



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:08 AM GMT

PDB ID : 2F9N  
Title : Crystal Structure of the Recombinant Human Alpha I Trypsin Mutant K192Q/D216G in Complex with Leupeptin  
Authors : Rohr, K.B.; Selwood, T.; Marquardt, U.; Huber, R.; Schechter, N.M.; Bode, W.; Than, M.E.  
Deposited on : 2005-12-06  
Resolution : 1.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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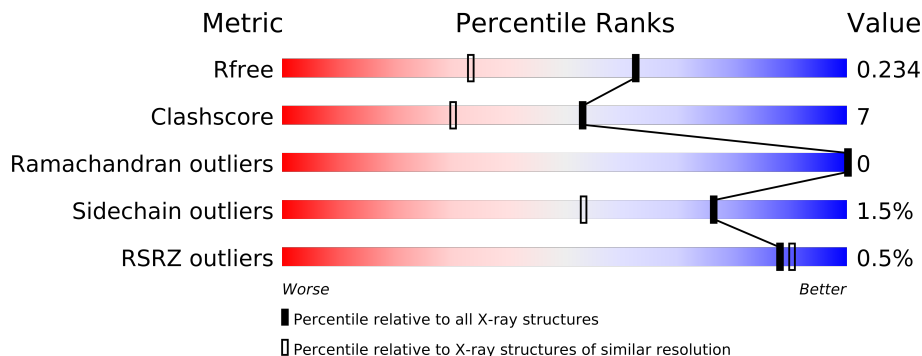
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
1	C	245	
1	D	245	
2	E	4	
2	F	4	
2	G	4	
2	H	4	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9588 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alpha I tryptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	30	13	0
			2033	1304	351	364	14			
1	B	243	Total	C	N	O	S	28	13	0
			2029	1300	354	361	14			
1	C	243	Total	C	N	O	S	30	12	0
			2027	1298	350	365	14			
1	D	243	Total	C	N	O	S	33	15	0
			2049	1311	359	365	14			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	VAL	LEU	ENGINEERED	UNP P15157
A	186	SER	THR	VARIANT	UNP P15157
A	187	GLN	ARG	VARIANT	UNP P15157
A	192	GLN	LYS	ENGINEERED	UNP P15157
A	216	GLY	ASP	ENGINEERED	UNP P15157
B	59	VAL	LEU	ENGINEERED	UNP P15157
B	186	SER	THR	VARIANT	UNP P15157
B	187	GLN	ARG	VARIANT	UNP P15157
B	192	GLN	LYS	ENGINEERED	UNP P15157
B	216	GLY	ASP	ENGINEERED	UNP P15157
C	59	VAL	LEU	ENGINEERED	UNP P15157
C	186	SER	THR	VARIANT	UNP P15157
C	187	GLN	ARG	VARIANT	UNP P15157
C	192	GLN	LYS	ENGINEERED	UNP P15157
C	216	GLY	ASP	ENGINEERED	UNP P15157
D	59	VAL	LEU	ENGINEERED	UNP P15157
D	186	SER	THR	VARIANT	UNP P15157
D	187	GLN	ARG	VARIANT	UNP P15157
D	192	GLN	LYS	ENGINEERED	UNP P15157
D	216	GLY	ASP	ENGINEERED	UNP P15157

- Molecule 2 is a protein called Leupeptin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			30	20	6	4			
2	F	4	Total	C	N	O	1	0	0
			30	20	6	4			
2	G	4	Total	C	N	O	0	0	0
			30	20	6	4			
2	H	4	Total	C	N	O	0	0	0
			30	20	6	4			

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total	C	N	O	4	0
			48	28	2	18		
3	D	4	Total	C	N	O	1	0
			48	28	2	18		

There are 10 discrepancies between the modelled and reference sequences:

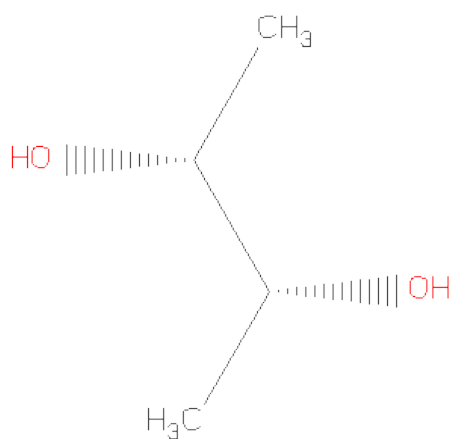
Chain	Residue	Modelled	Actual	Comment	Reference
B	59	VAL	LEU	ENGINEERED	UNP P15157
B	186	SER	THR	VARIANT	UNP P15157
B	187	GLN	ARG	VARIANT	UNP P15157
B	192	GLN	LYS	ENGINEERED	UNP P15157
B	216	GLY	ASP	ENGINEERED	UNP P15157
D	59	VAL	LEU	ENGINEERED	UNP P15157
D	186	SER	THR	VARIANT	UNP P15157
D	187	GLN	ARG	VARIANT	UNP P15157
D	192	GLN	LYS	ENGINEERED	UNP P15157
D	216	GLY	ASP	ENGINEERED	UNP P15157

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	6	0
			14	8	1	5		

- Molecule 5 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	4	2		
5	D	1	Total	C	O	0	0
			6	4	2		

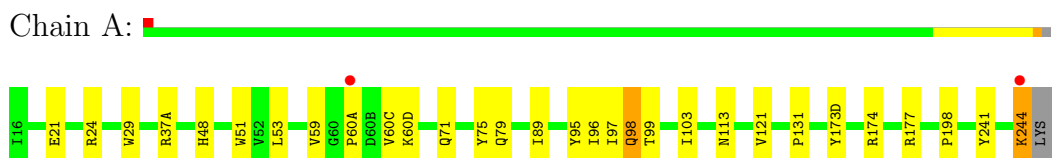
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	293	Total	O	0	1
			294	294		
6	B	294	Total	O	0	1
			295	295		
6	C	294	Total	O	0	1
			295	295		
6	D	272	Total	O	0	1
			273	273		
6	E	7	Total	O	0	0
			7	7		
6	F	6	Total	O	0	0
			6	6		
6	G	6	Total	O	0	0
			6	6		
6	H	6	Total	O	0	0
			6	6		

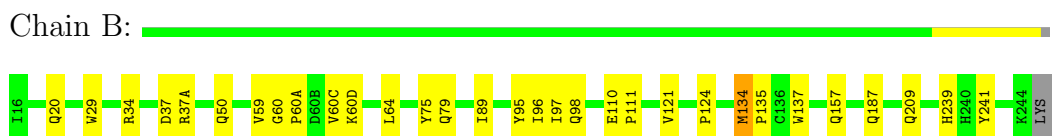
### 3 Residue-property plots

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.

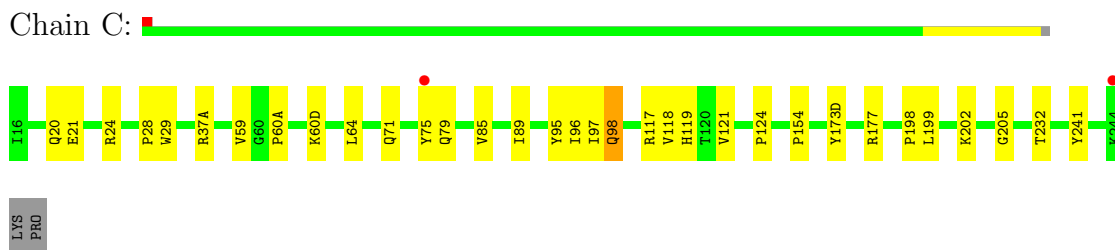
- Molecule 1: alpha I tryptase



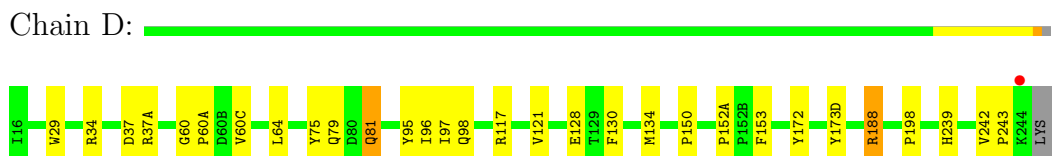
- Molecule 1: alpha I tryptase



- Molecule 1: alpha I tryptase



- Molecule 1: alpha I tryptase



- Molecule 2: Leupeptin



- Molecule 2: Leupeptin





- Molecule 2: Leupeptin

Chain G:



- Molecule 2: Leupeptin

Chain H:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.31Å 88.57Å 163.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.60 19.92 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.90-1.60) 99.0 (19.92-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.236 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	7659 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	6 of 156604 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 50.37 % 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 6.5342e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BU3, NAG, ACE, AR7

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	0.55	0/2103	0.75	0/2880
1	B	0.57	0/2100	0.75	0/2876
1	C	0.56	0/2095	0.75	1/2869 (0.0%)
1	D	0.55	0/2120	0.76	1/2902 (0.0%)
2	E	0.45	0/16	1.01	0/21
2	F	0.43	0/16	0.72	0/21
2	G	0.49	0/16	0.98	0/21
2	H	0.36	0/16	0.87	0/21
All	All	0.56	0/8482	0.75	2/11611 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	GLN	N-CA-C	-5.13	97.14	111.00
1	C	199	LEU	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2033	0	1954	30	0
1	B	2029	0	1942	33	0
1	C	2027	0	1945	35	0
1	D	2049	0	1960	33	0
2	E	30	0	38	6	0
2	F	30	0	38	4	0
2	G	30	0	38	5	0
2	H	30	0	38	2	0
3	B	48	0	43	0	0
3	D	48	0	43	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
5	A	6	0	10	0	0
5	B	6	0	10	0	0
5	C	6	0	10	0	0
5	D	6	0	10	0	0
6	A	294	0	0	5	0
6	B	295	0	0	4	0
6	C	295	0	0	6	0
6	D	273	0	0	3	0
6	E	7	0	0	0	0
6	F	6	0	0	0	0
6	G	6	0	0	0	0
6	H	6	0	0	0	0
All	All	9588	0	8105	114	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (114) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60(A)[B]:PRO:HG3	1:C:96:ILE:HG23	1.16	1.15
1:A:60(A)[B]:PRO:HG3	1:A:96:ILE:HG23	1.16	1.10
1:B:97:ILE:HD11	2:G:302:LEU:HB3	1.43	1.00
1:C:60(A)[B]:PRO:CG	1:C:96:ILE:HG23	1.93	0.97
1:A:60(A)[B]:PRO:CG	1:A:96:ILE:HG23	2.02	0.88
1:C:97:ILE:HD11	2:F:302:LEU:HB3	1.56	0.86
1:B:97:ILE:CD1	2:G:302:LEU:HB3	2.09	0.82
1:D:130:PHE:HA	1:D:134:MET:HE2	1.64	0.80
1:B:239:HIS:HD2	6:B:2539:HOH:O	1.66	0.79
1:A:21[A]:GLU:HG3	6:A:2500:HOH:O	1.82	0.78
1:C:75[A]:TYR:CD2	1:C:79[A]:GLN:HG2	2.20	0.76
1:A:173(D)[B]:TYR:HE2	1:D:60[B]:GLY:HA2	1.52	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:97:ILE:CD1	2:F:302:LEU:HB3	2.16	0.75
1:D:97:ILE:HD11	2:E:302:LEU:HB3	1.69	0.74
1:B:20:GLN:HE21	1:B:157:GLN:HE21	1.36	0.73
1:C:95:TYR:O	1:C:98:GLN:HG3	1.91	0.70
1:C:177:ARG:NE	6:C:2524:HOH:O	2.26	0.68
1:B:60[B]:GLY:CA	1:C:173(D)[B]:TYR:HE2	2.06	0.68
1:A:75[A]:TYR:CD2	1:A:79[A]:GLN:HG2	2.28	0.67
1:A:173(D)[B]:TYR:CE2	1:D:60[B]:GLY:HA2	2.29	0.67
1:A:97:ILE:HD11	2:H:302:LEU:HB3	1.76	0.66
1:B:60[B]:GLY:HA2	1:C:173(D)[B]:TYR:HE2	1.60	0.65
1:B:97:ILE:HD11	2:G:302:LEU:CB	2.25	0.63
1:B:97:ILE:HG12	2:G:302:LEU:HD13	1.79	0.63
1:A:97:ILE:CD1	2:H:302:LEU:HB3	2.29	0.63
1:C:24:ARG:HG3	6:C:2343:HOH:O	2.00	0.61
1:D:97:ILE:CD1	2:E:302:LEU:HB3	2.30	0.61
1:B:239:HIS:CD2	6:B:2539:HOH:O	2.46	0.61
1:B:137[B]:TRP:HH2	6:B:2356:HOH:O	1.85	0.60
1:A:95:TYR:O	1:A:98:GLN:HG3	2.01	0.60
1:D:97:ILE:HD11	2:E:302:LEU:HD22	1.83	0.60
1:C:75[B]:TYR:O	1:C:79[B]:GLN:HB2	2.01	0.59
1:B:59[B]:VAL:O	1:B:60(D):LYS:HE2	2.02	0.58
1:B:60[B]:GLY:CA	1:C:173(D)[B]:TYR:CE2	2.87	0.57
1:C:59[B]:VAL:O	1:C:60(D):LYS:HE2	2.05	0.56
1:B:60(C)[A]:VAL:HA	1:C:173(D)[A]:TYR:CE2	2.41	0.56
1:A:173(D)[A]:TYR:CE2	1:D:60(C)[A]:VAL:HA	2.40	0.56
1:C:37(A):ARG:NH1	1:D:150:PRO:O	2.33	0.55
1:B:187:GLN:HG3	6:B:2543:HOH:O	2.06	0.55
1:D:29:TRP:CD2	1:D:121:VAL:HB	2.42	0.54
1:A:71:GLN:NE2	6:A:2500:HOH:O	2.42	0.53
1:D:95:TYR:O	1:D:98:GLN:HG3	2.08	0.52
1:A:24:ARG:CZ	1:A:71:GLN:HG2	2.39	0.52
1:C:177:ARG:NH2	6:C:2496:HOH:O	2.42	0.52
1:A:173(D)[B]:TYR:CE2	1:D:60[B]:GLY:CA	2.93	0.52
1:C:117:ARG:HG3	1:C:118:VAL:HG23	1.92	0.52
1:C:98:GLN:NE2	6:C:2377:HOH:O	2.42	0.51
1:B:60(A)[B]:PRO:HG3	1:B:96:ILE:HB	1.92	0.51
1:C:97:ILE:HD11	2:F:302:LEU:HD22	1.92	0.51
1:B:50:GLN:OE1	1:B:111:PRO:HG3	2.09	0.51
1:B:134:MET:HE2	1:B:135:PRO:HD2	1.92	0.51
1:C:29:TRP:CG	1:C:121:VAL:HB	2.46	0.50
1:C:71:GLN:NE2	6:C:2537:HOH:O	2.45	0.50
1:A:75[B]:TYR:O	1:A:79[B]:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:60[B]:GLY:HA3	1:C:173(D)[B]:TYR:CE2	2.46	0.49
1:C:64[A]:LEU:CD2	1:C:85:VAL:HG21	2.43	0.48
1:C:29:TRP:CD2	1:C:121:VAL:HB	2.47	0.48
1:C:202:LYS:HE2	1:C:205:GLY:HA2	1.94	0.48
1:D:60(A)[B]:PRO:HG3	1:D:96:ILE:HB	1.94	0.48
1:B:89:ILE:HD13	1:B:241:TYR:CD1	2.49	0.48
1:A:37(A):ARG:NH2	6:A:2467:HOH:O	2.47	0.48
1:D:239:HIS:HD2	6:D:2416:HOH:O	1.97	0.48
1:D:188[A]:ARG:HG2	1:D:188[A]:ARG:NH1	2.29	0.47
1:D:188[A]:ARG:HG2	1:D:188[A]:ARG:HH11	1.78	0.47
1:D:97:ILE:HD11	2:E:302:LEU:CD2	2.45	0.46
1:A:29:TRP:CG	1:A:121:VAL:HB	2.50	0.46
1:B:134:MET:CE	1:B:135:PRO:HD2	2.46	0.46
1:D:97:ILE:CD1	2:E:302:LEU:HD22	2.46	0.46
1:D:29:TRP:CG	1:D:121:VAL:HB	2.50	0.46
1:A:75[A]:TYR:HB2	1:B:75[A]:TYR:CD2	2.52	0.45
1:B:124:PRO:HD3	1:B:209:GLN:O	2.16	0.45
1:A:75[A]:TYR:HB2	1:B:75[A]:TYR:CE2	2.51	0.45
1:D:37:ASP:O	1:D:37(A):ARG:HB2	2.17	0.45
1:D:97:ILE:CG1	2:E:302:LEU:HD22	2.47	0.45
1:D:75[B]:TYR:O	1:D:79[B]:GLN:HB2	2.17	0.44
1:A:29:TRP:CD2	1:A:121:VAL:HB	2.52	0.44
1:A:53:LEU:HD11	1:A:103:ILE:HD11	1.99	0.44
1:D:75[B]:TYR:CD2	1:D:79[B]:GLN:HG3	2.52	0.44
1:B:110:GLU:HG3	1:B:111:PRO:HD2	2.00	0.44
1:C:21[A]:GLU:HG3	6:C:2537:HOH:O	2.17	0.44
1:B:29:TRP:CD2	1:B:121:VAL:HB	2.53	0.44
1:B:20:GLN:NE2	1:B:137[A]:TRP:HZ3	2.15	0.43
1:C:75[A]:TYR:CE2	1:C:79[A]:GLN:HG2	2.52	0.43
1:B:97:ILE:HD11	2:G:302:LEU:HD22	2.01	0.43
1:B:75[B]:TYR:CD2	1:B:79[B]:GLN:HG3	2.53	0.43
1:C:64[A]:LEU:HD23	1:C:85:VAL:HG21	2.00	0.43
1:C:89:ILE:HD13	1:C:241:TYR:CD1	2.53	0.43
1:A:99:THR:HG23	1:D:97:ILE:CG2	2.49	0.42
1:B:37:ASP:O	1:B:37(A):ARG:HB2	2.19	0.42
1:C:124:PRO:HG2	1:C:232:THR:HG22	2.02	0.42
1:A:60(C)[B]:VAL:HA	1:D:173(D):TYR:CE2	2.54	0.42
1:A:244:LYS:HG2	1:A:244:LYS:H	1.35	0.42
1:C:75[B]:TYR:O	1:C:79[B]:GLN:CB	2.67	0.42
1:B:34:ARG:O	1:B:64:LEU:HD12	2.20	0.42
1:A:48:HIS:HB3	1:A:51:TRP:HB2	2.01	0.42
1:D:242:VAL:HA	1:D:243:PRO:HD3	1.78	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21[B]:GLU:HG2	1:C:154:PRO:CG	2.49	0.41
1:A:96:ILE:HD11	1:D:172:TYR:CD2	2.55	0.41
1:A:89:ILE:HD13	1:A:241:TYR:CD1	2.54	0.41
1:D:128:GLU:HB2	6:D:2379:HOH:O	2.20	0.41
1:A:59[B]:VAL:O	1:A:60(D):LYS:NZ	2.51	0.41
1:C:75[A]:TYR:HB2	1:D:75[A]:TYR:CE2	2.56	0.41
1:D:96:ILE:HG12	1:D:97:ILE:HG13	2.03	0.41
1:B:96:ILE:HG12	1:B:97:ILE:HG13	2.03	0.41
1:A:21[A]:GLU:CG	6:A:2500:HOH:O	2.54	0.41
1:A:131:PRO:HB3	6:A:2492:HOH:O	2.21	0.41
1:C:97:ILE:HD11	2:F:302:LEU:CB	2.39	0.40
1:C:28:PRO:HG3	1:C:119:HIS:NE2	2.36	0.40
1:D:34:ARG:O	1:D:64:LEU:HD12	2.21	0.40
1:B:110:GLU:HG3	1:B:111:PRO:CD	2.50	0.40
1:D:152(A):PRO:HG3	1:D:153:PHE:CZ	2.55	0.40
1:A:60(C)[A]:VAL:HA	1:D:173(D):TYR:CE2	2.57	0.40
1:B:95:TYR:O	1:B:98:GLN:HG3	2.21	0.40
1:D:81:GLN:NE2	6:D:2403:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 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	254/245 (104%)	245 (96%)	9 (4%)	0	100	100
1	B	254/245 (104%)	245 (96%)	9 (4%)	0	100	100
1	C	253/245 (103%)	247 (98%)	6 (2%)	0	100	100
1	D	256/245 (104%)	246 (96%)	10 (4%)	0	100	100
2	E	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
2	F	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
2	G	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
2	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1025/996 (103%)	987 (96%)	38 (4%)	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	223/213 (105%)	217 (97%)	6 (3%)	57	26
1	B	221/213 (104%)	220 (100%)	1 (0%)	94	87
1	C	222/213 (104%)	219 (99%)	3 (1%)	78	57
1	D	223/213 (105%)	219 (98%)	4 (2%)	71	44
2	E	2/2 (100%)	2 (100%)	0	100	100
2	F	2/2 (100%)	2 (100%)	0	100	100
2	G	2/2 (100%)	2 (100%)	0	100	100
2	H	2/2 (100%)	2 (100%)	0	100	100
All	All	897/860 (104%)	883 (98%)	14 (2%)	76	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	113	ASN
1	A	174	ARG
1	A	177	ARG
1	A	198	PRO
1	A	244	LYS
1	B	134	MET
1	C	20	GLN
1	C	98	GLN
1	C	198	PRO
1	D	117	ARG
1	D	188[A]	ARG
1	D	188[B]	ARG

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Mol	Chain	Res	Type
1	D	198	PRO

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

Mol	Chain	Res	Type
1	A	93	GLN
1	A	98	GLN
1	A	223	ASN
1	B	20	GLN
1	C	98	GLN
1	C	209	GLN
1	D	30	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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
2	AR7	E	304	2	10,10,11	4.98	2 (20%)	8,11,13	0.33	0
2	AR7	F	304	2	10,10,11	5.37	2 (20%)	8,11,13	0.34	0
2	AR7	G	304	2	10,10,11	5.37	2 (20%)	8,11,13	0.59	0
2	AR7	H	304	2	10,10,11	5.56	2 (20%)	8,11,13	0.37	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	AR7	E	304	2	-	0/7/9/11	0/0/0/0
2	AR7	F	304	2	-	0/7/9/11	0/0/0/0
2	AR7	G	304	2	-	0/7/9/11	0/0/0/0
2	AR7	H	304	2	-	0/7/9/11	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	304	AR7	O-C	17.03	1.44	1.25
2	F	304	AR7	O-C	16.73	1.43	1.25
2	G	304	AR7	O-C	16.56	1.43	1.25
2	E	304	AR7	O-C	15.54	1.42	1.25
2	H	304	AR7	C-CA	4.26	1.56	1.53
2	G	304	AR7	C-CA	3.62	1.56	1.53
2	F	304	AR7	C-CA	2.75	1.55	1.53
2	E	304	AR7	C-CA	2.44	1.55	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

8 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	$\# Z  > 2$
3	NAG	B	1000	1,3	12,14,15	0.67	0	15,19,21	0.60	0
3	NAG	B	1001	3	12,14,15	0.47	0	15,19,21	0.62	0
3	FUC	B	1002	3	9,10,11	0.72	0	10,14,16	0.56	0
3	FUC	B	1003	3	9,10,11	0.57	0	10,14,16	0.37	0
3	NAG	D	1000	1,3	12,14,15	0.47	0	15,19,21	0.78	0
3	NAG	D	1001	3	12,14,15	0.55	0	15,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FUC	D	1002	3	9,10,11	0.57	0	10,14,16	0.60	0
3	FUC	D	1003	3	9,10,11	0.54	0	10,14,16	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1000	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	3	-	0/6/23/26	0/1/1/1
3	FUC	B	1002	3	-	0/0/17/20	0/1/1/1
3	FUC	B	1003	3	-	0/0/17/20	0/1/1/1
3	NAG	D	1000	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1001	3	-	0/6/23/26	0/1/1/1
3	FUC	D	1002	3	-	0/0/17/20	0/1/1/1
3	FUC	D	1003	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

6 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
5	BU3	A	2250	-	5,5,5	0.44	0	6,6,6	0.33	0
4	NAG	B	1004	1	12,14,15	0.75	0	15,19,21	0.90	0
5	BU3	B	2251	-	5,5,5	0.47	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BU3	C	2252	-	5,5,5	0.44	0	6,6,6	0.33	0
4	NAG	D	1004	1	12,14,15	0.51	0	15,19,21	0.65	0
5	BU3	D	2253	-	5,5,5	0.48	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BU3	A	2250	-	-	0/4/4/4	0/0/0/0
4	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
5	BU3	B	2251	-	-	0/4/4/4	0/0/0/0
5	BU3	C	2252	-	-	0/4/4/4	0/0/0/0
4	NAG	D	1004	1	-	0/6/23/26	0/1/1/1
5	BU3	D	2253	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	243/245 (99%)	-0.40	2 (0%) 83 86	12, 19, 36, 51	8 (3%)
1	B	243/245 (99%)	-0.49	0 100 100	12, 18, 32, 40	8 (3%)
1	C	243/245 (99%)	-0.40	2 (0%) 83 86	12, 19, 36, 56	7 (2%)
1	D	243/245 (99%)	-0.39	1 (0%) 90 91	12, 20, 34, 47	10 (4%)
2	E	4/4 (100%)	-0.51	0 100 100	15, 16, 30, 32	0
2	F	4/4 (100%)	-0.57	0 100 100	14, 15, 26, 37	1 (25%)
2	G	4/4 (100%)	-0.49	0 100 100	14, 15, 28, 31	0
2	H	4/4 (100%)	-0.35	0 100 100	15, 18, 29, 33	0
All	All	988/996 (99%)	-0.42	5 (0%) 88 90	12, 19, 36, 56	34 (3%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	LYS	2.7
1	A	244	LYS	2.5
1	D	244	LYS	2.4
1	A	60(A)[A]	PRO	2.0
1	C	75[A]	TYR	2.0

### 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. 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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AR7	E	304	11/12	0.08	-	11,13,16,19	0
2	AR7	H	304	11/12	0.08	-	12,13,16,18	0
2	AR7	F	304	11/12	0.06	-	10,13,15,18	0
2	AR7	G	304	11/12	0.07	-	12,12,16,16	0

### 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	1001	14/15	0.22	-	54,58,60,62	1
3	FUC	D	1002	10/11	0.13	-	31,42,46,52	0
3	NAG	D	1000	14/15	0.15	-	40,47,57,63	0
3	NAG	B	1000	14/15	0.14	-	38,45,57,62	0
3	FUC	B	1002	10/11	0.14	-	36,43,46,47	0
3	FUC	B	1003	10/11	0.23	-	63,64,64,64	4
3	FUC	D	1003	10/11	0.28	-	67,70,73,75	0
3	NAG	B	1001	14/15	0.26	-	55,60,65,66	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<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BU3	B	2251	6/6	0.06	-	23,24,25,26	0
5	BU3	A	2250	6/6	0.09	-	20,24,25,29	0
4	NAG	B	1004	14/15	0.26	-	53,59,64,64	0
4	NAG	D	1004	14/15	0.41	-	63,67,70,72	6
5	BU3	D	2253	6/6	0.07	-	21,25,28,30	0
5	BU3	C	2252	6/6	0.09	-	19,23,25,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.