wwPDB X-ray Structure Validation Summary Report (i)

Sep 26, 2024 – 04:06 PM EDT

PDB ID	:	9AXQ
Title	:	Crystal Structure of HY11-7E1_Hu3 Fab in the Apo Conformation
Authors	:	Rodarte, J.V.; Pancera, M.; Hannon, B.
Deposited on	:	2024-03-06
Resolution	:	2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

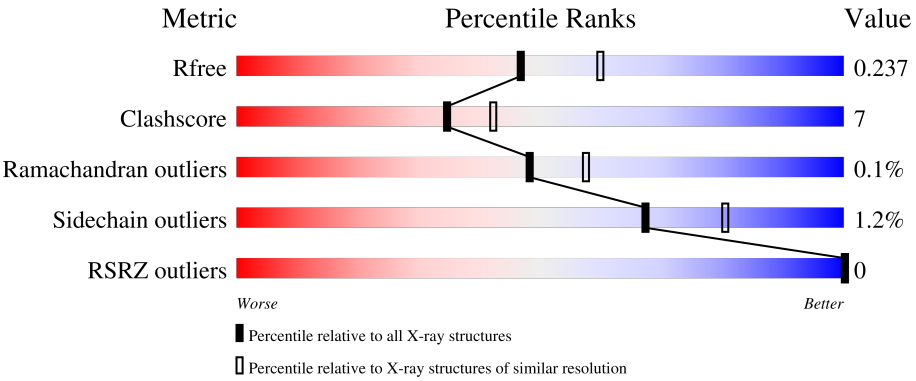
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 <=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	232	83% 9% 7%
1	C	232	78% 14% 8%
1	E	232	75% 16% 8%
1	H	232	79% 12% • 7%
2	B	214	82% 16% ••

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Mol	Chain	Length	Quality of chain
2	D	214	80% 19%
2	F	214	82% 16%
2	L	214	83% 16%

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	ACT	A	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13485 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.

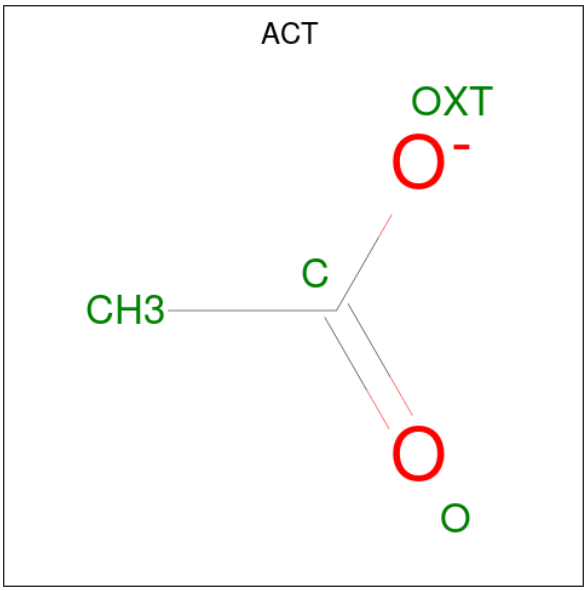
- Molecule 1 is a protein called HY11-7E1_Hu3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	215	Total	C	N	O	S	0	2	0
			1634	1039	266	322	7			
1	A	215	Total	C	N	O	S	0	1	0
			1643	1044	270	322	7			
1	C	214	Total	C	N	O	S	0	0	0
			1618	1027	268	316	7			
1	E	214	Total	C	N	O	S	0	0	0
			1629	1035	268	319	7			

- Molecule 2 is a protein called HY11-7E1_Hu3 Fab Light Chain.

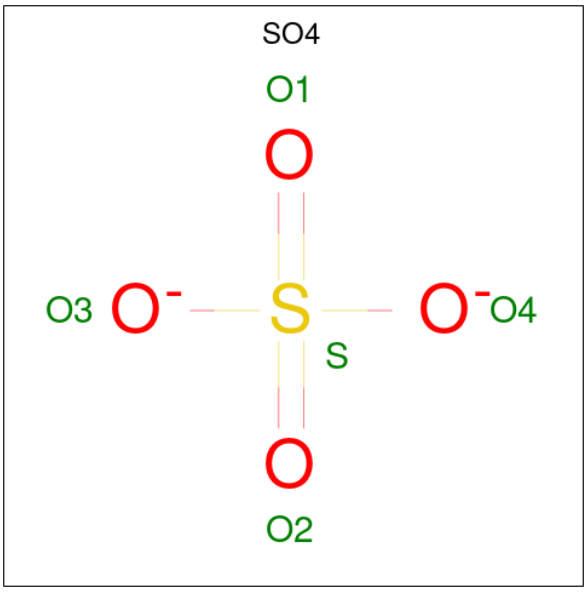
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1624	1017	272	330	5			
2	B	212	Total	C	N	O	S	0	0	0
			1624	1017	272	330	5			
2	D	212	Total	C	N	O	S	0	0	0
			1628	1020	273	330	5			
2	F	212	Total	C	N	O	S	0	0	0
			1628	1020	273	330	5			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

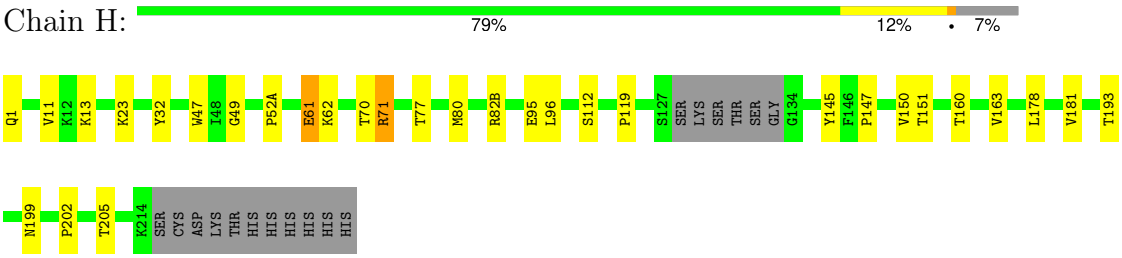
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	45	Total O 45 45	0	0
5	L	51	Total O 51 51	0	0
5	A	61	Total O 61 61	0	0
5	C	25	Total O 25 25	0	0
5	E	40	Total O 40 40	0	0
5	B	60	Total O 60 60	0	0
5	D	52	Total O 52 52	0	0
5	F	59	Total O 59 59	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

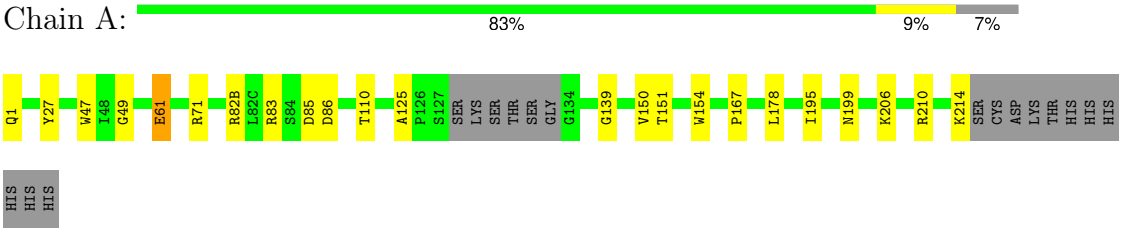
• Molecule 1: HY11-7E1_Hu3 Fab Heavy Chain

Chain H:



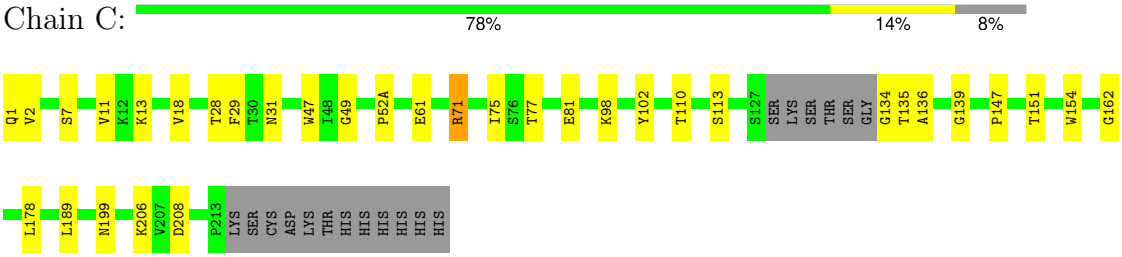
• Molecule 1: HY11-7E1_Hu3 Fab Heavy Chain

Chain A:



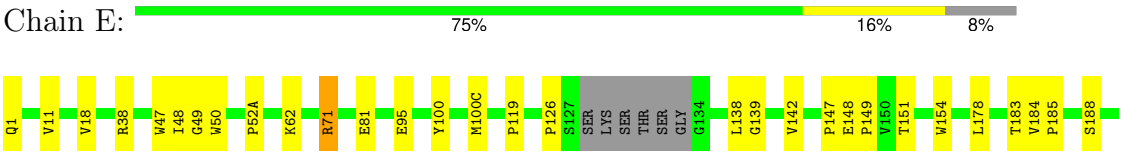
• Molecule 1: HY11-7E1_Hu3 Fab Heavy Chain

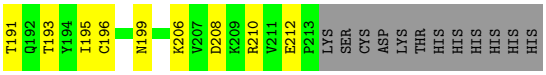
Chain C:



• Molecule 1: HY11-7E1_Hu3 Fab Heavy Chain

Chain E:



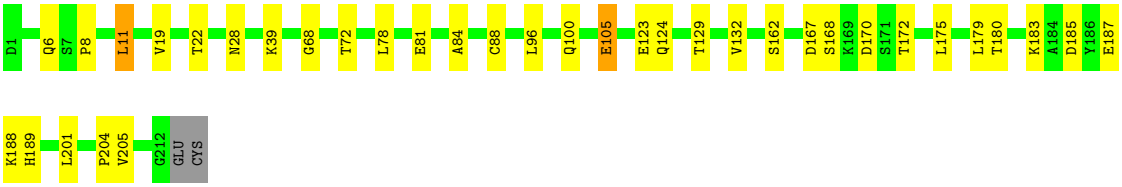


• Molecule 2: HY11-7E1_Hu3 Fab Light Chain

Chain L:

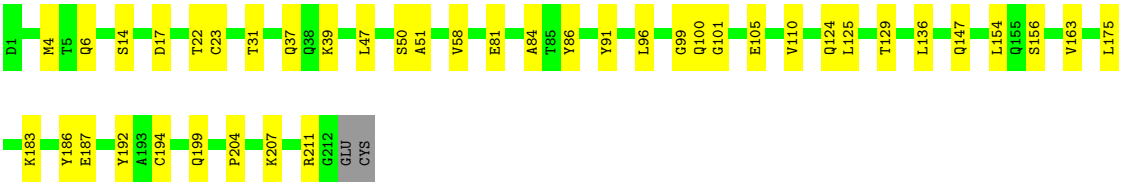
• Molecule 2: HY11-7E1_Hu3 Fab Light Chain

Chain B:



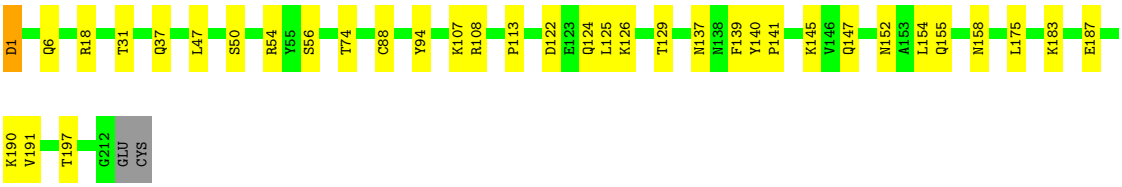
• Molecule 2: HY11-7E1_Hu3 Fab Light Chain

Chain D:



• Molecule 2: HY11-7E1_Hu3 Fab Light Chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.58Å 151.10Å 104.60Å 90.00° 91.14° 90.00°	Depositor
Resolution (Å)	42.83 – 2.20 42.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (42.83-2.20) 90.7 (42.83-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.238 0.208 , 0.237	Depositor DCC
R_{free} test set	5437 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.290 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13485	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.74 % 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 6.5878e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: ACT, PCA, SO4

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	0.29	0/1679	0.53	0/2289
1	C	0.26	0/1650	0.50	0/2251
1	E	0.28	0/1662	0.52	0/2267
1	H	0.26	0/1673	0.49	0/2284
2	B	0.28	0/1660	0.50	0/2255
2	D	0.28	0/1664	0.50	0/2259
2	F	0.28	0/1664	0.52	0/2259
2	L	0.28	0/1660	0.51	0/2255
All	All	0.28	0/13312	0.51	0/18119

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	1643	0	1610	17	0
1	C	1618	0	1582	26	0
1	E	1629	0	1593	28	0
1	H	1634	0	1588	19	0
2	B	1624	0	1569	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1628	0	1580	26	0
2	F	1628	0	1580	27	0
2	L	1624	0	1569	26	0
3	A	4	0	3	2	0
3	B	8	0	6	0	0
3	C	4	0	3	1	0
3	D	8	0	6	0	0
3	F	8	0	6	0	0
3	H	4	0	3	0	0
3	L	8	0	6	0	0
4	F	10	0	0	0	0
4	L	10	0	0	0	0
5	A	61	0	0	3	0
5	B	60	0	0	4	0
5	C	25	0	0	4	0
5	D	52	0	0	4	0
5	E	40	0	0	1	0
5	F	59	0	0	2	0
5	H	45	0	0	0	0
5	L	51	0	0	0	0
All	All	13485	0	12704	190	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 7.

The worst 5 of 190 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:L:123:GLU:OE1	2:L:123:GLU:N	2.09	0.85
1:E:50:TRP:HH2	2:D:110:VAL:HG21	1.47	0.80
1:A:110:THR:HG21	5:A:444:HOH:O	1.84	0.75
2:D:186:TYR:CE2	2:D:211:ARG:HD3	2.20	0.75
2:L:183:LYS:O	2:L:187:GLU:HG2	1.87	0.73

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	212/232 (91%)	207 (98%)	5 (2%)	0	100 100
1	C	210/232 (90%)	205 (98%)	5 (2%)	0	100 100
1	E	210/232 (90%)	205 (98%)	5 (2%)	0	100 100
1	H	213/232 (92%)	208 (98%)	5 (2%)	0	100 100
2	B	210/214 (98%)	206 (98%)	4 (2%)	0	100 100
2	D	210/214 (98%)	203 (97%)	7 (3%)	0	100 100
2	F	210/214 (98%)	202 (96%)	7 (3%)	1 (0%)	25 28
2	L	210/214 (98%)	203 (97%)	7 (3%)	0	100 100
All	All	1685/1784 (94%)	1639 (97%)	45 (3%)	1 (0%)	48 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	152	ASN

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	183/198 (92%)	180 (98%)	3 (2%)	58 73
1	C	179/198 (90%)	177 (99%)	2 (1%)	70 82
1	E	181/198 (91%)	180 (99%)	1 (1%)	84 91
1	H	181/198 (91%)	177 (98%)	4 (2%)	47 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	184/187 (98%)	182 (99%)	2 (1%)	70	82
2	D	185/187 (99%)	183 (99%)	2 (1%)	70	82
2	F	185/187 (99%)	184 (100%)	1 (0%)	86	93
2	L	184/187 (98%)	182 (99%)	2 (1%)	70	82
All	All	1462/1540 (95%)	1445 (99%)	17 (1%)	67	80

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	105	GLU
2	F	1	ASP
1	A	71	ARG
1	A	82(B)	ARG
1	C	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	199	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	PCA	C	1	1	7,8,9	1.96	1 (14%)	9,10,12	2.29	5 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	1.91	1 (14%)	9,10,12	2.14	5 (55%)
1	PCA	H	1	1	7,8,9	1.92	1 (14%)	9,10,12	2.15	5 (55%)
1	PCA	E	1	1	7,8,9	1.95	1 (14%)	9,10,12	2.23	5 (55%)

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	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CD-N	5.03	1.47	1.34
1	E	1	PCA	CD-N	5.02	1.47	1.34
1	H	1	PCA	CD-N	4.95	1.46	1.34
1	A	1	PCA	CD-N	4.95	1.46	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1	PCA	OE-CD-CG	-3.14	121.11	126.72
1	A	1	PCA	OE-CD-CG	-3.08	121.22	126.72
1	C	1	PCA	CB-CA-C	-3.08	108.44	112.66
1	E	1	PCA	OE-CD-CG	-3.01	121.35	126.72
1	H	1	PCA	OE-CD-CG	-2.91	121.53	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

15 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	$\#\|Z\| > 2$
4	SO4	F	301	-	4,4,4	0.22	0	6,6,6	0.11	0
3	ACT	L	303	-	3,3,3	1.13	0	3,3,3	0.76	0
3	ACT	D	301	-	3,3,3	1.02	0	3,3,3	0.83	0
3	ACT	C	301	-	3,3,3	1.34	0	3,3,3	1.51	0
4	SO4	L	302	-	4,4,4	0.48	0	6,6,6	0.58	0
3	ACT	A	301	-	3,3,3	1.02	0	3,3,3	0.94	0
3	ACT	D	302	-	3,3,3	1.09	0	3,3,3	0.82	0
3	ACT	F	304	-	3,3,3	1.29	1 (33%)	3,3,3	0.76	0
3	ACT	F	303	-	3,3,3	1.15	0	3,3,3	0.81	0
4	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.25	0
4	SO4	F	302	-	4,4,4	0.23	0	6,6,6	0.08	0
3	ACT	H	301	-	3,3,3	1.05	0	3,3,3	0.79	0
3	ACT	B	302	-	3,3,3	1.09	0	3,3,3	1.62	1 (33%)
3	ACT	L	304	-	3,3,3	1.03	0	3,3,3	0.84	0
3	ACT	B	301	-	3,3,3	1.04	0	3,3,3	0.82	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	304	ACT	OXT-C	-2.01	1.21	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	ACT	O-C-CH3	-2.01	114.27	122.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	ACT	1	0
3	A	301	ACT	2	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, 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	214/232 (92%)	-1.15	0	100	100	27, 52, 80, 94	1 (0%)
1	C	213/232 (91%)	-1.11	0	100	100	43, 56, 78, 97	0
1	E	213/232 (91%)	-1.10	0	100	100	41, 58, 92, 108	0
1	H	214/232 (92%)	-1.14	0	100	100	28, 56, 79, 97	2 (0%)
2	B	212/214 (99%)	-1.11	0	100	100	38, 50, 73, 81	0
2	D	212/214 (99%)	-1.14	0	100	100	38, 50, 71, 83	0
2	F	212/214 (99%)	-1.09	0	100	100	36, 51, 79, 90	0
2	L	212/214 (99%)	-1.10	0	100	100	37, 50, 77, 86	0
All	All	1702/1784 (95%)	-1.12	0	100	100	27, 53, 79, 108	3 (0%)

There are no RSRZ outliers to report.

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

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, 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	B-factors(Å^2)	Q<0.9
1	PCA	H	1	8/9	0.97	0.05	60,66,72,76	0
1	PCA	C	1	8/9	0.98	0.07	60,68,71,72	0
1	PCA	A	1	8/9	0.99	0.05	46,53,59,69	0
1	PCA	E	1	8/9	0.99	0.06	48,49,58,58	0

6.3 Carbohydrates

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, 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	B-factors(Å^2)	Q<0.9
3	ACT	D	301	4/4	0.91	0.06	80,82,83,87	0
3	ACT	L	304	4/4	0.95	0.10	62,65,76,76	0
3	ACT	B	301	4/4	0.96	0.07	87,89,92,96	0
3	ACT	B	302	4/4	0.96	0.12	64,67,73,74	0
3	ACT	L	303	4/4	0.96	0.10	60,68,68,79	0
3	ACT	C	301	4/4	0.97	0.07	60,63,69,69	0
3	ACT	D	302	4/4	0.97	0.06	71,77,80,85	0
4	SO4	F	302	5/5	0.97	0.03	97,101,107,111	0
3	ACT	H	301	4/4	0.98	0.07	58,61,66,74	0
3	ACT	F	304	4/4	0.98	0.06	55,64,65,71	0
3	ACT	A	301	4/4	0.98	0.05	46,54,55,59	0
4	SO4	L	301	5/5	0.99	0.03	39,43,49,50	0
4	SO4	L	302	5/5	0.99	0.17	30,30,30,30	0
4	SO4	F	301	5/5	0.99	0.02	38,41,51,52	0
3	ACT	F	303	4/4	0.99	0.06	50,59,59,60	0

6.5 Other polymers (i)

There are no such residues in this entry.