



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:08 AM UTC

PDB ID : 4GFV / pdb_00004gfv
Title : PTPN18 in complex with HER2-pY1196 phosphor-peptides
Authors : Wang, H.M.; Yang, F.; Du, Y.J.; Yang, D.X.; Zhang, Y.; Yu, X.; Sun, J.P.
Deposited on : 2012-08-04
Resolution : 2.10 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

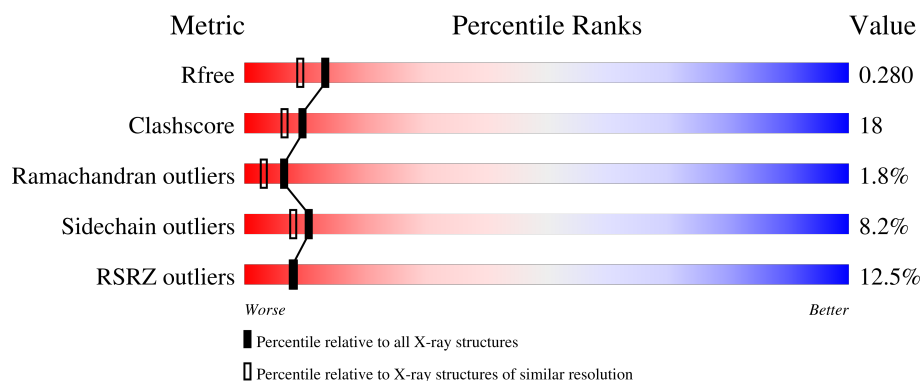
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	297	9% 63% 26% 6% ..
1	B	297	13% 52% 33% 11% ..
2	E	6	50% 33% 17% 33% 17%
2	F	6	50% 33% 17% 33% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	E	1196	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4816 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	286	Total	C	N	O	S	0	1	0
			2291	1449	410	415	17			
1	B	288	Total	C	N	O	S	0	1	0
			2305	1457	411	420	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	-	expression tag	UNP Q99952
A	5	ALA	-	expression tag	UNP Q99952
A	229	SER	CYS	engineered mutation	UNP Q99952
B	4	ALA	-	expression tag	UNP Q99952
B	5	ALA	-	expression tag	UNP Q99952
B	229	SER	CYS	engineered mutation	UNP Q99952

- Molecule 2 is a protein called HER2-pY1196 phosphor-peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	P	0	0	0
			54	34	6	13	1			
2	F	5	Total	C	N	O	P	0	0	0
			47	29	5	12	1			

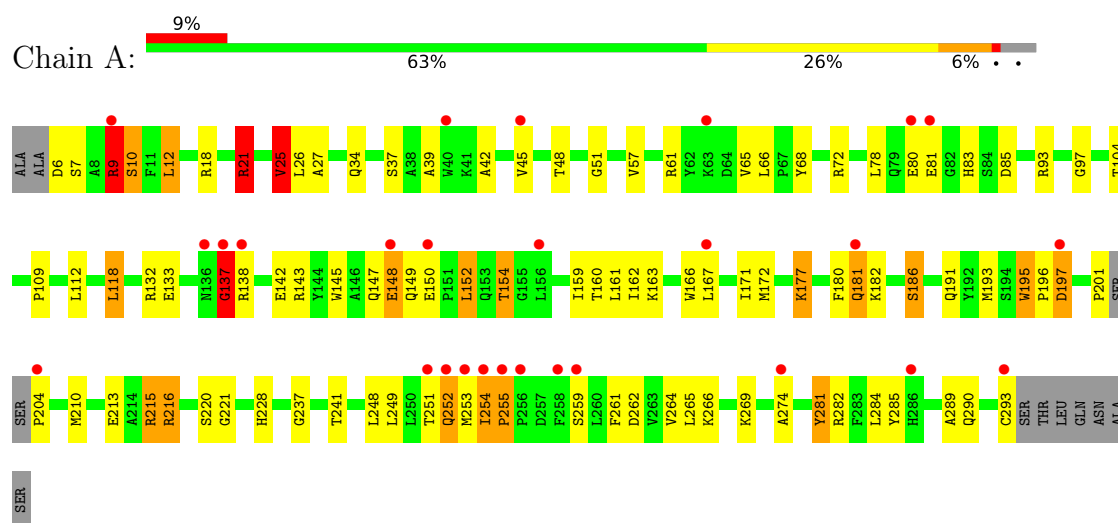
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	52	Total	O	0	0
			52	52		
3	F	2	Total	O	0	0
			2	2		

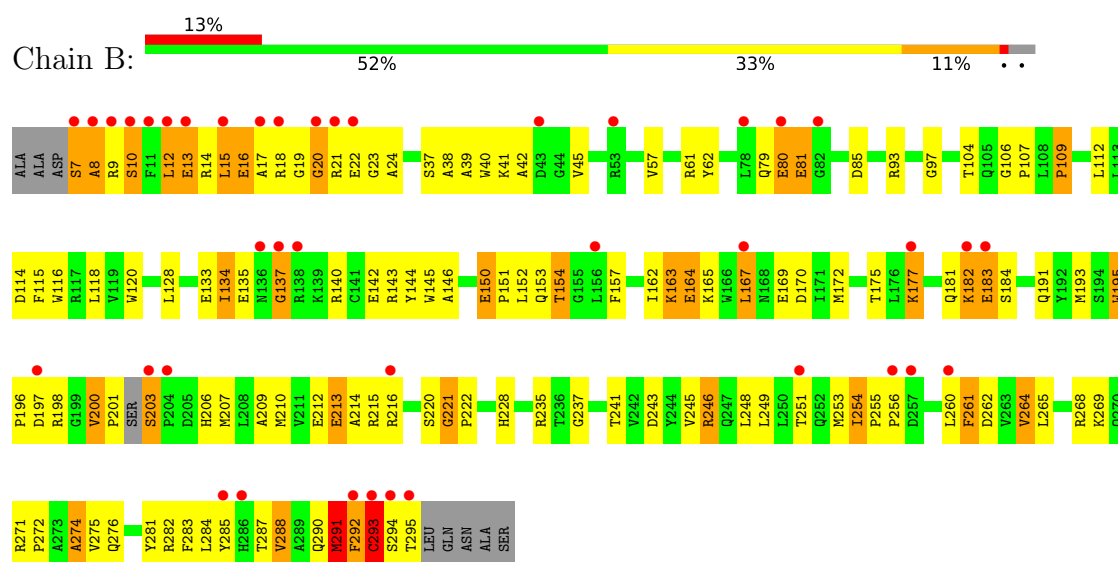
3 Residue-property plots

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.

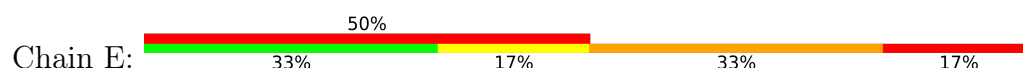
- Molecule 1: Tyrosine-protein phosphatase non-receptor type 18

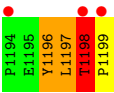


- Molecule 1: Tyrosine-protein phosphatase non-receptor type 18

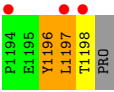
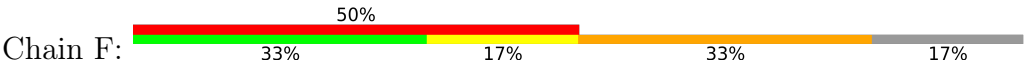


- Molecule 2: HER2-pY1196 phosphor-peptide





● Molecule 2: HER2-pY1196 phosphor-peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.35Å 91.34Å 92.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.10 49.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.00-2.10) 95.2 (49.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.246 , 0.293 0.249 , 0.280	Depositor DCC
R_{free} test set	1810 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.893	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4816	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 53.31 % 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 4.2927e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	1.58	34/2343 (1.5%)	1.18	15/3165 (0.5%)
1	B	1.76	59/2354 (2.5%)	1.26	19/3182 (0.6%)
2	E	0.63	0/38	1.00	0/50
2	F	0.45	0/30	0.57	0/38
All	All	1.67	93/4765 (2.0%)	1.21	34/6435 (0.5%)

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	3
1	B	0	1
All	All	0	4

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216[A]	ARG	CA-C	8.51	1.64	1.52
1	A	216[B]	ARG	CA-C	8.51	1.64	1.52
1	B	146	ALA	CA-CB	-8.07	1.40	1.53
1	A	133	GLU	C-O	-8.05	1.14	1.24
1	A	195	TRP	C-O	-7.94	1.17	1.25
1	B	144	TYR	C-O	-7.42	1.14	1.24
1	A	7	SER	C-O	-7.34	1.15	1.24
1	B	246	ARG	C-O	-7.23	1.15	1.24
1	B	268	ARG	C-O	-7.21	1.15	1.24
1	A	281	TYR	C-O	-7.19	1.15	1.24
1	B	195	TRP	C-O	-7.17	1.16	1.24
1	B	163	LYS	C-O	-7.03	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	VAL	C-O	-6.97	1.16	1.24
1	B	61	ARG	C-O	-6.96	1.15	1.24
1	B	133	GLU	C-O	-6.80	1.16	1.24
1	B	264	VAL	C-O	-6.76	1.16	1.24
1	A	197	ASP	CB-CG	-6.74	1.35	1.52
1	A	215	ARG	C-O	-6.72	1.16	1.24
1	B	262	ASP	C-O	-6.69	1.15	1.24
1	B	209	ALA	C-O	-6.55	1.16	1.24
1	B	255	PRO	C-N	6.34	1.40	1.34
1	B	169	GLU	C-O	-6.34	1.16	1.24
1	B	62	TYR	C-O	-6.29	1.16	1.24
1	B	213	GLU	C-O	-6.21	1.17	1.24
1	B	214	ALA	CA-CB	-6.07	1.44	1.53
1	A	249	LEU	C-O	-6.05	1.17	1.24
1	A	27	ALA	C-O	-6.03	1.17	1.24
1	B	39	ALA	C-O	-5.86	1.17	1.24
1	B	254	ILE	C-N	5.86	1.40	1.33
1	A	216[A]	ARG	N-CA	5.82	1.53	1.46
1	A	216[B]	ARG	N-CA	5.82	1.53	1.46
1	B	214	ALA	C-O	-5.81	1.17	1.24
1	A	9	ARG	C-O	-5.81	1.16	1.24
1	B	288	VAL	C-O	-5.75	1.17	1.24
1	B	157	PHE	C-O	-5.72	1.17	1.23
1	B	285	TYR	C-O	-5.71	1.17	1.24
1	B	287	THR	C-O	-5.68	1.17	1.24
1	B	115	PHE	C-O	-5.67	1.17	1.24
1	A	180	PHE	C-O	-5.67	1.17	1.23
1	B	261	PHE	C-O	-5.65	1.17	1.24
1	A	25	VAL	C-O	-5.64	1.16	1.24
1	B	200	VAL	C-O	-5.62	1.20	1.24
1	B	116	TRP	C-O	-5.61	1.17	1.24
1	A	197	ASP	CA-CB	-5.60	1.44	1.53
1	B	164	GLU	N-CA	-5.57	1.39	1.46
1	A	21	ARG	CB-CG	-5.56	1.35	1.52
1	B	274	ALA	CA-CB	-5.53	1.44	1.53
1	B	243	ASP	C-O	-5.52	1.17	1.24
1	B	114	ASP	C-O	-5.49	1.17	1.24
1	B	175	THR	C-O	-5.49	1.17	1.24
1	B	195	TRP	C-N	5.48	1.40	1.33
1	B	209	ALA	CA-CB	-5.45	1.44	1.53
1	A	61	ARG	C-O	-5.42	1.17	1.24
1	A	285	TYR	C-O	-5.41	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ILE	C-N	5.40	1.39	1.33
1	A	163	LYS	C-O	-5.38	1.17	1.23
1	A	221	GLY	C-N	5.36	1.39	1.34
1	A	39	ALA	C-O	-5.35	1.17	1.24
1	B	17	ALA	CA-CB	-5.35	1.44	1.53
1	B	37	SER	C-O	-5.34	1.18	1.24
1	A	132	ARG	C-O	-5.33	1.17	1.23
1	B	109	PRO	N-CD	5.32	1.55	1.47
1	B	18	ARG	CA-CB	-5.29	1.45	1.52
1	B	245	VAL	C-O	-5.29	1.18	1.24
1	B	255	PRO	N-CD	5.28	1.55	1.47
1	B	203	SER	C-N	5.28	1.41	1.33
1	B	212	GLU	C-O	-5.27	1.18	1.24
1	B	210	MET	C-O	-5.25	1.18	1.24
1	B	154	THR	CA-C	-5.24	1.46	1.52
1	B	291	MET	C-O	-5.22	1.18	1.24
1	B	40	TRP	C-O	-5.20	1.18	1.24
1	A	282	ARG	C-O	-5.19	1.18	1.24
1	B	276	GLN	C-O	-5.19	1.17	1.24
1	B	170	ASP	C-O	-5.17	1.17	1.24
1	B	81	GLU	C-O	-5.16	1.18	1.24
1	A	37	SER	C-O	-5.14	1.18	1.24
1	B	42	ALA	C-O	-5.14	1.17	1.24
1	A	34	GLN	C-O	-5.14	1.18	1.24
1	A	42	ALA	C-O	-5.13	1.18	1.24
1	A	289	ALA	CA-CB	-5.12	1.45	1.53
1	B	134	ILE	C-O	-5.10	1.18	1.24
1	B	207	MET	C-O	-5.10	1.18	1.24
1	B	290	GLN	C-O	-5.08	1.18	1.24
1	B	256	PRO	N-CD	5.07	1.54	1.47
1	A	26	LEU	C-O	-5.07	1.18	1.24
1	B	133	GLU	CB-CG	-5.06	1.37	1.52
1	A	180	PHE	N-CA	-5.05	1.40	1.46
1	B	151	PRO	C-O	-5.05	1.17	1.23
1	A	290	GLN	C-O	-5.04	1.18	1.24
1	B	38	ALA	C-O	-5.04	1.18	1.24
1	B	107	PRO	N-CD	5.03	1.54	1.47
1	A	161	LEU	C-O	-5.02	1.18	1.24
1	A	186	SER	C-O	-5.01	1.17	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216[A]	ARG	CA-C-O	-12.26	106.24	120.10
1	A	216[B]	ARG	CA-C-O	-12.26	106.24	120.10
1	B	254	ILE	CA-C-N	-7.38	112.78	120.38
1	B	254	ILE	C-N-CA	-7.38	112.78	120.38
1	A	154	THR	CB-CA-C	-7.11	97.21	109.65
1	A	254	ILE	CA-C-N	-7.00	113.17	120.38
1	A	254	ILE	C-N-CA	-7.00	113.17	120.38
1	B	221	GLY	CA-C-N	6.60	127.16	120.04
1	B	221	GLY	C-N-CA	6.60	127.16	120.04
1	B	196	PRO	CA-N-CD	-6.39	103.05	112.00
1	B	255	PRO	CA-C-N	-6.28	113.26	120.04
1	B	255	PRO	C-N-CA	-6.28	113.26	120.04
1	A	195	TRP	CA-C-N	-6.27	113.49	120.14
1	A	195	TRP	C-N-CA	-6.27	113.49	120.14
1	A	197	ASP	N-CA-CB	-6.19	100.48	109.83
1	A	221	GLY	O-C-N	5.97	127.74	121.77
1	B	151	PRO	CA-N-CD	-5.83	103.84	112.00
1	B	203	SER	CA-C-N	-5.41	113.19	119.47
1	B	203	SER	C-N-CA	-5.41	113.19	119.47
1	A	221	GLY	CA-C-N	-5.34	114.27	120.04
1	A	221	GLY	C-N-CA	-5.34	114.27	120.04
1	B	12	LEU	CA-C-N	5.33	128.81	120.82
1	B	12	LEU	C-N-CA	5.33	128.81	120.82
1	B	150	GLU	CA-C-N	-5.31	114.47	119.89
1	B	150	GLU	C-N-CA	-5.31	114.47	119.89
1	B	292	PHE	N-CA-C	5.22	121.91	110.80
1	B	24	ALA	N-CA-C	5.21	117.38	111.02
1	A	216[A]	ARG	N-CA-C	5.17	117.66	111.71
1	A	216[B]	ARG	N-CA-C	5.17	117.66	111.71
1	A	196	PRO	CA-N-CD	-5.17	104.76	112.00
1	B	162	ILE	N-CA-C	5.16	116.62	111.00
1	B	106	GLY	CA-C-N	-5.13	114.66	119.89
1	B	106	GLY	C-N-CA	-5.13	114.66	119.89
1	A	255	PRO	CA-N-CD	-5.11	104.84	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	GLY	Peptide
1	A	216[A]	ARG	Mainchain
1	A	216[B]	ARG	Mainchain
1	B	293	CYS	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	2291	0	2276	67	0
1	B	2305	0	2285	93	0
2	E	54	0	45	10	0
2	F	47	0	38	7	0
3	A	65	0	0	2	0
3	B	52	0	0	3	0
3	F	2	0	0	0	0
All	All	4816	0	4644	166	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 18.

All (166) 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:149:GLN:N	1:A:150:GLU:OE1	1.87	1.07
1:B:197:ASP:OD2	2:E:1196:PTR:CZ	2.03	1.05
1:B:197:ASP:OD2	2:E:1196:PTR:CE1	2.04	1.05
1:A:137:GLY:HA3	1:A:138:ARG:HG2	1.39	1.01
1:B:197:ASP:OD1	3:B:411:HOH:O	1.80	1.00
1:B:20:GLY:O	1:B:22:GLU:N	1.95	0.99
1:B:8:ALA:HA	1:B:10:SER:N	1.81	0.94
1:B:8:ALA:HA	1:B:10:SER:H	1.30	0.92
1:B:23:GLY:HA2	1:B:282:ARG:HH12	1.35	0.89
1:B:163:LYS:HD2	1:B:164:GLU:H	1.39	0.87
1:A:148:GLU:HG2	1:A:149:GLN:HG3	1.57	0.86
2:F:1197:LEU:O	2:F:1198:THR:HG23	1.76	0.85
1:B:293:CYS:SG	3:B:425:HOH:O	2.09	0.85
1:A:237:GLY:HA3	1:A:274:ALA:O	1.82	0.80
1:A:137:GLY:CA	1:A:138:ARG:HG2	2.11	0.80
1:B:246:ARG:HA	1:B:291:MET:HE3	1.64	0.80
1:B:165:LYS:HZ1	1:B:167:LEU:HD23	1.47	0.79
1:A:21:ARG:HD3	3:A:463:HOH:O	1.82	0.79
1:B:23:GLY:HA2	1:B:282:ARG:NH1	1.97	0.78
2:E:1196:PTR:HD2	2:E:1197:LEU:HD13	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:SER:HB2	1:B:14:ARG:NH1	2.00	0.77
1:B:15:LEU:C	1:B:15:LEU:HD13	2.10	0.76
1:B:8:ALA:CA	1:B:10:SER:H	2.00	0.74
1:B:165:LYS:NZ	1:B:167:LEU:HD23	2.01	0.74
2:E:1196:PTR:HD2	2:E:1197:LEU:CD1	2.17	0.73
1:B:8:ALA:N	1:B:9:ARG:HB3	2.02	0.73
1:B:10:SER:HB2	1:B:14:ARG:HH12	1.55	0.72
2:F:1196:PTR:HD2	2:F:1197:LEU:CD1	2.20	0.72
1:B:241:THR:HG21	1:B:284:LEU:HD21	1.72	0.72
1:B:237:GLY:HA3	1:B:274:ALA:O	1.90	0.71
1:B:197:ASP:CG	2:E:1196:PTR:OH	2.32	0.71
1:B:152:LEU:C	1:B:152:LEU:HD23	2.15	0.71
1:A:9:ARG:N	1:A:9:ARG:HD3	2.07	0.69
1:B:15:LEU:HD13	1:B:16:GLU:N	2.06	0.69
1:B:197:ASP:OD2	2:E:1196:PTR:OH	2.10	0.69
1:B:292:PHE:O	1:B:295:THR:HG22	1.94	0.68
1:B:152:LEU:HD23	1:B:153:GLN:N	2.08	0.68
1:B:79:GLN:C	1:B:81:GLU:H	2.02	0.67
1:A:251:THR:HG21	1:A:253:MET:HG3	1.77	0.67
1:A:251:THR:HG22	1:A:253:MET:HG2	1.77	0.67
2:E:1198:THR:OG1	2:E:1199:PRO:HD3	1.94	0.66
1:A:220:SER:HA	1:B:253:MET:CE	2.26	0.66
1:B:293:CYS:HA	1:B:295:THR:H	1.62	0.65
1:B:249:LEU:HD13	1:B:292:PHE:CE1	2.32	0.65
1:A:241:THR:HG21	1:A:284:LEU:HD13	1.80	0.64
1:A:220:SER:HA	1:B:253:MET:HE3	1.80	0.63
1:B:249:LEU:HD13	1:B:292:PHE:CD1	2.32	0.63
1:B:12:LEU:O	1:B:15:LEU:HD12	2.00	0.61
1:A:149:GLN:C	1:A:150:GLU:HG3	2.25	0.61
1:A:251:THR:CG2	1:A:253:MET:HG3	2.31	0.61
1:B:293:CYS:HA	1:B:295:THR:N	2.16	0.61
1:B:8:ALA:H	1:B:9:ARG:HB3	1.64	0.61
1:B:80:GLU:C	1:B:81:GLU:HG3	2.26	0.60
1:A:259:SER:HB3	1:A:262:ASP:OD2	2.02	0.60
1:A:255:PRO:HA	1:B:220:SER:OG	2.01	0.60
1:B:9:ARG:NH1	1:B:13:GLU:OE2	2.35	0.59
1:B:213:GLU:OE2	1:B:216[B]:ARG:NH2	2.28	0.59
1:A:252:GLN:C	1:A:253:MET:HG2	2.27	0.58
1:A:6:ASP:O	1:A:10:SER:HB2	2.03	0.58
1:A:251:THR:HG22	1:A:253:MET:CG	2.34	0.58
1:A:195:TRP:CE2	1:A:201:PRO:HD3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLY:HA3	1:A:138:ARG:CG	2.24	0.57
1:A:251:THR:C	1:A:252:GLN:HG3	2.30	0.57
1:A:248:LEU:HB3	1:A:254:ILE:CD1	2.35	0.56
1:B:15:LEU:HD22	1:B:15:LEU:O	2.04	0.56
1:A:118:LEU:C	1:A:118:LEU:HD23	2.30	0.56
1:A:152:LEU:HD23	1:A:159:ILE:HG13	1.88	0.56
1:B:203:SER:HB2	1:B:206:HIS:HB2	1.88	0.56
1:B:79:GLN:O	1:B:81:GLU:N	2.39	0.56
1:B:163:LYS:HD2	1:B:164:GLU:N	2.16	0.56
1:A:12:LEU:HD11	1:A:293:CYS:SG	2.46	0.55
1:A:149:GLN:O	1:A:150:GLU:HG3	2.06	0.55
1:B:246:ARG:CA	1:B:291:MET:HE3	2.34	0.55
1:B:118:LEU:C	1:B:118:LEU:HD23	2.32	0.55
1:A:251:THR:CG2	1:A:253:MET:CG	2.86	0.54
1:B:10:SER:O	1:B:14:ARG:HG3	2.08	0.53
1:A:171:ILE:HD13	1:A:210:MET:HB2	1.90	0.53
1:A:204:PRO:N	3:A:419:HOH:O	2.41	0.53
1:A:248:LEU:HB3	1:A:254:ILE:HD13	1.90	0.53
1:B:8:ALA:CA	1:B:10:SER:N	2.64	0.52
1:B:20:GLY:C	1:B:22:GLU:H	2.08	0.52
1:B:200:VAL:HG11	1:B:283:PHE:HB2	1.92	0.52
1:B:23:GLY:CA	1:B:282:ARG:HH12	2.16	0.51
1:B:13:GLU:HA	1:B:16:GLU:HG3	1.92	0.51
1:A:261:PHE:O	1:A:265:LEU:HB2	2.10	0.51
1:A:152:LEU:HD23	1:A:159:ILE:CG1	2.40	0.51
1:B:197:ASP:OD2	2:E:1196:PTR:HE1	2.05	0.51
1:A:181:GLN:O	1:A:182:LYS:HB2	2.11	0.50
1:A:78:LEU:HB3	1:A:83:HIS:CD2	2.46	0.50
1:A:264:VAL:HG21	1:A:281:TYR:HE1	1.77	0.50
1:A:213:GLU:OE1	1:A:213:GLU:HA	2.11	0.49
1:A:147:GLN:O	1:A:150:GLU:HB2	2.11	0.49
1:B:8:ALA:N	1:B:10:SER:H	2.11	0.49
1:B:271:ARG:HD2	1:B:272:PRO:HD2	1.93	0.49
1:A:149:GLN:C	1:A:150:GLU:CG	2.85	0.49
1:B:80:GLU:C	1:B:81:GLU:CG	2.85	0.49
1:B:163:LYS:CD	1:B:164:GLU:H	2.19	0.49
1:B:248:LEU:HB3	1:B:254:ILE:HD13	1.95	0.49
1:A:259:SER:CB	1:A:262:ASP:OD2	2.61	0.48
1:B:261:PHE:O	1:B:265:LEU:HB2	2.13	0.48
1:B:7:SER:O	1:B:8:ALA:HB3	2.14	0.48
1:B:135:GLU:HB2	1:B:140:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:N	1:A:142:GLU:HG3	2.28	0.48
1:B:195:TRP:CE2	1:B:235:ARG:HG2	2.49	0.48
1:A:166:TRP:CZ2	1:A:172:MET:HE2	2.49	0.48
1:B:172:MET:HB3	1:B:193:MET:CE	2.43	0.48
1:A:18:ARG:HD2	1:A:25:VAL:HG11	1.96	0.48
1:A:143:ARG:HG3	1:A:145:TRP:CE2	2.49	0.47
1:B:182:LYS:HA	1:B:182:LYS:HD2	1.53	0.47
2:F:1196:PTR:HD2	2:F:1197:LEU:HD12	1.94	0.47
1:A:9:ARG:N	1:A:9:ARG:CD	2.78	0.47
1:A:215:ARG:HD3	1:A:215:ARG:HA	1.70	0.47
1:A:252:GLN:O	1:A:253:MET:HG2	2.15	0.46
1:A:220:SER:HA	1:B:253:MET:HE1	1.96	0.46
1:A:162:ILE:HD11	1:A:177:LYS:NZ	2.29	0.46
1:B:128:LEU:N	1:B:128:LEU:HD12	2.29	0.46
1:B:264:VAL:HG21	1:B:281:TYR:HE1	1.81	0.46
1:A:253:MET:HB3	1:A:253:MET:HE3	1.77	0.46
1:B:109:PRO:N	1:B:142:GLU:HG3	2.31	0.46
1:B:197:ASP:OD1	1:B:198:ARG:N	2.49	0.46
1:B:165:LYS:NZ	1:B:167:LEU:HA	2.32	0.45
1:A:65:VAL:C	1:A:66:LEU:HD23	2.41	0.45
1:A:51:GLY:C	1:A:66:LEU:HD13	2.41	0.45
1:A:93:ARG:HD2	1:A:97:GLY:O	2.17	0.45
1:B:120:TRP:HH2	1:B:183:GLU:HG3	1.81	0.45
1:B:293:CYS:HA	1:B:295:THR:HG22	1.98	0.45
1:B:134:ILE:CG2	1:B:137:GLY:HA2	2.47	0.44
1:B:172:MET:HE2	1:B:172:MET:HB2	1.82	0.44
2:F:1196:PTR:HD2	2:F:1197:LEU:HD11	1.97	0.44
1:A:162:ILE:HD11	1:A:177:LYS:HZ1	1.82	0.44
1:B:260:LEU:HD11	1:B:288:VAL:HG21	1.98	0.44
1:B:177:LYS:HD3	1:B:184:SER:CB	2.48	0.44
1:B:177:LYS:HD3	1:B:184:SER:HB3	1.99	0.44
1:B:191:GLN:OE1	1:B:193:MET:HE1	2.18	0.44
1:A:68:TYR:O	1:A:72:ARG:HB3	2.17	0.43
2:F:1197:LEU:O	2:F:1198:THR:CG2	2.59	0.43
1:A:48:THR:HB	1:A:66:LEU:HD12	2.01	0.43
2:E:1198:THR:CB	2:E:1199:PRO:HD3	2.48	0.43
1:B:104:THR:O	1:B:228:HIS:HB2	2.19	0.43
2:F:1197:LEU:CD1	2:F:1197:LEU:N	2.82	0.43
1:B:200:VAL:HG11	1:B:283:PHE:CB	2.47	0.43
1:B:251:THR:O	1:B:251:THR:HG22	2.18	0.42
1:A:147:GLN:HB2	1:A:150:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:HD2	1:A:182:LYS:HA	1.80	0.42
1:B:13:GLU:O	1:B:16:GLU:HG3	2.19	0.42
1:B:93:ARG:HD2	1:B:97:GLY:O	2.19	0.42
1:A:191:GLN:OE1	1:A:193:MET:HE1	2.21	0.41
1:B:264:VAL:HG21	1:B:281:TYR:CE1	2.55	0.41
1:A:143:ARG:HG3	1:A:145:TRP:CD2	2.56	0.41
1:B:292:PHE:C	1:B:293:CYS:SG	2.93	0.41
1:A:85:ASP:OD1	1:A:85:ASP:C	2.64	0.41
1:A:264:VAL:HG21	1:A:281:TYR:CE1	2.55	0.41
1:B:13:GLU:CA	1:B:16:GLU:HG3	2.49	0.41
1:A:104:THR:O	1:A:228:HIS:HB2	2.21	0.41
1:A:197:ASP:OD1	2:F:1196:PTR:HE1	2.20	0.41
1:B:85:ASP:OD1	1:B:85:ASP:C	2.64	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.71	0.40
1:A:241:THR:HG21	1:A:284:LEU:CD1	2.49	0.40
1:B:7:SER:O	1:B:8:ALA:CB	2.70	0.40
1:B:112:LEU:HB2	3:B:415:HOH:O	2.22	0.40
1:B:195:TRP:CE2	1:B:201:PRO:HD3	2.56	0.40
1:B:197:ASP:CG	2:E:1196:PTR:CZ	2.83	0.40
1:B:143:ARG:HG3	1:B:145:TRP:CE2	2.56	0.40
1:B:215:ARG:HA	1:B:215:ARG:HD3	1.90	0.40
1:B:221:GLY:HA2	1:B:222:PRO:HD3	1.70	0.40
1:A:171:ILE:CD1	1:A:210:MET:HB2	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	283/297 (95%)	267 (94%)	13 (5%)	3 (1%)	11 8
1	B	285/297 (96%)	268 (94%)	11 (4%)	6 (2%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3/6 (50%)	2 (67%)	0	1 (33%)	0	0
2	F	2/6 (33%)	2 (100%)	0	0	100	100
All	All	573/606 (95%)	539 (94%)	24 (4%)	10 (2%)	6	3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	148	GLU
1	B	21	ARG
1	B	8	ALA
1	B	80	GLU
1	B	19	GLY
1	B	137	GLY
1	B	20	GLY
2	E	1198	THR
1	A	137	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/255 (96%)	227 (92%)	19 (8%)	12	9
1	B	248/255 (97%)	229 (92%)	19 (8%)	12	9
2	E	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	F	4/5 (80%)	3 (75%)	1 (25%)	0	0
All	All	503/520 (97%)	462 (92%)	41 (8%)	10	8

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	10	SER

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Mol	Chain	Res	Type
1	A	12	LEU
1	A	21	ARG
1	A	25	VAL
1	A	45	VAL
1	A	57	VAL
1	A	81	GLU
1	A	118	LEU
1	A	152	LEU
1	A	154	THR
1	A	160	THR
1	A	167	LEU
1	A	177	LYS
1	A	181	GLN
1	A	186	SER
1	A	252	GLN
1	A	266	LYS
1	A	269	LYS
1	B	7	SER
1	B	10	SER
1	B	13	GLU
1	B	15	LEU
1	B	16	GLU
1	B	41	LYS
1	B	45	VAL
1	B	57	VAL
1	B	150	GLU
1	B	154	THR
1	B	167	LEU
1	B	177	LYS
1	B	181	GLN
1	B	182	LYS
1	B	183	GLU
1	B	269	LYS
1	B	291	MET
1	B	293	CYS
1	B	294	SER
2	E	1197	LEU
2	E	1198	THR
2	F	1197	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	252	GLN
1	B	83	HIS
1	B	147	GLN
1	B	247	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	1196	2	15,16,17	2.19	1 (6%)	17,22,24	0.84	1 (5%)
2	PTR	E	1196	2	15,16,17	1.98	1 (6%)	17,22,24	0.80	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	1196	2	-	1/10/11/13	0/1/1/1
2	PTR	E	1196	2	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1196	PTR	OH-CZ	-7.86	1.23	1.40
2	E	1196	PTR	OH-CZ	-7.43	1.23	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1196	PTR	O2P-P-OH	2.66	113.20	105.32
2	E	1196	PTR	O2P-P-OH	2.46	112.61	105.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1196	PTR	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1196	PTR	4	0
2	E	1196	PTR	8	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 [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	286/297 (96%)	0.68	27 (9%) 14 14	15, 26, 44, 61	1 (0%)
1	B	288/297 (96%)	0.76	40 (13%) 6 6	13, 26, 50, 62	1 (0%)
2	E	5/6 (83%)	2.86	3 (60%) 0 0	30, 49, 57, 73	0
2	F	4/6 (66%)	3.42	3 (75%) 0 0	37, 46, 55, 60	0
All	All	583/606 (96%)	0.75	73 (12%) 8 8	13, 26, 49, 73	2 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	CYS	6.6
1	B	197	ASP	6.4
1	B	256	PRO	5.2
2	E	1199	PRO	4.6
2	F	1194	PRO	4.5
1	A	197	ASP	4.5
2	E	1194	PRO	4.1
1	B	285	TYR	4.0
2	F	1198	THR	4.0
1	B	294	SER	3.9
1	B	203	SER	3.9
1	A	148	GLU	3.7
1	A	259	SER	3.7
1	B	9	ARG	3.6
1	B	8	ALA	3.5
1	A	204	PRO	3.4
2	F	1197	LEU	3.4
1	B	137	GLY	3.2
1	B	18	ARG	3.1
1	B	13	GLU	3.1
1	A	63	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	182	LYS	3.1
1	B	11	PHE	3.0
1	A	45	VAL	3.0
1	A	251	THR	3.0
1	B	15	LEU	2.9
1	B	286	HIS	2.9
1	B	156	LEU	2.9
1	B	7	SER	2.9
1	B	80	GLU	2.8
1	B	293	CYS	2.8
1	A	253	MET	2.7
1	B	21	ARG	2.7
1	A	40	TRP	2.7
1	B	295	THR	2.7
1	A	150	GLU	2.7
1	B	22	GLU	2.7
1	A	9	ARG	2.7
1	A	252	GLN	2.6
2	E	1198	THR	2.6
1	B	292	PHE	2.5
1	B	251	THR	2.5
1	B	260	LEU	2.5
1	A	256	PRO	2.5
1	B	136	ASN	2.5
1	A	181	GLN	2.4
1	A	156	LEU	2.4
1	B	12	LEU	2.4
1	B	20	GLY	2.4
1	B	43	ASP	2.4
1	B	177	LYS	2.4
1	A	286	HIS	2.4
1	A	138	ARG	2.3
1	B	10	SER	2.3
1	A	80	GLU	2.3
1	A	81	GLU	2.3
1	A	136	ASN	2.3
1	A	274	ALA	2.3
1	A	255	PRO	2.2
1	A	167	LEU	2.2
1	B	183	GLU	2.2
1	A	254	ILE	2.2
1	B	82	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	53	ARG	2.2
1	B	138	ARG	2.2
1	B	78	LEU	2.2
1	B	204	PRO	2.1
1	B	167	LEU	2.1
1	B	216[A]	ARG	2.1
1	A	258	PHE	2.0
1	B	17	ALA	2.0
1	B	257	ASP	2.0
1	A	137	GLY	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($\text{\AA}^2$)	Q<0.9
2	PTR	F	1196	16/17	0.95	0.10	13,19,29,38	0
2	PTR	E	1196	16/17	0.97	0.10	15,20,33,34	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.