Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:43 am BST

PDB ID	:	2GCH
Title	:	REFINED CRYSTAL STRUCTURE OF GAMMA-CHYMOTRYPSIN AT 1.9 ANGSTROMS RESOLUTION
Authors	:	Cohen, G.H.; Davies, D.R.; Silverton, E.W.
Deposited on	:	1980-05-21
Resolution	:	1.90 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 ①) were used in the production of this report:

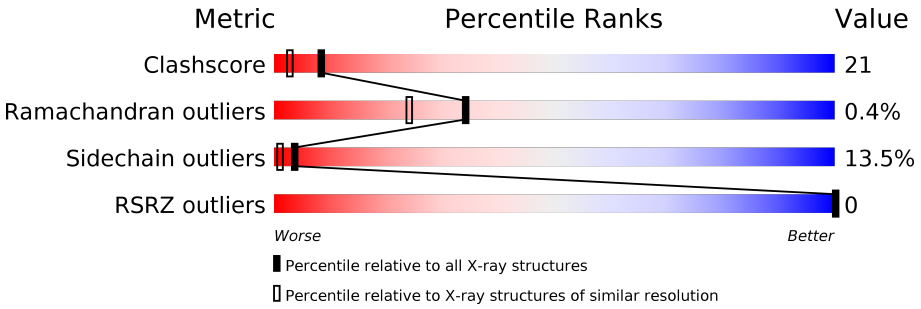
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	E	13	23% 38% 8% 15% 15%
2	F	131	41% 37% 20% .
3	G	97	40% 39% 14% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1889 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 GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	11	Total	C	N	O	S	0	0	1
			69	45	12	11	1			

- Molecule 2 is a protein called GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	131	Total	C	N	O	S	0	0	0
			980	618	162	196	4			

- Molecule 3 is a protein called GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	95	Total	C	N	O	S	0	0	0
			689	429	120	133	7			

- Molecule 4 is water.

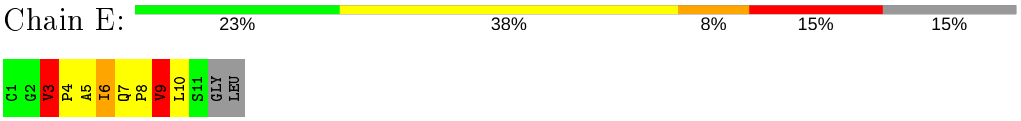
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	4	Total	O	0	0
			4	4		
4	F	83	Total	O	0	0
			83	83		
4	G	64	Total	O	0	0
			64	64		

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.

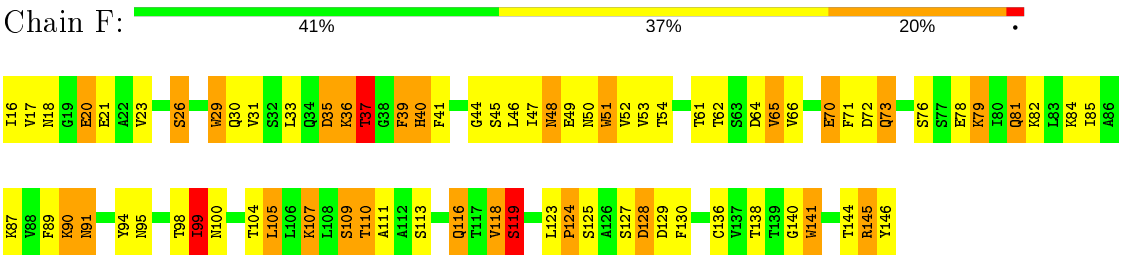
- Molecule 1: GAMMA-CHYMOTRYPSIN A

Chain E:



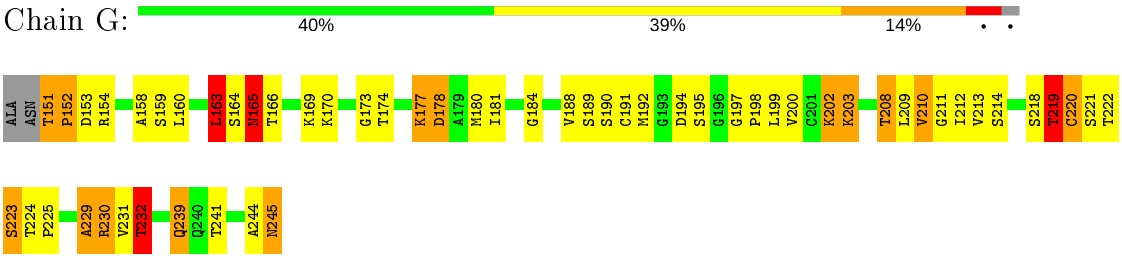
- Molecule 2: GAMMA-CHYMOTRYPSIN A

Chain F:



- Molecule 3: GAMMA-CHYMOTRYPSIN A

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	69.60Å 69.60Å 97.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90 7.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.90) 78.2 (7.16-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available) 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	9.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 71.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	1889	wwPDB-VP
Average B, all atoms (Å^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] 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

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	E	1.76	0/70	2.54	8/97 (8.2%)
2	F	2.00	28/1000 (2.8%)	2.50	75/1361 (5.5%)
3	G	1.91	10/702 (1.4%)	2.44	44/955 (4.6%)
All	All	1.96	38/1772 (2.1%)	2.48	127/2413 (5.3%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	26	SER	CB-OG	-10.34	1.28	1.42
2	F	119	SER	CB-OG	-8.69	1.30	1.42
2	F	70	GLU	CD-OE2	8.08	1.34	1.25
3	G	195	SER	CB-OG	7.07	1.51	1.42
2	F	40	HIS	CG-CD2	7.05	1.47	1.35
2	F	47	ILE	C-O	6.69	1.36	1.23
2	F	20	GLU	CD-OE2	6.63	1.32	1.25
3	G	177	LYS	CE-NZ	6.61	1.65	1.49
2	F	109	SER	CB-OG	-6.44	1.33	1.42
3	G	214	SER	CB-OG	-6.33	1.34	1.42
2	F	130	PHE	CE1-CZ	6.16	1.49	1.37
2	F	82	LYS	CE-NZ	6.15	1.64	1.49
3	G	165	ASN	CB-CG	6.15	1.65	1.51
2	F	30	GLN	C-O	6.10	1.34	1.23
2	F	94	TYR	CA-CB	5.93	1.67	1.53
2	F	71	PHE	CA-CB	5.81	1.66	1.53
3	G	159	SER	CB-OG	-5.71	1.34	1.42
3	G	202	LYS	CA-CB	-5.70	1.41	1.53
2	F	51	TRP	CG-CD2	5.65	1.53	1.43
2	F	65	VAL	C-O	-5.64	1.12	1.23
2	F	29	TRP	CG-CD1	5.55	1.44	1.36
2	F	30	GLN	C-N	-5.54	1.21	1.34
2	F	72	ASP	CG-OD1	-5.46	1.12	1.25
2	F	70	GLU	CG-CD	-5.45	1.43	1.51
3	G	170	LYS	CE-NZ	5.39	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	21	GLU	CG-CD	5.36	1.59	1.51
3	G	198	PRO	N-CD	5.33	1.55	1.47
3	G	164	SER	CB-OG	5.29	1.49	1.42
2	F	127	SER	CA-CB	5.20	1.60	1.52
3	G	222	THR	CB-OG1	-5.20	1.32	1.43
2	F	20	GLU	CG-CD	-5.17	1.44	1.51
2	F	141	TRP	CD1-NE1	5.11	1.46	1.38
2	F	41	PHE	CG-CD2	5.09	1.46	1.38
2	F	94	TYR	CE1-CZ	5.07	1.45	1.38
2	F	110	THR	CA-CB	5.04	1.66	1.53
2	F	62	THR	CB-OG1	5.03	1.53	1.43
2	F	78	GLU	CD-OE1	-5.03	1.20	1.25
2	F	44	GLY	CA-C	5.00	1.59	1.51

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	202	LYS	CA-CB-CG	13.97	144.13	113.40
3	G	244	ALA	CB-CA-C	12.98	129.58	110.10
2	F	145	ARG	NE-CZ-NH1	-12.20	114.20	120.30
3	G	154	ARG	NE-CZ-NH1	11.34	125.97	120.30
2	F	128	ASP	CB-CG-OD2	10.60	127.84	118.30
2	F	61	THR	CA-CB-CG2	10.47	127.06	112.40
2	F	94	TYR	CB-CG-CD2	-10.30	114.82	121.00
3	G	229	ALA	O-C-N	10.16	138.95	122.70
2	F	73	GLN	CB-CG-CD	9.82	137.12	111.60
2	F	20	GLU	CG-CD-OE1	9.66	137.63	118.30
2	F	146	TYR	CB-CG-CD1	-9.25	115.45	121.00
2	F	128	ASP	CB-CG-OD1	-8.67	110.50	118.30
3	G	163	LEU	CA-CB-CG	8.64	135.17	115.30
2	F	51	TRP	CB-CG-CD1	8.35	137.85	127.00
2	F	37	THR	CA-CB-CG2	8.28	123.99	112.40
1	E	3	VAL	CA-CB-CG1	8.06	123.00	110.90
3	G	224	THR	CA-CB-OG1	-7.66	92.92	109.00
3	G	202	LYS	N-CA-CB	7.59	124.27	110.60
2	F	116	GLN	CA-CB-CG	-7.59	96.70	113.40
2	F	51	TRP	CD1-CG-CD2	-7.55	100.26	106.30
3	G	153	ASP	CA-CB-CG	7.51	129.91	113.40
2	F	21	GLU	OE1-CD-OE2	7.48	132.27	123.30
3	G	210	VAL	CG1-CB-CG2	7.44	122.81	110.90
3	G	192	MET	CG-SD-CE	7.44	112.10	100.20
3	G	154	ARG	NH1-CZ-NH2	-7.29	111.38	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	146	TYR	CB-CG-CD2	7.18	125.31	121.00
2	F	70	GLU	CG-CD-OE1	7.13	132.55	118.30
3	G	244	ALA	N-CA-CB	-7.11	100.14	110.10
2	F	91	ASN	O-C-N	-7.01	111.48	122.70
3	G	223	SER	O-C-N	6.93	133.79	122.70
2	F	145	ARG	NE-CZ-NH2	6.92	123.76	120.30
3	G	230	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	E	10	LEU	N-CA-CB	-6.83	96.73	110.40
3	G	189	SER	CB-CA-C	-6.83	97.13	110.10
2	F	20	GLU	O-C-N	6.69	133.40	122.70
2	F	76	SER	O-C-N	6.65	133.34	122.70
3	G	199	LEU	N-CA-CB	6.65	123.70	110.40
2	F	94	TYR	CB-CG-CD1	6.62	124.97	121.00
2	F	46	LEU	O-C-N	6.60	133.26	122.70
2	F	73	GLN	CA-CB-CG	6.57	127.86	113.40
2	F	54	THR	CA-CB-CG2	6.57	121.60	112.40
2	F	138	THR	O-C-N	-6.48	112.33	122.70
3	G	178	ASP	CB-CG-OD2	6.47	124.13	118.30
2	F	109	SER	CB-CA-C	-6.46	97.82	110.10
2	F	91	ASN	N-CA-CB	-6.44	99.02	110.60
2	F	76	SER	CA-C-O	-6.42	106.62	120.10
2	F	36	LYS	CA-CB-CG	6.41	127.50	113.40
2	F	110	THR	CA-CB-CG2	6.40	121.36	112.40
3	G	159	SER	N-CA-CB	6.39	120.08	110.50
3	G	244	ALA	O-C-N	-6.38	112.50	122.70
3	G	152	PRO	N-CD-CG	-6.36	93.66	103.20
2	F	20	GLU	OE1-CD-OE2	-6.28	115.77	123.30
3	G	194	ASP	N-CA-CB	6.24	121.82	110.60
1	E	10	LEU	CB-CA-C	6.20	121.98	110.20
2	F	39	PHE	CG-CD1-CE1	-6.19	113.99	120.80
2	F	39	PHE	CB-CG-CD1	-6.16	116.49	120.80
2	F	84	LYS	CG-CD-CE	6.13	130.28	111.90
1	E	10	LEU	CA-C-N	6.08	130.57	117.20
2	F	51	TRP	CG-CD2-CE3	-6.00	128.50	133.90
3	G	180	MET	CG-SD-CE	-6.00	90.60	100.20
3	G	223	SER	N-CA-CB	5.99	119.48	110.50
3	G	165	ASN	CA-CB-CG	-5.98	100.24	113.40
2	F	98	THR	CA-CB-CG2	5.95	120.74	112.40
2	F	119	SER	N-CA-CB	5.92	119.39	110.50
3	G	189	SER	O-C-N	5.90	132.14	122.70
3	G	158	ALA	CB-CA-C	-5.87	101.29	110.10
2	F	20	GLU	CG-CD-OE2	-5.86	106.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	64	ASP	CB-CG-OD1	5.84	123.55	118.30
1	E	6	ILE	CB-CG1-CD1	5.79	130.11	113.90
2	F	110	THR	CA-CB-OG1	-5.71	97.02	109.00
3	G	203	LYS	N-CA-CB	-5.70	100.34	110.60
2	F	79	LYS	CB-CA-C	5.70	121.80	110.40
2	F	70	GLU	CG-CD-OE2	-5.67	106.95	118.30
2	F	116	GLN	CB-CG-CD	-5.65	96.91	111.60
2	F	89	PHE	CB-CG-CD2	-5.64	116.85	120.80
2	F	110	THR	N-CA-CB	-5.62	99.62	110.30
3	G	151	THR	CA-CB-OG1	5.62	120.79	109.00
2	F	116	GLN	OE1-CD-NE2	5.61	134.81	121.90
2	F	109	SER	N-CA-CB	5.59	118.89	110.50
3	G	219	THR	O-C-N	-5.58	113.77	122.70
2	F	35	ASP	CB-CG-OD2	5.57	123.31	118.30
2	F	113	SER	CB-CA-C	5.57	120.68	110.10
3	G	154	ARG	CD-NE-CZ	5.56	131.39	123.60
2	F	81	GLN	CG-CD-OE1	5.55	132.70	121.60
2	F	31	VAL	CG1-CB-CG2	5.53	119.74	110.90
3	G	178	ASP	OD1-CG-OD2	-5.51	112.84	123.30
3	G	190	SER	O-C-N	-5.50	113.91	122.70
2	F	118	VAL	CG1-CB-CG2	-5.48	102.12	110.90
2	F	140	GLY	O-C-N	5.47	131.44	122.70
2	F	128	ASP	CA-CB-CG	5.41	125.30	113.40
2	F	123	LEU	CB-CG-CD2	-5.34	101.91	111.00
3	G	212	ILE	CA-CB-CG1	5.32	121.11	111.00
3	G	208	THR	CA-CB-CG2	5.31	119.84	112.40
3	G	241	THR	CA-CB-OG1	-5.31	97.85	109.00
2	F	129	ASP	CA-CB-CG	-5.28	101.78	113.40
2	F	51	TRP	O-C-N	5.28	131.15	122.70
2	F	39	PHE	C-N-CA	5.27	134.87	121.70
1	E	9	VAL	CA-CB-CG2	5.25	118.77	110.90
2	F	29	TRP	CG-CD2-CE3	-5.21	129.21	133.90
2	F	118	VAL	CA-CB-CG2	5.20	118.70	110.90
3	G	184	GLY	O-C-N	5.19	131.00	122.70
3	G	178	ASP	CB-CG-OD1	5.19	122.97	118.30
3	G	220	CYS	CA-CB-SG	-5.17	104.70	114.00
2	F	91	ASN	CB-CA-C	5.16	120.72	110.40
2	F	107	LYS	N-CA-CB	-5.15	101.32	110.60
3	G	174	THR	OG1-CB-CG2	5.15	121.85	110.00
2	F	104	THR	N-CA-CB	5.13	120.05	110.30
1	E	10	LEU	CA-C-O	-5.13	109.33	120.10
2	F	71	PHE	O-C-N	-5.13	114.49	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	87	LYS	CA-CB-CG	-5.13	102.11	113.40
3	G	244	ALA	CA-C-N	5.11	128.44	117.20
2	F	30	GLN	C-N-CA	5.10	134.46	121.70
3	G	214	SER	N-CA-CB	5.10	118.15	110.50
2	F	39	PHE	CG-CD2-CE2	5.09	126.40	120.80
3	G	160	LEU	O-C-N	5.09	130.77	121.10
2	F	94	TYR	CA-CB-CG	-5.08	103.75	113.40
2	F	20	GLU	N-CA-CB	5.08	119.74	110.60
3	G	231	VAL	CG1-CB-CG2	-5.07	102.78	110.90
2	F	105	LEU	CB-CG-CD1	-5.07	102.38	111.00
2	F	37	THR	CA-CB-OG1	-5.05	98.39	109.00
1	E	7	GLN	CG-CD-OE1	5.04	131.69	121.60
2	F	99	ILE	O-C-N	5.04	130.77	122.70
2	F	52	VAL	CG1-CB-CG2	-5.04	102.83	110.90
2	F	37	THR	N-CA-CB	-5.02	100.76	110.30
2	F	39	PHE	CZ-CE2-CD2	-5.01	114.09	120.10
2	F	130	PHE	CB-CA-C	5.01	120.42	110.40
3	G	232	THR	C-N-CA	5.01	134.22	121.70

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	E	69	0	76	11	0
2	F	980	0	949	49	0
3	G	689	0	687	26	0
4	E	4	0	0	0	0
4	F	83	0	0	14	0
4	G	64	0	0	6	0
All	All	1889	0	1712	72	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 21.

All (72) 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:F:40:HIS:HD2	4:F:161:HOH:O	1.29	1.12
1:E:5:ALA:HB3	2:F:116:GLN:HG3	1.40	1.03
2:F:73:GLN:NE2	4:F:216:HOH:O	1.98	0.96
2:F:48:ASN:HD22	2:F:50:ASN:H	1.11	0.94
2:F:16:ILE:HD13	4:F:196:HOH:O	1.69	0.93
1:E:5:ALA:CB	2:F:116:GLN:HG3	1.99	0.93
3:G:239:GLN:HA	3:G:239:GLN:HE21	1.34	0.91
2:F:17:VAL:O	2:F:18:ASN:HB2	1.76	0.84
2:F:48:ASN:ND2	2:F:50:ASN:H	1.80	0.80
2:F:70:GLU:OE1	4:F:208:HOH:O	1.98	0.78
2:F:51:TRP:CZ2	2:F:107:LYS:HD3	2.20	0.77
2:F:53:VAL:HG12	2:F:105:LEU:HD23	1.69	0.74
2:F:40:HIS:CD2	4:F:161:HOH:O	2.15	0.73
3:G:178:ASP:OD1	4:G:284:HOH:O	2.09	0.70
2:F:35:ASP:OD2	2:F:37:THR:HB	1.92	0.70
3:G:239:GLN:HA	3:G:239:GLN:NE2	2.06	0.70
2:F:16:ILE:CD1	4:F:196:HOH:O	2.33	0.69
2:F:17:VAL:O	2:F:18:ASN:CB	2.40	0.69
3:G:165:ASN:ND2	4:G:294:HOH:O	2.20	0.67
1:E:9:VAL:HB	2:F:23:VAL:HG21	1.75	0.67
2:F:33:LEU:CD2	2:F:66:VAL:HG22	2.26	0.66
3:G:218:SER:OG	4:G:308:HOH:O	2.12	0.65
2:F:119:SER:HB2	4:F:185:HOH:O	1.96	0.65
2:F:16:ILE:CG2	4:F:196:HOH:O	2.46	0.64
2:F:95:ASN:O	2:F:99:ILE:N	2.31	0.64
2:F:125:SER:HB2	2:F:128:ASP:CG	2.19	0.63
2:F:53:VAL:HG12	2:F:105:LEU:CD2	2.28	0.63
2:F:111:ALA:HB1	4:F:199:HOH:O	2.00	0.60
1:E:6:ILE:HD11	2:F:116:GLN:HG2	1.85	0.58
1:E:6:ILE:CD1	2:F:116:GLN:HG2	2.34	0.58
2:F:16:ILE:HG21	4:F:196:HOH:O	2.02	0.57
3:G:232:THR:HB	4:G:251:HOH:O	2.05	0.57
3:G:245:ASN:ND2	3:G:245:ASN:H	2.01	0.57
2:F:144:THR:HG23	3:G:152:PRO:HD3	1.87	0.56
2:F:141:TRP:O	3:G:151:THR:HB	2.05	0.56
2:F:125:SER:HB2	2:F:128:ASP:OD2	2.06	0.56
2:F:124:PRO:HD3	3:G:209:LEU:O	2.06	0.55
2:F:18:ASN:HB3	3:G:188:VAL:HG12	1.89	0.55
3:G:220:CYS:HA	4:G:285:HOH:O	2.07	0.54
3:G:211:GLY:HA2	3:G:229:ALA:O	2.10	0.51
2:F:36:LYS:NZ	4:F:201:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:HB	2:F:23:VAL:CG2	2.41	0.50
2:F:37:THR:HG22	2:F:39:PHE:HB2	1.95	0.49
2:F:90:LYS:O	2:F:91:ASN:C	2.51	0.48
1:E:9:VAL:HG12	1:E:9:VAL:O	2.13	0.48
3:G:181:ILE:HD13	3:G:181:ILE:HG21	1.57	0.48
3:G:239:GLN:HB3	4:G:267:HOH:O	2.12	0.48
2:F:16:ILE:CG1	4:F:196:HOH:O	2.59	0.48
3:G:169:LYS:HG2	3:G:173:GLY:O	2.12	0.48
3:G:245:ASN:ND2	3:G:245:ASN:N	2.62	0.48
2:F:136:CYS:HB3	3:G:200:VAL:O	2.15	0.47
3:G:219:THR:O	3:G:220:CYS:HB2	2.16	0.46
3:G:230:ARG:HG2	3:G:232:THR:HG22	1.98	0.45
3:G:163:LEU:HD11	3:G:225:PRO:HB3	1.99	0.44
2:F:145:ARG:NH1	4:F:228:HOH:O	2.49	0.44
1:E:3:VAL:CG2	1:E:3:VAL:O	2.65	0.43
2:F:16:ILE:O	2:F:144:THR:HA	2.17	0.43
2:F:79:LYS:O	2:F:79:LYS:HG2	2.17	0.43
2:F:100:ASN:ND2	3:G:177:LYS:HB2	2.34	0.43
2:F:81:GLN:NE2	2:F:118:VAL:HG21	2.33	0.43
2:F:116:GLN:O	2:F:116:GLN:CG	2.67	0.43
3:G:197:GLY:O	3:G:213:VAL:HG23	2.19	0.43
2:F:85:ILE:HD13	2:F:85:ILE:HG21	1.77	0.42
3:G:210:VAL:HG12	3:G:210:VAL:O	2.19	0.42
2:F:29:TRP:O	2:F:45:SER:HA	2.20	0.41
1:E:5:ALA:HB1	2:F:116:GLN:HG3	1.94	0.41
3:G:165:ASN:ND2	3:G:230:ARG:HH11	2.19	0.41
2:F:16:ILE:HG21	2:F:16:ILE:HD13	1.74	0.41
3:G:169:LYS:HA	3:G:173:GLY:H	1.86	0.41
2:F:79:LYS:N	4:F:203:HOH:O	2.40	0.41
1:E:4:PRO:HG2	1:E:8:PRO:HD3	2.04	0.40
1:E:8:PRO:HA	2:F:26:SER:CB	2.52	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	E	9/13 (69%)	9 (100%)	0	0	100 100
2	F	129/131 (98%)	123 (95%)	5 (4%)	1 (1%)	19 9
3	G	93/97 (96%)	90 (97%)	3 (3%)	0	100 100
All	All	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	34 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	99	ILE

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	E	8/10 (80%)	6 (75%)	2 (25%)	0 0
2	F	109/109 (100%)	98 (90%)	11 (10%)	7 2
3	G	76/77 (99%)	63 (83%)	13 (17%)	2 0
All	All	193/196 (98%)	167 (86%)	26 (14%)	4 1

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	VAL
1	E	9	VAL
2	F	20	GLU
2	F	37	THR
2	F	48	ASN
2	F	49	GLU
2	F	65	VAL
2	F	90	LYS
2	F	99	ILE

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Mol	Chain	Res	Type
2	F	109	SER
2	F	110	THR
2	F	119	SER
2	F	124	PRO
3	G	163	LEU
3	G	165	ASN
3	G	166	THR
3	G	191	CYS
3	G	202	LYS
3	G	203	LYS
3	G	208	THR
3	G	219	THR
3	G	221	SER
3	G	223	SER
3	G	232	THR
3	G	239	GLN
3	G	245	ASN

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

Mol	Chain	Res	Type
2	F	48	ASN
2	F	100	ASN
3	G	165	ASN
3	G	239	GLN
3	G	245	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	E	11/13 (84%)	0.13	0	100	100	8, 10, 25, 27	0
2	F	131/131 (100%)	-0.53	0	100	100	2, 7, 16, 20	0
3	G	95/97 (97%)	-0.46	0	100	100	2, 6, 16, 21	0
All	All	237/241 (98%)	-0.47	0	100	100	2, 7, 18, 27	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.