



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:10 PM JST

PDB ID : 5XR3
Title : SAV0551 with glyoxylate
Authors : Kim, H.J.; Kwon, A.R.; Lee, B.J.
Deposited on : 2017-06-08
Resolution : 3.01 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

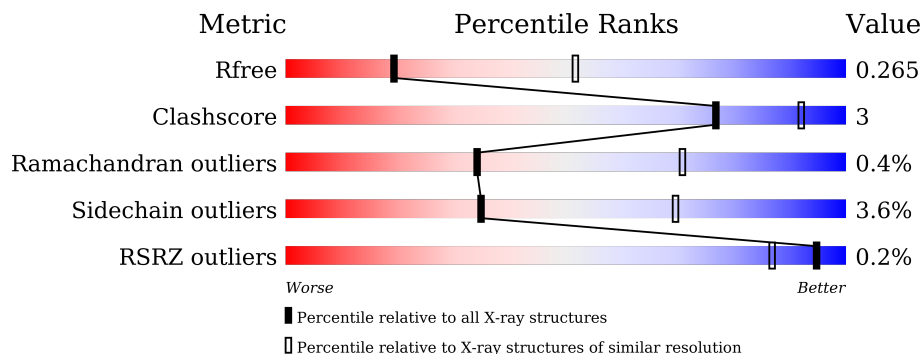
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 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	300	84% 11% 5%
1	B	300	85% 9% 5%
1	C	300	86% 10% 5%
1	D	300	81% 13% 5%
1	E	300	88% 6% 5%
1	F	300	83% 10% 5%

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Mol	Chain	Length	Quality of chain
1	G	300	 91% 5% . .
1	H	300	 86% 9% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17842 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 Protein/nucleic acid deglycase HchA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	286	Total 2220	C 1415	N 364	O 432	S 9	0	0	0
1	B	287	Total 2227	C 1417	N 364	O 437	S 9	0	0	0
1	C	290	Total 2256	C 1435	N 371	O 441	S 9	0	0	0
1	D	284	Total 2204	C 1404	N 360	O 431	S 9	0	0	0
1	E	285	Total 2212	C 1409	N 363	O 431	S 9	0	0	0
1	F	284	Total 2204	C 1404	N 360	O 431	S 9	0	0	0
1	G	292	Total 2273	C 1446	N 375	O 443	S 9	0	0	0
1	H	287	Total 2229	C 1418	N 366	O 436	S 9	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	LEU	-	expression tag	UNP P64312
A	294	GLU	-	expression tag	UNP P64312
A	295	HIS	-	expression tag	UNP P64312
A	296	HIS	-	expression tag	UNP P64312
A	297	HIS	-	expression tag	UNP P64312
A	298	HIS	-	expression tag	UNP P64312
A	299	HIS	-	expression tag	UNP P64312
A	300	HIS	-	expression tag	UNP P64312
B	293	LEU	-	expression tag	UNP P64312
B	294	GLU	-	expression tag	UNP P64312
B	295	HIS	-	expression tag	UNP P64312
B	296	HIS	-	expression tag	UNP P64312
B	297	HIS	-	expression tag	UNP P64312

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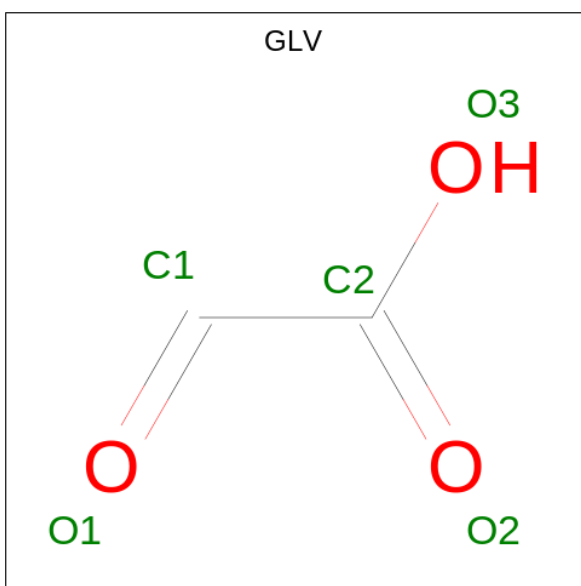
Chain	Residue	Modelled	Actual	Comment	Reference
B	298	HIS	-	expression tag	UNP P64312
B	299	HIS	-	expression tag	UNP P64312
B	300	HIS	-	expression tag	UNP P64312
C	293	LEU	-	expression tag	UNP P64312
C	294	GLU	-	expression tag	UNP P64312
C	295	HIS	-	expression tag	UNP P64312
C	296	HIS	-	expression tag	UNP P64312
C	297	HIS	-	expression tag	UNP P64312
C	298	HIS	-	expression tag	UNP P64312
C	299	HIS	-	expression tag	UNP P64312
C	300	HIS	-	expression tag	UNP P64312
D	293	LEU	-	expression tag	UNP P64312
D	294	GLU	-	expression tag	UNP P64312
D	295	HIS	-	expression tag	UNP P64312
D	296	HIS	-	expression tag	UNP P64312
D	297	HIS	-	expression tag	UNP P64312
D	298	HIS	-	expression tag	UNP P64312
D	299	HIS	-	expression tag	UNP P64312
D	300	HIS	-	expression tag	UNP P64312
E	293	LEU	-	expression tag	UNP P64312
E	294	GLU	-	expression tag	UNP P64312
E	295	HIS	-	expression tag	UNP P64312
E	296	HIS	-	expression tag	UNP P64312
E	297	HIS	-	expression tag	UNP P64312
E	298	HIS	-	expression tag	UNP P64312
E	299	HIS	-	expression tag	UNP P64312
E	300	HIS	-	expression tag	UNP P64312
F	293	LEU	-	expression tag	UNP P64312
F	294	GLU	-	expression tag	UNP P64312
F	295	HIS	-	expression tag	UNP P64312
F	296	HIS	-	expression tag	UNP P64312
F	297	HIS	-	expression tag	UNP P64312
F	298	HIS	-	expression tag	UNP P64312
F	299	HIS	-	expression tag	UNP P64312
F	300	HIS	-	expression tag	UNP P64312
G	293	LEU	-	expression tag	UNP P64312
G	294	GLU	-	expression tag	UNP P64312
G	295	HIS	-	expression tag	UNP P64312
G	296	HIS	-	expression tag	UNP P64312
G	297	HIS	-	expression tag	UNP P64312
G	298	HIS	-	expression tag	UNP P64312
G	299	HIS	-	expression tag	UNP P64312

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Chain	Residue	Modelled	Actual	Comment	Reference
G	300	HIS	-	expression tag	UNP P64312
H	293	LEU	-	expression tag	UNP P64312
H	294	GLU	-	expression tag	UNP P64312
H	295	HIS	-	expression tag	UNP P64312
H	296	HIS	-	expression tag	UNP P64312
H	297	HIS	-	expression tag	UNP P64312
H	298	HIS	-	expression tag	UNP P64312
H	299	HIS	-	expression tag	UNP P64312
H	300	HIS	-	expression tag	UNP P64312

- Molecule 2 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C₂H₂O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total	0	0
			5		
2	E	1	Total	0	0
			5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total	0	0
			3		
3	F	2	Total	0	0
			2		
3	G	1	Total	0	0
			1		

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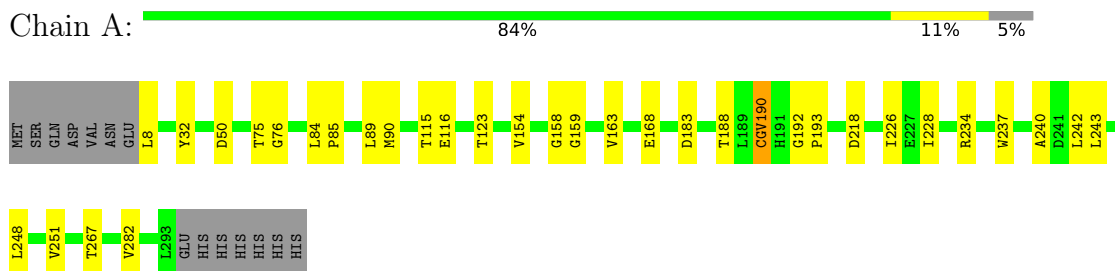
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	O	0	0
			1	1		

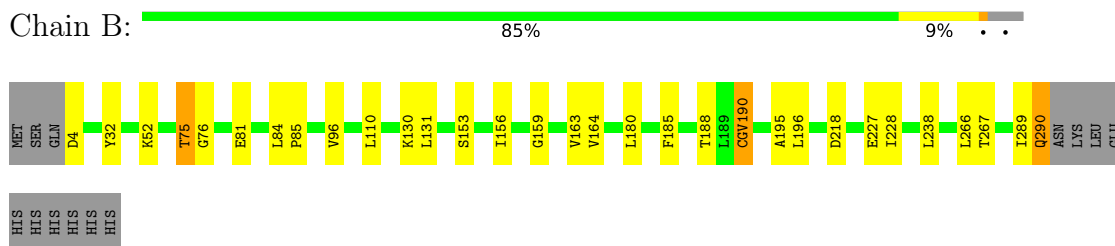
3 Residue-property plots [i](#)

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.

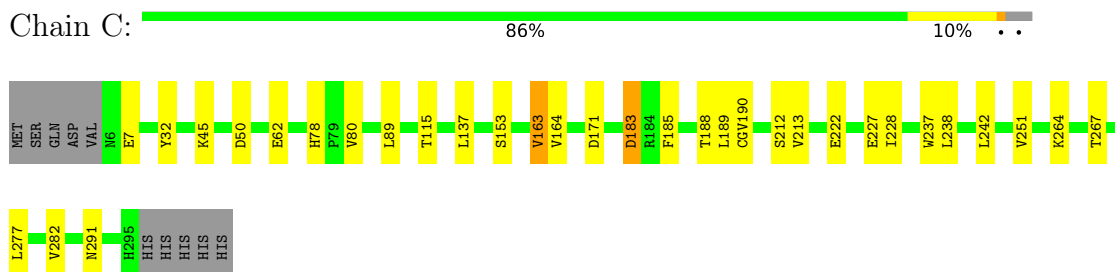
- Molecule 1: Protein/nucleic acid deglycase HchA



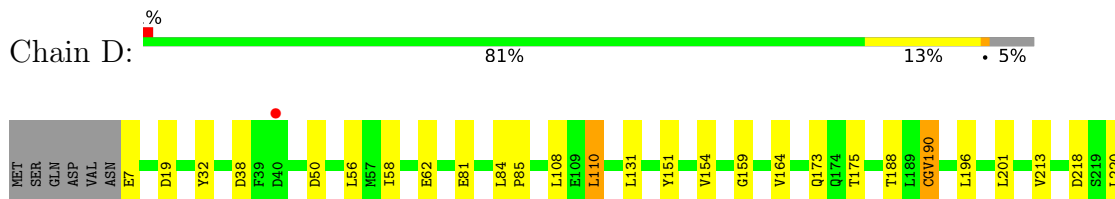
- Molecule 1: Protein/nucleic acid deglycase HchA

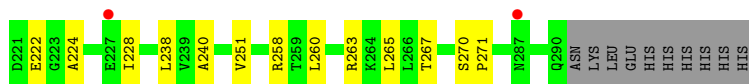


- Molecule 1: Protein/nucleic acid deglycase HchA

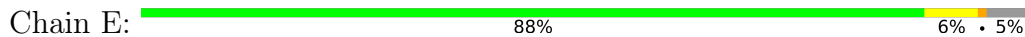


- Molecule 1: Protein/nucleic acid deglycase HchA

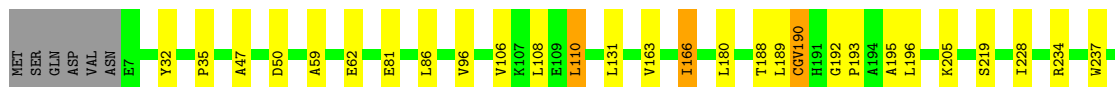
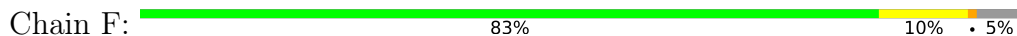




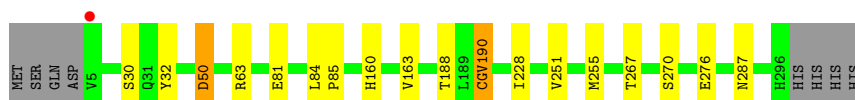
• Molecule 1: Protein/nucleic acid deglycase HchA



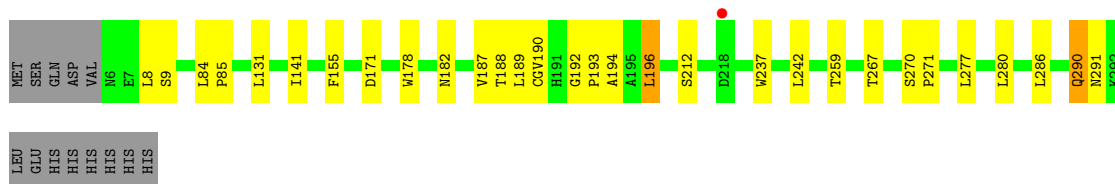
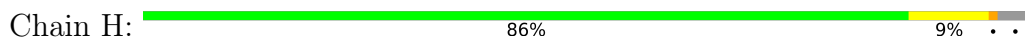
• Molecule 1: Protein/nucleic acid deglycase HchA



• Molecule 1: Protein/nucleic acid deglycase HchA



• Molecule 1: Protein/nucleic acid deglycase HchA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.20Å 130.12Å 187.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.01 48.81 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.01-3.01) 99.2 (48.81-3.01)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.50 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.269 0.183 , 0.265	Depositor DCC
R_{free} test set	2428 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17842	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0477e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CGV, GLV

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	0.56	0/2255	0.74	0/3058
1	B	0.55	0/2262	0.72	0/3069
1	C	0.55	0/2292	0.72	0/3108
1	D	0.52	0/2239	0.71	0/3037
1	E	0.55	0/2247	0.74	0/3047
1	F	0.55	0/2239	0.71	0/3037
1	G	0.57	0/2310	0.73	0/3133
1	H	0.55	0/2264	0.72	0/3070
All	All	0.55	0/18108	0.72	0/24559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2220	0	2215	18	0
1	B	2227	0	2210	13	0
1	C	2256	0	2240	14	0
1	D	2204	0	2191	19	0
1	E	2212	0	2204	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2204	0	2191	17	0
1	G	2273	0	2256	8	0
1	H	2229	0	2216	11	0
2	A	5	0	1	0	0
2	E	5	0	1	0	0
3	A	3	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	17842	0	17725	107	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 (107) 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:B:81:GLU:OE1	1:B:190:CGV:H6	1.85	0.75
1:C:213:VAL:HG12	1:C:267:THR:HG21	1.72	0.71
1:G:81:GLU:OE1	1:G:190:CGV:H6	1.91	0.69
1:A:159:GLY:N	1:A:190:CGV:OD2	2.26	0.68
1:F:166:ILE:CG2	1:F:195:ALA:HB2	2.27	0.64
1:F:192:GLY:N	1:F:193:PRO:CD	2.60	0.64
1:B:156:ILE:HD13	1:B:195:ALA:CB	2.29	0.63
1:G:32:TYR:CE2	1:G:228:ILE:HD11	2.34	0.63
1:H:286:LEU:O	1:H:290:GLN:NE2	2.34	0.60
1:B:289:ILE:O	1:B:290:GLN:NE2	2.36	0.59
1:D:213:VAL:CG1	1:D:265:LEU:HD21	2.34	0.57
1:E:78:HIS:HD2	1:E:80:VAL:H	1.52	0.57
1:F:188:THR:HG23	1:F:267:THR:HG22	1.86	0.57
1:C:163:VAL:HG22	1:C:237:TRP:CH2	2.41	0.56
1:D:108:LEU:HB2	1:D:110:LEU:CD1	2.38	0.54
1:F:81:GLU:OE1	1:F:190:CGV:H6	2.07	0.54
1:A:237:TRP:CE3	1:A:242:LEU:HD22	2.43	0.54
1:A:115:THR:HG23	1:A:116:GLU:HG3	1.90	0.53
1:D:32:TYR:CE2	1:D:228:ILE:HD11	2.44	0.53
1:E:63:ARG:O	1:E:63:ARG:HG3	2.07	0.53
1:A:188:THR:HG23	1:A:267:THR:HG22	1.91	0.52
1:B:153:SER:HB2	1:B:185:PHE:HB2	1.91	0.52
1:E:75:THR:OG1	1:E:76:GLY:N	2.41	0.52
1:C:78:HIS:HD2	1:C:80:VAL:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HD22	1:A:248:LEU:HD22	1.91	0.52
1:F:166:ILE:HG22	1:F:195:ALA:HB2	1.92	0.51
1:A:218:ASP:OD1	1:A:240:ALA:HB3	2.10	0.51
1:E:107:LYS:NZ	1:F:62:GLU:OE1	2.36	0.51
1:B:75:THR:OG1	1:B:76:GLY:N	2.44	0.51
1:A:90:MET:CE	1:A:123:THR:HG23	2.41	0.50
1:F:32:TYR:CE2	1:F:228:ILE:HD11	2.47	0.50
1:F:188:THR:CG2	1:F:267:THR:HG22	2.40	0.50
1:F:86:LEU:HD22	1:F:96:VAL:HG21	1.92	0.50
1:C:62:GLU:HG2	1:C:164:VAL:HG11	1.94	0.49
1:D:222:GLU:HG2	1:D:238:LEU:HD11	1.95	0.49
1:D:188:THR:HG23	1:D:267:THR:HG22	1.95	0.49
1:G:160:HIS:O	1:G:163:VAL:HB	2.13	0.49
1:C:188:THR:HG22	1:C:267:THR:HG22	1.95	0.48
1:D:58:ILE:HD11	1:D:175:THR:HG21	1.94	0.48
1:B:84:LEU:HB3	1:B:85:PRO:HD3	1.94	0.48
1:C:189:LEU:N	1:C:189:LEU:HD23	2.28	0.48
1:A:226:ILE:HD11	1:A:234:ARG:HA	1.96	0.47
1:D:81:GLU:OE1	1:D:190:CGV:H6	2.15	0.47
1:B:159:GLY:H	1:B:190:CGV:H9	1.80	0.47
1:C:237:TRP:CE3	1:C:242:LEU:HD22	2.49	0.47
1:H:193:PRO:O	1:H:196:LEU:N	2.45	0.47
1:B:153:SER:CB	1:B:185:PHE:HB2	2.44	0.47
1:D:108:LEU:HB2	1:D:110:LEU:HD13	1.97	0.47
1:A:32:TYR:CE2	1:A:228:ILE:HD11	2.49	0.46
1:G:188:THR:O	1:G:267:THR:HA	2.15	0.46
1:C:222:GLU:CG	1:C:238:LEU:HD11	2.46	0.46
1:B:156:ILE:HD13	1:B:195:ALA:HB1	1.97	0.45
1:C:183:ASP:OD2	1:C:264:LYS:HE3	2.15	0.45
1:D:84:LEU:HB3	1:D:85:PRO:HD3	1.99	0.45
1:E:159:GLY:H	1:E:190:CGV:CD1	2.30	0.45
1:G:84:LEU:HB3	1:G:85:PRO:HD3	1.98	0.45
1:C:89:LEU:HD23	1:C:282:VAL:HG22	1.99	0.45
1:C:137:LEU:HD23	1:C:171:ASP:HB3	1.99	0.44
1:D:251:VAL:HG11	1:D:260:LEU:HD22	1.99	0.44
1:E:189:LEU:HD22	1:E:277:LEU:HD23	1.99	0.44
1:H:237:TRP:CE3	1:H:242:LEU:HD12	2.53	0.44
1:E:159:GLY:H	1:E:190:CGV:H9	1.83	0.44
1:E:84:LEU:HB3	1:E:85:PRO:HD3	2.00	0.44
1:D:159:GLY:H	1:D:190:CGV:H9	1.83	0.44
1:A:75:THR:OG1	1:A:76:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:THR:HG23	1:B:267:THR:HG22	1.99	0.43
1:H:84:LEU:HB3	1:H:85:PRO:HD3	1.99	0.43
1:H:189:LEU:N	1:H:189:LEU:HD23	2.33	0.43
1:A:192:GLY:N	1:A:193:PRO:CD	2.81	0.43
1:A:90:MET:HE2	1:A:123:THR:HG23	2.00	0.43
1:F:190:CGV:O	1:F:193:PRO:HD2	2.18	0.43
1:A:115:THR:HG21	1:F:35:PRO:HD2	2.00	0.43
1:A:158:GLY:HA3	1:A:190:CGV:H5	2.00	0.43
1:D:222:GLU:CG	1:D:238:LEU:HD11	2.49	0.43
1:B:96:VAL:O	1:B:130:LYS:NZ	2.46	0.43
1:D:270:SER:HB2	1:D:271:PRO:HD2	1.99	0.43
1:A:84:LEU:HB3	1:A:85:PRO:HD3	2.01	0.42
1:A:163:VAL:HG13	1:A:237:TRP:CZ2	2.53	0.42
1:F:188:THR:O	1:F:267:THR:HA	2.19	0.42
1:B:218:ASP:HB3	1:B:238:LEU:HD13	2.01	0.42
1:G:255:MET:HG3	1:G:270:SER:CB	2.49	0.42
1:C:153:SER:HB2	1:C:185:PHE:HB2	2.02	0.42
1:D:220:LEU:HD23	1:D:224:ALA:HB3	2.00	0.42
1:B:32:TYR:CE2	1:B:228:ILE:HD11	2.54	0.42
1:C:189:LEU:HD13	1:C:277:LEU:HD22	2.02	0.42
1:F:108:LEU:HB2	1:F:110:LEU:CD1	2.50	0.42
1:G:81:GLU:CD	1:G:190:CGV:H6	2.40	0.42
1:H:141:ILE:HD11	1:H:171:ASP:O	2.20	0.42
1:D:173:GLN:NE2	1:D:201:LEU:O	2.52	0.42
1:H:189:LEU:HD22	1:H:277:LEU:CD2	2.50	0.42
1:D:218:ASP:OD1	1:D:240:ALA:HB3	2.20	0.41
1:G:50:ASP:OD1	1:G:50:ASP:N	2.53	0.41
1:H:155:PHE:HA	1:H:187:VAL:O	2.21	0.41
1:H:178:TRP:CD1	1:H:182:ASN:ND2	2.87	0.41
1:C:32:TYR:CE2	1:C:228:ILE:HD11	2.56	0.41
1:F:81:GLU:HG2	1:F:189:LEU:HD11	2.03	0.41
1:F:163:VAL:HG13	1:F:237:TRP:CZ2	2.56	0.41
1:D:188:THR:O	1:D:267:THR:HA	2.21	0.41
1:F:196:LEU:HD21	1:F:265:LEU:HD11	2.03	0.41
1:H:259:THR:CG2	1:H:280:LEU:HD22	2.50	0.41
1:A:89:LEU:HD23	1:A:282:VAL:HG22	2.03	0.41
1:E:237:TRP:CE3	1:E:242:LEU:HD22	2.56	0.40
1:A:188:THR:CG2	1:A:267:THR:HG22	2.51	0.40
1:D:251:VAL:HG11	1:D:260:LEU:CD2	2.51	0.40
1:F:59:ALA:HB3	1:F:106:VAL:HG22	2.03	0.40
1:D:56:LEU:HB2	1:D:151:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:270:SER:HB2	1:H:271:PRO:HD2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/300 (94%)	270 (95%)	13 (5%)	0	100	100
1	B	284/300 (95%)	260 (92%)	23 (8%)	1 (0%)	34	71
1	C	287/300 (96%)	273 (95%)	14 (5%)	0	100	100
1	D	281/300 (94%)	259 (92%)	19 (7%)	3 (1%)	14	48
1	E	282/300 (94%)	259 (92%)	22 (8%)	1 (0%)	34	71
1	F	281/300 (94%)	261 (93%)	18 (6%)	2 (1%)	22	59
1	G	289/300 (96%)	271 (94%)	18 (6%)	0	100	100
1	H	284/300 (95%)	257 (90%)	25 (9%)	2 (1%)	22	59
All	All	2271/2400 (95%)	2110 (93%)	152 (7%)	9 (0%)	34	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	263	ARG
1	E	39	PHE
1	D	258	ARG
1	F	47	ALA
1	H	194	ALA
1	B	164	VAL
1	D	164	VAL
1	H	192	GLY
1	F	166	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	242/256 (94%)	236 (98%)	6 (2%)	47 78
1	B	243/256 (95%)	232 (96%)	11 (4%)	27 63
1	C	246/256 (96%)	236 (96%)	10 (4%)	30 66
1	D	240/256 (94%)	231 (96%)	9 (4%)	33 68
1	E	241/256 (94%)	233 (97%)	8 (3%)	38 72
1	F	240/256 (94%)	229 (95%)	11 (5%)	27 62
1	G	248/256 (97%)	242 (98%)	6 (2%)	49 79
1	H	243/256 (95%)	234 (96%)	9 (4%)	34 69
All	All	1943/2048 (95%)	1873 (96%)	70 (4%)	35 69

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	50	ASP
1	A	154	VAL
1	A	168	GLU
1	A	183	ASP
1	A	251	VAL
1	B	4	ASP
1	B	52	LYS
1	B	75	THR
1	B	110	LEU
1	B	131	LEU
1	B	163	VAL
1	B	180	LEU
1	B	196	LEU
1	B	227	GLU
1	B	266	LEU
1	B	290	GLN
1	C	7	GLU
1	C	45	LYS

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Mol	Chain	Res	Type
1	C	50	ASP
1	C	115	THR
1	C	163	VAL
1	C	183	ASP
1	C	212	SER
1	C	227	GLU
1	C	251	VAL
1	C	291	ASN
1	D	7	GLU
1	D	19	ASP
1	D	38	ASP
1	D	50	ASP
1	D	62	GLU
1	D	110	LEU
1	D	131	LEU
1	D	154	VAL
1	D	196	LEU
1	E	63	ARG
1	E	75	THR
1	E	95	ASP
1	E	188	THR
1	E	244	THR
1	E	251	VAL
1	E	267	THR
1	E	290	GLN
1	F	50	ASP
1	F	110	LEU
1	F	131	LEU
1	F	180	LEU
1	F	205	LYS
1	F	219	SER
1	F	234	ARG
1	F	258	ARG
1	F	259	THR
1	F	264	LYS
1	F	290	GLN
1	G	30	SER
1	G	50	ASP
1	G	63	ARG
1	G	251	VAL
1	G	276	GLU
1	G	287	ASN

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Mol	Chain	Res	Type
1	H	8	LEU
1	H	9	SER
1	H	131	LEU
1	H	188	THR
1	H	196	LEU
1	H	212	SER
1	H	267	THR
1	H	290	GLN
1	H	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	HIS
1	B	290	GLN
1	C	78	HIS
1	D	78	HIS
1	E	78	HIS
1	E	291	ASN
1	F	78	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CGV	C	190	1	6,10,11	1.15	0	6,12,14	3.27	3 (50%)
1	CGV	F	190	1	6,10,11	1.18	1 (16%)	6,12,14	3.26	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGV	E	190	1	6,10,11	1.11	0	6,12,14	2.98	4 (66%)
1	CGV	D	190	1	6,10,11	1.40	1 (16%)	6,12,14	2.73	4 (66%)
1	CGV	G	190	1	6,10,11	1.45	1 (16%)	6,12,14	2.86	2 (33%)
1	CGV	A	190	1	6,10,11	1.64	1 (16%)	6,12,14	3.28	4 (66%)
1	CGV	B	190	1	6,10,11	1.20	0	6,12,14	2.55	3 (50%)
1	CGV	H	190	1	6,10,11	1.20	1 (16%)	6,12,14	4.48	4 (66%)

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
1	CGV	C	190	1	-	6/7/11/13	-
1	CGV	F	190	1	-	6/7/11/13	-
1	CGV	E	190	1	-	2/7/11/13	-
1	CGV	D	190	1	-	4/7/11/13	-
1	CGV	G	190	1	-	5/7/11/13	-
1	CGV	A	190	1	-	4/7/11/13	-
1	CGV	B	190	1	-	6/7/11/13	-
1	CGV	H	190	1	-	3/7/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	CGV	CB-SG	-3.22	1.78	1.82
1	D	190	CGV	CB-SG	-2.13	1.79	1.82
1	H	190	CGV	OZ3-CE1	2.06	1.28	1.22
1	F	190	CGV	O-C	2.03	1.28	1.19
1	G	190	CGV	CB-SG	-2.00	1.79	1.82

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	190	CGV	CB-SG-CD1	7.44	115.35	101.25
1	H	190	CGV	CE1-CD1-SG	6.61	120.06	108.50
1	F	190	CGV	CB-SG-CD1	5.96	112.55	101.25
1	C	190	CGV	CB-SG-CD1	5.91	112.46	101.25
1	G	190	CGV	CB-SG-CD1	5.49	111.66	101.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	CGV	CE1-CD1-SG	4.86	117.00	108.50
1	A	190	CGV	OZ2-CE1-CD1	4.69	121.96	113.12
1	B	190	CGV	CB-SG-CD1	4.65	110.07	101.25
1	F	190	CGV	CE1-CD1-SG	4.26	115.96	108.50
1	E	190	CGV	OZ2-CE1-CD1	4.16	120.96	113.12
1	C	190	CGV	CE1-CD1-SG	3.96	115.42	108.50
1	A	190	CGV	CB-SG-CD1	3.86	108.57	101.25
1	G	190	CGV	CE1-CD1-SG	3.84	115.21	108.50
1	D	190	CGV	OZ2-CE1-CD1	3.76	120.21	113.12
1	H	190	CGV	OZ2-CE1-CD1	3.76	120.21	113.12
1	D	190	CGV	CE1-CD1-SG	3.72	115.01	108.50
1	A	190	CGV	CE1-CD1-SG	3.69	114.94	108.50
1	A	190	CGV	OZ3-CE1-CD1	-3.27	116.47	122.69
1	D	190	CGV	OZ3-CE1-CD1	-3.23	116.54	122.69
1	C	190	CGV	OZ2-CE1-CD1	3.11	118.98	113.12
1	B	190	CGV	OZ2-CE1-CD1	2.86	118.50	113.12
1	F	190	CGV	OZ2-CE1-CD1	2.68	118.17	113.12
1	H	190	CGV	OZ3-CE1-CD1	-2.51	117.91	122.69
1	B	190	CGV	CE1-CD1-SG	2.48	112.84	108.50
1	D	190	CGV	CB-SG-CD1	2.45	105.89	101.25
1	E	190	CGV	OZ3-CE1-CD1	-2.24	118.42	122.69
1	E	190	CGV	CB-SG-CD1	2.03	105.09	101.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	190	CGV	OD2-CD1-CE1-OZ2
1	B	190	CGV	C-CA-CB-SG
1	B	190	CGV	OD2-CD1-CE1-OZ2
1	B	190	CGV	OD2-CD1-CE1-OZ3
1	C	190	CGV	SG-CD1-CE1-OZ2
1	C	190	CGV	SG-CD1-CE1-OZ3
1	F	190	CGV	N-CA-CB-SG
1	F	190	CGV	C-CA-CB-SG
1	F	190	CGV	SG-CD1-CE1-OZ2
1	F	190	CGV	SG-CD1-CE1-OZ3
1	G	190	CGV	N-CA-CB-SG
1	G	190	CGV	C-CA-CB-SG
1	G	190	CGV	OD2-CD1-CE1-OZ2
1	H	190	CGV	OD2-CD1-CE1-OZ3
1	D	190	CGV	OD2-CD1-CE1-OZ2

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Mol	Chain	Res	Type	Atoms
1	H	190	CGV	OD2-CD1-CE1-OZ2
1	C	190	CGV	OD2-CD1-CE1-OZ2
1	F	190	CGV	OD2-CD1-CE1-OZ2
1	F	190	CGV	OD2-CD1-CE1-OZ3
1	G	190	CGV	OD2-CD1-CE1-OZ3
1	B	190	CGV	N-CA-CB-SG
1	B	190	CGV	CA-CB-SG-CD1
1	C	190	CGV	CA-CB-SG-CD1
1	D	190	CGV	CA-CB-SG-CD1
1	E	190	CGV	CA-CB-SG-CD1
1	A	190	CGV	SG-CD1-CE1-OZ3
1	B	190	CGV	SG-CD1-CE1-OZ3
1	H	190	CGV	SG-CD1-CE1-OZ3
1	A	190	CGV	OD2-CD1-CE1-OZ3
1	C	190	CGV	OD2-CD1-CE1-OZ3
1	D	190	CGV	OD2-CD1-CE1-OZ3
1	A	190	CGV	N-CA-CB-SG
1	C	190	CGV	N-CA-CB-SG
1	D	190	CGV	N-CA-CB-SG
1	E	190	CGV	OD2-CD1-CE1-OZ2
1	G	190	CGV	SG-CD1-CE1-OZ3

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	190	CGV	2	0
1	E	190	CGV	2	0
1	D	190	CGV	2	0
1	G	190	CGV	2	0
1	A	190	CGV	2	0
1	B	190	CGV	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	GLV	A	401	-	4,4,4	1.16	0	3,4,4	1.75	2 (66%)
2	GLV	E	401	-	4,4,4	1.20	0	3,4,4	1.35	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	GLV	A	401	-	-	0/0/2/2	-
2	GLV	E	401	-	-	0/0/2/2	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GLV	O2-C2-C1	-2.21	116.79	123.83
2	A	401	GLV	O3-C2-C1	2.04	119.79	113.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/300 (95%)	-0.53	0 100 100	25, 37, 59, 92	0
1	B	286/300 (95%)	-0.34	0 100 100	27, 50, 72, 83	0
1	C	289/300 (96%)	-0.51	0 100 100	25, 39, 65, 105	0
1	D	283/300 (94%)	-0.18	3 (1%) 80 55	30, 60, 83, 103	0
1	E	284/300 (94%)	-0.47	0 100 100	24, 42, 65, 81	0
1	F	283/300 (94%)	-0.37	0 100 100	28, 51, 72, 100	0
1	G	291/300 (97%)	-0.44	1 (0%) 94 83	25, 38, 61, 102	0
1	H	286/300 (95%)	-0.30	1 (0%) 94 83	28, 53, 76, 93	0
All	All	2287/2400 (95%)	-0.39	5 (0%) 95 87	24, 45, 72, 105	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	287	ASN	3.4
1	G	5	VAL	2.6
1	D	227	GLU	2.4
1	H	218	ASP	2.3
1	D	40	ASP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CGV	E	190	11/12	0.87	0.32	33,65,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CGV	B	190	11/12	0.90	0.25	34,63,77,82	0
1	CGV	G	190	11/12	0.90	0.28	32,47,67,72	0
1	CGV	C	190	11/12	0.91	0.30	36,57,73,73	0
1	CGV	H	190	11/12	0.91	0.20	36,61,76,83	0
1	CGV	F	190	11/12	0.92	0.18	43,68,83,90	0
1	CGV	A	190	11/12	0.93	0.20	36,50,66,78	0
1	CGV	D	190	11/12	0.93	0.33	55,75,86,86	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLV	A	401	5/5	0.93	0.23	47,48,52,57	0
2	GLV	E	401	5/5	0.95	0.15	48,49,54,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.