



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:14 PM UTC

PDB ID : 4NND / pdb_00004nnd
Title : Structural basis of PTPN18 fingerprint on distinct HER2 tyrosine phosphorylation sites
Authors : Wang, H.; Yang, F.; Yang, D.; Du, Y.
Deposited on : 2013-11-17
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
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

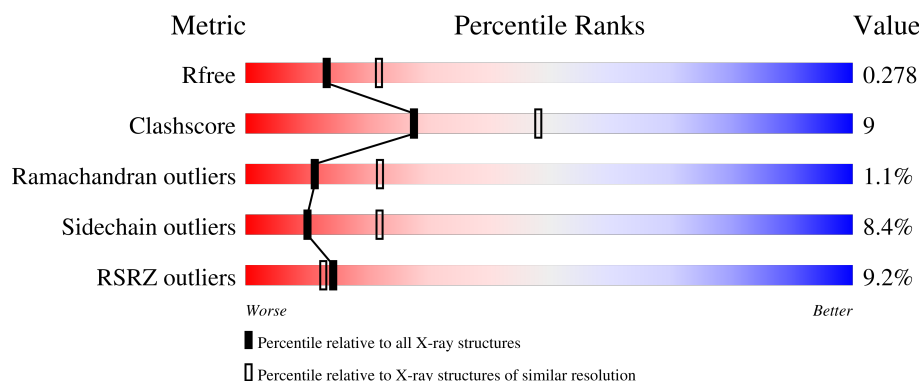
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	290	5% 72% 19% 6% ..
1	B	290	6% 79% 15% ..
1	D	290	9% 73% 17% 7% .
1	G	290	12% 64% 25% 6% .
2	C	6	33% 50% 17% 17% 17%

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Mol	Chain	Length	Quality of chain
2	E	6	50% 33% 50% 17%
2	F	6	33% 33% 17% 17%
2	H	6	67% 33% 33% 17% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9330 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 Tyrosine-protein phosphatase non-receptor type 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	1	0	0
			2270	1437	401	415	17			
1	B	283	Total	C	N	O	S	0	0	0
			2274	1439	402	416	17			
1	D	281	Total	C	N	O	S	10	0	0
			2255	1429	396	413	17			
1	G	278	Total	C	N	O	S	23	0	0
			2239	1420	394	408	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	SER	CYS	engineered mutation	UNP Q99952
B	229	SER	CYS	engineered mutation	UNP Q99952
D	229	SER	CYS	engineered mutation	UNP Q99952
G	229	SER	CYS	engineered mutation	UNP Q99952

- Molecule 2 is a protein called Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	6	Total	C	N	O	P	0	0	0
			59	34	10	14	1			
2	C	6	Total	C	N	O	P	0	0	0
			59	34	10	14	1			
2	E	5	Total	C	N	O	P	4	0	0
			50	29	9	11	1			
2	H	5	Total	C	N	O	P	0	0	0
			50	29	9	11	1			

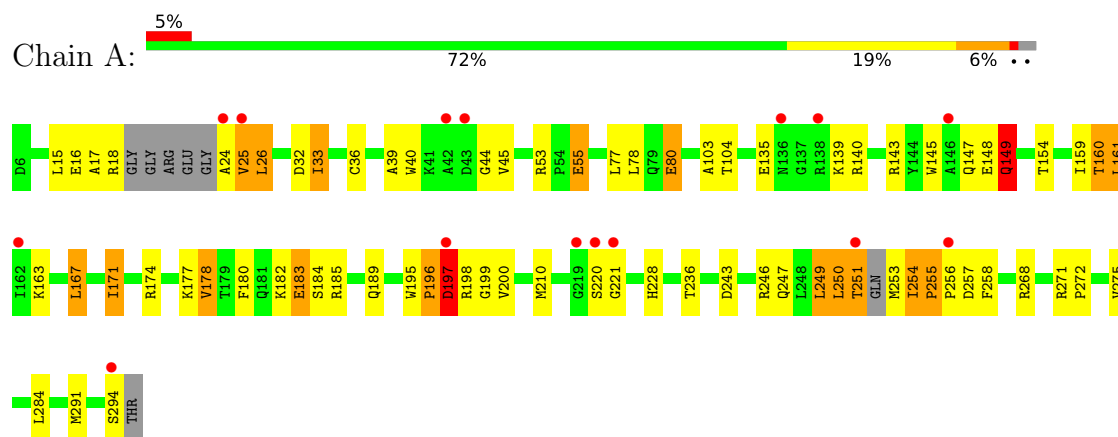
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	22	Total 22	O 22	0	0
3	D	16	Total 16	O 16	0	0
3	G	13	Total 13	O 13	0	0
3	H	1	Total 1	O 1	0	0

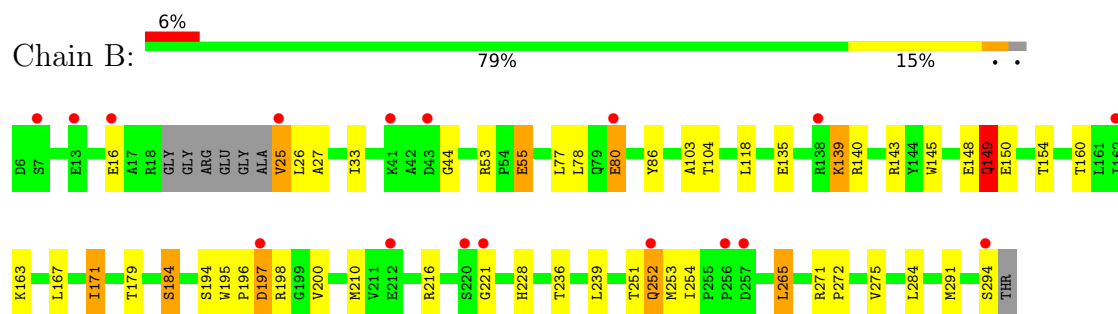
3 Residue-property plots [i](#)

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.

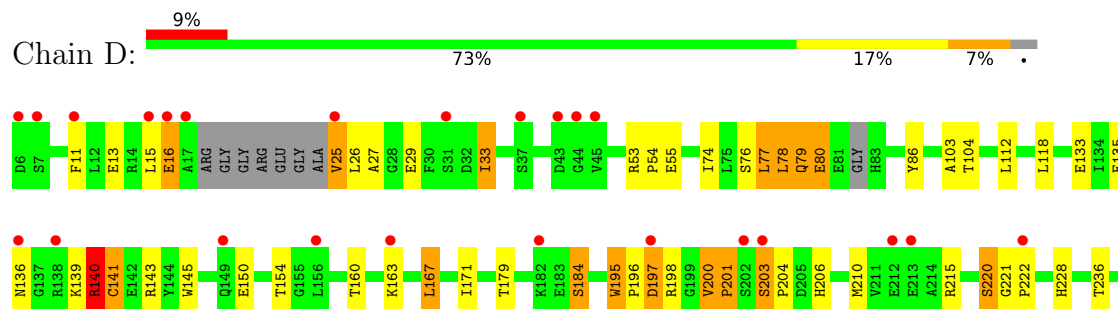
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 18

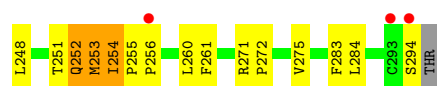


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 18

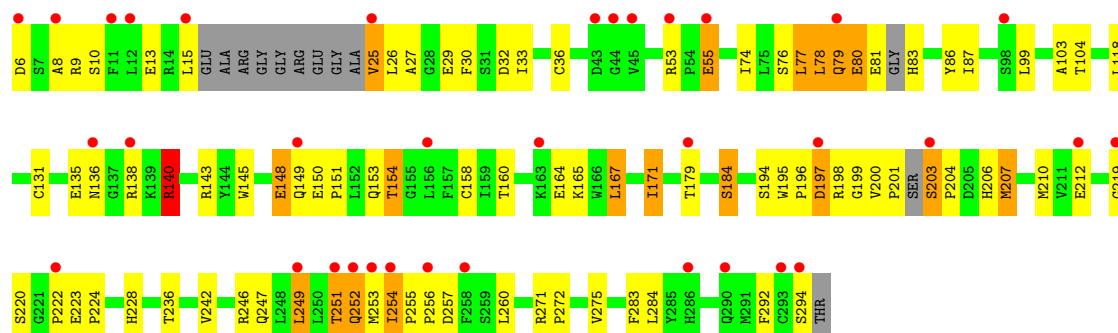


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 18

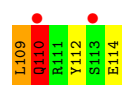




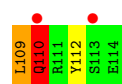
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 18



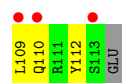
- Molecule 2: Receptor tyrosine-protein kinase erbB-2



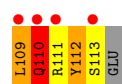
- Molecule 2: Receptor tyrosine-protein kinase erbB-2



- Molecule 2: Receptor tyrosine-protein kinase erbB-2



- Molecule 2: Receptor tyrosine-protein kinase erbB-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 95.28Å 88.16Å 90.00° 94.02° 90.00°	Depositor
Resolution (Å)	34.96 – 2.50 34.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (34.96-2.50) 91.9 (34.96-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	26.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.262 , 0.291 0.255 , 0.278	Depositor DCC
R_{free} test set	2055 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9330	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4147e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

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	1.29	16/2318 (0.7%)	1.10	16/3134 (0.5%)
1	B	0.90	7/2323 (0.3%)	1.02	13/3142 (0.4%)
1	D	1.24	15/2303 (0.7%)	1.10	23/3115 (0.7%)
1	G	1.42	17/2286 (0.7%)	1.14	24/3090 (0.8%)
2	C	0.61	0/41	0.88	0/51
2	E	1.14	0/32	1.00	0/39
2	F	0.52	0/41	0.87	0/51
2	H	1.21	0/32	1.41	1/39 (2.6%)
All	All	1.22	55/9376 (0.6%)	1.09	77/12661 (0.6%)

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	A	0	1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	254	ILE	C-N	8.74	1.41	1.33
1	A	178	VAL	CA-CB	8.25	1.64	1.54
1	B	275	VAL	C-O	-7.09	1.15	1.23
1	A	159	ILE	C-O	-7.02	1.16	1.24
1	G	77	LEU	C-O	-6.55	1.16	1.24
1	D	254	ILE	C-N	6.44	1.41	1.33
1	G	74	ILE	C-O	-6.39	1.17	1.24
1	A	139	LYS	C-O	-6.33	1.16	1.24
1	B	139	LYS	C-O	-6.29	1.16	1.24
1	G	87	ILE	C-O	-6.22	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	223	GLU	C-N	6.11	1.40	1.33
1	A	254	ILE	C-N	6.05	1.40	1.33
1	D	255	PRO	C-N	5.93	1.40	1.34
1	D	74	ILE	C-O	-5.90	1.17	1.24
1	G	203	SER	C-N	5.88	1.41	1.33
1	A	180	PHE	C-O	-5.87	1.17	1.23
1	B	271	ARG	C-O	-5.82	1.18	1.25
1	D	260	LEU	C-O	-5.82	1.16	1.24
1	D	140	ARG	C-O	-5.64	1.16	1.24
1	A	32	ASP	C-O	-5.51	1.17	1.24
1	D	195	TRP	C-N	5.48	1.39	1.33
1	A	185	ARG	C-O	-5.48	1.17	1.23
1	D	53	ARG	C-O	-5.46	1.17	1.24
1	D	221	GLY	C-N	5.46	1.39	1.34
1	A	36	CYS	C-O	-5.42	1.17	1.24
1	A	195	TRP	C-N	5.42	1.40	1.33
1	G	140	ARG	C-O	-5.39	1.17	1.24
1	B	196	PRO	C-O	-5.38	1.17	1.23
1	B	200	VAL	C-N	5.38	1.40	1.33
1	D	77	LEU	C-O	-5.38	1.17	1.24
1	B	195	TRP	C-N	5.33	1.40	1.33
1	G	222	PRO	N-CD	5.32	1.55	1.47
1	D	200	VAL	C-N	5.31	1.40	1.33
1	D	222	PRO	N-CD	5.29	1.55	1.47
1	G	158	CYS	C-O	-5.27	1.18	1.24
1	G	165	LYS	C-O	-5.27	1.17	1.23
1	G	195	TRP	C-O	-5.27	1.20	1.24
1	A	256	PRO	N-CD	5.24	1.55	1.47
1	A	255	PRO	C-N	5.23	1.40	1.34
1	D	141	CYS	C-O	-5.22	1.17	1.23
1	G	150	GLU	C-N	5.21	1.39	1.33
1	G	36	CYS	C-O	-5.18	1.17	1.24
1	D	53	ARG	C-N	5.17	1.40	1.34
1	D	256	PRO	N-CD	5.17	1.54	1.47
1	G	32	ASP	C-O	-5.16	1.17	1.24
1	A	246	ARG	C-O	-5.15	1.18	1.24
1	A	161	LEU	C-O	-5.14	1.17	1.24
1	G	256	PRO	N-CD	5.14	1.54	1.47
1	G	154	THR	C-O	-5.13	1.18	1.24
1	G	160	THR	C-O	-5.13	1.17	1.24
1	A	250	LEU	C-O	-5.12	1.18	1.24
1	A	200	VAL	C-O	-5.11	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	ARG	CA-C	-5.08	1.48	1.52
1	D	261	PHE	C-O	-5.07	1.18	1.24
1	A	196	PRO	C-O	-5.05	1.18	1.23

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	254	ILE	CA-C-N	-7.45	114.22	119.66
1	G	254	ILE	C-N-CA	-7.45	114.22	119.66
1	G	255	PRO	O-C-N	6.93	124.50	121.31
1	D	86	TYR	N-CA-C	6.77	120.27	109.24
1	A	39	ALA	N-CA-C	6.75	118.64	111.28
1	D	167	LEU	N-CA-C	-6.71	104.04	111.36
1	G	150	GLU	CA-C-N	-6.62	113.48	120.03
1	G	150	GLU	C-N-CA	-6.62	113.48	120.03
1	A	182	LYS	N-CA-C	6.53	120.82	112.86
1	D	255	PRO	CA-C-N	-6.47	113.05	120.04
1	D	255	PRO	C-N-CA	-6.47	113.05	120.04
1	D	195	TRP	CA-C-N	-6.46	113.97	120.31
1	D	195	TRP	C-N-CA	-6.46	113.97	120.31
1	B	200	VAL	CA-C-N	-6.46	113.64	120.03
1	B	200	VAL	C-N-CA	-6.46	113.64	120.03
1	D	201	PRO	N-CA-C	6.43	120.53	111.33
1	G	255	PRO	CA-C-N	-6.42	113.15	119.64
1	G	255	PRO	C-N-CA	-6.42	113.15	119.64
1	G	167	LEU	N-CA-C	-6.36	104.43	111.36
1	G	223	GLU	CA-C-N	-6.33	114.02	120.85
1	G	223	GLU	C-N-CA	-6.33	114.02	120.85
1	B	195	TRP	CA-C-N	-6.30	113.46	120.14
1	B	195	TRP	C-N-CA	-6.30	113.46	120.14
1	G	86	TYR	N-CA-C	6.17	119.29	109.24
2	H	110	GLN	N-CA-C	6.15	123.90	110.80
1	B	221	GLY	CA-C-N	6.12	126.65	120.04
1	B	221	GLY	C-N-CA	6.12	126.65	120.04
1	D	254	ILE	CA-C-N	-6.09	114.11	120.38
1	D	254	ILE	C-N-CA	-6.09	114.11	120.38
1	B	275	VAL	CB-CA-C	6.04	118.92	111.25
1	A	255	PRO	CA-C-N	-6.03	113.60	119.87
1	A	255	PRO	C-N-CA	-6.03	113.60	119.87
1	B	272	PRO	CA-N-CD	-5.98	103.63	112.00
1	G	203	SER	CA-C-N	-5.91	113.53	119.56
1	G	203	SER	C-N-CA	-5.91	113.53	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	GLY	CA-C-N	-5.88	113.69	120.04
1	D	221	GLY	C-N-CA	-5.88	113.69	120.04
1	D	201	PRO	CA-N-CD	-5.88	103.77	112.00
1	A	195	TRP	CA-C-N	-5.82	113.97	120.14
1	A	195	TRP	C-N-CA	-5.82	113.97	120.14
1	A	196	PRO	CA-N-CD	-5.76	103.94	112.00
1	G	195	TRP	CA-C-N	-5.68	114.11	119.85
1	G	195	TRP	C-N-CA	-5.68	114.11	119.85
1	A	25	VAL	N-CA-C	5.63	116.64	106.61
1	G	197	ASP	N-CA-C	5.57	118.55	110.42
1	A	254	ILE	CA-C-N	-5.55	114.66	120.38
1	A	254	ILE	C-N-CA	-5.55	114.66	120.38
1	G	201	PRO	CA-N-CD	-5.55	104.23	112.00
1	D	196	PRO	CA-N-CD	-5.50	104.30	112.00
1	D	203	SER	CA-C-N	-5.43	113.05	119.84
1	D	203	SER	C-N-CA	-5.43	113.05	119.84
1	G	151	PRO	CA-N-CD	-5.42	104.41	112.00
1	G	196	PRO	CA-N-CD	-5.42	104.41	112.00
1	A	255	PRO	CA-N-CD	-5.39	104.45	112.00
1	G	255	PRO	CA-N-CD	-5.39	104.45	112.00
1	D	200	VAL	CA-C-N	-5.31	114.16	120.11
1	D	200	VAL	C-N-CA	-5.31	114.16	120.11
1	G	204	PRO	CA-N-CD	-5.30	104.58	112.00
1	D	54	PRO	CA-N-CD	-5.30	104.59	112.00
1	A	171	ILE	N-CA-C	5.29	115.60	107.77
1	G	171	ILE	N-CA-C	5.27	115.49	108.11
1	A	221	GLY	CA-C-N	5.25	125.71	120.04
1	A	221	GLY	C-N-CA	5.25	125.71	120.04
1	B	86	TYR	N-CA-C	5.23	117.76	109.24
1	D	204	PRO	CA-N-CD	-5.21	104.70	112.00
1	D	53	ARG	CA-C-N	-5.14	114.36	119.56
1	D	53	ARG	C-N-CA	-5.14	114.36	119.56
1	B	196	PRO	CA-N-CD	-5.13	104.81	112.00
1	B	271	ARG	CA-C-N	-5.13	114.47	119.76
1	B	271	ARG	C-N-CA	-5.13	114.47	119.76
1	D	255	PRO	CA-N-CD	-5.12	104.83	112.00
1	A	183	GLU	N-CA-C	-5.08	101.88	109.95
1	G	197	ASP	CB-CA-C	-5.06	102.68	109.71
1	A	167	LEU	N-CA-C	-5.05	105.86	111.36
1	G	255	PRO	N-CA-C	5.01	115.28	110.47
1	D	197	ASP	N-CA-C	5.01	117.60	110.24
1	B	171	ILE	N-CA-C	5.00	115.17	107.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	PRO	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	2270	0	2252	40	1
1	B	2274	0	2256	31	1
1	D	2255	0	2233	39	1
1	G	2239	0	2222	52	1
2	C	59	0	49	2	0
2	E	50	0	43	2	0
2	F	59	0	49	2	0
2	H	50	0	43	7	0
3	A	22	0	0	1	0
3	B	22	0	0	1	0
3	D	16	0	0	0	0
3	G	13	0	0	0	0
3	H	1	0	0	0	0
All	All	9330	0	9147	165	2

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 9.

All (165) 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:148:GLU:O	1:B:149:GLN:HB2	1.52	1.09
1:B:252:GLN:NE2	1:G:219:GLY:O	1.89	1.05
1:A:135:GLU:HB2	1:A:140:ARG:HG3	1.44	0.99
1:B:135:GLU:HB2	1:B:140:ARG:HG3	1.44	0.98
1:G:25:VAL:HA	1:G:27:ALA:H	1.33	0.93
1:B:25:VAL:HA	1:B:27:ALA:H	1.32	0.91
1:D:25:VAL:HA	1:D:27:ALA:H	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:THR:HG22	1:G:253:MET:HG2	1.53	0.88
2:F:109:LEU:O	2:F:110:GLN:HG3	1.76	0.85
1:B:251:THR:HG22	1:B:253:MET:HG2	1.58	0.84
1:G:6:ASP:O	1:G:9:ARG:N	2.11	0.84
2:C:109:LEU:O	2:C:110:GLN:HG3	1.79	0.83
1:A:247:GLN:O	1:A:251:THR:HB	1.83	0.79
1:D:203:SER:HB3	1:D:206:HIS:HB2	1.66	0.77
1:G:251:THR:CG2	1:G:253:MET:HG2	2.15	0.76
1:G:25:VAL:HA	1:G:27:ALA:N	2.01	0.76
1:B:25:VAL:HA	1:B:27:ALA:N	2.02	0.75
1:A:220:SER:HA	1:D:253:MET:HE3	1.68	0.75
1:A:249:LEU:C	1:A:249:LEU:HD12	2.11	0.75
1:A:25:VAL:HA	1:A:26:LEU:CB	2.18	0.73
1:D:25:VAL:HA	1:D:27:ALA:N	2.04	0.72
1:G:247:GLN:O	1:G:251:THR:HB	1.92	0.68
1:G:251:THR:HG22	1:G:253:MET:CG	2.23	0.68
1:G:80:GLU:H	1:G:80:GLU:CD	2.02	0.67
1:A:148:GLU:O	1:A:149:GLN:HB2	1.94	0.67
1:G:25:VAL:HG12	1:G:27:ALA:HB3	1.76	0.66
1:D:271:ARG:HD2	1:D:272:PRO:HD2	1.78	0.65
1:A:160:THR:HG22	1:A:177:LYS:HB3	1.77	0.65
1:B:25:VAL:N	1:B:26:LEU:HB2	2.11	0.65
1:D:11:PHE:CZ	1:D:15:LEU:HD11	2.31	0.65
1:A:25:VAL:CA	1:A:26:LEU:HB2	2.26	0.65
1:B:148:GLU:O	1:B:149:GLN:CB	2.36	0.65
1:D:80:GLU:CD	1:D:80:GLU:H	2.05	0.65
1:D:25:VAL:HG12	1:D:27:ALA:HB3	1.78	0.64
1:G:148:GLU:O	1:G:149:GLN:HB2	1.97	0.64
1:G:271:ARG:HD2	1:G:272:PRO:HD2	1.81	0.63
1:D:77:LEU:O	1:D:78:LEU:HB2	1.98	0.63
1:G:77:LEU:O	1:G:78:LEU:HB2	1.97	0.63
1:A:25:VAL:O	1:A:25:VAL:HG23	1.99	0.62
1:D:203:SER:HB3	1:D:206:HIS:CB	2.30	0.62
1:A:249:LEU:HD12	1:A:249:LEU:O	2.00	0.61
2:H:110:GLN:HE22	2:H:111:ARG:HE	1.47	0.61
1:D:15:LEU:HD12	1:D:15:LEU:N	2.15	0.61
1:D:203:SER:HB3	1:D:206:HIS:CG	2.36	0.61
1:A:220:SER:HA	1:D:253:MET:CE	2.30	0.60
2:C:109:LEU:C	2:C:110:GLN:HG3	2.25	0.60
2:H:110:GLN:NE2	2:H:111:ARG:HE	1.99	0.60
1:G:254:ILE:HG23	1:G:254:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ARG:HD2	1:A:272:PRO:HD2	1.83	0.60
1:A:80:GLU:H	1:A:80:GLU:CD	2.09	0.60
2:F:109:LEU:C	2:F:110:GLN:HG3	2.26	0.59
1:B:80:GLU:H	1:B:80:GLU:CD	2.10	0.59
1:A:25:VAL:HA	1:A:26:LEU:HB2	1.81	0.59
1:D:140:ARG:HH22	2:E:109:LEU:N	2.00	0.59
1:G:25:VAL:N	1:G:26:LEU:HB2	2.17	0.59
1:D:25:VAL:N	1:D:26:LEU:HB2	2.17	0.59
1:A:148:GLU:HB2	1:A:161:LEU:CD2	2.33	0.59
1:G:203:SER:HB3	1:G:206:HIS:HB2	1.84	0.58
1:G:29:GLU:O	1:G:33:ILE:HD12	2.03	0.58
1:G:138:ARG:HE	2:H:109:LEU:HG	1.68	0.58
1:D:252:GLN:O	1:D:252:GLN:HG3	2.02	0.57
1:D:251:THR:HG22	1:D:251:THR:O	2.04	0.57
1:B:25:VAL:HG12	1:B:27:ALA:HB3	1.87	0.56
1:B:171:ILE:HD13	1:B:210:MET:HB2	1.86	0.56
1:G:252:GLN:O	1:G:252:GLN:HG3	2.05	0.56
1:B:251:THR:HG22	1:B:251:THR:O	2.05	0.55
1:G:143:ARG:HG3	1:G:145:TRP:CE2	2.41	0.55
1:D:139:LYS:HE2	1:D:141:CYS:O	2.06	0.55
1:D:140:ARG:NH2	2:E:109:LEU:N	2.56	0.54
1:G:212:GLU:HG2	1:G:246:ARG:NH2	2.23	0.54
1:G:30:PHE:HA	1:G:33:ILE:HD12	1.88	0.54
1:B:251:THR:HG22	1:B:253:MET:CG	2.34	0.54
1:B:197:ASP:O	1:B:198:ARG:HB2	2.08	0.54
1:D:143:ARG:HG3	1:D:145:TRP:CE2	2.43	0.53
1:G:104:THR:O	1:G:228:HIS:HB2	2.08	0.53
1:G:251:THR:CG2	1:G:253:MET:CG	2.85	0.53
1:B:252:GLN:HG3	1:B:252:GLN:O	2.09	0.53
1:D:248:LEU:HB3	1:D:254:ILE:HD13	1.91	0.53
1:D:248:LEU:HB3	1:D:254:ILE:CD1	2.39	0.52
1:A:77:LEU:O	1:A:78:LEU:HB2	2.10	0.52
1:A:257:ASP:OD1	1:A:257:ASP:N	2.43	0.52
1:D:104:THR:O	1:D:228:HIS:HB2	2.09	0.52
1:G:103:ALA:HB1	1:G:236:THR:HG21	1.92	0.52
1:G:99:LEU:O	1:G:224:PRO:HB3	2.10	0.51
1:B:143:ARG:HG3	1:B:145:TRP:CE2	2.45	0.51
1:G:257:ASP:OD1	1:G:257:ASP:N	2.42	0.51
1:B:77:LEU:O	1:B:78:LEU:HB2	2.11	0.51
1:G:78:LEU:O	1:G:83:HIS:HB2	2.11	0.51
1:D:76:SER:O	1:D:79:GLN:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LEU:C	1:D:118:LEU:HD23	2.36	0.50
1:A:44:GLY:HA2	3:A:304:HOH:O	2.11	0.50
1:A:143:ARG:HG3	1:A:145:TRP:CE2	2.47	0.50
1:G:171:ILE:HD13	1:G:210:MET:HB2	1.95	0.49
1:A:171:ILE:HD13	1:A:210:MET:HB2	1.94	0.48
1:B:103:ALA:HB1	1:B:236:THR:HG21	1.95	0.48
2:H:112:PTR:HD2	2:H:113:SER:HB3	1.96	0.47
2:H:111:ARG:CZ	2:H:111:ARG:HB2	2.44	0.47
1:G:179:THR:HG22	1:G:184:SER:OG	2.13	0.47
1:A:103:ALA:HB1	1:A:236:THR:HG21	1.97	0.47
1:A:148:GLU:HB2	1:A:161:LEU:HD22	1.95	0.47
1:A:254:ILE:O	1:D:220:SER:HB3	2.14	0.47
1:D:171:ILE:HD13	1:D:210:MET:HB2	1.95	0.47
1:G:135:GLU:HB2	1:G:140:ARG:HG3	1.96	0.47
1:G:53:ARG:HH21	1:G:55:GLU:CD	2.23	0.47
1:D:139:LYS:HA	1:D:139:LYS:HD2	1.65	0.46
1:B:179:THR:HG22	1:B:184:SER:OG	2.15	0.46
1:D:179:THR:HG22	1:D:184:SER:OG	2.14	0.46
1:B:44:GLY:HA2	3:B:304:HOH:O	2.16	0.46
1:G:138:ARG:NE	2:H:109:LEU:HG	2.31	0.46
1:G:76:SER:O	1:G:79:GLN:HB3	2.16	0.46
1:A:148:GLU:HB2	1:A:161:LEU:HD23	1.96	0.46
1:A:104:THR:O	1:A:228:HIS:HB2	2.15	0.46
1:B:104:THR:O	1:B:228:HIS:HB2	2.16	0.45
1:D:200:VAL:HG11	1:D:283:PHE:HB2	1.98	0.45
1:B:216:ARG:HA	1:G:252:GLN:HE22	1.81	0.45
1:G:212:GLU:HG2	1:G:246:ARG:HH21	1.79	0.45
1:D:103:ALA:HB1	1:D:236:THR:HG21	1.99	0.45
1:A:243:ASP:O	1:A:247:GLN:HG2	2.16	0.45
1:G:207:MET:HE3	1:G:207:MET:HB3	1.82	0.45
1:G:197:ASP:O	1:G:198:ARG:HB2	2.17	0.44
1:B:139:LYS:HD2	1:B:139:LYS:HA	1.61	0.44
1:G:6:ASP:C	1:G:8:ALA:N	2.73	0.44
1:G:118:LEU:C	1:G:118:LEU:HD23	2.42	0.44
1:A:17:ALA:O	1:A:18:ARG:HB2	2.17	0.44
1:A:255:PRO:HD2	1:A:258:PHE:HD1	1.82	0.44
1:G:207:MET:HE1	1:G:242:VAL:HG21	2.00	0.44
1:A:197:ASP:O	1:A:198:ARG:HB2	2.18	0.43
1:D:197:ASP:O	1:D:198:ARG:HB2	2.18	0.43
1:D:29:GLU:O	1:D:33:ILE:HD12	2.18	0.43
1:G:200:VAL:HG11	1:G:283:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:THR:O	1:D:251:THR:CG2	2.66	0.43
1:B:265:LEU:HD12	1:B:265:LEU:HA	1.88	0.43
1:G:246:ARG:HG2	1:G:246:ARG:HH11	1.83	0.43
1:G:197:ASP:C	1:G:199:GLY:H	2.26	0.43
1:A:40:TRP:HB3	1:A:45:VAL:HG23	2.01	0.42
1:D:195:TRP:CE2	1:D:201:PRO:HD3	2.54	0.42
1:A:24:ALA:C	1:A:26:LEU:HB2	2.44	0.42
1:A:255:PRO:HD2	1:A:258:PHE:CD1	2.55	0.42
1:B:150:GLU:O	1:B:150:GLU:OE1	2.37	0.42
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.81	0.42
1:D:133:GLU:HB3	1:D:139:LYS:HE3	2.02	0.42
1:A:53:ARG:HH21	1:A:55:GLU:CD	2.28	0.42
1:A:251:THR:HG22	1:A:253:MET:HB3	2.01	0.42
1:G:55:GLU:CD	1:G:55:GLU:H	2.28	0.42
2:H:110:GLN:H	2:H:110:GLN:HG3	1.59	0.42
1:D:215:ARG:HA	1:D:215:ARG:HD3	1.82	0.42
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.77	0.42
1:B:291:MET:HE3	1:B:291:MET:HB2	1.75	0.42
1:G:249:LEU:HD12	1:G:292:PHE:CD1	2.55	0.42
1:A:174:ARG:HD2	1:A:189:GLN:OE1	2.20	0.41
1:B:254:ILE:O	1:G:220:SER:HB3	2.20	0.41
1:G:260:LEU:HD12	1:G:260:LEU:HA	1.87	0.41
1:G:79:GLN:C	1:G:81:GLU:N	2.76	0.41
1:A:291:MET:HE3	1:A:291:MET:HB2	1.78	0.41
1:B:251:THR:O	1:B:251:THR:CG2	2.68	0.41
1:B:53:ARG:HH21	1:B:55:GLU:CD	2.29	0.41
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.91	0.41
1:D:150:GLU:O	1:D:150:GLU:OE1	2.38	0.41
1:G:246:ARG:HG2	1:G:246:ARG:NH1	2.35	0.40
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.78	0.40
1:G:26:LEU:HD12	1:G:26:LEU:HA	1.92	0.40
1:A:197:ASP:C	1:A:199:GLY:H	2.29	0.40
1:B:118:LEU:HD23	1:B:118:LEU:C	2.46	0.40
1:G:131:CYS:HB2	1:G:135:GLU:OE2	2.22	0.40
1:A:33:ILE:CG2	1:A:268:ARG:HD2	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:OE1	1:D:135:GLU:O[2_544]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:OE1	1:G:135:GLU:O[2_544]	1.87	0.33

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	277/290 (96%)	264 (95%)	10 (4%)	3 (1%)	11	22
1	B	279/290 (96%)	265 (95%)	12 (4%)	2 (1%)	18	34
1	D	275/290 (95%)	261 (95%)	11 (4%)	3 (1%)	11	22
1	G	270/290 (93%)	249 (92%)	20 (7%)	1 (0%)	30	49
2	C	3/6 (50%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	E	2/6 (33%)	2 (100%)	0	0	100	100
2	F	3/6 (50%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	H	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	1111/1184 (94%)	1044 (94%)	55 (5%)	12 (1%)	11	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	110	GLN
1	A	149	GLN
1	B	149	GLN
1	A	197	ASP
2	F	110	GLN
2	C	110	GLN
1	D	220	SER
1	B	197	ASP
1	D	16	GLU
1	D	275	VAL
1	A	275	VAL

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Mol	Chain	Res	Type
1	G	275	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	247/251 (98%)	228 (92%)	19 (8%)	12	25
1	B	248/251 (99%)	233 (94%)	15 (6%)	17	36
1	D	246/251 (98%)	227 (92%)	19 (8%)	12	25
1	G	245/251 (98%)	222 (91%)	23 (9%)	8	18
2	C	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	E	4/5 (80%)	3 (75%)	1 (25%)	0	1
2	F	5/5 (100%)	2 (40%)	3 (60%)	0	0
2	H	4/5 (80%)	2 (50%)	2 (50%)	0	0
All	All	1004/1024 (98%)	920 (92%)	84 (8%)	10	22

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	33	ILE
1	A	55	GLU
1	A	80	GLU
1	A	147	GLN
1	A	149	GLN
1	A	154	THR
1	A	160	THR
1	A	163	LYS
1	A	167	LEU
1	A	178	VAL
1	A	183	GLU
1	A	184	SER
1	A	197	ASP

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Mol	Chain	Res	Type
1	A	249	LEU
1	A	250	LEU
1	A	251	THR
1	A	284	LEU
1	A	294	SER
2	F	109	LEU
2	F	110	GLN
2	F	114	GLU
1	B	25	VAL
1	B	33	ILE
1	B	55	GLU
1	B	80	GLU
1	B	149	GLN
1	B	154	THR
1	B	160	THR
1	B	163	LYS
1	B	167	LEU
1	B	184	SER
1	B	194	SER
1	B	252	GLN
1	B	265	LEU
1	B	284	LEU
1	B	294	SER
2	C	109	LEU
2	C	110	GLN
1	D	13	GLU
1	D	16	GLU
1	D	25	VAL
1	D	33	ILE
1	D	55	GLU
1	D	78	LEU
1	D	79	GLN
1	D	80	GLU
1	D	136	ASN
1	D	140	ARG
1	D	154	THR
1	D	160	THR
1	D	163	LYS
1	D	167	LEU
1	D	184	SER
1	D	252	GLN
1	D	253	MET

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Mol	Chain	Res	Type
1	D	284	LEU
1	D	294	SER
2	E	110	GLN
1	G	10	SER
1	G	13	GLU
1	G	15	LEU
1	G	25	VAL
1	G	55	GLU
1	G	78	LEU
1	G	79	GLN
1	G	80	GLU
1	G	136	ASN
1	G	140	ARG
1	G	148	GLU
1	G	153	GLN
1	G	154	THR
1	G	164	GLU
1	G	167	LEU
1	G	184	SER
1	G	194	SER
1	G	207	MET
1	G	249	LEU
1	G	251	THR
1	G	252	GLN
1	G	284	LEU
1	G	294	SER
2	H	109	LEU
2	H	110	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
2	F	110	GLN
1	B	147	GLN
2	C	110	GLN
1	D	56	ASN
1	D	83	HIS
1	D	147	GLN
1	D	252	GLN
2	E	110	GLN
1	G	56	ASN

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Mol	Chain	Res	Type
1	G	83	HIS
1	G	153	GLN
1	G	247	GLN
1	G	252	GLN
2	H	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PTR	F	112	2	15,16,17	2.07	1 (6%)	17,22,24	0.66	0
2	PTR	E	112	2	15,16,17	3.08	5 (33%)	17,22,24	0.75	0
2	PTR	H	112	2	15,16,17	2.98	6 (40%)	17,22,24	1.19	1 (5%)
2	PTR	C	112	2	15,16,17	2.15	1 (6%)	17,22,24	0.86	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	F	112	2	-	0/10/11/13	0/1/1/1
2	PTR	E	112	2	-	0/10/11/13	0/1/1/1
2	PTR	H	112	2	-	0/10/11/13	0/1/1/1
2	PTR	C	112	2	-	0/10/11/13	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	112	PTR	OH-CZ	-8.85	1.20	1.40
2	H	112	PTR	OH-CZ	-8.46	1.21	1.40
2	C	112	PTR	OH-CZ	-7.89	1.22	1.40
2	F	112	PTR	OH-CZ	-7.41	1.24	1.40
2	H	112	PTR	P-O3P	-4.55	1.37	1.54
2	E	112	PTR	P-O3P	-4.55	1.37	1.54
2	E	112	PTR	P-O2P	-3.55	1.41	1.54
2	H	112	PTR	P-O1P	-3.15	1.40	1.50
2	H	112	PTR	P-O2P	-3.02	1.43	1.54
2	E	112	PTR	P-O1P	-2.92	1.41	1.50
2	H	112	PTR	CE2-CZ	-2.48	1.34	1.38
2	H	112	PTR	P-OH	-2.15	1.55	1.59
2	E	112	PTR	CE2-CZ	-2.09	1.34	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	112	PTR	O2P-P-OH	3.70	116.27	105.32
2	C	112	PTR	O2P-P-O1P	-2.08	102.75	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	112	PTR	1	0

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 ⓘ

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	283/290 (97%)	0.24	15 (5%)	32	28	14, 30, 56, 66	1 (0%)
1	B	283/290 (97%)	0.26	17 (6%)	27	24	12, 30, 57, 68	0
1	D	281/290 (96%)	0.65	27 (9%)	13	11	16, 33, 65, 82	5 (1%)
1	G	278/290 (95%)	0.66	35 (12%)	8	6	14, 33, 65, 86	6 (2%)
2	C	5/6 (83%)	1.91	2 (40%)	1	0	52, 52, 56, 66	0
2	E	4/6 (66%)	2.55	3 (75%)	0	0	31, 49, 55, 67	1 (25%)
2	F	5/6 (83%)	1.90	2 (40%)	1	0	51, 53, 61, 65	0
2	H	4/6 (66%)	2.81	4 (100%)	0	0	44, 52, 62, 63	0
All	All	1143/1184 (96%)	0.48	105 (9%)	14	13	12, 31, 60, 86	13 (1%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	219	GLY	10.6
1	D	17	ALA	9.9
1	G	197	ASP	6.7
1	G	15	LEU	6.7
1	G	203	SER	5.8
1	B	197	ASP	5.4
1	D	197	ASP	5.3
1	A	197	ASP	5.2
1	D	25	VAL	4.9
1	D	203	SER	4.9
1	D	202	SER	4.9
1	D	15	LEU	4.8
1	G	294	SER	4.6
1	D	294	SER	4.5
1	D	11	PHE	3.9
1	A	24	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	25	VAL	3.9
1	A	294	SER	3.7
1	A	146	ALA	3.7
1	D	149	GLN	3.7
1	G	6	ASP	3.6
2	H	113	SER	3.6
1	D	16	GLU	3.5
1	B	25	VAL	3.5
1	D	6	ASP	3.4
1	G	43	ASP	3.4
1	G	156	LEU	3.4
2	E	113	SER	3.4
2	E	109	LEU	3.4
1	G	163	LYS	3.3
2	H	109	LEU	3.3
1	D	138	ARG	3.2
1	A	220	SER	3.1
1	A	138	ARG	3.1
1	B	220	SER	3.1
2	F	113	SER	3.0
1	A	162	ILE	2.9
1	G	11	PHE	2.9
1	G	256	PRO	2.9
1	D	293	CYS	2.9
1	G	149	GLN	2.9
1	B	16	GLU	2.9
1	G	249	LEU	2.8
1	A	25	VAL	2.8
1	G	138	ARG	2.8
1	D	31	SER	2.8
2	C	113	SER	2.7
1	B	294	SER	2.7
1	B	43	ASP	2.6
1	B	221	GLY	2.6
1	G	251	THR	2.6
1	G	222	PRO	2.6
1	B	138	ARG	2.6
1	G	290	GLN	2.6
1	G	12	LEU	2.5
1	G	179	THR	2.5
1	D	256	PRO	2.5
1	D	43	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	42	ALA	2.5
1	B	252	GLN	2.4
1	A	251	THR	2.4
1	A	219	GLY	2.4
1	A	221	GLY	2.4
2	C	110	GLN	2.4
1	B	80	GLU	2.4
1	B	162	ILE	2.3
1	D	222	PRO	2.3
1	B	256	PRO	2.3
1	G	44	GLY	2.3
1	G	79	GLN	2.3
1	D	37	SER	2.3
1	G	136	ASN	2.2
2	H	110	GLN	2.2
1	G	45	VAL	2.2
1	D	212	GLU	2.2
1	G	53	ARG	2.2
2	E	110	GLN	2.2
1	G	286	HIS	2.2
1	G	293	CYS	2.2
1	G	55	GLU	2.2
1	G	212	GLU	2.2
1	D	136	ASN	2.1
1	B	13	GLU	2.1
1	B	257	ASP	2.1
1	D	213	GLU	2.1
1	D	182	LYS	2.1
1	G	8	ALA	2.1
1	D	156	LEU	2.1
1	A	43	ASP	2.1
1	B	7	SER	2.1
1	G	258	PHE	2.1
2	F	110	GLN	2.1
1	D	45	VAL	2.1
1	A	136	ASN	2.1
1	D	44	GLY	2.1
2	H	111	ARG	2.1
1	B	212	GLU	2.1
1	A	256	PRO	2.1
1	G	253	MET	2.1
1	B	41	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	163	LYS	2.0
1	G	254	ILE	2.0
1	D	7	SER	2.0
1	G	252	GLN	2.0
1	G	98	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PTR	C	112	16/17	0.94	0.11	20,28,47,48	0
2	PTR	E	112	16/17	0.95	0.10	24,30,43,50	0
2	PTR	F	112	16/17	0.96	0.09	14,26,47,49	0
2	PTR	H	112	16/17	0.96	0.09	21,28,52,53	0

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.