



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:15 AM UTC

PDB ID : 1FYH / pdb_00001fyh
Title : 1:1 COMPLEX BETWEEN AN INTERFERON GAMMA SINGLE-CHAIN
VARIANT AND ITS RECEPTOR
Authors : Randal, M.; Kossiakoff, A.A.
Deposited on : 2000-09-29
Resolution : 2.04 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

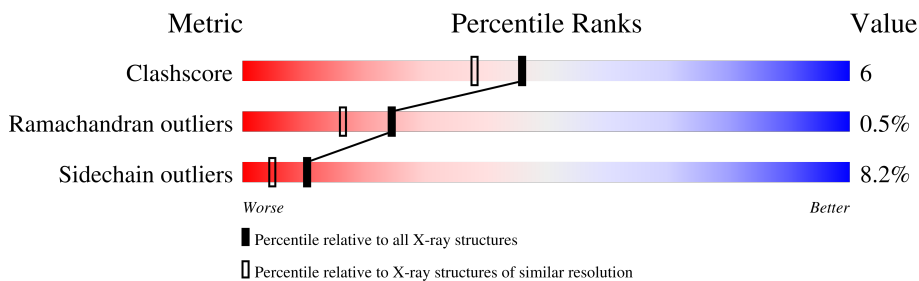
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	258	 68% 19% 7% 6%
1	D	258	 76% 16% • 7%
2	B	229	 72% 14% • 12%
2	E	229	 67% 18% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7687 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 Interferon gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	80	0	0
			1996	1272	333	384	7			
1	D	240	Total	C	N	O	S	24	0	0
			1984	1267	331	379	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01579
A	111	ASP	HIS	engineered mutation	UNP P01579
A	121	GLY	-	linker	UNP P01579
A	122	ALA	-	linker	UNP P01579
A	123	ASN	-	linker	UNP P01579
A	124	VAL	-	linker	UNP P01579
A	201	SER	-	linker	UNP P01579
A	202	GLY	-	linker	UNP P01579
A	203	GLU	-	linker	UNP P01579
A	204	PHE	-	linker	UNP P01579
D	0	MET	-	initiating methionine	UNP P01579
D	111	ASP	HIS	engineered mutation	UNP P01579
D	121	GLY	-	linker	UNP P01579
D	122	ALA	-	linker	UNP P01579
D	123	ASN	-	linker	UNP P01579
D	124	VAL	-	linker	UNP P01579
D	201	SER	-	linker	UNP P01579
D	202	GLY	-	linker	UNP P01579
D	203	GLU	-	linker	UNP P01579
D	204	PHE	-	linker	UNP P01579

- Molecule 2 is a protein called Interferon gamma receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	201	Total	C	N	O	S	49	0	0
			1612	1025	267	308	12			
2	E	201	Total	C	N	O	S	92	0	0
			1613	1028	266	307	12			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

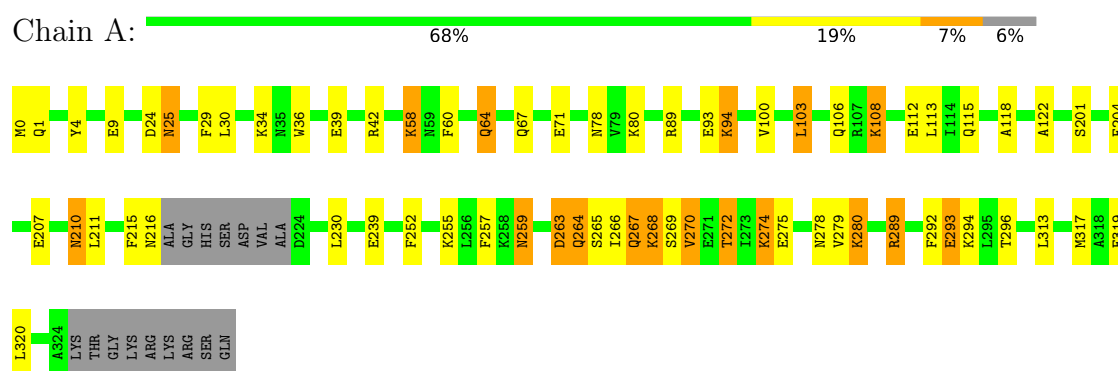
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	139	Total	O	0	0
			139	139		
4	D	143	Total	O	0	0
			143	143		
4	E	94	Total	O	0	0
			94	94		

3 Residue-property plots

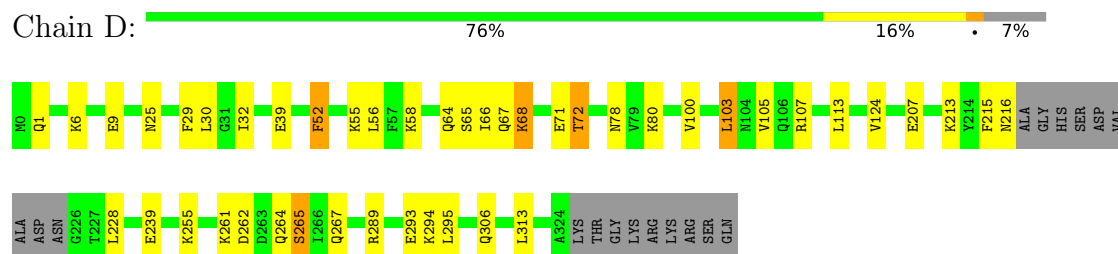
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

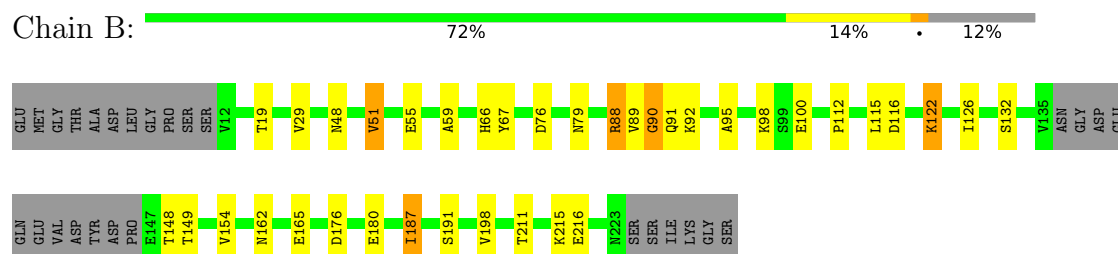
- Molecule 1: Interferon gamma



- Molecule 1: Interferon gamma

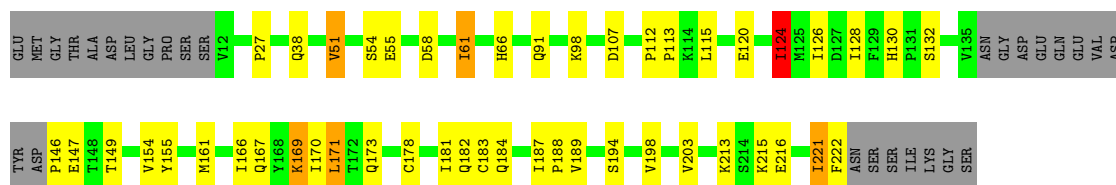


- Molecule 2: Interferon gamma receptor 1



- Molecule 2: Interferon gamma receptor 1





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.94Å 107.60Å 85.08Å 90.00° 97.94° 90.00°	Depositor
Resolution (Å)	15.00 – 2.04	Depositor
% Data completeness (in resolution range)	95.2 (15.00-2.04)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.86	0/2028	1.25	22/2712 (0.8%)
1	D	0.84	0/2016	1.14	19/2694 (0.7%)
2	B	0.95	2/1649 (0.1%)	1.26	15/2242 (0.7%)
2	E	0.91	4/1651 (0.2%)	1.26	18/2245 (0.8%)
All	All	0.89	6/7344 (0.1%)	1.23	74/9893 (0.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	51	VAL	CA-CB	8.36	1.62	1.54
2	E	120	GLU	C-N	-7.72	1.23	1.33
2	E	54	SER	C-O	5.61	1.32	1.23
2	E	181	ILE	C-O	5.57	1.29	1.23
2	B	55	GLU	C-N	5.20	1.41	1.33
2	B	162	ASN	CA-C	5.13	1.58	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	GLN	OE1-CD-NE2	-9.83	112.77	122.60
2	E	91	GLN	OE1-CD-NE2	-9.80	112.80	122.60
2	B	91	GLN	OE1-CD-NE2	-9.80	112.80	122.60
2	E	173	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	267	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	67	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	A	264	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	A	30	LEU	N-CA-C	8.10	119.74	111.07
1	A	113	LEU	N-CA-C	7.75	120.71	111.33
1	D	239	GLU	N-CA-C	7.66	119.63	111.28
2	B	66	HIS	N-CA-C	7.55	122.51	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	GLU	CA-C-O	7.44	129.06	120.80
2	B	112	PRO	N-CA-C	7.42	119.75	110.70
2	E	112	PRO	N-CA-C	7.28	119.58	110.70
1	A	39	GLU	N-CA-C	7.13	119.91	111.71
2	E	182	GLN	N-CA-C	7.05	118.47	108.74
2	B	187	ILE	CB-CA-C	-6.91	103.42	110.13
2	E	120	GLU	CA-C-O	-6.78	110.81	120.51
1	A	313	LEU	N-CA-C	6.74	119.20	111.11
1	A	267	GLN	CG-CD-NE2	6.71	126.46	116.40
1	A	60	PHE	CA-C-N	6.68	129.54	120.38
1	A	60	PHE	C-N-CA	6.68	129.54	120.38
2	E	91	GLN	CG-CD-NE2	6.68	126.42	116.40
2	E	173	GLN	CG-CD-NE2	6.67	126.41	116.40
1	D	264	GLN	CG-CD-NE2	6.67	126.41	116.40
2	B	91	GLN	CG-CD-NE2	6.65	126.38	116.40
1	A	67	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	264	GLN	CG-CD-NE2	6.61	126.31	116.40
1	A	80	LYS	N-CA-C	6.59	118.47	111.28
2	B	95	ALA	N-CA-C	-6.31	102.04	110.55
2	E	55	GLU	CA-C-O	6.31	128.17	120.92
2	E	124	ILE	N-CA-C	-6.28	99.38	108.36
2	B	76	ASP	N-CA-C	-6.09	102.10	109.72
2	B	100	GLU	N-CA-C	-6.06	102.71	110.53
1	D	113	LEU	N-CA-C	6.05	118.37	111.11
1	A	1	GLN	N-CA-C	6.04	119.48	109.46
1	D	30	LEU	N-CA-C	5.98	117.79	111.28
1	A	25	ASN	N-CA-C	5.97	123.52	110.80
1	D	64	GLN	N-CA-C	5.96	119.38	111.75
2	E	66	HIS	N-CA-C	5.92	120.94	111.81
2	B	215	LYS	CA-C-O	-5.89	114.57	121.16
1	A	230	LEU	N-CA-C	5.87	117.68	111.28
1	D	25	ASN	N-CA-C	5.87	123.31	110.80
1	D	9	GLU	CA-C-N	5.87	128.62	120.29
1	D	9	GLU	C-N-CA	5.87	128.62	120.29
1	A	263	ASP	CA-C-N	5.85	132.71	121.54
1	A	263	ASP	C-N-CA	5.85	132.71	121.54
1	D	80	LYS	N-CA-C	5.76	117.64	111.36
1	D	1	GLN	N-CA-C	5.76	118.11	108.96
2	E	113	PRO	N-CA-C	-5.75	102.56	111.13
1	D	265	SER	N-CA-C	5.68	118.24	111.71
1	A	29	PHE	N-CA-C	5.59	120.59	113.55
2	E	198	VAL	N-CA-C	5.54	116.65	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	TRP	N-CA-C	5.51	117.50	108.52
1	D	29	PHE	N-CA-C	5.50	120.86	114.04
2	B	198	VAL	N-CA-C	5.45	116.58	108.46
2	B	211	THR	N-CA-C	-5.41	102.89	110.35
1	A	210	ASN	N-CA-C	-5.36	105.12	110.97
2	E	130	HIS	N-CA-C	5.36	117.29	109.84
2	B	176	ASP	CA-C-N	5.30	128.37	120.31
2	B	176	ASP	C-N-CA	5.30	128.37	120.31
1	D	66	ILE	CB-CA-C	-5.30	104.62	111.20
1	A	239	GLU	N-CA-C	5.29	117.05	111.28
1	D	313	LEU	N-CA-C	5.27	117.43	111.11
2	E	215	LYS	CA-C-O	-5.26	115.05	121.05
2	E	107	ASP	N-CA-C	5.26	119.97	113.50
2	E	54	SER	CA-C-N	5.19	129.78	122.09
2	E	54	SER	C-N-CA	5.19	129.78	122.09
1	D	213	LYS	N-CA-C	-5.18	105.55	111.14
1	D	124	VAL	N-CA-C	5.09	116.58	109.80
1	D	65	SER	N-CA-C	5.08	117.72	111.82
2	E	27	PRO	N-CA-C	5.04	118.42	110.80
1	D	215	PHE	N-CA-C	5.03	119.17	113.19
2	B	59	ALA	N-CA-C	-5.00	104.91	111.96

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	1996	0	1988	33	0
1	D	1984	0	1989	17	0
2	B	1612	0	1568	11	0
2	E	1613	0	1577	20	0
3	A	1	0	0	0	0
4	A	105	0	0	2	0
4	B	139	0	0	1	0
4	D	143	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	94	0	0	1	0
All	All	7687	0	7122	80	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 6.

All (80) 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:A:207:GLU:HG3	1:A:272:THR:HG21	1.67	0.76
1:A:275:GLU:O	1:A:279:VAL:HG23	1.88	0.74
1:D:289:ARG:O	1:D:293:GLU:HG3	1.89	0.72
2:E:124:ILE:HD12	2:E:189:VAL:HG22	1.75	0.69
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.59	0.67
1:A:42:ARG:HH22	1:A:319:GLU:HB3	1.60	0.67
1:A:292:PHE:O	1:A:296:THR:HG23	1.95	0.66
4:A:522:HOH:O	2:B:149:THR:HG21	1.94	0.66
2:E:221:ILE:O	2:E:222:PHE:HB2	1.96	0.66
1:D:103:LEU:HD23	1:D:107:ARG:NH1	2.13	0.63
1:D:293:GLU:HG2	4:D:444:HOH:O	2.00	0.60
1:A:89:ARG:HH12	1:A:93:GLU:HB3	1.66	0.60
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.18	0.58
1:A:89:ARG:NH1	1:A:93:GLU:HB3	2.18	0.58
1:A:259:ASN:HD22	1:A:259:ASN:N	2.01	0.58
1:D:103:LEU:HD23	1:D:107:ARG:HH12	1.70	0.57
1:D:100:VAL:CG1	1:D:255:LYS:HD2	2.35	0.56
1:A:268:LYS:HE2	4:A:605:HOH:O	2.06	0.56
4:D:422:HOH:O	2:E:149:THR:HG21	2.04	0.56
1:A:268:LYS:O	1:A:268:LYS:NZ	2.39	0.56
1:D:100:VAL:HG11	1:D:255:LYS:HD2	1.87	0.56
1:A:215:PHE:O	1:A:216:ASN:HB2	2.06	0.55
1:A:263:ASP:O	1:A:267:GLN:HB3	2.07	0.55
1:D:306:GLN:NE2	4:D:352:HOH:O	2.40	0.55
1:D:207:GLU:HA	1:D:207:GLU:OE1	2.07	0.55
2:E:58:ASP:OD2	2:E:61:ILE:HD11	2.08	0.54
1:A:108:LYS:O	1:A:112:GLU:HG3	2.07	0.53
1:A:274:LYS:HD2	1:A:274:LYS:C	2.33	0.53
2:B:126:ILE:HD11	2:B:187:ILE:CD1	2.38	0.53
2:B:180:GLU:H	2:B:180:GLU:CD	2.16	0.52
2:E:154:VAL:HG23	2:E:170:ILE:O	2.10	0.52
1:D:107:ARG:HE	1:D:216:ASN:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG21	1:A:255:LYS:HG2	1.93	0.51
1:D:68:LYS:O	1:D:72:THR:HG23	2.10	0.51
1:D:68:LYS:O	1:D:68:LYS:HE3	2.12	0.50
1:D:32:ILE:HD13	1:D:295:LEU:HG	1.93	0.49
1:A:103:LEU:HA	1:A:106:GLN:OE1	2.12	0.48
1:A:252:PHE:C	1:A:252:PHE:CD1	2.91	0.48
2:E:58:ASP:CG	2:E:61:ILE:HD11	2.37	0.48
2:E:187:ILE:HG23	2:E:188:PRO:HD2	1.95	0.48
1:A:266:ILE:O	1:A:270:VAL:HG23	2.13	0.48
1:D:52:PHE:C	1:D:52:PHE:CD1	2.92	0.48
1:D:56:LEU:HD13	1:D:306:GLN:HG2	1.95	0.47
2:B:90:GLY:HA2	4:B:325:HOH:O	2.15	0.47
1:A:289:ARG:O	1:A:293:GLU:HG3	2.14	0.47
2:E:124:ILE:CD1	2:E:189:VAL:HG22	2.44	0.47
2:E:146:PRO:O	2:E:147:GLU:HB2	2.14	0.47
1:A:122:ALA:HB2	1:A:280:LYS:HG2	1.97	0.47
1:A:211:LEU:HD21	1:A:269:SER:HB2	1.95	0.46
1:A:269:SER:O	1:A:272:THR:N	2.49	0.46
4:D:341:HOH:O	2:E:98:LYS:HD2	2.16	0.46
2:E:221:ILE:HG22	2:E:222:PHE:N	2.29	0.46
2:E:167:GLN:OE1	2:E:169:LYS:NZ	2.45	0.46
2:B:48:ASN:O	2:B:51:VAL:HG23	2.16	0.45
2:B:88:ARG:HG3	2:B:89:VAL:N	2.31	0.45
1:A:100:VAL:HG12	1:A:252:PHE:CE2	2.52	0.45
2:E:126:ILE:HD11	2:E:187:ILE:HD12	1.98	0.45
1:A:58:LYS:HB3	1:A:58:LYS:HE3	1.86	0.45
1:D:32:ILE:HD11	1:D:294:LYS:HD3	1.99	0.45
1:D:261:LYS:HE3	1:D:261:LYS:HB2	1.60	0.44
1:A:257:PHE:HD2	1:A:274:LYS:HG2	1.81	0.44
2:E:154:VAL:HG12	2:E:203:VAL:HB	2.00	0.43
1:A:210:ASN:ND2	1:A:269:SER:OG	2.51	0.43
1:A:270:VAL:O	1:A:274:LYS:HB2	2.19	0.43
2:E:154:VAL:HG22	2:E:155:TYR:N	2.34	0.43
1:A:115:GLN:O	1:A:118:ALA:HB3	2.19	0.43
2:E:126:ILE:CD1	2:E:187:ILE:HD12	2.49	0.43
1:A:204:PHE:C	1:A:204:PHE:CD1	2.97	0.42
1:D:105:VAL:HG13	1:D:228:LEU:HD21	2.01	0.42
2:B:126:ILE:HD11	2:B:187:ILE:HD11	2.02	0.42
1:A:24:ASP:O	1:A:25:ASN:HB2	2.20	0.42
1:A:94:LYS:HB2	1:A:94:LYS:HE2	1.81	0.42
2:E:171:LEU:HG	4:E:292:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:LYS:HB2	2:B:122:LYS:NZ	2.35	0.41
1:A:201:SER:HA	2:E:188:PRO:HG2	2.02	0.41
2:B:29:VAL:O	2:B:67:TYR:HA	2.21	0.41
1:A:4:TYR:CD1	1:A:4:TYR:C	2.98	0.41
1:A:278:ASN:ND2	1:A:289:ARG:NH2	2.69	0.41
2:E:128:ILE:HD12	2:E:170:ILE:HD12	2.02	0.41
2:E:128:ILE:HD12	2:E:170:ILE:CD1	2.51	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	238/258 (92%)	225 (94%)	10 (4%)	3 (1%)	9	3
1	D	236/258 (92%)	234 (99%)	2 (1%)	0	100	100
2	B	197/229 (86%)	185 (94%)	11 (6%)	1 (0%)	24	16
2	E	197/229 (86%)	182 (92%)	15 (8%)	0	100	100
All	All	868/974 (89%)	826 (95%)	38 (4%)	4 (0%)	24	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	264	GLN
2	B	90	GLY
1	A	270	VAL

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	223/236 (94%)	202 (91%)	21 (9%)	8	3
1	D	222/236 (94%)	208 (94%)	14 (6%)	16	9
2	B	185/209 (88%)	170 (92%)	15 (8%)	11	5
2	E	186/209 (89%)	169 (91%)	17 (9%)	9	4
All	All	816/890 (92%)	749 (92%)	67 (8%)	10	5

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	9	GLU
1	A	34	LYS
1	A	58	LYS
1	A	64	GLN
1	A	71	GLU
1	A	78	ASN
1	A	94	LYS
1	A	103	LEU
1	A	108	LYS
1	A	259	ASN
1	A	265	SER
1	A	268	LYS
1	A	272	THR
1	A	274	LYS
1	A	280	LYS
1	A	289	ARG
1	A	293	GLU
1	A	294	LYS
1	A	317	MET
1	A	320	LEU
2	B	19	THR
2	B	51	VAL
2	B	79	ASN

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Mol	Chain	Res	Type
2	B	88	ARG
2	B	92	LYS
2	B	98	LYS
2	B	115	LEU
2	B	116	ASP
2	B	122	LYS
2	B	132	SER
2	B	148	THR
2	B	154	VAL
2	B	165	GLU
2	B	191	SER
2	B	216	GLU
1	D	6	LYS
1	D	39	GLU
1	D	52	PHE
1	D	55	LYS
1	D	58	LYS
1	D	67	GLN
1	D	68	LYS
1	D	71	GLU
1	D	72	THR
1	D	78	ASN
1	D	103	LEU
1	D	262	ASP
1	D	265	SER
1	D	267	GLN
2	E	38	GLN
2	E	51	VAL
2	E	61	ILE
2	E	115	LEU
2	E	124	ILE
2	E	132	SER
2	E	161	MET
2	E	166	ILE
2	E	169	LYS
2	E	171	LEU
2	E	178	CYS
2	E	183	CYS
2	E	184	GLN
2	E	194	SER
2	E	213	LYS
2	E	216	GLU

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Mol	Chain	Res	Type
2	E	221	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	210	ASN
1	A	259	ASN
1	A	304	ASN
2	B	38	GLN
2	B	182	GLN
1	D	259	ASN
1	D	304	ASN
1	D	306	GLN
2	E	184	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.