



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:37 AM EDT

PDB ID : 4FZQ / pdb_00004fzq
Title : Crystal structure of HP0197-G5
Authors : Yuan, Z.; Yan, X.
Deposited on : 2012-07-07
Resolution : 2.50 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

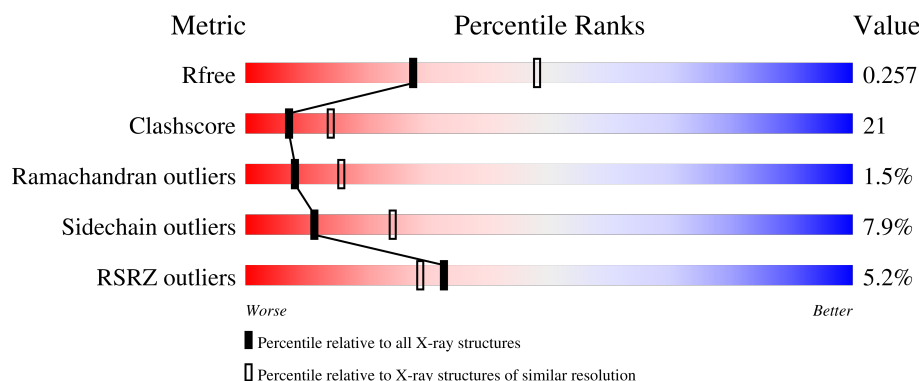
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	79	0% 62% 30% 8%
1	B	79	3% 67% 25% 6%
1	C	79	4% 71% 27%
1	D	79	4% 61% 28% 8%
1	E	79	13% 57% 30% 8%

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Mol	Chain	Length	Quality of chain
1	F	79	6% 61% 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3943 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 Uncharacterized protein conserved in bacteria.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	0	0	0
			616	389	102	124	1			
1	B	78	Total	C	N	O	S	0	0	0
			606	384	101	120	1			
1	C	79	Total	C	N	O	S	0	0	0
			616	389	102	124	1			
1	D	76	Total	C	N	O	S	0	0	0
			592	375	99	117	1			
1	E	76	Total	C	N	O	S	0	0	0
			592	375	99	117	1			
1	F	76	Total	C	N	O	S	0	0	0
			592	375	99	117	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	SER	-	expression tag	UNP A4VZ16
A	416	GLU	-	expression tag	UNP A4VZ16
A	470	MET	VAL	engineered mutation	UNP A4VZ16
B	415	SER	-	expression tag	UNP A4VZ16
B	416	GLU	-	expression tag	UNP A4VZ16
B	470	MET	VAL	engineered mutation	UNP A4VZ16
C	415	SER	-	expression tag	UNP A4VZ16
C	416	GLU	-	expression tag	UNP A4VZ16
C	470	MET	VAL	engineered mutation	UNP A4VZ16
D	415	SER	-	expression tag	UNP A4VZ16
D	416	GLU	-	expression tag	UNP A4VZ16
D	470	MET	VAL	engineered mutation	UNP A4VZ16
E	415	SER	-	expression tag	UNP A4VZ16
E	416	GLU	-	expression tag	UNP A4VZ16
E	470	MET	VAL	engineered mutation	UNP A4VZ16
F	416	SER	-	expression tag	UNP A4VZ16
F	417	GLU	-	expression tag	UNP A4VZ16

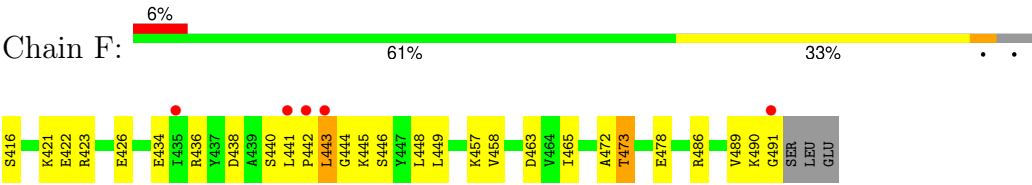
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Chain	Residue	Modelled	Actual	Comment	Reference
F	471	MET	VAL	engineered mutation	UNP A4VZ16

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	58	Total O 58 58	0	0
2	C	25	Total O 25 25	0	0
2	D	53	Total O 53 53	0	0
2	E	51	Total O 51 51	0	0
2	F	76	Total O 76 76	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.59Å 114.59Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 2.50 34.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.88-2.50) 97.7 (34.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.255 , 0.278 0.256 , 0.257	Depositor DCC
R_{free} test set	1507 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3943	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.45	0/621	0.95	1/832 (0.1%)
1	B	0.45	0/611	0.94	3/820 (0.4%)
1	C	0.41	0/621	0.91	1/832 (0.1%)
1	D	0.42	0/597	0.93	1/801 (0.1%)
1	E	0.37	0/597	1.12	3/801 (0.4%)
1	F	0.44	0/597	0.90	1/801 (0.1%)
All	All	0.42	0/3644	0.96	10/4887 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	437	ASP	N-CA-C	12.94	125.06	107.73
1	E	438	ALA	N-CA-C	-8.48	92.74	110.80
1	E	436	TYR	N-CA-C	8.08	124.94	114.75
1	A	485	ARG	N-CA-C	-6.91	97.99	109.46
1	D	481	GLU	N-CA-C	6.55	124.74	110.80
1	B	485	ARG	N-CA-C	-6.29	99.02	109.46
1	F	486	ARG	N-CA-C	-5.64	99.99	108.96
1	B	416	GLU	N-CA-C	-5.44	101.99	110.42
1	B	463	VAL	N-CA-C	-5.42	100.53	108.11
1	C	485	ARG	N-CA-C	-5.21	100.68	108.96

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	616	0	642	27	0
1	B	606	0	636	22	0
1	C	616	0	642	21	0
1	D	592	0	620	29	0
1	E	592	0	620	38	0
1	F	592	0	620	23	0
2	A	66	0	0	2	0
2	B	58	0	0	0	0
2	C	25	0	0	1	0
2	D	53	0	0	0	0
2	E	51	0	0	2	0
2	F	76	0	0	1	0
All	All	3943	0	3780	154	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 (154) 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:433:GLU:HB3	1:A:486:ILE:HD12	1.42	1.01
1:B:449:GLN:HB3	1:B:486:ILE:HD13	1.46	0.95
1:A:425:GLU:HG2	1:A:457:VAL:HG22	1.49	0.95
1:D:473:ASN:HD21	1:E:417:PHE:H	1.20	0.90
1:D:430:ILE:H	1:D:430:ILE:HD13	1.36	0.89
1:B:425:GLU:HG2	1:B:457:VAL:HG22	1.54	0.88
1:F:443:LEU:H	1:F:443:LEU:HD23	1.41	0.82
1:E:451:GLY:HA2	1:E:483:GLN:HG3	1.60	0.82
1:A:434:ILE:HD13	1:A:487:LEU:HB3	1.64	0.80
1:E:451:GLY:H	1:E:483:GLN:HE21	1.31	0.78
1:C:464:ILE:HD13	1:C:469:VAL:HA	1.66	0.76
1:A:447:LEU:HD12	1:A:447:LEU:O	1.86	0.74
1:A:462:ASP:OD2	1:A:472:THR:HB	1.87	0.74
1:D:432:GLU:HG2	1:D:485:ARG:HB3	1.71	0.73
1:E:462:ASP:OD1	1:E:472:THR:HB	1.89	0.71
1:D:420:LYS:HG2	1:D:464:ILE:HD11	1.74	0.69
1:D:433:GLU:HB3	1:D:486:ILE:HD12	1.74	0.69
1:B:485:ARG:C	1:B:486:ILE:HD12	2.19	0.68
1:D:442:LEU:HD23	1:D:443:GLY:N	2.07	0.68
1:D:430:ILE:H	1:D:430:ILE:CD1	2.08	0.67
1:E:462:ASP:HB3	1:E:469:VAL:HG13	1.77	0.66
1:B:449:GLN:CB	1:B:486:ILE:HD13	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:LYS:HE3	1:F:478:GLU:CD	2.21	0.66
1:E:449:GLN:HB3	1:E:486:ILE:HD13	1.76	0.66
1:D:433:GLU:HB3	1:D:486:ILE:CD1	2.27	0.65
1:E:442:LEU:HD11	2:E:521:HOH:O	1.96	0.65
1:F:463:ASP:OD2	1:F:473:THR:HB	1.95	0.65
1:A:442:LEU:H	1:A:442:LEU:HD23	1.63	0.64
1:C:448:LEU:HD23	1:C:486:ILE:HG21	1.78	0.64
1:B:430:ILE:HD11	1:B:453:ALA:HB2	1.78	0.64
1:C:437:ASP:HB2	1:C:488:VAL:CG1	2.28	0.63
1:E:449:GLN:CB	1:E:486:ILE:HD13	2.28	0.63
1:E:438:ALA:HB3	1:E:440:LEU:HD11	1.79	0.62
1:D:417:PHE:CE2	1:E:463:VAL:HG23	2.35	0.61
1:D:425:GLU:HG2	1:D:457:VAL:HG22	1.81	0.61
1:D:448:LEU:HD23	1:D:448:LEU:O	2.01	0.61
1:A:425:GLU:OE1	1:A:455:LYS:HD3	2.01	0.60
1:F:449:LEU:HG	1:F:489:VAL:HG23	1.82	0.60
1:E:489:LYS:HD3	1:E:490:GLY:N	2.15	0.60
1:A:434:ILE:HD12	1:A:487:LEU:HD23	1.83	0.60
1:D:473:ASN:HD21	1:E:417:PHE:N	1.97	0.60
1:E:435:ARG:HB2	1:E:488:VAL:HG22	1.82	0.60
1:A:420:LYS:HE3	1:A:464:ILE:HD11	1.83	0.60
1:E:434:ILE:H	1:E:434:ILE:HD13	1.66	0.60
1:A:423:LYS:NZ	1:A:423:LYS:HB2	2.17	0.60
1:D:485:ARG:O	1:D:486:ILE:HD13	2.01	0.60
1:E:434:ILE:O	1:E:434:ILE:HG12	2.02	0.59
1:E:464:ILE:HD11	1:E:469:VAL:HG22	1.83	0.59
1:C:465:VAL:HB	1:C:470:MET:HE3	1.83	0.59
1:D:432:GLU:HG3	1:D:485:ARG:HD3	1.84	0.59
1:E:486:ILE:HD12	1:E:486:ILE:N	2.19	0.58
1:B:486:ILE:HD12	1:B:486:ILE:N	2.18	0.58
1:A:434:ILE:CD1	1:A:487:LEU:HD23	2.34	0.58
1:E:464:ILE:HD13	1:E:469:VAL:HA	1.85	0.58
1:A:442:LEU:HG	1:A:443:GLY:N	2.18	0.57
1:F:442:PRO:HG2	1:F:445:LYS:HG3	1.87	0.57
1:D:462:ASP:OD1	1:D:472:THR:HB	2.05	0.57
1:F:441:LEU:HD11	1:F:490:LYS:O	2.05	0.57
1:A:452:LYS:H	1:A:483:GLN:HB3	1.69	0.56
1:B:468:LYS:HD2	1:B:468:LYS:N	2.19	0.56
1:B:435:ARG:HB2	1:B:488:VAL:HG12	1.87	0.56
1:E:440:LEU:H	1:E:440:LEU:HD12	1.71	0.56
1:E:438:ALA:HB3	1:E:440:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:GLN:HB3	1:E:486:ILE:CD1	2.36	0.55
1:D:430:ILE:HD13	1:D:430:ILE:N	2.16	0.55
1:B:467:GLY:C	1:B:468:LYS:HD2	2.32	0.55
1:C:449:GLN:HB3	1:C:486:ILE:HG12	1.88	0.54
1:D:464:ILE:HD12	1:D:464:ILE:N	2.23	0.53
1:E:450:GLU:HG2	2:E:540:HOH:O	2.08	0.53
1:A:434:ILE:CD1	1:A:487:LEU:HB3	2.36	0.53
1:E:484:ASN:O	1:E:486:ILE:HD12	2.08	0.53
1:C:432:GLU:OE1	1:C:485:ARG:HD3	2.09	0.52
1:C:442:LEU:HD23	1:C:491:SER:HB3	1.92	0.52
1:A:442:LEU:HG	1:A:443:GLY:H	1.75	0.52
1:F:441:LEU:HD12	1:F:442:PRO:O	2.10	0.52
1:E:437:ASP:HB3	1:E:439:SER:H	1.74	0.51
1:C:450:GLU:H	1:C:450:GLU:CD	2.18	0.51
1:A:485:ARG:C	1:A:486:ILE:HD13	2.35	0.51
1:A:461:GLN:NE2	2:A:527:HOH:O	2.42	0.51
1:B:423:LYS:HE2	1:B:425:GLU:OE2	2.11	0.51
1:A:485:ARG:HD2	2:A:519:HOH:O	2.12	0.50
1:E:449:GLN:HG2	1:E:483:GLN:NE2	2.25	0.50
1:F:449:LEU:HG	1:F:489:VAL:CG2	2.41	0.50
1:F:465:ILE:HD12	1:F:465:ILE:N	2.27	0.50
1:E:464:ILE:HD11	1:E:469:VAL:CG2	2.42	0.49
1:F:423:ARG:HD3	1:F:463:ASP:OD1	2.12	0.49
1:C:440:LEU:HD22	1:C:444:LYS:HG3	1.94	0.49
1:D:463:VAL:HG21	1:E:463:VAL:HG11	1.95	0.49
1:C:449:GLN:HG2	1:C:483:GLN:HE21	1.77	0.48
1:D:437:ASP:O	1:D:490:GLY:HA2	2.12	0.48
1:F:436:ARG:O	1:F:489:VAL:HA	2.14	0.48
1:E:449:GLN:CD	1:E:486:ILE:HD13	2.39	0.48
1:C:450:GLU:CD	1:C:450:GLU:N	2.72	0.48
1:D:452:LYS:HB3	1:D:483:GLN:H	1.80	0.47
1:B:434:ILE:HD12	1:B:434:ILE:N	2.30	0.47
1:B:462:ASP:OD2	1:B:472:THR:HB	2.15	0.47
1:D:442:LEU:HD23	1:D:442:LEU:C	2.40	0.47
1:E:418:THR:HG23	1:E:464:ILE:HB	1.96	0.47
1:E:455:LYS:HG3	1:E:480:VAL:HB	1.97	0.47
1:E:464:ILE:HD13	1:E:469:VAL:CA	2.45	0.47
1:F:438:ASP:CG	1:F:440:SER:HB3	2.39	0.47
1:C:449:GLN:NE2	1:C:483:GLN:HG2	2.30	0.47
1:B:430:ILE:CD1	1:B:453:ALA:HB2	2.45	0.47
1:B:461:GLN:O	1:B:472:THR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:LEU:HD12	1:E:440:LEU:N	2.29	0.47
1:F:446:SER:OG	1:F:490:LYS:HG3	2.14	0.47
1:D:448:LEU:HB2	1:D:488:VAL:HG23	1.98	0.46
1:F:438:ASP:OD2	1:F:440:SER:HB3	2.14	0.46
1:A:424:VAL:HG22	1:D:426:GLU:HG2	1.97	0.46
1:C:449:GLN:HE21	1:C:483:GLN:HG2	1.81	0.46
1:D:463:VAL:O	1:D:463:VAL:HG13	2.15	0.46
1:B:448:LEU:HD11	1:B:488:VAL:CG1	2.45	0.46
1:B:486:ILE:N	1:B:486:ILE:CD1	2.79	0.45
1:C:450:GLU:O	1:C:485:ARG:NH1	2.49	0.45
1:F:416:SER:HB3	2:F:555:HOH:O	2.15	0.45
1:A:423:LYS:HB2	1:A:423:LYS:HZ2	1.81	0.45
1:A:441:PRO:HD2	1:A:444:LYS:CB	2.47	0.45
1:A:465:VAL:HG12	1:A:466:ASP:OD2	2.15	0.45
1:D:463:VAL:CG1	1:D:471:ALA:HB3	2.47	0.45
1:F:443:LEU:H	1:F:443:LEU:CD2	2.19	0.45
1:C:442:LEU:CD2	1:C:491:SER:HB3	2.47	0.44
1:E:451:GLY:H	1:E:483:GLN:NE2	2.07	0.44
1:C:464:ILE:HD13	1:C:469:VAL:CA	2.41	0.44
1:F:490:LYS:HB3	1:F:491:GLY:H	1.49	0.44
1:C:440:LEU:HD11	1:C:446:TYR:HE1	1.82	0.44
1:A:447:LEU:HD12	1:A:447:LEU:C	2.43	0.44
1:E:434:ILE:HD13	1:E:434:ILE:N	2.31	0.44
1:C:440:LEU:HD11	1:C:446:TYR:CE1	2.53	0.43
1:F:441:LEU:HD12	1:F:441:LEU:C	2.43	0.43
1:A:425:GLU:CD	1:A:455:LYS:HD3	2.43	0.43
1:A:442:LEU:H	1:A:442:LEU:CD2	2.31	0.43
1:B:449:GLN:OE1	1:B:486:ILE:CD1	2.67	0.43
1:E:486:ILE:HD12	1:E:486:ILE:H	1.84	0.42
1:F:448:LEU:C	1:F:448:LEU:HD13	2.45	0.42
1:E:437:ASP:CB	1:E:439:SER:H	2.31	0.42
1:B:448:LEU:HG	1:B:488:VAL:HG13	2.00	0.42
1:F:446:SER:HA	1:F:489:VAL:O	2.20	0.42
1:B:448:LEU:HD11	1:B:488:VAL:HG11	2.02	0.42
1:C:449:GLN:CG	1:C:483:GLN:HE21	2.33	0.41
1:C:445:SER:HB3	1:C:489:LYS:HB3	2.02	0.41
1:D:432:GLU:CG	1:D:485:ARG:HD3	2.48	0.41
1:F:434:GLU:OE2	1:F:436:ARG:HD3	2.20	0.41
1:D:423:LYS:HB3	1:D:423:LYS:HE2	1.78	0.41
1:B:444:LYS:HE3	1:B:446:TYR:CZ	2.55	0.41
1:C:429:PRO:HA	2:C:502:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:PHE:CZ	1:E:463:VAL:HG23	2.56	0.41
1:F:472:ALA:C	1:F:473:THR:HG22	2.46	0.41
1:A:440:LEU:HD21	1:A:446:TYR:CE1	2.55	0.40
1:D:475:LEU:HD12	1:D:475:LEU:HA	1.95	0.40
1:A:441:PRO:O	1:A:490:GLY:HA3	2.21	0.40
1:B:475:LEU:HD12	1:B:475:LEU:HA	1.94	0.40
1:B:433:GLU:C	1:B:434:ILE:HD12	2.46	0.40
1:F:426:GLU:HG2	1:F:458:VAL:HG22	2.03	0.40
1:E:434:ILE:HA	1:E:487:LEU:O	2.21	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	77/79 (98%)	73 (95%)	2 (3%)	2 (3%)	4	7
1	B	76/79 (96%)	76 (100%)	0	0	100	100
1	C	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
1	D	74/79 (94%)	72 (97%)	1 (1%)	1 (1%)	9	17
1	E	74/79 (94%)	66 (89%)	5 (7%)	3 (4%)	2	3
1	F	74/79 (94%)	70 (95%)	3 (4%)	1 (1%)	9	17
All	All	452/474 (95%)	430 (95%)	15 (3%)	7 (2%)	8	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	438	ALA
1	E	441	PRO
1	D	481	GLU

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Mol	Chain	Res	Type
1	F	444	GLY
1	A	441	PRO
1	E	442	LEU
1	A	451	GLY

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	69/69 (100%)	63 (91%)	6 (9%)	9	21
1	B	68/69 (99%)	62 (91%)	6 (9%)	9	20
1	C	69/69 (100%)	66 (96%)	3 (4%)	26	51
1	D	66/69 (96%)	60 (91%)	6 (9%)	9	19
1	E	66/69 (96%)	59 (89%)	7 (11%)	6	14
1	F	66/69 (96%)	62 (94%)	4 (6%)	17	35
All	All	404/414 (98%)	372 (92%)	32 (8%)	11	24

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	423	LYS
1	A	444	LYS
1	A	448	LEU
1	A	472	THR
1	A	475	LEU
1	A	486	ILE
1	B	423	LYS
1	B	440	LEU
1	B	470	MET
1	B	472	THR
1	B	475	LEU
1	B	486	ILE
1	C	415	SER
1	C	450	GLU

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Mol	Chain	Res	Type
1	C	475	LEU
1	D	415	SER
1	D	426	GLU
1	D	430	ILE
1	D	432	GLU
1	D	472	THR
1	D	475	LEU
1	E	418	THR
1	E	434	ILE
1	E	447	LEU
1	E	448	LEU
1	E	455	LYS
1	E	472	THR
1	E	475	LEU
1	F	421	LYS
1	F	422	GLU
1	F	443	LEU
1	F	473	THR

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	449	GLN
1	A	461	GLN
1	C	449	GLN
1	C	461	GLN
1	C	483	GLN
1	D	449	GLN
1	D	473	ASN
1	D	483	GLN
1	E	483	GLN
1	F	450	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	79/79 (100%)	0.31	1 (1%) 75 71	21, 34, 62, 90	0
1	B	78/79 (98%)	0.12	2 (2%) 57 52	18, 34, 55, 60	0
1	C	79/79 (100%)	0.49	3 (3%) 44 39	19, 40, 75, 99	0
1	D	76/79 (96%)	0.41	3 (3%) 43 38	18, 39, 70, 76	0
1	E	76/79 (96%)	1.00	10 (13%) 7 6	29, 49, 90, 104	0
1	F	76/79 (96%)	0.41	5 (6%) 24 21	17, 37, 75, 113	0
All	All	464/474 (97%)	0.45	24 (5%) 33 29	17, 39, 72, 113	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	442	LEU	6.1
1	F	443	LEU	6.1
1	E	438	ALA	5.3
1	F	491	GLY	5.2
1	E	490	GLY	5.1
1	F	441	LEU	4.7
1	E	442	LEU	4.5
1	E	436	TYR	4.1
1	F	435	ILE	3.8
1	C	442	LEU	3.5
1	D	448	LEU	3.3
1	E	439	SER	3.1
1	E	437	ASP	3.0
1	C	490	GLY	3.0
1	D	450	GLU	2.9
1	E	434	ILE	2.7
1	B	492	LEU	2.7
1	D	490	GLY	2.7
1	C	469	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	451	GLY	2.5
1	E	489	LYS	2.4
1	B	415	SER	2.2
1	E	426	GLU	2.0
1	F	442	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.