



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 09:27 pm 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

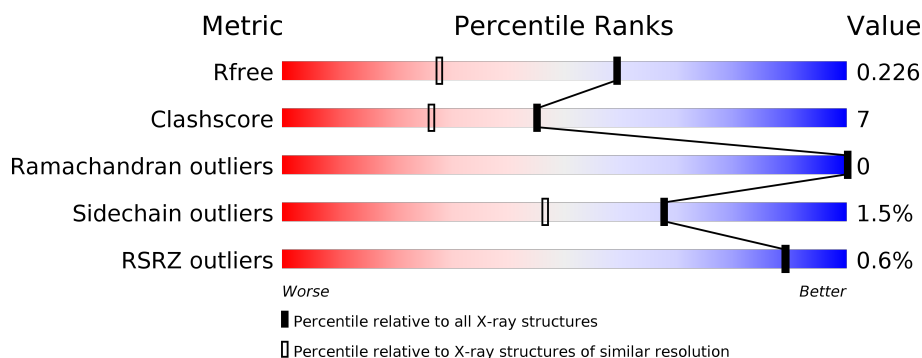
1 Overall quality at a glance

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}	111664	2957 (1.60-1.60)
Clashscore	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)
RSRZ outliers	108989	2883 (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	245	<div> <div></div> <div>87% 11% ..</div> </div>
1	B	245	<div> <div></div> <div>87% 12% .</div> </div>
1	C	245	<div> <div></div> <div>86% 13% .</div> </div>
1	D	245	<div> <div></div> <div>87% 11% ..</div> </div>
2	E	4	<div> <div></div> <div>75% 25%</div> </div>
2	F	4	<div> <div></div> <div>75% 25%</div> </div>

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Mol	Chain	Length	Quality of chain	
2	G	4		
2	H	4		

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
4	NAG	D	1004	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9588 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 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			

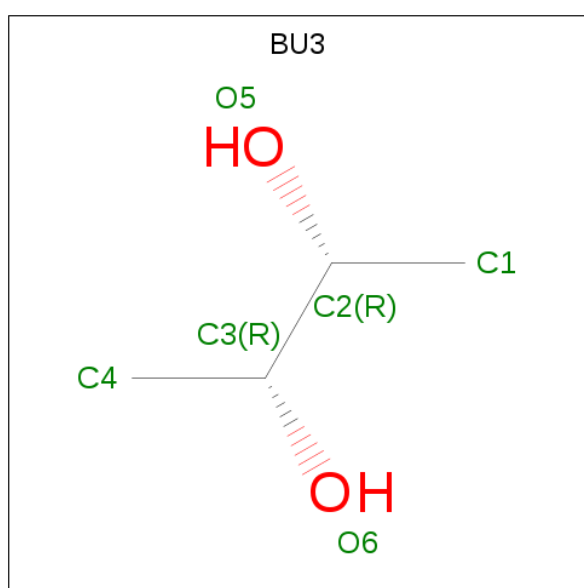
There are 20 discrepancies between the modelled and reference sequences:

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 (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C₄H₁₀O₂).



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

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	4	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

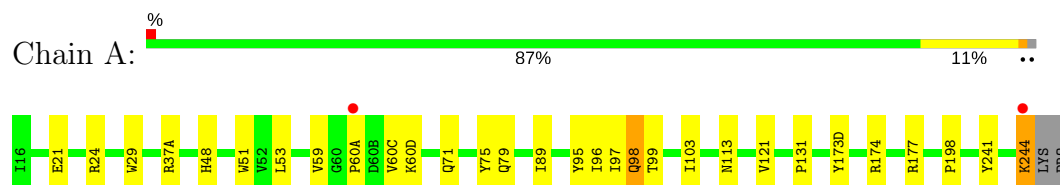
- Molecule 6 is water.

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		

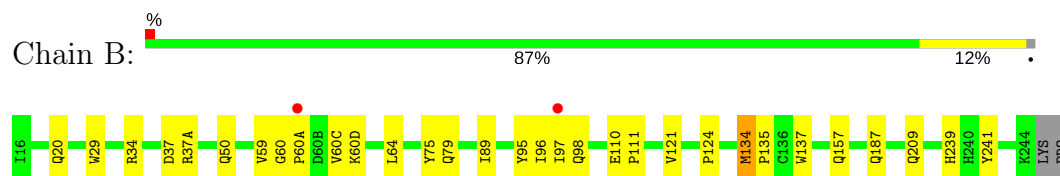
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

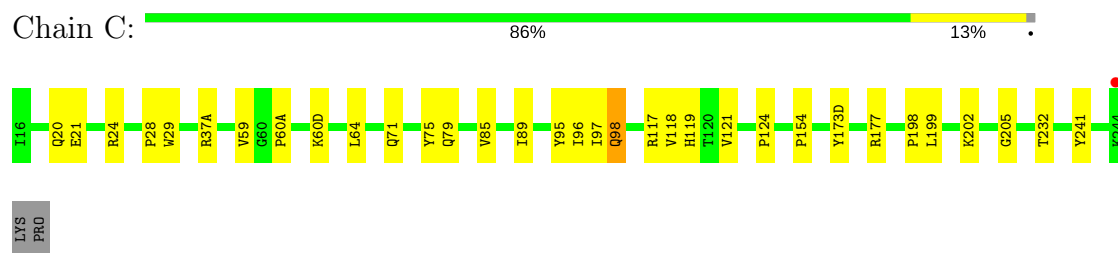
- Molecule 1: alpha I tryptase



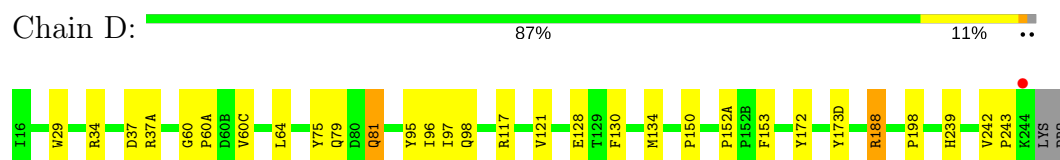
- Molecule 1: alpha I tryptase



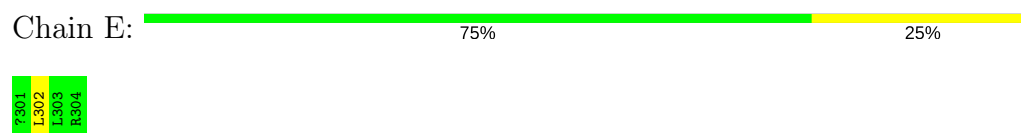
- Molecule 1: alpha I tryptase




- Molecule 1: alpha I tryptase



- Molecule 2: Leupeptin




- Molecule 2: Leupeptin

Chain F:  75% 25%


L301
L302
L303
R304

- Molecule 2: Leupeptin

Chain G:  75% 25%


L301
L302
L303
R304

- Molecule 2: Leupeptin

Chain H:  75% 25%


L301
L302
L303
R304

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.60Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.236 0.184 , 0.226	Depositor DCC
R_{free} test set	7659 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9588	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2033	0	1954	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	A	6	0	10	0	0
3	B	6	0	10	0	0
3	C	6	0	10	0	0
3	D	6	0	10	0	0
4	B	42	0	36	0	0
4	D	42	0	36	0	0
5	B	20	0	20	0	0
5	D	20	0	20	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

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.

All (114) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:95:TYR:O	1:A:98:GLN:HG3	2.01	0.60
1:B:137[B]:TRP:HH2	6:B:2356:HOH:O	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:37(A):ARG:NH2	6:A:2467:HOH:O	2.47	0.48
1:B:89:ILE:HD13	1:B:241:TYR:CD1	2.49	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:A:29:TRP:CG	1:A:121:VAL:HB	2.50	0.46
1:D:97:ILE:HD11	2:E:302:LEU:CD2	2.45	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:B:124:PRO:HD3	1:B:209:GLN:O	2.16	0.45
1:A:75[A]:TYR:HB2	1:B:75[A]:TYR:CD2	2.52	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:B:29:TRP:CD2	1:B:121:VAL:HB	2.53	0.44
1:C:21[A]:GLU:HG3	6:C:2537:HOH:O	2.17	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:A:244:LYS:HG2	1:A:244:LYS:H	1.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75[B]:TYR:O	1:C:79[B]:GLN:CB	2.67	0.42
1:A:48:HIS:HB3	1:A:51:TRP:HB2	2.01	0.42
1:B:34:ARG:O	1:B:64:LEU:HD12	2.20	0.42
1:D:242:VAL:HA	1:D:243:PRO:HD3	1.78	0.42
1:C:21[B]:GLU:HG2	1:C:154:PRO:CG	2.49	0.41
1:A:89:ILE:HD13	1:A:241:TYR:CD1	2.54	0.41
1:A:96:ILE:HD11	1:D:172:TYR:CD2	2.55	0.41
1:A:59[B]:VAL:O	1:A:60(D):LYS:NZ	2.51	0.41
1:D:128:GLU:HB2	6:D:2379:HOH:O	2.20	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:28:PRO:HG3	1:C:119:HIS:NE2	2.36	0.40
1:C:97:ILE:HD11	2:F:302:LEU:CB	2.39	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 [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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	48	21
1	B	221/213 (104%)	220 (100%)	1 (0%)	90	82
1	C	222/213 (104%)	219 (99%)	3 (1%)	69	50
1	D	223/213 (105%)	219 (98%)	4 (2%)	62	38
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%)	67	44

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

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Mol	Chain	Res	Type
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
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 molecules 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	0.64	0	8,11,13	0.39	0
2	AR7	F	304	2	10,10,11	0.67	0	8,11,13	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AR7	G	304	2	10,10,11	0.78	1 (10%)	8,11,13	0.65	0
2	AR7	H	304	2	10,10,11	0.89	1 (10%)	8,11,13	0.42	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	-	0/9/9/11	0/0/0/0
2	AR7	F	304	2	-	0/9/9/11	0/0/0/0
2	AR7	G	304	2	-	0/9/9/11	0/0/0/0
2	AR7	H	304	2	-	0/9/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	304	AR7	C-CA	2.33	1.56	1.52
2	H	304	AR7	C-CA	2.65	1.56	1.52

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
3	BU3	A	2250	-	4,5,5	0.35	0	6,6,6	0.41	0
4	NAG	B	1000	1,5,4	14,14,15	0.84	0	17,19,21	0.71	0
4	NAG	B	1001	4	14,14,15	0.75	0	17,19,21	0.63	0
5	FUC	B	1002	4	9,10,11	0.98	0	13,14,16	0.83	1 (7%)
5	FUC	B	1003	4	9,10,11	0.78	0	13,14,16	0.62	0
4	NAG	B	1004	1	14,14,15	0.96	0	17,19,21	1.10	2 (11%)
3	BU3	B	2251	-	4,5,5	0.42	0	6,6,6	0.39	0
3	BU3	C	2252	-	4,5,5	0.34	0	6,6,6	0.41	0
4	NAG	D	1000	1,5,4	14,14,15	0.60	0	17,19,21	0.80	0
4	NAG	D	1001	4	14,14,15	0.68	0	17,19,21	0.71	0
5	FUC	D	1002	4	9,10,11	0.73	0	13,14,16	0.74	0
5	FUC	D	1003	4	9,10,11	0.69	0	13,14,16	0.39	0
4	NAG	D	1004	1	14,14,15	0.85	0	17,19,21	0.76	0
3	BU3	D	2253	-	4,5,5	0.41	0	6,6,6	0.42	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	BU3	A	2250	-	-	0/4/4/4	0/0/0/0
4	NAG	B	1000	1,5,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1001	4	-	0/6/23/26	0/1/1/1
5	FUC	B	1002	4	-	0/0/17/20	0/1/1/1
5	FUC	B	1003	4	-	0/0/17/20	0/1/1/1
4	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
3	BU3	B	2251	-	-	0/4/4/4	0/0/0/0
3	BU3	C	2252	-	-	0/4/4/4	0/0/0/0
4	NAG	D	1000	1,5,4	-	0/6/23/26	0/1/1/1
4	NAG	D	1001	4	-	0/6/23/26	0/1/1/1
5	FUC	D	1002	4	-	0/0/17/20	0/1/1/1
5	FUC	D	1003	4	-	0/0/17/20	0/1/1/1
4	NAG	D	1004	1	-	0/6/23/26	0/1/1/1
3	BU3	D	2253	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	NAG	C4-C3-C2	-2.91	106.76	111.02
4	B	1004	NAG	C2-N2-C7	-2.13	119.83	122.94
5	B	1002	FUC	C1-C2-C3	2.14	112.37	109.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	243/245 (99%)	-0.30	2 (0%) 86 86	12, 19, 36, 51	8 (3%)
1	B	243/245 (99%)	-0.39	2 (0%) 86 86	12, 18, 32, 40	8 (3%)
1	C	243/245 (99%)	-0.30	1 (0%) 92 92	12, 19, 36, 56	7 (2%)
1	D	243/245 (99%)	-0.30	1 (0%) 92 92	12, 20, 34, 47	10 (4%)
2	E	2/4 (50%)	-0.23	0 100 100	16, 16, 16, 30	0
2	F	2/4 (50%)	-0.56	0 100 100	15, 15, 15, 26	1 (50%)
2	G	2/4 (50%)	0.03	0 100 100	15, 15, 15, 28	0
2	H	2/4 (50%)	0.02	0 100 100	18, 18, 18, 29	0
All	All	980/996 (98%)	-0.32	6 (0%) 89 89	12, 19, 36, 56	34 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	LYS	2.9
1	A	244	LYS	2.7
1	D	244	LYS	2.5
1	A	60(A)[A]	PRO	2.3
1	B	97	ILE	2.1
1	B	60(A)[A]	PRO	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AR7	H	304	11/12	0.94	0.09	12,13,16,18	0
2	AR7	G	304	11/12	0.94	0.08	12,12,16,16	0
2	AR7	F	304	11/12	0.95	0.07	10,13,15,18	0
2	AR7	E	304	11/12	0.95	0.09	11,13,16,19	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	1004	14/15	0.32	0.41	63,67,70,72	6
4	NAG	B	1004	14/15	0.53	0.31	53,59,64,64	0
5	FUC	B	1003	10/11	0.60	0.23	63,64,64,64	4
4	NAG	D	1001	14/15	0.77	0.22	54,58,60,62	1
4	NAG	B	1000	14/15	0.78	0.17	38,45,57,62	0
5	FUC	B	1002	10/11	0.78	0.17	36,43,46,47	0
4	NAG	D	1000	14/15	0.79	0.18	40,47,57,63	0
5	FUC	D	1003	10/11	0.82	0.32	67,70,73,75	0
4	NAG	B	1001	14/15	0.84	0.29	55,60,65,66	0
5	FUC	D	1002	10/11	0.90	0.14	31,42,46,52	0
3	BU3	A	2250	6/6	0.91	0.10	20,24,25,29	0
3	BU3	C	2252	6/6	0.93	0.09	19,23,25,28	0
3	BU3	D	2253	6/6	0.97	0.07	21,25,28,30	0
3	BU3	B	2251	6/6	0.98	0.06	23,24,25,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.