wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 01:42 AM EDT

PDB ID	:	5OYM
Title	:	HIV Integrase Binding Domain of Lens Epithelium-Derived Growth Factor
Authors	:	Rabbitts, T.H.; Phillips, S.E.V.; Cruz-Migoni, A.; Carr, S.B.; Hannon, C.
Deposited on	:	2017-09-11
Resolution	:	2.05 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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

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 2.05 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		3.1%
RSRZ outliers		2.8%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
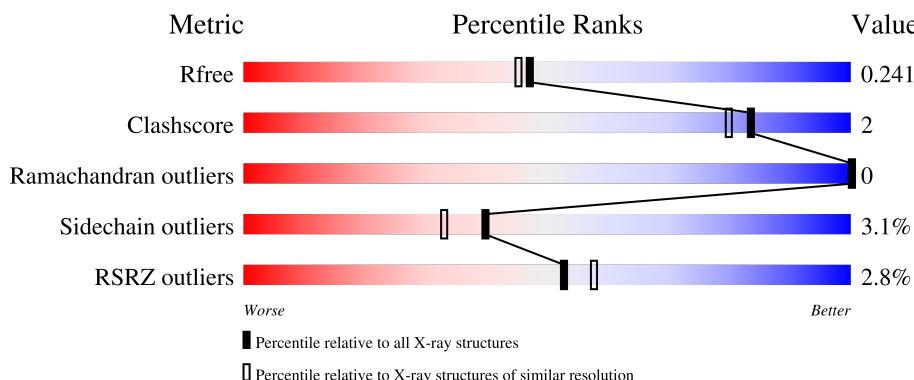
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	111	2% 72% · · 23%
1	B	111	3% 70% 5% · 24%
1	C	111	2% 71% 5% · 23%
1	D	111	% 74% · · 22%
1	E	111	5% 73% 5% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	111	3% 70% 7% · 22%
1	G	111	2% 71% 7% · 21%
1	H	111	.% 69% 7% 23%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6129 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 PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	85	Total	C	N	O	S	0	0	0
			696	436	124	129	7			
1	G	88	Total	C	N	O	S	0	4	0
			738	462	132	135	9			
1	A	85	Total	C	N	O	S	0	1	0
			704	441	127	129	7			
1	B	84	Total	C	N	O	S	0	2	0
			703	438	127	130	8			
1	C	85	Total	C	N	O	S	0	0	0
			696	436	124	129	7			
1	D	87	Total	C	N	O	S	0	2	0
			719	450	129	132	8			
1	E	86	Total	C	N	O	S	0	0	0
			700	438	125	130	7			
1	F	87	Total	C	N	O	S	0	3	0
			728	456	131	133	8			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	321	GLY	-	expression tag	UNP O75475
H	322	GLY	-	expression tag	UNP O75475
H	323	SER	-	expression tag	UNP O75475
H	324	MET	-	expression tag	UNP O75475
H	325	GLY	-	expression tag	UNP O75475
H	326	SER	-	expression tag	UNP O75475
H	327	GLY	-	expression tag	UNP O75475
H	328	GLY	-	expression tag	UNP O75475
H	329	GLY	-	expression tag	UNP O75475
H	330	GLY	-	expression tag	UNP O75475
H	331	SER	-	expression tag	UNP O75475
H	332	GLY	-	expression tag	UNP O75475
H	333	GLY	-	expression tag	UNP O75475

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	334	GLY	-	expression tag	UNP O75475
H	335	GLY	-	expression tag	UNP O75475
H	336	SER	-	expression tag	UNP O75475
H	337	GLY	-	expression tag	UNP O75475
H	338	GLY	-	expression tag	UNP O75475
H	339	GLY	-	expression tag	UNP O75475
H	340	GLY	-	expression tag	UNP O75475
H	341	ALA	-	expression tag	UNP O75475
H	342	ALA	-	expression tag	UNP O75475
H	343	ALA	-	expression tag	UNP O75475
H	344	MET	-	expression tag	UNP O75475
G	321	GLY	-	expression tag	UNP O75475
G	322	GLY	-	expression tag	UNP O75475
G	323	SER	-	expression tag	UNP O75475
G	324	MET	-	expression tag	UNP O75475
G	325	GLY	-	expression tag	UNP O75475
G	326	SER	-	expression tag	UNP O75475
G	327	GLY	-	expression tag	UNP O75475
G	328	GLY	-	expression tag	UNP O75475
G	329	GLY	-	expression tag	UNP O75475
G	330	GLY	-	expression tag	UNP O75475
G	331	SER	-	expression tag	UNP O75475
G	332	GLY	-	expression tag	UNP O75475
G	333	GLY	-	expression tag	UNP O75475
G	334	GLY	-	expression tag	UNP O75475
G	335	GLY	-	expression tag	UNP O75475
G	336	SER	-	expression tag	UNP O75475
G	337	GLY	-	expression tag	UNP O75475
G	338	GLY	-	expression tag	UNP O75475
G	339	GLY	-	expression tag	UNP O75475
G	340	GLY	-	expression tag	UNP O75475
G	341	ALA	-	expression tag	UNP O75475
G	342	ALA	-	expression tag	UNP O75475
G	343	ALA	-	expression tag	UNP O75475
G	344	MET	-	expression tag	UNP O75475
A	321	GLY	-	expression tag	UNP O75475
A	322	GLY	-	expression tag	UNP O75475
A	323	SER	-	expression tag	UNP O75475
A	324	MET	-	expression tag	UNP O75475
A	325	GLY	-	expression tag	UNP O75475
A	326	SER	-	expression tag	UNP O75475
A	327	GLY	-	expression tag	UNP O75475

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	GLY	-	expression tag	UNP O75475
A	329	GLY	-	expression tag	UNP O75475
A	330	GLY	-	expression tag	UNP O75475
A	331	SER	-	expression tag	UNP O75475
A	332	GLY	-	expression tag	UNP O75475
A	333	GLY	-	expression tag	UNP O75475
A	334	GLY	-	expression tag	UNP O75475
A	335	GLY	-	expression tag	UNP O75475
A	336	SER	-	expression tag	UNP O75475
A	337	GLY	-	expression tag	UNP O75475
A	338	GLY	-	expression tag	UNP O75475
A	339	GLY	-	expression tag	UNP O75475
A	340	GLY	-	expression tag	UNP O75475
A	341	ALA	-	expression tag	UNP O75475
A	342	ALA	-	expression tag	UNP O75475
A	343	ALA	-	expression tag	UNP O75475
A	344	MET	-	expression tag	UNP O75475
B	321	GLY	-	expression tag	UNP O75475
B	322	GLY	-	expression tag	UNP O75475
B	323	SER	-	expression tag	UNP O75475
B	324	MET	-	expression tag	UNP O75475
B	325	GLY	-	expression tag	UNP O75475
B	326	SER	-	expression tag	UNP O75475
B	327	GLY	-	expression tag	UNP O75475
B	328	GLY	-	expression tag	UNP O75475
B	329	GLY	-	expression tag	UNP O75475
B	330	GLY	-	expression tag	UNP O75475
B	331	SER	-	expression tag	UNP O75475
B	332	GLY	-	expression tag	UNP O75475
B	333	GLY	-	expression tag	UNP O75475
B	334	GLY	-	expression tag	UNP O75475
B	335	GLY	-	expression tag	UNP O75475
B	336	SER	-	expression tag	UNP O75475
B	337	GLY	-	expression tag	UNP O75475
B	338	GLY	-	expression tag	UNP O75475
B	339	GLY	-	expression tag	UNP O75475
B	340	GLY	-	expression tag	UNP O75475
B	341	ALA	-	expression tag	UNP O75475
B	342	ALA	-	expression tag	UNP O75475
B	343	ALA	-	expression tag	UNP O75475
B	344	MET	-	expression tag	UNP O75475
C	321	GLY	-	expression tag	UNP O75475

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	322	GLY	-	expression tag	UNP O75475
C	323	SER	-	expression tag	UNP O75475
C	324	MET	-	expression tag	UNP O75475
C	325	GLY	-	expression tag	UNP O75475
C	326	SER	-	expression tag	UNP O75475
C	327	GLY	-	expression tag	UNP O75475
C	328	GLY	-	expression tag	UNP O75475
C	329	GLY	-	expression tag	UNP O75475
C	330	GLY	-	expression tag	UNP O75475
C	331	SER	-	expression tag	UNP O75475
C	332	GLY	-	expression tag	UNP O75475
C	333	GLY	-	expression tag	UNP O75475
C	334	GLY	-	expression tag	UNP O75475
C	335	GLY	-	expression tag	UNP O75475
C	336	SER	-	expression tag	UNP O75475
C	337	GLY	-	expression tag	UNP O75475
C	338	GLY	-	expression tag	UNP O75475
C	339	GLY	-	expression tag	UNP O75475
C	340	GLY	-	expression tag	UNP O75475
C	341	ALA	-	expression tag	UNP O75475
C	342	ALA	-	expression tag	UNP O75475
C	343	ALA	-	expression tag	UNP O75475
C	344	MET	-	expression tag	UNP O75475
D	321	GLY	-	expression tag	UNP O75475
D	322	GLY	-	expression tag	UNP O75475
D	323	SER	-	expression tag	UNP O75475
D	324	MET	-	expression tag	UNP O75475
D	325	GLY	-	expression tag	UNP O75475
D	326	SER	-	expression tag	UNP O75475
D	327	GLY	-	expression tag	UNP O75475
D	328	GLY	-	expression tag	UNP O75475
D	329	GLY	-	expression tag	UNP O75475
D	330	GLY	-	expression tag	UNP O75475
D	331	SER	-	expression tag	UNP O75475
D	332	GLY	-	expression tag	UNP O75475
D	333	GLY	-	expression tag	UNP O75475
D	334	GLY	-	expression tag	UNP O75475
D	335	GLY	-	expression tag	UNP O75475
D	336	SER	-	expression tag	UNP O75475
D	337	GLY	-	expression tag	UNP O75475
D	338	GLY	-	expression tag	UNP O75475
D	339	GLY	-	expression tag	UNP O75475

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	340	GLY	-	expression tag	UNP O75475
D	341	ALA	-	expression tag	UNP O75475
D	342	ALA	-	expression tag	UNP O75475
D	343	ALA	-	expression tag	UNP O75475
D	344	MET	-	expression tag	UNP O75475
E	321	GLY	-	expression tag	UNP O75475
E	322	GLY	-	expression tag	UNP O75475
E	323	SER	-	expression tag	UNP O75475
E	324	MET	-	expression tag	UNP O75475
E	325	GLY	-	expression tag	UNP O75475
E	326	SER	-	expression tag	UNP O75475
E	327	GLY	-	expression tag	UNP O75475
E	328	GLY	-	expression tag	UNP O75475
E	329	GLY	-	expression tag	UNP O75475
E	330	GLY	-	expression tag	UNP O75475
E	331	SER	-	expression tag	UNP O75475
E	332	GLY	-	expression tag	UNP O75475
E	333	GLY	-	expression tag	UNP O75475
E	334	GLY	-	expression tag	UNP O75475
E	335	GLY	-	expression tag	UNP O75475
E	336	SER	-	expression tag	UNP O75475
E	337	GLY	-	expression tag	UNP O75475
E	338	GLY	-	expression tag	UNP O75475
E	339	GLY	-	expression tag	UNP O75475
E	340	GLY	-	expression tag	UNP O75475
E	341	ALA	-	expression tag	UNP O75475
E	342	ALA	-	expression tag	UNP O75475
E	343	ALA	-	expression tag	UNP O75475
E	344	MET	-	expression tag	UNP O75475
F	321	GLY	-	expression tag	UNP O75475
F	322	GLY	-	expression tag	UNP O75475
F	323	SER	-	expression tag	UNP O75475
F	324	MET	-	expression tag	UNP O75475
F	325	GLY	-	expression tag	UNP O75475
F	326	SER	-	expression tag	UNP O75475
F	327	GLY	-	expression tag	UNP O75475
F	328	GLY	-	expression tag	UNP O75475
F	329	GLY	-	expression tag	UNP O75475
F	330	GLY	-	expression tag	UNP O75475
F	331	SER	-	expression tag	UNP O75475
F	332	GLY	-	expression tag	UNP O75475
F	333	GLY	-	expression tag	UNP O75475

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	334	GLY	-	expression tag	UNP O75475
F	335	GLY	-	expression tag	UNP O75475
F	336	SER	-	expression tag	UNP O75475
F	337	GLY	-	expression tag	UNP O75475
F	338	GLY	-	expression tag	UNP O75475
F	339	GLY	-	expression tag	UNP O75475
F	340	GLY	-	expression tag	UNP O75475
F	341	ALA	-	expression tag	UNP O75475
F	342	ALA	-	expression tag	UNP O75475
F	343	ALA	-	expression tag	UNP O75475
F	344	MET	-	expression tag	UNP O75475

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	53	Total 53	O 53	0	0
2	G	70	Total 70	O 70	0	0
2	A	48	Total 48	O 48	0	0
2	B	65	Total 65	O 65	0	0
2	C	54	Total 54	O 54	0	0
2	D	72	Total 72	O 72	0	0
2	E	32	Total 32	O 32	0	0
2	F	51	Total 51	O 51	0	0

3 Residue-property plots ⓘ

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: PC4 and SFRS1-interacting protein
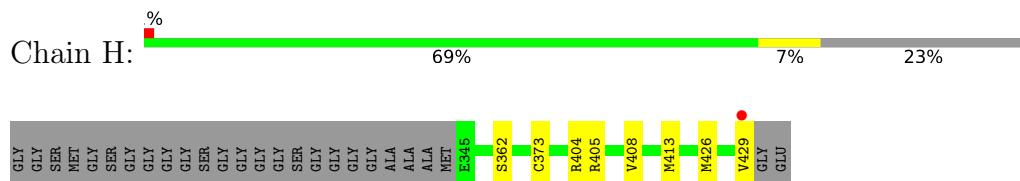
Chain H:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain G:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain A:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain B:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain C:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain D:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain E:

• Molecule 1: PC4 and SFRS1-interacting protein

Chain F:
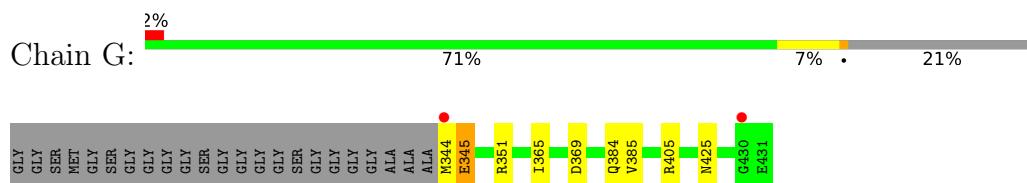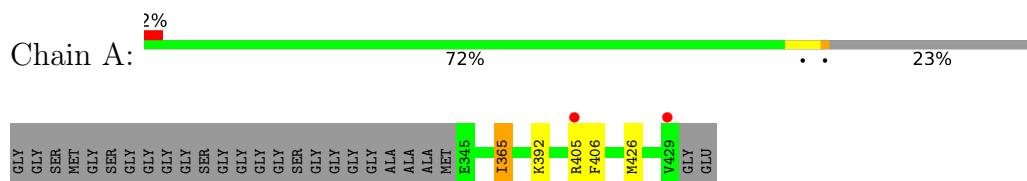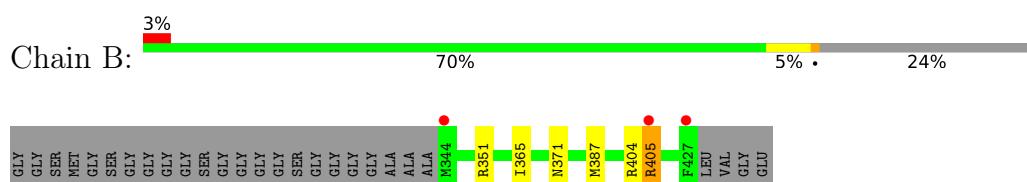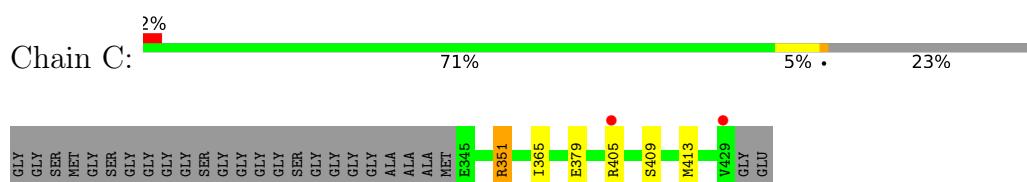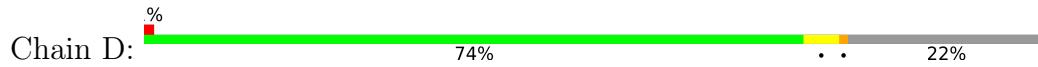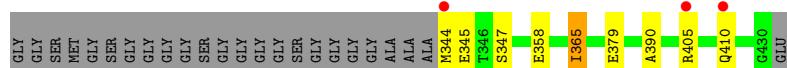
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.18Å 54.81Å 118.00Å 90.00° 91.23° 90.00°	Depositor
Resolution (Å)	14.98 – 2.05 14.98 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.3 (14.98-2.05) 96.6 (14.98-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.182 , 0.236 0.189 , 0.241	Depositor DCC
R_{free} test set	2800 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.1	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6129	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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	A	0.85	0/712	0.91	0/949
1	B	0.84	0/711	0.92	0/946
1	C	0.86	0/701	0.98	2/935 (0.2%)
1	D	0.90	0/730	0.95	1/972 (0.1%)
1	E	0.74	0/705	0.91	0/940
1	F	0.90	3/742 (0.4%)	0.92	0/988
1	G	0.91	0/752	1.01	4/1001 (0.4%)
1	H	0.83	0/701	0.95	0/935
All	All	0.86	3/5754 (0.1%)	0.94	7/7666 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	347	SER	CB-OG	-6.00	1.34	1.42
1	F	379	GLU	CD-OE1	5.51	1.31	1.25
1	F	358	GLU	CD-OE1	5.09	1.31	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	354	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	G	369	ASP	CB-CG-OD1	7.09	124.68	118.30
1	G	351[A]	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	G	351[B]	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	351	ARG	NE-CZ-NH1	6.06	123.33	120.30

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	704	0	746	5	0
1	B	703	0	739	7	0
1	C	696	0	733	3	0
1	D	719	0	763	2	0
1	E	700	0	736	3	0
1	F	728	0	774	4	0
1	G	738	0	781	5	0
1	H	696	0	733	5	0
2	A	48	0	0	1	0
2	B	65	0	0	5	0
2	C	54	0	0	1	0
2	D	72	0	0	1	0
2	E	32	0	0	0	0
2	F	51	0	0	0	0
2	G	70	0	0	4	0
2	H	53	0	0	1	0
All	All	6129	0	6005	28	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 2.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ARG:HD3	2:B:513:HOH:O	1.95	0.64
1:B:404:ARG:HG3	2:B:504:HOH:O	1.96	0.64
1:B:351[B]:ARG:HD3	2:B:518:HOH:O	1.99	0.63
1:A:365:ILE:HD13	1:A:365:ILE:O	1.99	0.62
1:D:365:ILE:HD13	1:D:365:ILE:O	2.02	0.60

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	84/111 (76%)	81 (96%)	3 (4%)	0	100	100
1	B	84/111 (76%)	82 (98%)	2 (2%)	0	100	100
1	C	83/111 (75%)	81 (98%)	2 (2%)	0	100	100
1	D	87/111 (78%)	86 (99%)	1 (1%)	0	100	100
1	E	84/111 (76%)	82 (98%)	2 (2%)	0	100	100
1	F	88/111 (79%)	85 (97%)	3 (3%)	0	100	100
1	G	90/111 (81%)	88 (98%)	2 (2%)	0	100	100
1	H	83/111 (75%)	81 (98%)	2 (2%)	0	100	100
All	All	683/888 (77%)	666 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	82/88 (93%)	80 (98%)	2 (2%)	49	42
1	B	82/88 (93%)	81 (99%)	1 (1%)	71	70
1	C	81/88 (92%)	79 (98%)	2 (2%)	47	40
1	D	84/88 (96%)	81 (96%)	3 (4%)	35	28
1	E	81/88 (92%)	79 (98%)	2 (2%)	47	40
1	F	85/88 (97%)	81 (95%)	4 (5%)	26	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	86/88 (98%)	81 (94%)	5 (6%)	20	11
1	H	81/88 (92%)	80 (99%)	1 (1%)	71	70
All	All	662/704 (94%)	642 (97%)	20 (3%)	40	34

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	365	ILE
1	F	345	GLU
1	F	405	ARG
1	F	365	ILE
1	A	365	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	367	ASN
1	E	353	GLN
1	B	367	ASN
1	C	353	GLN
1	C	391	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no monosaccharides 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, 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(Å²)	Q<0.9
1	A	85/111 (76%)	-0.19	2 (2%)	59	63	20, 34, 54, 80	0
1	B	84/111 (75%)	-0.21	3 (3%)	42	46	21, 31, 63, 91	0
1	C	85/111 (76%)	-0.17	2 (2%)	59	63	19, 34, 59, 86	0
1	D	87/111 (78%)	-0.20	1 (1%)	80	82	20, 30, 53, 73	0
1	E	86/111 (77%)	0.05	5 (5%)	23	25	26, 42, 75, 90	0
1	F	87/111 (78%)	-0.07	3 (3%)	45	49	18, 34, 64, 84	0
1	G	88/111 (79%)	-0.15	2 (2%)	60	64	19, 30, 55, 86	0
1	H	85/111 (76%)	-0.06	1 (1%)	79	81	23, 36, 61, 72	0
All	All	687/888 (77%)	-0.13	19 (2%)	53	58	18, 34, 66, 91	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	344	MET	7.6
1	H	429	VAL	5.3
1	B	344	MET	5.3
1	F	344	MET	5.0
1	D	344	MET	4.4

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 monosaccharides 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.