



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 PM UTC

PDB ID : 2GEF / pdb_00002gef
Title : Crystal structure of a Novel viral protease with a serine/lysine catalytic dyad mechanism
Authors : Paetzel, M.; Feldman, A.R.; Lee, J.; Delmas, B.
Deposited on : 2006-03-20
Resolution : 2.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

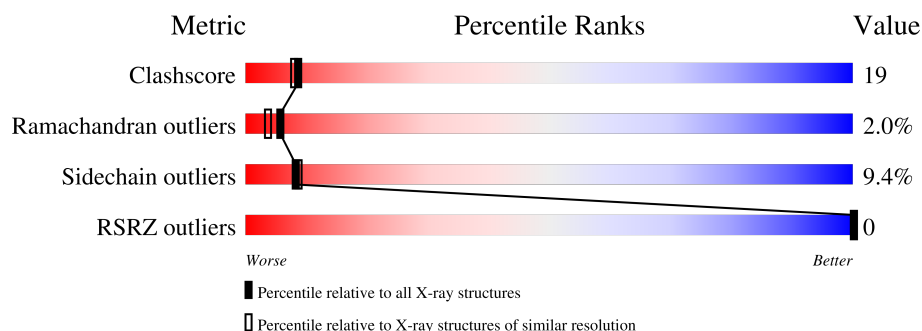
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	217	
1	B	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3285 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 Protease VP4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	Se	0	0	0
			1488	935	258	289	2	4			
1	B	203	Total	C	N	O	S	Se	0	0	0
			1519	954	263	296	2	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	557	MET	-	initiating methionine	UNP Q8AZM0
A	615	MSE	MET	modified residue	UNP Q8AZM0
A	685	MSE	MET	modified residue	UNP Q8AZM0
A	743	MSE	MET	modified residue	UNP Q8AZM0
A	767	MSE	MET	modified residue	UNP Q8AZM0
B	557	MET	-	initiating methionine	UNP Q8AZM0
B	615	MSE	MET	modified residue	UNP Q8AZM0
B	685	MSE	MET	modified residue	UNP Q8AZM0
B	743	MSE	MET	modified residue	UNP Q8AZM0
B	767	MSE	MET	modified residue	UNP Q8AZM0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	162	Total	O	0	0
			162	162		
2	B	116	Total	O	0	0
			116	116		

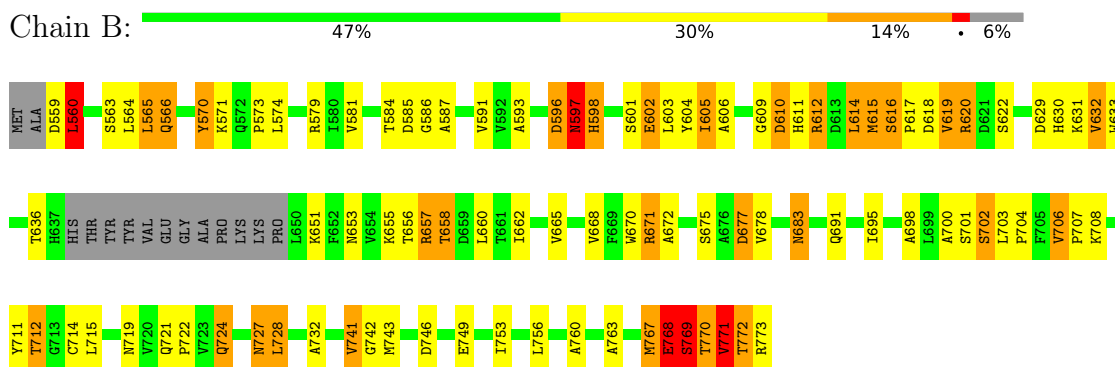
3 Residue-property plots

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: Protease VP4



• Molecule 1: Protease VP4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	144.07 Å 144.07 Å 144.07 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.41 – 2.20 29.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.41-2.20) 99.9 (29.41-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.15 (at 2.20 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.267 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.329 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3285	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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	2.16	43/1516 (2.8%)	1.76	37/2060 (1.8%)
1	B	1.92	36/1547 (2.3%)	1.81	33/2104 (1.6%)
All	All	2.04	79/3063 (2.6%)	1.79	70/4164 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	695	ILE	CA-CB	-11.47	1.41	1.54
1	B	597	ASN	N-CA	11.20	1.60	1.46
1	B	632	VAL	CA-CB	9.85	1.64	1.53
1	A	562	ILE	CA-CB	9.83	1.66	1.54
1	B	770	THR	C-O	8.66	1.34	1.24
1	A	607	VAL	N-CA	8.39	1.56	1.46
1	B	606	ALA	CA-C	8.01	1.62	1.52
1	B	763	ALA	CA-CB	-7.92	1.41	1.53
1	B	770	THR	CB-OG1	7.66	1.56	1.43
1	B	620	ARG	N-CA	7.56	1.55	1.46
1	A	653	ASN	CA-C	7.50	1.62	1.52
1	A	731	ARG	C-O	-7.47	1.15	1.24
1	B	770	THR	CA-C	7.24	1.62	1.52
1	A	589	PHE	CA-C	7.23	1.60	1.52
1	B	610	ASP	CA-CB	7.12	1.61	1.52
1	A	601	SER	C-O	7.12	1.32	1.23
1	A	736	ILE	C-O	-6.97	1.15	1.24
1	A	590	PRO	CA-C	-6.96	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	722	PRO	CA-C	6.73	1.61	1.52
1	A	570	TYR	CZ-OH	6.60	1.51	1.38
1	A	681	VAL	CA-CB	6.55	1.64	1.54
1	B	770	THR	N-CA	6.50	1.54	1.46
1	B	706	VAL	CA-CB	6.46	1.60	1.53
1	A	705	PHE	C-O	6.39	1.31	1.23
1	A	690	GLY	C-O	6.36	1.32	1.23
1	A	760	ALA	CA-CB	6.33	1.63	1.53
1	A	665	VAL	CA-C	6.24	1.60	1.52
1	A	570	TYR	CA-CB	6.22	1.62	1.53
1	A	623	TYR	C-O	6.09	1.31	1.23
1	A	600	THR	C-O	-6.01	1.16	1.23
1	A	765	ASP	C-O	5.98	1.31	1.24
1	A	592	VAL	CA-C	5.97	1.60	1.52
1	B	570	TYR	CA-C	5.93	1.60	1.52
1	B	593	ALA	CA-C	5.92	1.59	1.52
1	B	560	LEU	N-CA	-5.89	1.40	1.45
1	B	662	ILE	N-CA	5.89	1.53	1.46
1	B	772	THR	CA-C	5.81	1.60	1.52
1	A	611	HIS	CA-C	-5.74	1.45	1.53
1	B	770	THR	C-N	5.65	1.41	1.33
1	B	602	GLU	N-CA	5.59	1.53	1.45
1	B	603	LEU	CA-C	5.57	1.59	1.52
1	A	657	ARG	CA-C	5.52	1.61	1.52
1	A	656	THR	CA-CB	-5.51	1.45	1.54
1	B	695	ILE	CA-CB	5.50	1.61	1.54
1	B	605	ILE	N-CA	5.49	1.52	1.46
1	A	605	ILE	C-O	-5.45	1.18	1.24
1	A	691	GLN	CA-CB	5.43	1.61	1.53
1	B	741	VAL	N-CA	-5.43	1.39	1.46
1	A	737	GLY	N-CA	5.40	1.53	1.45
1	A	577	ASN	CA-C	5.38	1.60	1.53
1	A	636	THR	CA-CB	5.37	1.66	1.53
1	A	606	ALA	CA-CB	-5.36	1.45	1.53
1	A	666	ALA	C-O	-5.35	1.17	1.24
1	A	664	PRO	C-O	-5.34	1.18	1.23
1	A	585	ASP	C-O	-5.29	1.17	1.23
1	B	763	ALA	CA-C	5.29	1.59	1.52
1	A	759	ALA	C-O	-5.28	1.18	1.24
1	B	698	ALA	CA-CB	-5.27	1.44	1.53
1	A	597	ASN	N-CA	5.26	1.52	1.46
1	B	712	THR	CA-C	5.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	560	LEU	CA-CB	5.26	1.60	1.54
1	A	695	ILE	N-CA	-5.21	1.40	1.46
1	B	707	PRO	C-O	5.20	1.29	1.23
1	B	587	ALA	CA-CB	5.19	1.63	1.53
1	A	606	ALA	C-O	5.19	1.30	1.24
1	A	594	PHE	N-CA	5.18	1.52	1.46
1	A	672	ALA	N-CA	5.18	1.52	1.46
1	B	701	SER	C-O	5.17	1.30	1.24
1	A	656	THR	CB-CG2	5.17	1.69	1.52
1	B	708	LYS	CA-C	5.14	1.59	1.53
1	A	603	LEU	CA-C	-5.10	1.46	1.52
1	B	677	ASP	CA-C	5.08	1.59	1.52
1	A	749	GLU	CA-CB	5.08	1.61	1.53
1	B	614	LEU	CA-C	5.07	1.59	1.52
1	A	654	VAL	CA-CB	5.06	1.59	1.54
1	B	727	ASN	CG-ND2	5.05	1.43	1.33
1	B	566	GLN	CD-NE2	-5.02	1.22	1.33
1	B	591	VAL	N-CA	5.02	1.52	1.46
1	B	596	ASP	C-O	-5.01	1.17	1.23

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	769	SER	N-CA-C	9.44	130.91	110.80
1	B	770	THR	N-CA-C	9.07	130.13	110.80
1	A	683	ASN	N-CA-C	-9.05	95.24	109.72
1	A	596	ASP	N-CA-C	-9.02	98.08	110.35
1	B	616	SER	CA-C-N	8.98	131.06	119.84
1	B	616	SER	C-N-CA	8.98	131.06	119.84
1	B	596	ASP	N-CA-C	-8.96	97.86	110.50
1	A	578	SER	N-CA-C	8.91	123.24	109.96
1	A	703	LEU	N-CA-C	8.41	120.51	109.83
1	A	562	ILE	CA-C-N	-8.16	111.28	122.30
1	A	562	ILE	C-N-CA	-8.16	111.28	122.30
1	B	721	GLN	CA-C-N	8.15	128.79	119.99
1	B	721	GLN	C-N-CA	8.15	128.79	119.99
1	B	619	VAL	CB-CA-C	8.11	119.72	110.88
1	B	596	ASP	CA-C-N	-7.99	106.28	121.54
1	B	596	ASP	C-N-CA	-7.99	106.28	121.54
1	B	560	LEU	N-CA-C	-7.92	95.30	109.09
1	A	562	ILE	N-CA-C	-7.69	97.36	108.36
1	B	658	THR	N-CA-C	7.69	120.76	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	ASP	O-C-N	-7.59	113.90	122.86
1	B	560	LEU	CB-CA-C	7.35	120.39	109.22
1	A	727	ASN	N-CA-C	7.24	119.80	111.11
1	B	683	ASN	N-CA-C	-7.16	98.70	109.94
1	B	615	MSE	N-CA-C	6.96	119.82	110.35
1	A	620	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	B	653	ASN	N-CA-C	-6.74	103.40	111.69
1	A	673	ASP	N-CA-C	6.69	121.05	113.02
1	B	724	GLN	N-CA-C	-6.66	100.66	110.52
1	B	760	ALA	N-CA-C	-6.51	103.69	111.69
1	B	767	MSE	N-CA-C	-6.26	105.62	113.20
1	A	653	ASN	N-CA-C	6.20	117.71	111.07
1	B	651	LYS	N-CA-C	6.18	118.53	110.43
1	A	574	LEU	N-CA-C	-6.17	100.51	109.59
1	B	598	HIS	N-CA-C	6.07	116.57	108.38
1	B	609	GLY	CA-C-O	-6.02	117.76	122.52
1	A	560	LEU	CB-CA-C	5.94	118.15	109.48
1	A	655	LYS	N-CA-C	-5.85	98.88	108.41
1	A	572	GLN	N-CA-C	-5.76	102.81	110.07
1	B	563	SER	CA-C-N	-5.74	111.82	121.75
1	B	563	SER	C-N-CA	-5.74	111.82	121.75
1	B	712	THR	N-CA-C	-5.73	99.27	108.55
1	A	619	VAL	N-CA-C	5.65	119.07	113.53
1	B	691	GLN	N-CA-C	-5.65	104.61	113.02
1	A	654	VAL	N-CA-C	5.64	117.58	109.51
1	B	610	ASP	N-CA-C	5.61	117.86	107.99
1	A	678	VAL	N-CA-C	-5.60	100.06	108.12
1	B	768	GLU	CA-C-N	5.54	132.13	121.54
1	B	768	GLU	C-N-CA	5.54	132.13	121.54
1	A	598	HIS	N-CA-C	5.53	117.47	109.07
1	A	564	LEU	N-CA-C	5.49	118.51	109.72
1	A	729	LYS	CA-C-O	-5.40	114.80	120.63
1	A	685	MSE	N-CA-C	-5.40	103.12	110.36
1	A	752	ARG	CB-CG-CD	-5.36	98.96	111.30
1	A	609	GLY	N-CA-C	-5.34	104.17	112.45
1	A	610	ASP	CB-CA-C	5.33	118.82	110.19
1	A	764	PHE	N-CA-C	-5.33	105.39	111.14
1	A	721	GLN	N-CA-C	5.26	118.26	110.32
1	A	756	LEU	N-CA-C	5.18	117.66	111.71
1	A	663	LEU	CA-C-N	-5.17	114.59	119.76
1	A	663	LEU	C-N-CA	-5.17	114.59	119.76
1	A	563	SER	CA-CB-OG	-5.16	100.77	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	LEU	CA-CB-CG	5.16	134.36	116.30
1	A	560	LEU	CA-C-N	5.16	125.09	119.78
1	A	560	LEU	C-N-CA	5.16	125.09	119.78
1	B	728	LEU	N-CA-C	5.15	116.89	111.28
1	A	608	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	A	653	ASN	CA-C-N	5.06	127.48	120.49
1	A	653	ASN	C-N-CA	5.06	127.48	120.49
1	B	671	ARG	CA-C-N	5.05	127.56	120.28
1	B	671	ARG	C-N-CA	5.05	127.56	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	636	THR	Peptide
1	B	769	SER	Peptide

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	1488	0	1434	50	0
1	B	1519	0	1461	71	0
2	A	162	0	0	8	0
2	B	116	0	0	9	0
All	All	3285	0	2895	111	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 19.

All (111) 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:573:PRO:HG2	1:B:602:GLU:HG3	1.31	1.12
1:B:722:PRO:HB3	1:B:743:MSE:HE2	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD22	1:B:565:LEU:CD2	1.86	1.05
1:A:565:LEU:HD22	1:B:565:LEU:HD22	1.38	1.05
1:A:752:ARG:NH2	2:A:216:HOH:O	1.89	1.05
1:B:611:HIS:HB3	1:B:614:LEU:HD12	1.34	1.04
1:B:584:THR:HA	1:B:675:SER:HB2	1.40	1.02
1:A:596:ASP:O	1:A:597:ASN:HB3	1.74	0.88
1:B:656:THR:O	1:B:657:ARG:HG2	1.77	0.83
1:B:727:ASN:OD1	2:B:235:HOH:O	1.97	0.81
1:B:559:ASP:HB3	1:B:560:LEU:HD23	1.62	0.80
1:B:596:ASP:O	1:B:597:ASN:CB	2.21	0.77
1:A:565:LEU:HD22	1:B:565:LEU:HD21	1.67	0.75
1:B:668:VAL:HG13	1:B:678:VAL:HG22	1.67	0.75
1:B:671:ARG:NH2	1:B:677:ASP:OD1	2.20	0.74
1:B:573:PRO:HG2	1:B:602:GLU:CG	2.14	0.74
1:B:596:ASP:O	1:B:597:ASN:HB3	1.87	0.73
1:A:745:GLN:HE22	1:B:597:ASN:HA	1.54	0.72
1:A:596:ASP:O	1:A:597:ASN:CB	2.32	0.72
1:A:560:LEU:HB2	1:A:561:PRO:HD2	1.70	0.71
1:A:580:ILE:HD13	1:A:580:ILE:N	2.05	0.71
1:B:584:THR:HA	1:B:675:SER:CB	2.19	0.71
1:B:672:ALA:O	2:B:234:HOH:O	2.09	0.69
1:B:629:ASP:O	2:B:259:HOH:O	2.11	0.68
1:A:651:LYS:CB	2:A:52:HOH:O	2.43	0.67
1:A:615:MSE:HE2	1:A:619:VAL:HG12	1.75	0.67
1:A:615:MSE:CE	1:A:619:VAL:HG12	2.25	0.65
1:A:560:LEU:CD2	2:A:202:HOH:O	2.44	0.65
1:B:722:PRO:CB	1:B:743:MSE:HE2	2.19	0.64
1:B:665:VAL:HG11	1:B:678:VAL:HG11	1.79	0.64
1:A:670:TRP:CE2	1:A:708:LYS:HG2	2.35	0.62
1:A:684:ASP:N	2:A:237:HOH:O	2.07	0.62
1:A:692:SER:HB3	1:A:723:VAL:HG21	1.82	0.62
1:B:656:THR:C	1:B:658:THR:H	2.08	0.61
1:B:614:LEU:HD11	2:B:146:HOH:O	2.00	0.61
1:B:711:TYR:HA	1:B:741:VAL:O	2.00	0.60
1:B:714:CYS:HB3	2:B:64:HOH:O	2.01	0.60
1:A:565:LEU:CD2	1:B:565:LEU:HD22	2.25	0.60
1:B:612:ARG:O	1:B:620:ARG:NE	2.33	0.60
1:B:586:GLY:HA2	1:B:700:ALA:HB1	1.84	0.59
1:B:584:THR:OG1	1:B:585:ASP:OD1	2.21	0.58
1:B:611:HIS:CB	1:B:614:LEU:HD12	2.23	0.58
1:B:772:THR:O	1:B:773:ARG:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:VAL:HG12	1:B:772:THR:H	1.69	0.58
1:B:722:PRO:HB3	1:B:743:MSE:CE	2.21	0.57
1:A:674:GLY:HA2	1:A:767:MSE:CE	2.34	0.56
1:B:574:LEU:O	2:B:62:HOH:O	2.17	0.56
1:A:612:ARG:O	1:A:620:ARG:HD3	2.06	0.55
1:B:630:HIS:HB3	1:B:658:THR:O	2.06	0.55
1:A:741:VAL:HG21	1:A:762:HIS:CE1	2.41	0.55
1:B:656:THR:C	1:B:658:THR:N	2.65	0.55
1:A:571:LYS:HB2	1:A:598:HIS:HD2	1.73	0.54
1:B:570:TYR:CE1	1:B:601:SER:HB3	2.43	0.54
1:B:612:ARG:HA	1:B:615:MSE:SE	2.58	0.54
1:A:668:VAL:HG13	1:A:678:VAL:HG22	1.90	0.54
1:A:566:GLN:HE22	1:B:728:LEU:H	1.54	0.54
1:B:767:MSE:O	1:B:768:GLU:C	2.51	0.54
1:B:749:GLU:O	1:B:749:GLU:HG2	2.07	0.53
1:B:604:TYR:OH	1:B:683:ASN:ND2	2.26	0.52
1:B:771:VAL:HG21	2:B:234:HOH:O	2.10	0.52
1:A:566:GLN:NE2	1:B:728:LEU:H	2.08	0.52
1:B:617:PRO:HA	1:B:620:ARG:HG3	1.92	0.51
1:B:670:TRP:NE1	1:B:706:VAL:O	2.39	0.51
1:A:573:PRO:HG2	1:A:602:GLU:CD	2.36	0.50
1:B:570:TYR:HE1	1:B:601:SER:HB3	1.76	0.50
1:A:573:PRO:HG2	1:A:602:GLU:HG3	1.93	0.49
1:A:615:MSE:HB2	1:A:620:ARG:HG2	1.93	0.49
1:B:605:ILE:HG23	1:B:605:ILE:O	2.13	0.49
1:B:715:LEU:HD21	1:B:756:LEU:HD13	1.94	0.49
1:B:657:ARG:HH22	1:B:702:SER:HB3	1.77	0.49
1:B:727:ASN:HB2	1:B:746:ASP:OD2	2.12	0.49
1:A:561:PRO:HD3	1:B:571:LYS:HE2	1.95	0.49
1:B:631:LYS:HD2	1:B:633:TRP:CZ2	2.48	0.48
1:B:671:ARG:NH1	2:B:75:HOH:O	2.34	0.48
1:B:769:SER:C	1:B:770:THR:HG22	2.38	0.48
1:B:665:VAL:CG1	1:B:678:VAL:HG11	2.42	0.48
1:A:561:PRO:HG3	2:B:80:HOH:O	2.14	0.48
1:A:619:VAL:O	1:A:619:VAL:CG1	2.61	0.47
1:A:685:MSE:HE2	2:A:9:HOH:O	2.14	0.47
1:B:586:GLY:HA2	1:B:700:ALA:CB	2.45	0.47
1:A:683:ASN:OD1	1:A:683:ASN:C	2.58	0.46
1:B:722:PRO:HA	1:B:743:MSE:HB3	1.98	0.45
1:B:616:SER:HA	1:B:617:PRO:HD2	1.77	0.45
1:A:580:ILE:N	1:A:580:ILE:CD1	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PHE:HB3	1:A:696:ALA:HB2	1.99	0.45
1:A:573:PRO:HG2	1:A:602:GLU:CG	2.46	0.44
1:A:582:HIS:CE1	1:A:675:SER:HB2	2.51	0.44
1:B:719:ASN:HD22	1:B:719:ASN:HA	1.57	0.43
1:A:560:LEU:HD21	2:A:202:HOH:O	2.13	0.43
1:A:735:LYS:NZ	2:A:190:HOH:O	2.50	0.43
1:A:560:LEU:CB	1:A:561:PRO:HD2	2.44	0.43
1:A:746:ASP:OD2	1:B:566:GLN:OE1	2.37	0.43
1:A:560:LEU:HD23	1:A:560:LEU:H	1.82	0.43
1:A:610:ASP:O	1:A:610:ASP:OD1	2.36	0.43
1:B:597:ASN:O	1:B:598:HIS:HB3	2.19	0.43
1:A:626:THR:HA	1:A:652:PHE:HB2	2.01	0.42
1:A:619:VAL:HG11	2:A:1:HOH:O	2.20	0.42
1:A:745:GLN:NE2	1:B:597:ASN:HA	2.26	0.42
1:A:582:HIS:HE1	1:A:675:SER:OG	2.02	0.42
1:B:630:HIS:CB	1:B:658:THR:O	2.67	0.41
1:A:734:HIS:NE2	1:A:750:ASP:OD2	2.35	0.41
1:B:656:THR:C	1:B:657:ARG:HG2	2.41	0.41
1:B:601:SER:OG	1:B:732:ALA:HB2	2.20	0.41
1:B:655:LYS:HZ3	1:B:655:LYS:HG3	1.70	0.41
1:A:590:PRO:HB2	1:A:729:LYS:HG2	2.02	0.41
1:B:585:ASP:OD1	1:B:585:ASP:N	2.52	0.41
1:A:657:ARG:NH1	1:A:657:ARG:HG3	2.36	0.41
1:B:703:LEU:HA	1:B:704:PRO:HD3	1.98	0.41
1:B:605:ILE:O	1:B:605:ILE:CG2	2.69	0.40
1:B:712:THR:O	1:B:742:GLY:HA3	2.22	0.40
1:A:743:MSE:HE3	1:A:752:ARG:CZ	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	A	194/217 (89%)	182 (94%)	9 (5%)	3 (2%)	8	6
1	B	199/217 (92%)	181 (91%)	13 (6%)	5 (2%)	4	2
All	All	393/434 (91%)	363 (92%)	22 (6%)	8 (2%)	6	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	GLU
1	B	768	GLU
1	B	769	SER
1	B	771	VAL
1	A	597	ASN
1	B	597	ASN
1	A	672	ALA
1	B	612	ARG

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	158/173 (91%)	145 (92%)	13 (8%)	10	12
1	B	161/173 (93%)	144 (89%)	17 (11%)	6	6
All	All	319/346 (92%)	289 (91%)	30 (9%)	8	9

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	560	LEU
1	A	563	SER
1	A	564	LEU
1	A	572	GLN
1	A	574	LEU
1	A	579	ARG
1	A	580	ILE
1	A	581	VAL

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Mol	Chain	Res	Type
1	A	598	HIS
1	A	610	ASP
1	A	657	ARG
1	A	704	PRO
1	A	768	GLU
1	B	560	LEU
1	B	564	LEU
1	B	565	LEU
1	B	579	ARG
1	B	581	VAL
1	B	610	ASP
1	B	618	ASP
1	B	619	VAL
1	B	622	SER
1	B	632	VAL
1	B	657	ARG
1	B	660	LEU
1	B	702	SER
1	B	724	GLN
1	B	753	ILE
1	B	769	SER
1	B	771	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	566	GLN
1	A	582	HIS
1	A	597	ASN
1	A	598	HIS
1	A	719	ASN
1	A	745	GLN
1	B	566	GLN
1	B	572	GLN
1	B	582	HIS
1	B	598	HIS
1	B	719	ASN
1	B	721	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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	194/217 (89%)	-1.39	0 100 100	6, 12, 24, 35	0
1	B	199/217 (91%)	-1.14	0 100 100	7, 24, 42, 48	0
All	All	393/434 (90%)	-1.26	0 100 100	6, 19, 39, 48	0

There are no RSRZ outliers to report.

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.