Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:55 PM GMT

PDB ID	:	4DUR
Title	:	The X-ray Crystal Structure of Full-Length type II Human Plasminogen
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Deposited on	:	2012-02-22
Resolution	:	2.45 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:

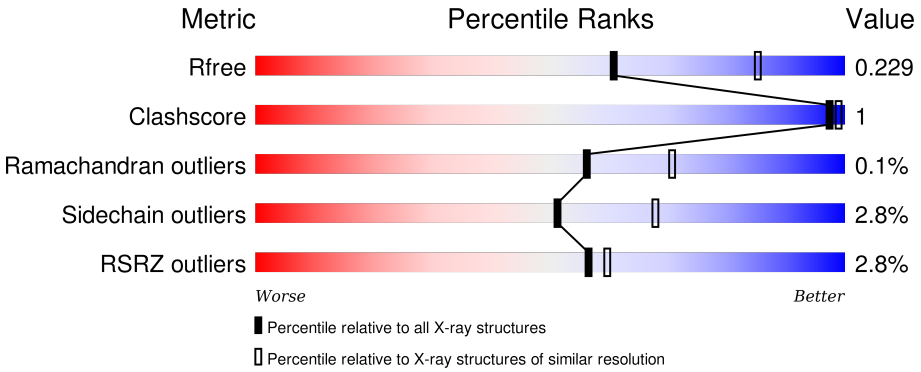
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

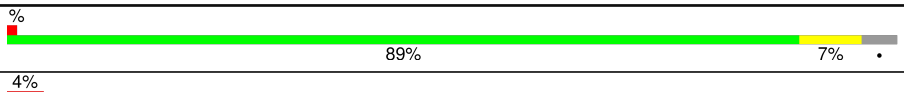
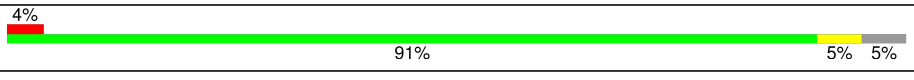
The reported resolution of this entry is 2.45 Å.

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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 <=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	791	
1	B	791	

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
5	ACT	A	807	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13246 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 Plasminogen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	4	0
			5894	3667	1042	1126	59			
1	B	754	Total	C	N	O	S	0	1	0
			5805	3623	1026	1099	57			

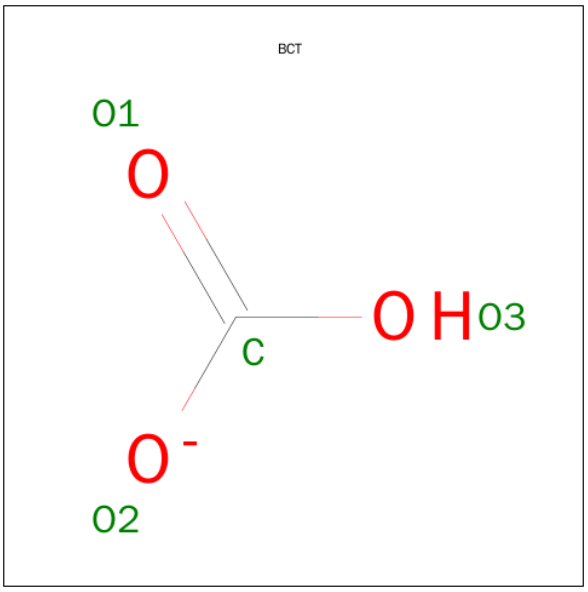
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cl	0	0
			3	3		
2	A	4	Total	Cl	0	0
			4	4		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

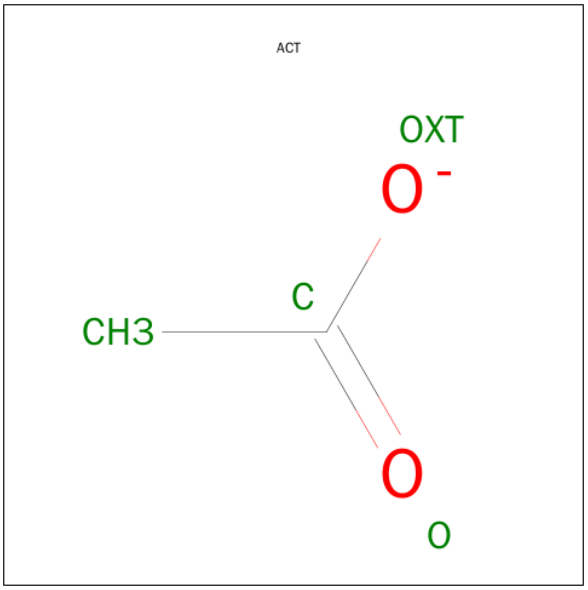
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			45	25	2	18		
6	B	3	Total	C	N	O	0	0
			45	25	2	18		

- Molecule 7 is water.

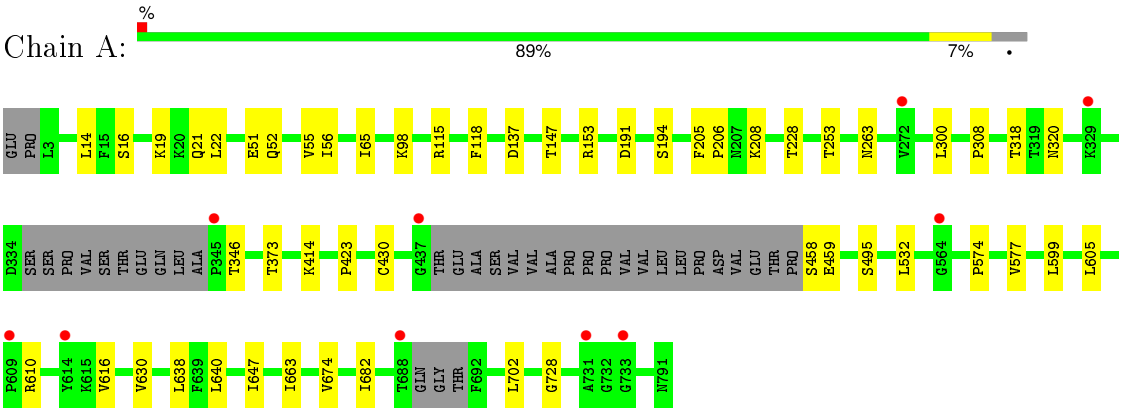
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	735	Total	O	0	0
			735	735		
7	B	701	Total	O	0	0
			701	701		

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.

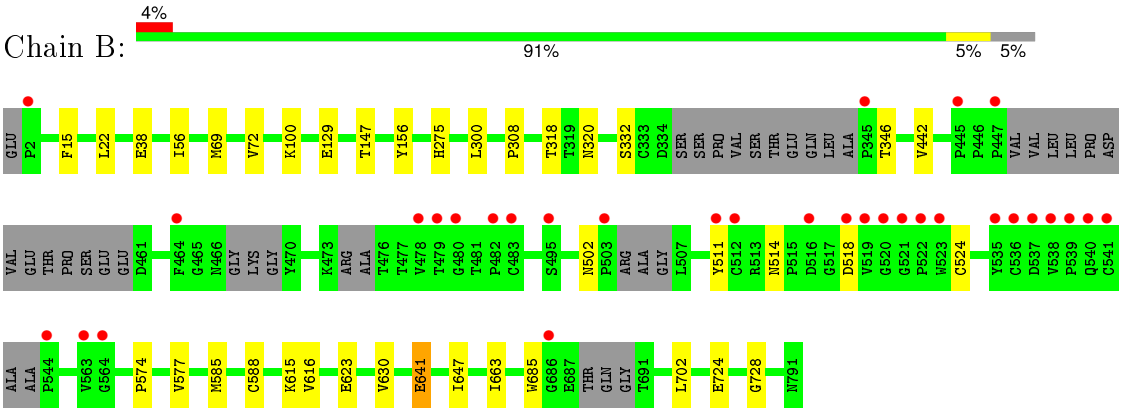
- Molecule 1: Plasminogen

Chain A:



- Molecule 1: Plasminogen

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.62Å 144.62Å 233.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	125.25 – 2.45 125.24 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (125.25-2.45) 99.8 (125.24-2.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.190 , 0.215 0.200 , 0.229	Depositor DCC
R_{free} test set	5236 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.8	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 104035 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13246	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, CL, K, SIA, GAL, ACT, BCT

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	0.35	0/6069	0.58	0/8253
1	B	0.35	0/5975	0.58	0/8133
All	All	0.35	0/12044	0.58	0/16386

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

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	5894	0	5504	16	0
1	B	5805	0	5367	12	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	1	0	0
4	B	4	0	1	0	0
5	A	4	0	3	0	0
6	A	45	0	38	0	0
6	B	45	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	735	0	0	0	0
7	B	701	0	0	0	0
All	All	13246	0	10952	27	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 1.

All (27) 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:318:THR:HG22	1:B:320:ASN:H	1.62	0.64
1:B:100:LYS:HE2	1:B:156:TYR:HB2	1.88	0.56
1:B:702:LEU:HD22	1:B:728:GLY:HA2	1.87	0.56
1:A:638[A]:LEU:HD12	1:B:442:VAL:HG22	1.88	0.55
1:A:52:GLN:HE22	1:A:495:SER:HB2	1.74	0.53
1:A:300:LEU:HD21	1:A:308:PRO:HG3	1.94	0.50
1:A:373:THR:HA	1:A:430:CYS:HA	1.95	0.48
1:A:21:GLN:HG3	1:A:55:VAL:HG22	1.96	0.48
1:A:206:PRO:HB2	1:A:423:PRO:HD2	1.96	0.48
1:A:16:SER:HB3	1:A:19:LYS:HD3	1.95	0.47
1:A:51:GLU:HG3	1:A:532:LEU:HD13	1.97	0.47
1:A:318:THR:HG22	1:A:320:ASN:H	1.80	0.46
1:A:574:PRO:HB2	1:A:663:ILE:H	1.79	0.46
1:B:275:HIS:HB3	1:B:318:THR:HG23	1.98	0.46
1:A:702:LEU:HD22	1:A:728:GLY:HA2	1.98	0.45
1:A:115:ARG:O	1:A:153:ARG:NH2	2.49	0.45
1:B:69:MET:HB3	1:B:72:VAL:HG11	1.99	0.45
1:B:300:LEU:HD21	1:B:308:PRO:HG3	1.99	0.45
1:B:641:GLU:HG2	1:B:647:ILE:HG22	1.97	0.44
1:B:623:GLU:HB2	1:B:685:TRP:CD1	2.52	0.44
1:A:118:PHE:CZ	1:A:137:ASP:HB3	2.53	0.44
1:B:574:PRO:HB2	1:B:663:ILE:H	1.84	0.43
1:A:599:LEU:HD21	1:A:647:ILE:HD11	2.01	0.43
1:B:514:ASN:HD21	1:B:518:ASP:H	1.67	0.42
1:A:205:PHE:HB3	1:A:208:LYS:HG3	2.01	0.42
1:A:577:VAL:HG13	1:A:616:VAL:HG13	2.03	0.41
1:B:577:VAL:HG13	1:B:616:VAL:HG13	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	752/791 (95%)	727 (97%)	25 (3%)	0	100 100
1	B	739/791 (93%)	709 (96%)	28 (4%)	2 (0%)	46 57
All	All	1491/1582 (94%)	1436 (96%)	53 (4%)	2 (0%)	56 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	ASN
1	B	38	GLU

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	647/694 (93%)	625 (97%)	22 (3%)	44 61
1	B	628/694 (90%)	613 (98%)	15 (2%)	57 73
All	All	1275/1388 (92%)	1238 (97%)	37 (3%)	51 66

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	22	LEU
1	A	56	ILE
1	A	65	ILE

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Mol	Chain	Res	Type
1	A	98	LYS
1	A	147	THR
1	A	191[A]	ASP
1	A	191[B]	ASP
1	A	194	SER
1	A	228	THR
1	A	253	THR
1	A	263	ASN
1	A	346	THR
1	A	414	LYS
1	A	458	SER
1	A	459	GLU
1	A	605	LEU
1	A	610	ARG
1	A	630	VAL
1	A	640	LEU
1	A	674	VAL
1	A	682	ILE
1	B	15	PHE
1	B	22	LEU
1	B	56	ILE
1	B	129	GLU
1	B	147	THR
1	B	332	SER
1	B	346	THR
1	B	511	TYR
1	B	524	CYS
1	B	585	MET
1	B	588	CYS
1	B	615	LYS
1	B	630	VAL
1	B	641	GLU
1	B	724	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	53	GLN
1	A	263	ASN
1	B	52	GLN
1	B	514	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

6 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	A	808	1,6	14,14,15	1.95	4 (28%)	15,19,21	1.79	4 (26%)
6	GAL	A	809	6	11,11,12	1.92	3 (27%)	14,15,17	2.94	4 (28%)
6	SIA	A	810	6	16,20,21	2.11	6 (37%)	18,28,31	1.33	2 (11%)
6	NAG	B	806	1,6	14,14,15	1.88	4 (28%)	15,19,21	1.81	5 (33%)
6	GAL	B	807	6	11,11,12	2.03	4 (36%)	14,15,17	2.15	5 (35%)
6	SIA	B	808	6	16,20,21	2.12	6 (37%)	18,28,31	1.23	1 (5%)

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	A	808	1,6	-	0/6/23/26	0/1/1/1
6	GAL	A	809	6	-	0/2/19/22	0/1/1/1
6	SIA	A	810	6	-	0/14/34/38	0/1/1/1
6	NAG	B	806	1,6	-	0/6/23/26	0/1/1/1
6	GAL	B	807	6	-	0/2/19/22	0/1/1/1
6	SIA	B	808	6	-	0/14/34/38	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	808	SIA	C10-N5	2.04	1.42	1.34
6	A	809	GAL	C4-C3	2.06	1.57	1.52
6	B	807	GAL	C4-C5	2.11	1.57	1.53
6	A	808	NAG	C3-C2	2.17	1.57	1.52
6	A	810	SIA	C10-N5	2.17	1.42	1.34
6	B	806	NAG	C4-C3	2.18	1.58	1.52
6	B	808	SIA	C3-C4	2.28	1.56	1.52
6	B	806	NAG	C3-C2	2.32	1.57	1.52
6	A	810	SIA	C3-C4	2.33	1.56	1.52
6	B	807	GAL	C4-C3	2.35	1.58	1.52
6	A	808	NAG	C4-C3	2.35	1.58	1.52
6	A	808	NAG	C4-C5	2.45	1.58	1.53
6	B	806	NAG	C4-C5	2.54	1.58	1.53
6	B	808	SIA	C3-C2	2.54	1.56	1.52
6	A	810	SIA	C3-C2	2.94	1.57	1.52
6	A	809	GAL	C1-C2	2.97	1.59	1.52
6	B	808	SIA	C8-C7	2.97	1.59	1.53
6	B	807	GAL	C1-C2	2.98	1.59	1.52
6	A	810	SIA	C8-C7	3.02	1.59	1.53
6	A	810	SIA	C6-C5	3.14	1.58	1.53
6	B	808	SIA	C6-C5	3.49	1.58	1.53
6	A	809	GAL	C2-C3	4.18	1.58	1.52
6	B	807	GAL	C2-C3	4.51	1.58	1.52
6	A	810	SIA	C7-C6	4.68	1.58	1.52
6	B	806	NAG	C1-C2	4.94	1.59	1.52
6	B	808	SIA	C7-C6	4.95	1.59	1.52
6	A	808	NAG	C1-C2	5.45	1.60	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	809	GAL	C3-C4-C5	-5.43	100.73	110.20
6	A	809	GAL	C1-C2-C3	-5.24	103.34	109.54
6	B	807	GAL	C3-C4-C5	-4.06	103.12	110.20
6	B	806	NAG	C3-C4-C5	-3.54	104.03	110.20
6	B	807	GAL	C1-C2-C3	-3.24	105.71	109.54
6	A	808	NAG	C3-C4-C5	-3.04	104.91	110.20
6	A	810	SIA	O9-C9-C8	-2.96	104.65	111.10
6	B	808	SIA	O9-C9-C8	-2.77	105.07	111.10
6	B	806	NAG	O4-C4-C3	-2.11	105.59	110.34
6	B	807	GAL	O2-C2-C3	-2.11	105.88	110.12
6	B	806	NAG	O3-C3-C2	2.08	113.23	109.11
6	B	806	NAG	O3-C3-C4	2.54	116.06	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	810	SIA	O6-C2-C3	2.59	114.83	109.86
6	B	807	GAL	C1-O5-C5	2.62	115.57	112.25
6	A	808	NAG	O3-C3-C4	2.74	116.50	110.34
6	A	808	NAG	O3-C3-C2	2.76	114.58	109.11
6	A	808	NAG	C1-O5-C5	3.71	116.95	112.25
6	B	806	NAG	C1-O5-C5	3.97	117.29	112.25
6	A	809	GAL	C1-O5-C5	4.22	117.60	112.25
6	B	807	GAL	O3-C3-C2	4.56	118.24	110.00
6	A	809	GAL	O3-C3-C2	5.80	120.47	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	BCT	A	806	-	0,3,3	0.00	-	0,3,3	0.00	-
5	ACT	A	807	-	1,3,3	4.13	1 (100%)	0,3,3	0.00	-
4	BCT	B	805	-	0,3,3	0.00	-	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
4	BCT	A	806	-	-	0/0/0/0	0/0/0/0
5	ACT	A	807	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCT	B	805	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	807	ACT	CH3-C	4.13	1.54	1.48

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	756/791 (95%)	0.10	10 (1%)	79	81	14, 28, 57, 99	0
1	B	754/791 (95%)	0.20	32 (4%)	40	43	12, 27, 99, 123	0
All	All	1510/1582 (95%)	0.15	42 (2%)	56	60	12, 28, 75, 123	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	PRO	6.7
1	B	479	THR	5.1
1	B	512	CYS	4.7
1	B	539	PRO	4.7
1	B	540	GLN	4.3
1	B	536	CYS	4.0
1	B	478	VAL	3.9
1	B	519	VAL	3.9
1	B	541	CYS	3.9
1	B	520	GLY	3.6
1	B	563	VAL	3.6
1	A	437	GLY	3.5
1	B	447	PRO	3.5
1	B	518	ASP	3.5
1	B	2	PRO	3.2
1	A	688	THR	3.1
1	B	511	TYR	3.1
1	B	523	TRP	2.9
1	B	495	SER	2.9
1	B	464	PHE	2.9
1	B	503	PRO	2.9
1	A	272	VAL	2.8
1	A	733	GLY	2.8
1	B	537	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	482	PRO	2.8
1	A	731	ALA	2.7
1	B	445	PRO	2.7
1	B	483	CYS	2.7
1	B	522	PRO	2.6
1	B	564	GLY	2.5
1	B	686	GLY	2.3
1	A	345	PRO	2.2
1	B	521	GLY	2.2
1	B	345	PRO	2.2
1	B	538	VAL	2.2
1	A	329	LYS	2.2
1	B	516	ASP	2.2
1	A	564	GLY	2.1
1	A	614	TYR	2.1
1	B	535	TYR	2.1
1	B	480	GLY	2.1
1	B	544	PRO	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, 95^{th} 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
6	NAG	A	808	14/15	0.79	0.21	0.82	71,73,76,79	0
6	GAL	A	809	11/12	0.82	0.21	-	81,83,84,87	0
6	NAG	B	806	14/15	0.82	0.21	-	76,78,79,82	0
6	SIA	B	808	20/21	0.85	0.16	-	88,89,89,89	0
6	GAL	B	807	11/12	0.88	0.17	-	83,85,86,88	0
6	SIA	A	810	20/21	0.81	0.25	-	87,89,90,90	0

6.4 Ligands

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, 95^{th} 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
5	ACT	A	807	4/4	0.98	0.20	2.37	34,35,35,36	0
4	BCT	A	806	4/4	0.74	0.19	0.24	66,66,67,67	0
4	BCT	B	805	4/4	0.74	0.16	-0.75	79,80,80,80	0
3	K	A	805	1/1	0.99	0.08	-2.20	42,42,42,42	0
2	CL	A	801	1/1	0.99	0.11	-2.57	25,25,25,25	0
2	CL	A	804	1/1	0.99	0.09	-2.88	35,35,35,35	0
2	CL	B	801	1/1	0.98	0.10	-4.97	24,24,24,24	0
3	K	B	804	1/1	0.98	0.09	-6.47	36,36,36,36	0
2	CL	B	803	1/1	0.98	0.09	-	28,28,28,28	0
2	CL	A	803	1/1	0.99	0.12	-	26,26,26,26	0
2	CL	B	802	1/1	0.99	0.13	-	25,25,25,25	0
2	CL	A	802	1/1	0.98	0.10	-	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.