/1/1/1
5	GAL	H	409	5	-	0/2/19/22	0/1/1/1
5	SIA	I	407	5	-	0/14/34/38	0/1/1/1
5	NAG	I	408	5	-	0/6/26/26	0/1/1/1
5	GAL	I	409	5	-	0/2/19/22	0/1/1/1
5	SIA	J	404	5	-	0/14/34/38	0/1/1/1
5	NAG	J	405	5	-	0/6/26/26	0/1/1/1
5	GAL	J	406	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	409	GAL	O5-C1	-2.00	1.40	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	406	NAG	O4-C4-C3	-2.73	104.19	110.34
5	J	405	NAG	O7-C7-C8	-2.55	117.39	122.06
5	E	406	NAG	C1-O5-C5	-2.43	108.98	113.47
5	E	407	GAL	O3-C3-C2	-2.37	105.71	110.00
5	H	408	NAG	O4-C4-C3	-2.32	105.11	110.34
5	E	406	NAG	O4-C4-C3	-2.20	105.39	110.34
5	I	408	NAG	O4-C4-C3	-2.08	105.66	110.34
5	A	410	NAG	O4-C4-C3	-2.04	105.75	110.34
5	F	409	GAL	C1-O5-C5	2.03	114.83	112.25
5	E	407	GAL	C1-O5-C5	2.15	114.98	112.25
5	G	406	NAG	C4-C3-C2	2.26	113.57	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	409	SIA	O6-C6-C5	2.30	112.25	108.48
5	G	407	GAL	C1-O5-C5	2.46	115.37	112.25
5	I	409	GAL	C1-O5-C5	2.46	115.37	112.25
5	F	408	NAG	C4-C3-C2	2.48	113.87	110.43
5	H	409	GAL	C1-C2-C3	2.56	112.57	109.54
5	J	405	NAG	C2-N2-C7	2.78	130.25	123.10
5	D	407	GAL	C1-O5-C5	3.10	116.18	112.25
5	J	405	NAG	C8-C7-N2	3.59	122.97	116.11
5	H	409	GAL	C1-O5-C5	3.86	117.14	112.25
5	B	409	GAL	C1-O5-C5	4.13	117.49	112.25
5	A	410	NAG	C4-C3-C2	4.74	117.00	110.43
5	J	405	NAG	C4-C3-C2	5.46	118.00	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	411	GAL	1	0
5	B	407	SIA	1	0
5	B	409	GAL	1	0
5	D	405	SIA	1	0
5	G	407	GAL	1	0
5	I	407	SIA	1	0
5	J	404	SIA	1	0
5	J	405	NAG	1	2

5.6 Ligand geometry

Of 50 ligands modelled in this entry, 10 are monoatomic - leaving 40 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	EDO	A	402	-	3,3,3	0.46	0	2,2,2	0.64	0
3	EDO	A	403	-	3,3,3	0.58	0	2,2,2	0.33	0
3	EDO	A	404	-	3,3,3	0.50	0	2,2,2	0.49	0
3	EDO	A	405	-	3,3,3	0.40	0	2,2,2	0.75	0
3	EDO	A	406	-	3,3,3	0.53	0	2,2,2	0.33	0
3	EDO	A	407	-	3,3,3	0.57	0	2,2,2	0.08	0
4	IPA	A	408	-	3,3,3	0.48	0	3,3,3	0.31	0
3	EDO	B	402	-	3,3,3	0.56	0	2,2,2	0.31	0
3	EDO	B	403	-	3,3,3	0.52	0	2,2,2	0.35	0
3	EDO	B	404	-	3,3,3	0.59	0	2,2,2	0.08	0
3	EDO	B	405	-	3,3,3	0.40	0	2,2,2	0.73	0
4	IPA	B	406	-	3,3,3	0.40	0	3,3,3	0.53	0
3	EDO	C	402	-	3,3,3	0.53	0	2,2,2	0.51	0
4	IPA	C	403	-	3,3,3	0.45	0	3,3,3	0.29	0
3	EDO	D	402	-	3,3,3	0.47	0	2,2,2	0.48	0
3	EDO	D	403	-	3,3,3	0.53	0	2,2,2	0.27	0
4	IPA	D	404	-	3,3,3	0.50	0	3,3,3	0.28	0
3	EDO	E	402	-	3,3,3	0.45	0	2,2,2	0.58	0
3	EDO	E	403	-	3,3,3	0.42	0	2,2,2	0.63	0
4	IPA	E	404	-	3,3,3	0.43	0	3,3,3	0.41	0
3	EDO	F	402	-	3,3,3	0.48	0	2,2,2	0.52	0
3	EDO	F	403	-	3,3,3	0.52	0	2,2,2	0.45	0
3	EDO	F	404	-	3,3,3	0.40	0	2,2,2	0.39	0
3	EDO	F	405	-	3,3,3	0.49	0	2,2,2	0.32	0
4	IPA	F	406	-	3,3,3	0.42	0	3,3,3	0.40	0
3	EDO	G	402	-	3,3,3	0.54	0	2,2,2	0.06	0
3	EDO	G	403	-	3,3,3	0.44	0	2,2,2	0.55	0
4	IPA	G	404	-	3,3,3	0.52	0	3,3,3	0.39	0
3	EDO	H	402	-	3,3,3	0.49	0	2,2,2	0.40	0
3	EDO	H	403	-	3,3,3	0.29	0	2,2,2	0.68	0
3	EDO	H	404	-	3,3,3	0.52	0	2,2,2	0.02	0
3	EDO	H	405	-	3,3,3	0.39	0	2,2,2	0.74	0
4	IPA	H	406	-	3,3,3	0.50	0	3,3,3	0.38	0
3	EDO	I	402	-	3,3,3	0.47	0	2,2,2	0.51	0
3	EDO	I	403	-	3,3,3	0.47	0	2,2,2	0.50	0
3	EDO	I	404	-	3,3,3	0.52	0	2,2,2	0.31	0
3	EDO	I	405	-	3,3,3	0.53	0	2,2,2	0.11	0
4	IPA	I	406	-	3,3,3	0.45	0	3,3,3	0.30	0
3	EDO	J	402	-	3,3,3	0.51	0	2,2,2	0.44	0
4	IPA	J	403	-	3,3,3	0.41	0	3,3,3	0.44	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
3	EDO	A	402	-	-	0/1/1/1	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0
3	EDO	A	404	-	-	0/1/1/1	0/0/0/0
3	EDO	A	405	-	-	0/1/1/1	0/0/0/0
3	EDO	A	406	-	-	0/1/1/1	0/0/0/0
3	EDO	A	407	-	-	0/1/1/1	0/0/0/0
4	IPA	A	408	-	-	0/0/0/0	0/0/0/0
3	EDO	B	402	-	-	0/1/1/1	0/0/0/0
3	EDO	B	403	-	-	0/1/1/1	0/0/0/0
3	EDO	B	404	-	-	0/1/1/1	0/0/0/0
3	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	IPA	B	406	-	-	0/0/0/0	0/0/0/0
3	EDO	C	402	-	-	0/1/1/1	0/0/0/0
4	IPA	C	403	-	-	0/0/0/0	0/0/0/0
3	EDO	D	402	-	-	0/1/1/1	0/0/0/0
3	EDO	D	403	-	-	0/1/1/1	0/0/0/0
4	IPA	D	404	-	-	0/0/0/0	0/0/0/0
3	EDO	E	402	-	-	0/1/1/1	0/0/0/0
3	EDO	E	403	-	-	0/1/1/1	0/0/0/0
4	IPA	E	404	-	-	0/0/0/0	0/0/0/0
3	EDO	F	402	-	-	0/1/1/1	0/0/0/0
3	EDO	F	403	-	-	0/1/1/1	0/0/0/0
3	EDO	F	404	-	-	0/1/1/1	0/0/0/0
3	EDO	F	405	-	-	0/1/1/1	0/0/0/0
4	IPA	F	406	-	-	0/0/0/0	0/0/0/0
3	EDO	G	402	-	-	0/1/1/1	0/0/0/0
3	EDO	G	403	-	-	0/1/1/1	0/0/0/0
4	IPA	G	404	-	-	0/0/0/0	0/0/0/0
3	EDO	H	402	-	-	0/1/1/1	0/0/0/0
3	EDO	H	403	-	-	0/1/1/1	0/0/0/0
3	EDO	H	404	-	-	0/1/1/1	0/0/0/0
3	EDO	H	405	-	-	0/1/1/1	0/0/0/0
4	IPA	H	406	-	-	0/0/0/0	0/0/0/0
3	EDO	I	402	-	-	0/1/1/1	0/0/0/0
3	EDO	I	403	-	-	0/1/1/1	0/0/0/0
3	EDO	I	404	-	-	0/1/1/1	0/0/0/0
3	EDO	I	405	-	-	0/1/1/1	0/0/0/0
4	IPA	I	406	-	-	0/0/0/0	0/0/0/0
3	EDO	J	402	-	-	0/1/1/1	0/0/0/0
4	IPA	J	403	-	-	0/0/0/0	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.

20 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	EDO	2	0
3	A	404	EDO	1	0
3	A	406	EDO	6	0
3	A	407	EDO	1	0
3	B	402	EDO	1	0
3	B	403	EDO	1	0
3	B	404	EDO	1	0
3	E	402	EDO	2	0
3	F	402	EDO	1	0
3	F	404	EDO	2	0
3	F	405	EDO	3	0
3	G	402	EDO	1	0
4	G	404	IPA	1	0
3	H	402	EDO	1	0
3	H	403	EDO	1	0
3	H	405	EDO	2	0
4	H	406	IPA	1	0
3	I	403	EDO	1	0
3	I	404	EDO	3	0
3	I	405	EDO	3	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	A	270/278 (97%)	-0.27	6 (2%) 65 66	17, 22, 43, 76	2 (0%)
1	B	270/278 (97%)	-0.52	1 (0%) 93 93	17, 23, 38, 57	1 (0%)
1	C	269/278 (96%)	-0.34	5 (1%) 70 70	19, 25, 46, 121	0
1	D	271/278 (97%)	-0.41	4 (1%) 76 77	20, 25, 43, 95	0
1	E	270/278 (97%)	-0.40	3 (1%) 82 83	16, 24, 45, 68	1 (0%)
1	F	272/278 (97%)	-0.46	0 100 100	19, 24, 36, 53	2 (0%)
1	G	270/278 (97%)	-0.30	7 (2%) 59 60	18, 24, 54, 132	2 (0%)
1	H	271/278 (97%)	-0.24	5 (1%) 71 72	16, 23, 44, 69	0
1	I	272/278 (97%)	-0.33	6 (2%) 65 66	17, 23, 48, 81	0
1	J	274/278 (98%)	-0.48	2 (0%) 89 89	18, 23, 44, 77	0
All	All	2709/2780 (97%)	-0.37	39 (1%) 78 78	16, 24, 44, 132	8 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	103	GLU	4.3
1	G	107	CYS	4.0
1	A	108	ASP	3.7
1	A	106	THR	3.7
1	C	103	GLU	3.7
1	A	103	GLU	3.6
1	I	103	GLU	3.6
1	G	105	MET	3.5
1	A	104	ASP	3.5
1	G	108	ASP	3.4
1	H	33	VAL	3.3
1	I	106	THR	3.3
1	G	301	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	106	THR	3.1
1	H	108	ASP	3.0
1	D	299	VAL	2.9
1	E	106	THR	2.9
1	D	298	VAL	2.9
1	G	33	VAL	2.8
1	I	108	ASP	2.7
1	J	106	THR	2.7
1	B	42	PRO	2.7
1	C	108	ASP	2.6
1	E	108	ASP	2.6
1	H	32	GLY	2.6
1	A	42	PRO	2.5
1	I	104	ASP	2.4
1	I	32	GLY	2.4
1	H	300	LYS	2.3
1	D	32	GLY	2.2
1	H	42	PRO	2.2
1	J	108	ASP	2.2
1	E	33	VAL	2.1
1	C	42	PRO	2.1
1	C	105	MET	2.1
1	I	179	ASP	2.1
1	C	106	THR	2.0
1	A	107	CYS	2.0
1	D	108	ASP	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](#)

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	GAL	J	406	11/12	0.95	0.17	4.60	23,25,29,34	0
5	GAL	G	407	11/12	0.94	0.16	3.49	27,30,37,40	0
5	GAL	D	407	11/12	0.88	0.21	3.19	40,42,47,49	0
5	GAL	A	411	11/12	0.92	0.16	2.52	38,44,46,49	0
5	GAL	B	409	11/12	0.94	0.16	2.23	24,26,34,39	0
5	SIA	A	409	20/21	0.93	0.14	1.99	29,33,35,35	0
5	SIA	B	407	20/21	0.96	0.11	0.89	19,22,25,25	0
5	SIA	J	404	20/21	0.96	0.11	0.86	20,23,27,29	0
5	GAL	H	409	11/12	0.94	0.10	0.76	23,26,29,31	0
5	SIA	D	405	20/21	0.92	0.13	0.64	25,34,37,38	0
5	NAG	D	406	15/15	0.80	0.26	0.27	50,58,64,69	0
5	GAL	I	409	11/12	0.94	0.10	0.21	27,30,34,38	0
5	SIA	G	405	20/21	0.95	0.09	0.20	20,24,25,27	0
5	SIA	I	407	20/21	0.96	0.09	0.08	19,22,26,26	0
5	GAL	F	409	11/12	0.96	0.10	-0.42	27,29,32,36	0
5	SIA	E	405	20/21	0.97	0.09	-0.44	19,21,25,25	0
5	SIA	F	407	20/21	0.97	0.08	-0.70	20,23,25,25	0
5	GAL	E	407	11/12	0.96	0.09	-0.75	23,25,28,36	0
5	SIA	H	407	20/21	0.97	0.07	-1.60	17,21,23,23	0
5	NAG	H	408	15/15	0.87	0.24	-	33,44,55,58	0
5	NAG	F	408	15/15	0.89	0.19	-	34,43,61,62	0
5	NAG	E	406	15/15	0.93	0.12	-	30,34,37,41	0
5	NAG	A	410	15/15	0.82	0.33	-	55,72,87,90	0
5	NAG	B	408	15/15	0.90	0.22	-	33,40,55,55	0
5	NAG	G	406	15/15	0.86	0.22	-	40,47,55,62	0
5	NAG	I	408	15/15	0.89	0.22	-	36,48,62,62	0
5	NAG	J	405	15/15	0.87	0.23	-	33,42,53,58	0

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	H	402	4/4	0.91	0.19	14.99	26,33,38,44	0
3	EDO	J	402	4/4	0.83	0.22	14.25	32,32,36,36	0
3	EDO	H	405	4/4	0.88	0.28	11.52	32,37,37,40	0
3	EDO	A	405	4/4	0.89	0.21	9.98	29,33,37,42	0
3	EDO	C	402	4/4	0.94	0.14	8.63	32,32,37,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	IPA	I	406	4/4	0.88	0.26	8.03	32,33,34,36	0
4	IPA	B	406	4/4	0.87	0.20	7.91	29,29,31,32	0
4	IPA	J	403	4/4	0.91	0.18	7.87	27,27,27,29	0
4	IPA	C	403	4/4	0.92	0.22	7.77	33,34,36,36	0
3	EDO	I	402	4/4	0.93	0.16	7.76	31,32,34,39	0
4	IPA	E	404	4/4	0.92	0.17	6.95	31,34,34,37	0
4	IPA	F	406	4/4	0.90	0.19	6.07	34,35,38,38	0
4	IPA	G	404	4/4	0.87	0.23	5.63	30,32,35,36	0
3	EDO	I	405	4/4	0.79	0.26	5.58	45,45,49,49	0
3	EDO	E	402	4/4	0.87	0.19	5.06	39,42,43,47	0
3	EDO	H	404	4/4	0.92	0.13	5.04	30,30,32,32	0
3	EDO	F	402	4/4	0.96	0.16	4.61	34,35,36,38	0
4	IPA	A	408	4/4	0.94	0.17	4.11	31,32,36,36	0
3	EDO	A	402	4/4	0.95	0.13	3.89	26,31,32,39	0
3	EDO	A	403	4/4	0.91	0.19	3.80	25,27,31,32	0
3	EDO	B	404	4/4	0.81	0.17	3.65	34,37,38,39	0
3	EDO	A	406	4/4	0.81	0.23	3.51	40,44,45,46	0
3	EDO	G	403	4/4	0.96	0.11	3.49	31,33,34,35	0
3	EDO	D	402	4/4	0.94	0.17	3.46	33,36,38,46	0
3	EDO	B	403	4/4	0.96	0.12	3.38	31,32,34,36	0
3	EDO	F	404	4/4	0.95	0.18	2.94	25,26,29,31	0
4	IPA	H	406	4/4	0.92	0.17	2.81	32,32,33,34	0
3	EDO	I	404	4/4	0.81	0.21	2.71	40,42,42,44	0
3	EDO	G	402	4/4	0.90	0.13	2.53	31,31,32,39	0
3	EDO	H	403	4/4	0.92	0.17	1.98	30,31,32,36	0
4	IPA	D	404	4/4	0.97	0.14	1.92	26,28,30,31	0
3	EDO	I	403	4/4	0.91	0.18	1.86	39,43,47,48	0
3	EDO	B	402	4/4	0.92	0.12	1.70	28,32,33,35	0
3	EDO	F	405	4/4	0.95	0.17	1.66	35,37,38,39	0
3	EDO	F	403	4/4	0.95	0.12	1.46	29,29,31,33	0
3	EDO	A	404	4/4	0.89	0.14	1.27	38,39,46,46	0
3	EDO	D	403	4/4	0.92	0.14	1.09	37,40,43,47	0
3	EDO	A	407	4/4	0.95	0.12	0.28	25,27,29,32	0
2	CA	A	401	1/1	0.97	0.05	-2.03	40,40,40,40	0
2	CA	D	401	1/1	0.97	0.04	-3.95	38,38,38,38	0
2	CA	G	401	1/1	0.98	0.04	-	33,33,33,33	0
2	CA	H	401	1/1	0.98	0.03	-	26,26,26,26	0
2	CA	E	401	1/1	0.98	0.04	-	35,35,35,35	0
2	CA	B	401	1/1	0.99	0.03	-	37,37,37,37	0
3	EDO	E	403	4/4	0.91	0.13	-	45,47,48,49	0
2	CA	I	401	1/1	0.99	0.03	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	F	401	1/1	0.99	0.03	-	38,38,38,38	0
2	CA	J	401	1/1	0.99	0.08	-	38,38,38,38	0
3	EDO	B	405	4/4	0.90	0.17	-	45,45,49,49	0
2	CA	C	401	1/1	0.96	0.08	-	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.