



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 PM GMT

PDB ID : 4AVV
Title : Structure of CPHPC bound to Serum Amyloid P Component
Authors : Kolstoe, S.E.; Jenvey, M.C.; Wood, S.P.
Deposited on : 2012-05-29
Resolution : 1.60 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

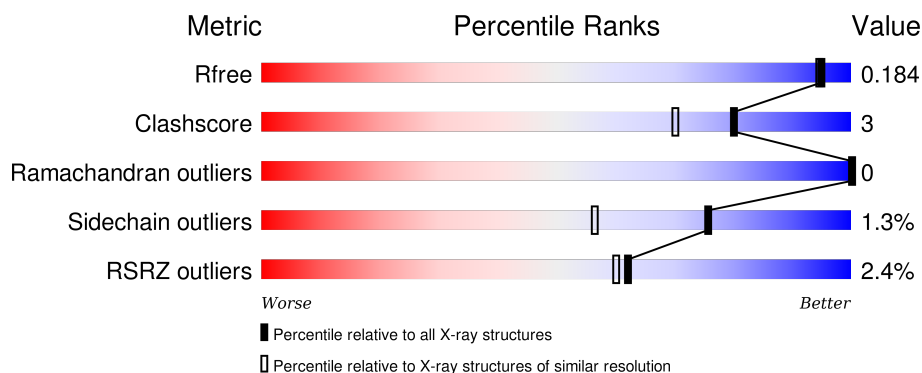
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	204	<div> <div>93%</div> <div>7%</div> </div>
1	B	204	<div> <div>94%</div> <div>6%</div> </div>
1	C	204	<div> <div>93%</div> <div>6%</div> </div>
1	D	204	<div> <div>94%</div> <div>6%</div> </div>
1	E	204	<div> <div>94%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	1206	-	-	X	-
2	ACT	A	1208	-	-	X	-
2	ACT	B	1208	-	-	X	-
2	ACT	E	1215	-	-	-	X
3	GHE	A	1207	-	-	-	X
3	GHE	B	1207	-	-	-	X
3	GHE	C	1207	-	-	-	X
3	GHE	D	1207	-	-	-	X
3	GHE	E	1207	-	-	-	X
5	NAG	C	1209	-	-	-	X
7	SIA	B	1213	-	-	-	X
8	GAL	D	1132	X	-	-	-
8	SIA	D	1205	-	-	-	X
9	SIA	D	6037	-	-	-	X

2 Entry composition [i](#)

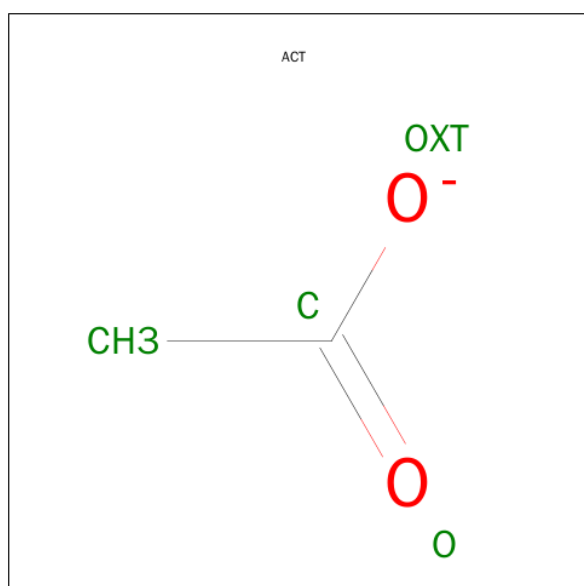
There are 10 unique types of molecules in this entry. The entry contains 10255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERUM AMYLOID P-COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total	C	N	O	S	0	8	0
			1710	1107	283	315	5			
1	B	204	Total	C	N	O	S	0	4	0
			1675	1086	276	308	5			
1	C	204	Total	C	N	O	S	0	4	0
			1675	1086	276	308	5			
1	D	204	Total	C	N	O	S	0	6	0
			1691	1093	279	314	5			
1	E	204	Total	C	N	O	S	0	4	0
			1675	1084	277	309	5			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



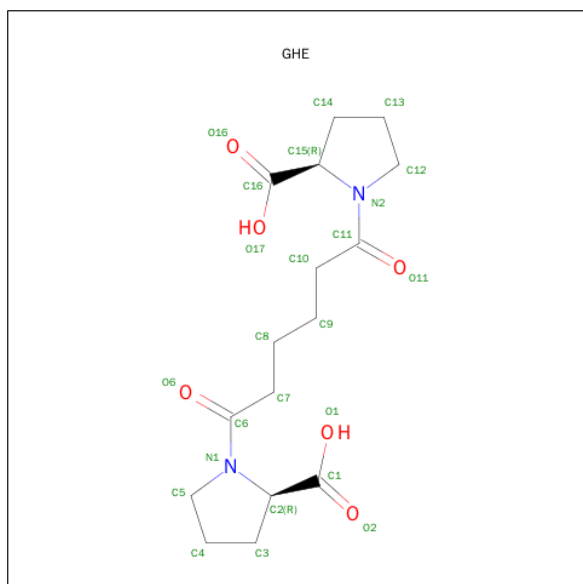
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is (2R)-1-[6-[(2R)-2-CARBOXYPYRROLIDIN-1-YL]-6-OXIDANYLIDENE-H EXANOYL]PYRROLIDINE-2-CARBOXYLIC ACID (three-letter code: GHE) (formula: $C_{16}H_{24}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	16	2	6		
3	B	1	Total	C	N	O	0	0
			24	16	2	6		
3	C	1	Total	C	N	O	0	0
			24	16	2	6		

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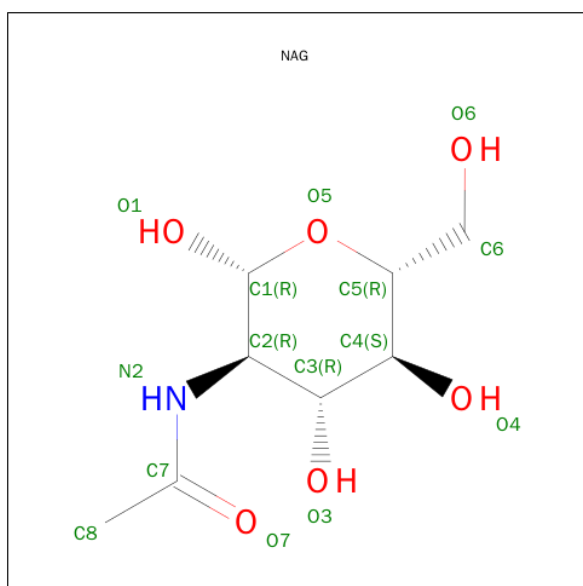
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			24	16	2	6		
3	E	1	Total	C	N	O	0	0
			24	16	2	6		

- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	7	Total	Cd	0	0
			7	7		
4	A	8	Total	Cd	0	0
			8	8		
4	D	5	Total	Cd	0	0
			5	5		
4	C	6	Total	Cd	0	0
			6	6		
4	E	9	Total	Cd	0	0
			9	9		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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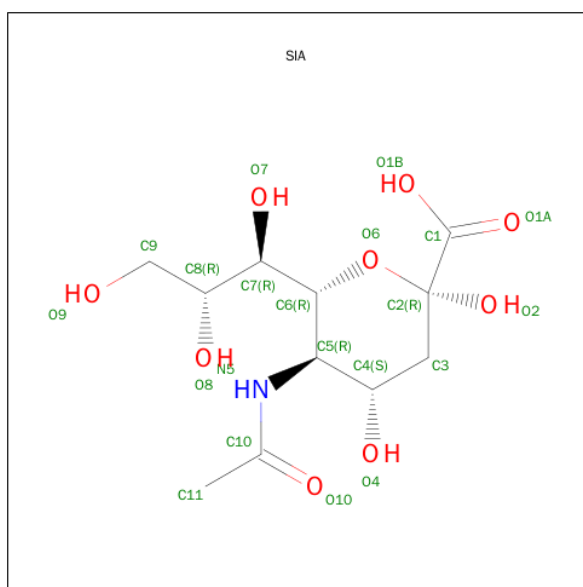
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (O-SIALIC ACID) (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	2	Total	C	N	O	0	0
			31	17	1	13		

- Molecule 9 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	9	Total	C	N	O	0	0
			120	67	5	48		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	327	Total 327	O 327	0	0
10	B	275	Total 275	O 275	0	0
10	C	283	Total 283	O 283	0	0
10	D	277	Total 277	O 277	0	0
10	E	239	Total 239	O 239	0	0

3 Residue-property plots [i](#)

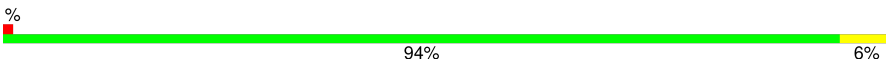
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: SERUM AMYLOID P-COMPONENT

Chain A: 

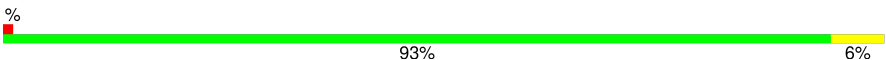


• Molecule 1: SERUM AMYLOID P-COMPONENT

Chain B: 



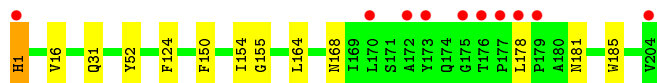
• Molecule 1: SERUM AMYLOID P-COMPONENT

Chain C: 

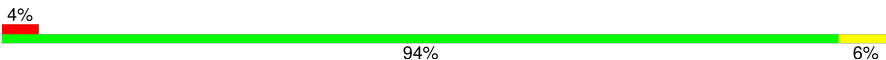


• Molecule 1: SERUM AMYLOID P-COMPONENT

Chain D: 



• Molecule 1: SERUM AMYLOID P-COMPONENT

Chain E: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.38Å 108.58Å 120.26Å 90.00° 138.53° 90.00°	Depositor
Resolution (Å)	37.87 – 1.60 80.56 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.87-1.60) 99.1 (80.56-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 1.60Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.150 , 0.175 0.159 , 0.184	Depositor DCC
R_{free} test set	2005 reflections (1.19%)	DCC
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.2	EDS
Estimated twinning fraction	0.011 for h+2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 170896 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CD, GHE, SIA, GAL, ACT, MAN

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	0.51	0/1757	0.71	0/2389
1	B	0.50	0/1722	0.70	0/2341
1	C	0.50	0/1722	0.70	0/2341
1	D	0.48	0/1738	0.69	0/2362
1	E	0.49	0/1722	0.69	1/2341 (0.0%)
All	All	0.50	0/8661	0.70	1/11774 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	D	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	77	ARG	NE-CZ-NH2	-5.17	117.72	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	D	1132	GAL	C1

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1710	0	1679	12	0
1	B	1675	0	1645	11	0
1	C	1675	0	1644	7	0
1	D	1691	0	1651	10	0
1	E	1675	0	1639	7	0
2	A	16	0	12	4	0
2	B	4	0	3	3	0
2	E	12	0	9	1	0
3	A	24	0	22	0	0
3	B	24	0	22	0	0
3	C	24	0	22	1	0
3	D	24	0	22	0	0
3	E	24	0	22	0	0
4	A	8	0	0	0	0
4	B	7	0	0	0	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
4	E	9	0	0	0	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	1	0
6	B	28	0	25	0	0
7	B	20	0	18	1	0
8	D	31	0	26	1	0
9	D	120	0	101	2	0
10	A	327	0	0	6	0
10	B	275	0	0	4	1
10	C	283	0	0	2	0
10	D	277	0	0	1	1
10	E	239	0	0	1	0
All	All	10255	0	8601	58	1

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 (58) 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)
2:A:1206:ACT:H3	10:A:7145:HOH:O	1.70	0.90
1:B:120:ARG:HH12	2:B:1208:ACT:H3	1.42	0.84
1:E:95[B]:CYS:SG	1:E:169:ILE:HD12	2.21	0.80
1:B:31:GLN:HG2	1:B:124:PHE:CE2	2.19	0.78
1:B:181:ASN:ND2	10:B:7228:HOH:O	2.20	0.74
10:A:7103:HOH:O	1:E:82:SER:CB	2.35	0.73
1:C:181:ASN:ND2	10:C:7228:HOH:O	2.27	0.68
1:B:82:SER:CB	10:B:7157:HOH:O	2.42	0.67
1:A:181:ASN:OD1	10:A:7289:HOH:O	2.14	0.66
1:A:181:ASN:CG	10:A:7289:HOH:O	2.35	0.64
1:D:181:ASN:ND2	10:D:7226:HOH:O	2.35	0.59
2:A:1205:ACT:OXT	2:A:1206:ACT:OXT	2.21	0.58
7:B:1213:SIA:O1B	7:B:1213:SIA:H6	2.04	0.57
1:B:82:SER:HB3	10:B:7157:HOH:O	2.01	0.56
2:A:1208:ACT:O	2:A:1215:ACT:OXT	2.22	0.56
1:E:201:LEU:HD21	1:E:204:VAL:HB	1.88	0.56
8:D:1205:SIA:H6	8:D:1205:SIA:O1B	2.07	0.54
1:C:150:PHE:CE2	1:C:154[A]:ILE:HG13	2.43	0.54
1:B:31:GLN:HG2	1:B:124:PHE:CD2	2.44	0.53
9:D:4032:MAN:O5	9:D:6035:BMA:O2	2.28	0.50
1:D:168:ASN:ND2	1:D:178:LEU:HD21	2.27	0.49
1:B:120:ARG:NH1	2:B:1208:ACT:H3	2.21	0.48
1:D:31:GLN:HG2	1:D:124:PHE:CE1	2.48	0.48
1:D:1:HIS:C	1:D:1:HIS:HD1	2.16	0.48
1:C:91:PRO:HB3	1:C:203:TRP:CE3	2.50	0.47
1:E:91:PRO:HB3	1:E:203:TRP:CE3	2.50	0.47
2:E:1206:ACT:OXT	2:E:1214:ACT:O	2.32	0.46
1:A:96:VAL:HA	1:A:106[B]:GLU:O	2.15	0.46
1:A:78:HIS:HE2	2:A:1208:ACT:C	2.29	0.46
1:A:150:PHE:CE2	1:A:154:ILE:HG13	2.51	0.45
1:E:38:ARG:HD3	1:E:204:VAL:HG21	1.97	0.45
9:D:4032:MAN:O3	9:D:5032:NAG:C7	2.64	0.45
1:E:95[B]:CYS:HG	1:E:169:ILE:HD12	1.77	0.45
3:C:1207:GHE:H102	10:C:7207:HOH:O	2.16	0.44
1:A:91:PRO:HB3	1:A:203:TRP:CE3	2.53	0.44
1:B:91:PRO:HB3	1:B:203:TRP:CE3	2.52	0.43
1:B:108:TRP:CD1	1:B:169[B]:ILE:HD13	2.53	0.43
1:C:155:GLY:HA2	1:C:185:TRP:CZ2	2.54	0.43
1:D:150:PHE:CE2	1:D:154:ILE:HG13	2.53	0.43
1:D:155:GLY:HA2	1:D:185:TRP:CZ2	2.54	0.42
2:B:1208:ACT:OXT	10:B:7264:HOH:O	2.21	0.42
1:A:147:SER:HB3	10:A:7263:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TRP:CE2	1:A:169[B]:ILE:HD13	2.54	0.42
1:A:38:ARG:HD3	1:A:204:VAL:CG2	2.50	0.41
1:A:108:TRP:CD1	1:A:169[B]:ILE:HD13	2.55	0.41
1:D:1:HIS:ND1	1:D:1:HIS:C	2.74	0.41
1:C:74:TYR:HA	1:C:78:HIS:O	2.20	0.41
10:A:7103:HOH:O	1:E:82:SER:HB3	2.09	0.41
1:B:31:GLN:CG	1:B:124:PHE:CE2	2.97	0.41
1:D:31:GLN:HG2	1:D:124:PHE:CD1	2.55	0.41
1:D:1:HIS:ND1	1:D:1:HIS:O	2.52	0.41
1:C:67:ARG:NH1	1:C:70:GLU:OE2	2.53	0.41
1:D:16:VAL:O	1:D:16:VAL:HG22	2.21	0.40
1:A:28:LYS:HE2	1:A:28:LYS:HB2	1.83	0.40
1:C:52:TYR:HB3	1:C:61:LEU:O	2.21	0.40
1:B:167:GLU:H	1:B:167:GLU:CD	2.23	0.40
1:A:108:TRP:NE1	1:A:169[B]:ILE:HD13	2.37	0.40
5:E:1213:NAG:C6	10:E:7151:HOH:O	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:7052:HOH:O	10:D:7209:HOH:O[2_557]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	210/204 (103%)	203 (97%)	7 (3%)	0	100	100
1	B	206/204 (101%)	199 (97%)	7 (3%)	0	100	100
1	C	206/204 (101%)	201 (98%)	5 (2%)	0	100	100
1	D	208/204 (102%)	203 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	206/204 (101%)	202 (98%)	4 (2%)	0	100	100
All	All	1036/1020 (102%)	1008 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/181 (104%)	187 (99%)	2 (1%)	80	63
1	B	185/181 (102%)	183 (99%)	2 (1%)	80	63
1	C	185/181 (102%)	183 (99%)	2 (1%)	80	63
1	D	187/181 (103%)	184 (98%)	3 (2%)	70	47
1	E	185/181 (102%)	182 (98%)	3 (2%)	70	47
All	All	931/905 (103%)	919 (99%)	12 (1%)	76	56

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	52	TYR
1	B	52	TYR
1	B	164	LEU
1	C	52	TYR
1	C	178	LEU
1	D	1	HIS
1	D	52	TYR
1	D	164	LEU
1	E	1	HIS
1	E	28	LYS
1	E	52	TYR

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

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 ⓘ

13 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$
6	NAG	B	1205	1,6	14,14,15	0.52	0	15,19,21	0.94	0
6	NAG	B	1206	6	14,14,15	0.38	0	15,19,21	0.99	1 (6%)
8	GAL	D	1132	9,8	11,11,12	0.56	0	14,15,17	0.61	0
8	SIA	D	1205	8	16,20,21	1.86	3 (18%)	18,28,31	0.99	2 (11%)
9	MAN	D	4032	9	11,11,12	0.94	0	14,15,17	4.89	5 (35%)
9	NAG	D	5032	9	14,14,15	0.39	0	15,19,21	1.22	3 (20%)
9	NAG	D	6033	1,9	14,14,15	0.62	0	15,19,21	0.78	0
9	NAG	D	6034	9	14,14,15	0.51	0	15,19,21	0.77	0
9	BMA	D	6035	9	11,11,12	2.01	3 (27%)	14,15,17	1.40	1 (7%)
9	GAL	D	6036	9	11,11,12	0.65	0	14,15,17	2.30	6 (42%)
9	SIA	D	6037	9	16,20,21	1.63	3 (18%)	18,28,31	1.10	1 (5%)
9	MAN	D	6038	9	11,11,12	0.68	0	14,15,17	1.11	2 (14%)
9	NAG	D	6039	9,8	14,14,15	0.28	0	15,19,21	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1205	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1206	6	-	0/6/23/26	0/1/1/1
8	GAL	D	1132	9,8	1/1/4/5	0/2/19/22	0/1/1/1
8	SIA	D	1205	8	-	0/14/34/38	0/1/1/1
9	MAN	D	4032	9	-	0/2/19/22	1/1/1/1
9	NAG	D	5032	9	-	0/6/23/26	0/1/1/1
9	NAG	D	6033	1,9	-	0/6/23/26	0/1/1/1
9	NAG	D	6034	9	-	0/6/23/26	0/1/1/1
9	BMA	D	6035	9	-	0/2/19/22	0/1/1/1
9	GAL	D	6036	9	-	0/2/19/22	0/1/1/1
9	SIA	D	6037	9	-	0/14/34/38	0/1/1/1
9	MAN	D	6038	9	-	0/2/19/22	0/1/1/1
9	NAG	D	6039	9,8	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1205	SIA	O6-C6	-4.26	1.36	1.43
9	D	6037	SIA	O6-C6	-3.45	1.38	1.43
9	D	6035	BMA	O5-C1	-2.19	1.40	1.43
9	D	6037	SIA	O8-C8	-2.10	1.38	1.43
8	D	1205	SIA	O8-C8	-2.08	1.38	1.43
9	D	6037	SIA	C10-N5	2.40	1.43	1.34
8	D	1205	SIA	C10-N5	2.42	1.43	1.34
9	D	6035	BMA	O3-C3	3.41	1.51	1.43
9	D	6035	BMA	C2-C3	4.80	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	4032	MAN	C1-C2-C3	-10.28	97.39	109.54
9	D	6036	GAL	C3-C4-C5	-3.23	104.57	110.20
9	D	4032	MAN	O5-C1-C2	-2.72	106.44	110.86
9	D	6037	SIA	C8-C7-C6	-2.69	107.59	113.01
9	D	4032	MAN	C2-C3-C4	-2.62	106.60	111.04
9	D	6036	GAL	O2-C2-C3	-2.59	104.90	110.12
9	D	6038	MAN	C1-C2-C3	-2.22	106.91	109.54
9	D	6038	MAN	C2-C3-C4	-2.13	107.43	111.04
8	D	1205	SIA	C3-C4-C5	-2.04	109.20	111.47
9	D	5032	NAG	C4-C3-C2	-2.01	108.10	111.23
9	D	6036	GAL	O6-C6-C5	2.03	118.05	111.33
9	D	6036	GAL	O2-C2-C1	2.05	113.32	109.21
8	D	1205	SIA	O6-C2-C3	2.07	113.85	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	5032	NAG	O4-C4-C5	2.20	115.07	109.24
6	B	1206	NAG	O5-C5-C6	2.29	112.30	107.35
9	D	5032	NAG	C1-O5-C5	2.30	115.17	112.25
9	D	4032	MAN	O2-C2-C3	2.53	115.20	110.12
9	D	6036	GAL	C1-C2-C3	3.49	113.67	109.54
9	D	6035	BMA	O3-C3-C2	4.76	118.60	110.00
9	D	6036	GAL	O5-C5-C6	5.69	119.67	107.35
9	D	4032	MAN	O2-C2-C1	14.12	137.51	109.21

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	D	1132	GAL	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	4032	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	1205	SIA	1	0
9	D	4032	MAN	2	0
9	D	5032	NAG	1	0
9	D	6035	BMA	1	0

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 35 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	1205	4	1,3,3	0.96	0	0,3,3	0.00	-
2	ACT	A	1206	4	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
3	GHE	A	1207	4	19,25,25	1.96	7 (36%)	22,34,34	0.49	0
2	ACT	A	1208	4	1,3,3	2.05	1 (100%)	0,3,3	0.00	-
5	NAG	A	1214	1	14,14,15	0.51	0	15,19,21	1.05	1 (6%)
2	ACT	A	1215	4	1,3,3	0.08	0	0,3,3	0.00	-
3	GHE	B	1207	4	19,25,25	1.74	7 (36%)	22,34,34	0.93	1 (4%)
2	ACT	B	1208	4	1,3,3	1.26	0	0,3,3	0.00	-
7	SIA	B	1213	-	16,20,21	1.06	1 (6%)	16,29,31	0.80	1 (6%)
3	GHE	C	1207	4	19,25,25	1.90	7 (36%)	22,34,34	0.83	0
5	NAG	C	1209	1	14,14,15	0.72	0	15,19,21	1.48	2 (13%)
3	GHE	D	1207	4	19,25,25	1.73	6 (31%)	22,34,34	0.87	0
2	ACT	E	1206	4	1,3,3	0.26	0	0,3,3	0.00	-
3	GHE	E	1207	4	19,25,25	1.97	7 (36%)	22,34,34	0.57	0
5	NAG	E	1213	1	14,14,15	0.52	0	15,19,21	1.01	1 (6%)
2	ACT	E	1214	4	1,3,3	3.09	1 (100%)	0,3,3	0.00	-
2	ACT	E	1215	4	1,3,3	0.75	0	0,3,3	0.00	-

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	ACT	A	1205	4	-	0/0/0/0	0/0/0/0
2	ACT	A	1206	4	-	0/0/0/0	0/0/0/0
3	GHE	A	1207	4	-	0/15/43/43	0/2/2/2
2	ACT	A	1208	4	-	0/0/0/0	0/0/0/0
5	NAG	A	1214	1	-	0/6/23/26	0/1/1/1
2	ACT	A	1215	4	-	0/0/0/0	0/0/0/0
3	GHE	B	1207	4	-	0/15/43/43	0/2/2/2
2	ACT	B	1208	4	-	0/0/0/0	0/0/0/0
7	SIA	B	1213	-	-	0/13/37/38	0/1/1/1
3	GHE	C	1207	4	-	0/15/43/43	0/2/2/2
5	NAG	C	1209	1	-	0/6/23/26	0/1/1/1
3	GHE	D	1207	4	-	0/15/43/43	0/2/2/2
2	ACT	E	1206	4	-	0/0/0/0	0/0/0/0
3	GHE	E	1207	4	-	0/15/43/43	0/2/2/2
5	NAG	E	1213	1	-	0/6/23/26	0/1/1/1
2	ACT	E	1214	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	E	1215	4	-	0/0/0/0	0/0/0/0

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1207	GHE	C3-C2	-3.53	1.44	1.54
3	A	1207	GHE	C3-C2	-3.51	1.44	1.54
3	C	1207	GHE	C3-C2	-3.49	1.44	1.54
3	E	1207	GHE	C15-N2	-3.43	1.42	1.47
3	D	1207	GHE	C3-C2	-3.42	1.45	1.54
3	B	1207	GHE	C3-C2	-3.20	1.45	1.54
3	A	1207	GHE	C15-N2	-3.11	1.42	1.47
2	E	1214	ACT	CH3-C	-3.09	1.44	1.48
3	C	1207	GHE	C12-N2	-3.03	1.41	1.47
3	B	1207	GHE	C12-N2	-2.99	1.41	1.47
3	C	1207	GHE	C15-N2	-2.97	1.43	1.47
3	D	1207	GHE	C12-N2	-2.68	1.42	1.47
3	C	1207	GHE	C5-N1	-2.62	1.42	1.47
3	D	1207	GHE	C5-N1	-2.57	1.42	1.47
3	A	1207	GHE	C2-N1	-2.57	1.43	1.47
3	A	1207	GHE	C12-N2	-2.56	1.42	1.47
3	E	1207	GHE	C12-N2	-2.50	1.42	1.47
3	B	1207	GHE	C5-N1	-2.26	1.43	1.47
3	E	1207	GHE	C5-N1	-2.20	1.43	1.47
3	E	1207	GHE	C2-N1	-2.17	1.44	1.47
3	D	1207	GHE	C15-N2	-2.16	1.44	1.47
3	C	1207	GHE	C2-N1	-2.12	1.44	1.47
3	A	1207	GHE	C5-N1	-2.10	1.43	1.47
3	B	1207	GHE	C15-N2	-2.09	1.44	1.47
2	A	1206	ACT	CH3-C	-2.02	1.46	1.48
2	A	1208	ACT	CH3-C	2.05	1.51	1.48
3	B	1207	GHE	O11-C11	2.18	1.28	1.23
3	B	1207	GHE	C11-N2	2.31	1.41	1.35
3	D	1207	GHE	C11-N2	2.43	1.41	1.35
3	C	1207	GHE	C11-N2	2.47	1.41	1.35
3	A	1207	GHE	C11-N2	2.97	1.42	1.35
3	D	1207	GHE	C6-N1	3.11	1.43	1.35
3	B	1207	GHE	C6-N1	3.23	1.43	1.35
3	E	1207	GHE	C11-N2	3.26	1.43	1.35
7	B	1213	SIA	O2-C2	3.37	1.43	1.40
3	C	1207	GHE	C6-N1	3.38	1.43	1.35
3	E	1207	GHE	C6-N1	3.79	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1207	GHE	C6-N1	3.94	1.45	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1213	NAG	C1-O5-C5	-2.58	108.97	112.25
7	B	1213	SIA	C7-C6-C5	-2.23	110.94	114.32
5	A	1214	NAG	C1-O5-C5	-2.18	109.48	112.25
5	C	1209	NAG	C4-C3-C2	2.03	114.38	111.23
3	B	1207	GHE	C2-N1-C6	2.12	126.70	121.35
5	C	1209	NAG	C3-C4-C5	3.79	116.81	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1205	ACT	1	0
2	A	1206	ACT	2	0
2	A	1208	ACT	2	0
2	A	1215	ACT	1	0
2	B	1208	ACT	3	0
7	B	1213	SIA	1	0
3	C	1207	GHE	1	0
2	E	1206	ACT	1	0
5	E	1213	NAG	1	0
2	E	1214	ACT	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	A	204/204 (100%)	-0.42	1 (0%) 91 91	10, 14, 24, 39	0
1	B	204/204 (100%)	-0.35	3 (1%) 76 75	10, 15, 30, 42	0
1	C	204/204 (100%)	-0.40	2 (0%) 84 84	10, 14, 26, 38	0
1	D	204/204 (100%)	-0.26	10 (4%) 33 30	10, 15, 34, 44	0
1	E	204/204 (100%)	-0.26	8 (3%) 43 40	10, 15, 32, 41	0
All	All	1020/1020 (100%)	-0.34	24 (2%) 62 60	10, 15, 31, 44	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	VAL	7.2
1	B	204	VAL	6.2
1	D	170	LEU	5.6
1	A	204	VAL	5.2
1	C	204	VAL	4.9
1	D	173	TYR	4.5
1	E	178	LEU	4.3
1	E	204	VAL	3.9
1	D	178	LEU	3.7
1	E	26	LEU	3.7
1	D	1	HIS	3.5
1	E	25	PRO	3.2
1	D	179	PRO	3.2
1	B	25	PRO	3.1
1	E	1	HIS	3.0
1	E	167	GLU	2.9
1	D	172	ALA	2.8
1	D	176	THR	2.7
1	E	173	TYR	2.4
1	D	177	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	178	LEU	2.1
1	E	27	GLU	2.1
1	D	175	GLY	2.1
1	C	26	LEU	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(Å ²)	Q<0.9
8	SIA	D	1205	20/21	0.78	0.18	5.06	16,24,31,33	20
9	SIA	D	6037	20/21	0.92	0.10	3.26	14,20,28,32	20
9	NAG	D	6033	14/15	0.81	0.11	0.71	21,27,30,30	14
9	GAL	D	6036	11/12	0.78	0.19	-	24,31,36,37	11
9	MAN	D	6038	11/12	0.77	0.28	-	35,38,43,49	11
9	NAG	D	6034	14/15	0.81	0.14	-	26,34,39,42	14
6	NAG	B	1205	14/15	0.84	0.16	-	23,31,38,42	0
8	GAL	D	1132	11/12	0.65	0.28	-	25,35,40,40	11
9	BMA	D	6035	11/12	0.70	0.19	-	34,39,42,44	11
9	MAN	D	4032	11/12	0.41	0.41	-	41,46,48,48	11
9	NAG	D	5032	14/15	0.67	0.24	-	25,31,38,44	13
6	NAG	B	1206	14/15	0.69	0.28	-	36,44,52,58	0
9	NAG	D	6039	14/15	0.02	0.78	-	25,28,33,36	14

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
7	SIA	B	1213	20/21	0.76	0.18	11.72	15,21,30,31	20
5	NAG	C	1209	14/15	0.77	0.20	5.62	26,34,42,47	14
3	GHE	D	1207	24/24	0.94	0.12	3.67	11,14,21,22	24
3	GHE	B	1207	24/24	0.94	0.12	3.43	11,14,21,22	24
3	GHE	E	1207	24/24	0.96	0.11	3.34	9,14,20,21	24
3	GHE	C	1207	24/24	0.94	0.11	3.19	10,13,23,24	24
3	GHE	A	1207	24/24	0.96	0.10	3.02	9,14,20,21	24
2	ACT	E	1215	4/4	0.86	0.11	2.25	14,16,22,24	4
2	ACT	A	1206	4/4	0.89	0.12	1.94	10,19,23,25	4
4	CD	A	1212	1/1	0.99	0.11	0.74	11,11,11,11	1
4	CD	E	1208	1/1	1.00	0.08	0.23	11,11,11,11	0
4	CD	B	1209	1/1	1.00	0.07	-0.62	12,12,12,12	0
4	CD	D	6041	1/1	1.00	0.07	-0.64	11,11,11,11	0
4	CD	E	1209	1/1	1.00	0.07	-0.68	12,12,12,12	0
4	CD	A	1210	1/1	1.00	0.07	-0.81	12,12,12,12	0
4	CD	D	6040	1/1	1.00	0.07	-1.15	12,12,12,12	0
4	CD	A	1209	1/1	1.00	0.07	-1.20	12,12,12,12	0
4	CD	C	1205	1/1	1.00	0.07	-1.25	13,13,13,13	0
4	CD	B	1210	1/1	1.00	0.07	-2.01	13,13,13,13	0
4	CD	C	1206	1/1	1.00	0.07	-2.03	13,13,13,13	0
2	ACT	B	1208	4/4	0.86	0.15	-	17,22,23,24	4
4	CD	E	1218	1/1	0.98	0.10	-	16,16,16,16	1
4	CD	E	1216	1/1	0.99	0.09	-	17,17,17,17	1
4	CD	E	1210	1/1	1.00	0.11	-	8,8,8,8	1
4	CD	A	1219	1/1	0.93	0.10	-	21,21,21,21	1
2	ACT	A	1205	4/4	0.81	0.15	-	16,17,19,26	4
2	ACT	A	1215	4/4	0.84	0.15	-	12,14,16,31	4
5	NAG	E	1213	14/15	0.67	0.22	-	31,38,49,51	14
4	CD	E	1211	1/1	0.99	0.11	-	11,11,11,11	1
4	CD	E	1219	1/1	0.99	0.04	-	19,19,19,19	1
4	CD	C	1212	1/1	0.99	0.06	-	23,23,23,23	1
4	CD	B	1212	1/1	1.00	0.12	-	11,11,11,11	1
4	CD	E	1212	1/1	0.98	0.12	-	16,16,16,16	1
4	CD	E	1217	1/1	0.99	0.12	-	13,13,13,13	1
4	CD	C	1208	1/1	0.99	0.11	-	13,13,13,13	1
4	CD	B	1214	1/1	0.98	0.10	-	16,16,16,16	1
2	ACT	E	1206	4/4	0.96	0.09	-	16,17,18,22	4
4	CD	A	1211	1/1	0.98	0.11	-	15,15,15,15	1
4	CD	B	1216	1/1	0.95	0.08	-	49,49,49,49	1
4	CD	D	6042	1/1	0.99	0.11	-	12,12,12,12	1
2	ACT	A	1208	4/4	0.86	0.19	-	15,19,21,29	4
4	CD	D	6044	1/1	0.99	0.07	-	15,15,15,15	1
4	CD	B	1211	1/1	0.98	0.12	-	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ACT	E	1214	4/4	0.88	0.15	-	8,18,22,33	0
4	CD	C	1211	1/1	0.99	0.08	-	16,16,16,16	1
4	CD	C	1210	1/1	0.98	0.12	-	15,15,15,15	1
4	CD	B	1215	1/1	0.99	0.07	-	22,22,22,22	1
4	CD	D	6043	1/1	0.98	0.11	-	16,16,16,16	1
5	NAG	A	1214	14/15	0.77	0.16	-	25,30,39,40	14
4	CD	A	1216	1/1	0.98	0.06	-	23,23,23,23	1
4	CD	A	1218	1/1	0.99	0.06	-	16,16,16,16	1
4	CD	A	1213	1/1	1.00	0.11	-	11,11,11,11	1

6.5 Other polymers [i](#)

There are no such residues in this entry.