



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:04 PM UTC

PDB ID : 6QHD / pdb_00006qhd
Title : Lysine acetylated and tyrosine phosphorylated STAT3 in a complex with DNA
Authors : Arbely, E.; Belo, Y.; Shahar, A.; Zarivach, R.
Deposited on : 2019-01-16
Resolution : 2.85 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

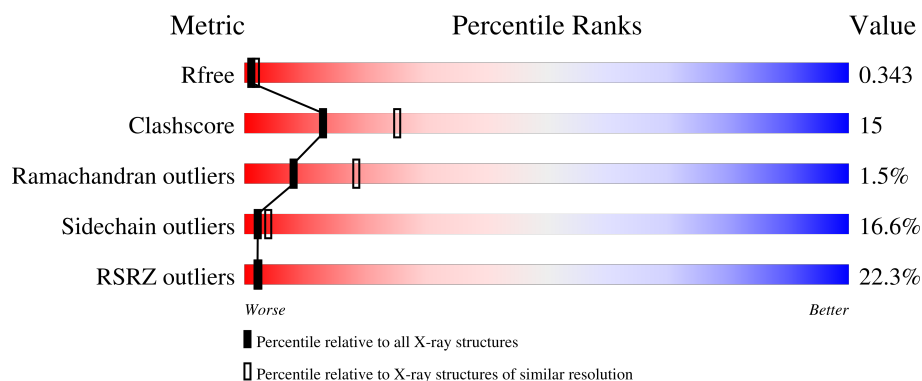
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	596	21% 54% 27% 6% 11%
1	B	596	20% 55% 25% 8% 11%
2	C	18	72% 17% 11%
3	D	18	56% 44%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9454 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 Signal transducer and activator of transcription 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	P	S	0	1	0
			4310	2756	728	796	1	29			
1	B	532	Total	C	N	O	P	S	0	0	0
			4323	2767	731	797	1	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	631	SER	LYS	conflict	UNP P40763
B	631	SER	LYS	conflict	UNP P40763

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*TP*TP*TP*AP*CP*GP*GP*GP*AP*AP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			372	178	74	103	17			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total	C	N	O	P	0	0	0
			360	175	59	109	17			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	36	Total	O	0	0
			36	36		

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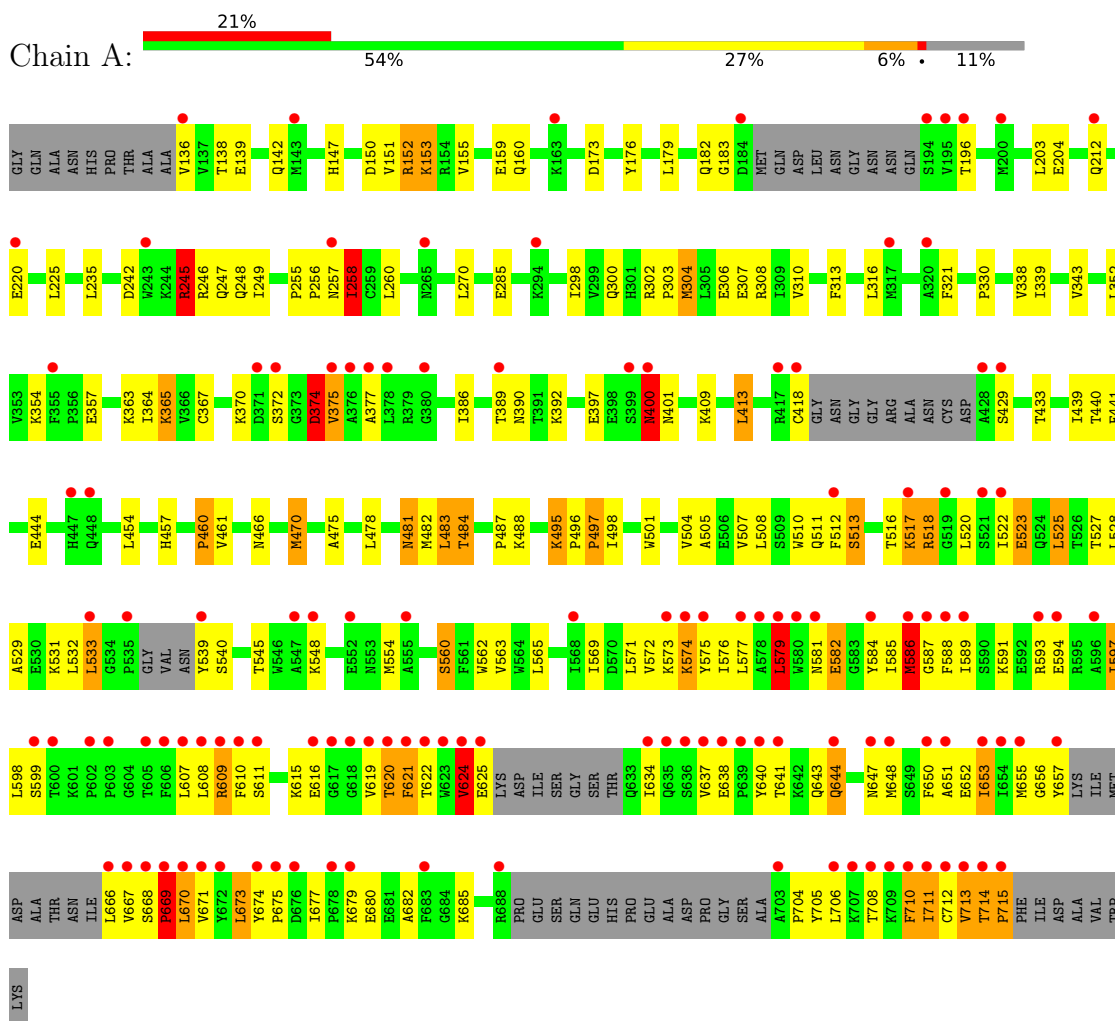
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	6	Total	O	0	0
			6	6		
4	D	5	Total	O	0	0
			5	5		

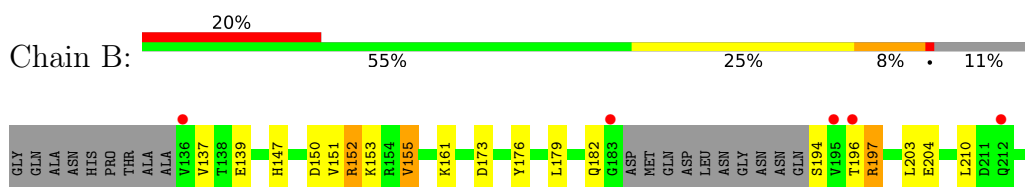
3 Residue-property plots [i](#)

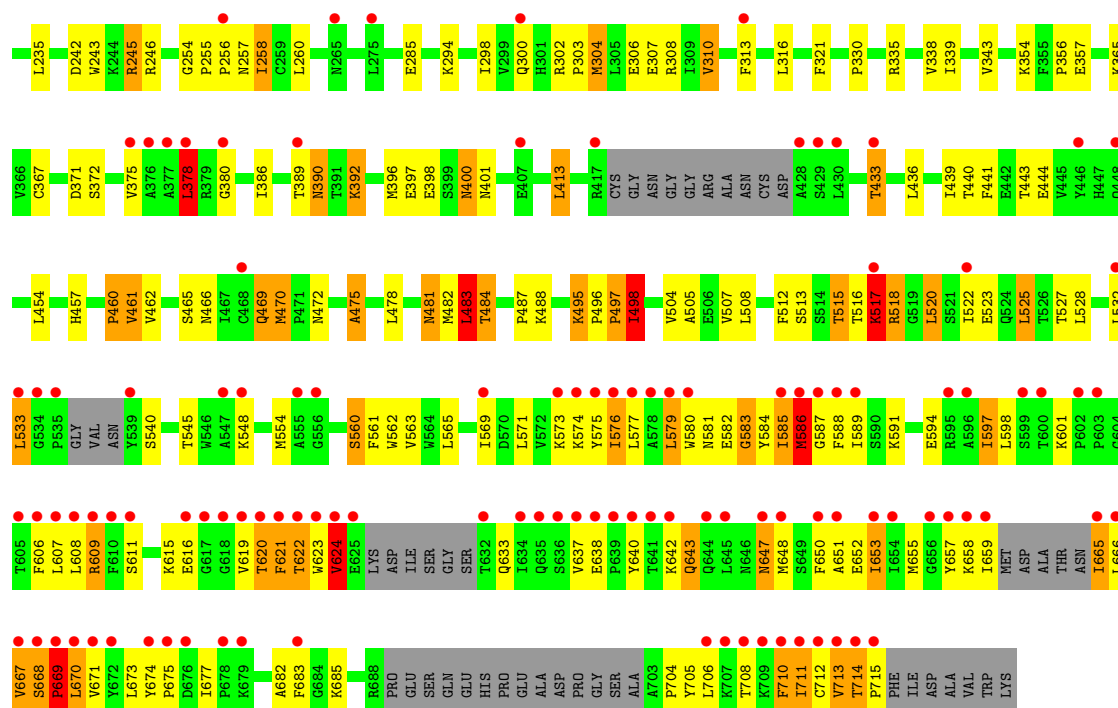
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Signal transducer and activator of transcription 3

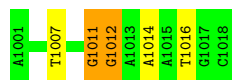


- Molecule 1: Signal transducer and activator of transcription 3





Chain C:



• Molecule 3: DNA (5'-D(*TP*GP*CP*AP*TP*TP*TP*CP*CP*CP*GP*TP*AP*AP*AP*TP*CP*T)-3')

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	175.49Å 175.49Å 79.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.85) 100.0 (50.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.294 , 0.343 0.294 , 0.343	Depositor DCC
R_{free} test set	2781 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å ²)	109.0	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 98.07 % 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 5.6998e-11. 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, ALY

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	1.32	11/4364 (0.3%)	1.40	34/5886 (0.6%)
1	B	1.33	13/4374 (0.3%)	1.38	33/5900 (0.6%)
2	C	0.72	0/419	1.29	4/646 (0.6%)
3	D	0.66	0/401	1.36	6/616 (1.0%)
All	All	1.28	24/9558 (0.3%)	1.38	77/13048 (0.6%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	ILE	C-O	-7.31	1.15	1.24
1	A	439	ILE	C-O	-7.28	1.15	1.24
1	A	365	LYS	C-O	-6.51	1.16	1.24
1	B	668	SER	N-CA	6.29	1.55	1.46
1	B	668	SER	CA-C	6.23	1.60	1.52
1	B	365	LYS	C-O	-5.83	1.17	1.24
1	A	478	LEU	CA-C	-5.76	1.45	1.52
1	A	669	PRO	CA-C	5.72	1.60	1.52
1	A	196	THR	CA-C	5.61	1.60	1.52
1	B	256	PRO	CA-CB	5.58	1.57	1.53
1	B	457	HIS	C-O	-5.54	1.16	1.23
1	B	666	LEU	CA-C	5.51	1.60	1.53
1	A	714	THR	N-CA	5.28	1.50	1.46
1	B	478	LEU	CA-C	-5.26	1.46	1.52
1	A	457	HIS	C-O	-5.25	1.17	1.23
1	B	469	GLN	CD-NE2	-5.16	1.22	1.33
1	A	481	ASN	CA-C	-5.14	1.45	1.52
1	A	258	ILE	N-CA	-5.11	1.40	1.46
1	B	481	ASN	C-O	-5.10	1.17	1.24
1	B	310	VAL	C-O	-5.07	1.18	1.24
1	B	443	THR	C-O	-5.06	1.18	1.24
1	A	245	ARG	C-O	-5.06	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	475	ALA	C-O	-5.04	1.18	1.24
1	A	375	VAL	N-CA	5.02	1.52	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	VAL	CB-CA-C	-9.08	102.97	111.05
1	B	624	VAL	N-CA-C	9.01	121.78	108.45
1	B	667	VAL	N-CA-C	8.81	121.70	109.45
1	A	671	VAL	CB-CA-C	-8.62	103.38	111.05
1	B	586	MET	N-CA-C	-8.20	101.40	111.40
1	A	586	MET	N-CA-C	-7.80	101.88	111.40
3	D	1012	DT	C4'-C3'-O3'	-7.73	98.41	110.00
1	B	671	VAL	N-CA-C	7.44	117.50	111.62
1	A	397	GLU	N-CA-C	7.39	119.84	110.24
1	A	582	GLU	N-CA-C	-7.30	104.23	113.72
3	D	1011	DG	C4'-C3'-O3'	-7.27	99.10	110.00
1	B	579	LEU	N-CA-C	-7.17	103.54	111.36
1	A	624	VAL	N-CA-C	7.01	119.64	108.85
2	C	1012	DG	C4'-C3'-O3'	-6.97	99.55	110.00
1	A	258	ILE	N-CA-CB	-6.91	103.38	112.36
1	B	256	PRO	CA-C-O	-6.85	116.24	121.31
1	A	671	VAL	N-CA-C	6.83	117.01	111.62
1	B	710	PHE	N-CA-C	6.68	119.10	109.14
1	A	579	LEU	N-CA-C	-6.52	104.25	111.36
1	A	484	THR	CB-CA-C	-6.51	96.45	110.45
1	B	484	THR	CB-CA-C	-6.47	96.54	110.45
1	A	668	SER	CA-C-N	6.44	127.89	119.84
1	A	668	SER	C-N-CA	6.44	127.89	119.84
2	C	1011	DG	C4'-C3'-O3'	-6.39	100.42	110.00
1	B	673	LEU	N-CA-C	-6.22	100.45	109.59
2	C	1016	DT	N1-C1'-C2'	6.18	122.77	113.50
1	A	258	ILE	CB-CA-C	6.17	117.72	110.93
1	B	498	ILE	CB-CA-C	6.15	119.73	110.63
1	A	374	ASP	N-CA-C	6.14	123.88	110.80
1	A	256	PRO	CA-C-O	-6.10	116.80	121.31
1	B	583	GLY	N-CA-C	-6.05	106.73	115.27
1	A	257	ASN	N-CA-CB	5.99	118.97	110.46
1	B	298	ILE	N-CA-C	-5.92	104.74	110.72
3	D	1016	DT	N1-C1'-C2'	5.92	122.39	113.50
1	A	496	PRO	N-CA-C	5.91	117.91	110.70
3	D	1003	DC	C2'-C3'-O3'	5.88	120.32	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	LYS	N-CA-CB	-5.87	101.35	110.57
1	A	298	ILE	N-CA-C	-5.86	104.80	110.72
1	A	673	LEU	N-CA-C	-5.86	100.98	109.59
1	B	357	GLU	N-CA-C	-5.73	106.29	113.28
3	D	1012	DT	C2'-C3'-O3'	5.69	120.04	111.50
1	B	496	PRO	N-CA-C	5.65	117.60	110.70
1	A	343	VAL	CB-CA-C	-5.63	103.29	111.68
1	A	470	MET	CA-C-N	-5.57	113.15	119.28
1	A	470	MET	C-N-CA	-5.57	113.15	119.28
1	A	357	GLU	N-CA-C	-5.56	106.49	113.28
1	A	400	ASN	N-CA-C	-5.56	104.91	110.97
1	B	517	LYS	N-CA-C	5.52	119.18	112.23
1	A	647	ASN	N-CA-C	5.50	117.36	111.36
1	B	316	LEU	N-CA-C	-5.46	105.41	111.36
1	B	343	VAL	CB-CA-C	-5.43	103.58	111.68
1	A	316	LEU	N-CA-C	-5.41	105.47	111.36
3	D	1005	DT	C2'-C3'-O3'	5.33	119.49	111.50
1	A	560	SER	CB-CA-C	-5.30	99.78	109.54
1	B	560	SER	CB-CA-C	-5.28	99.82	109.54
1	B	470	MET	CA-C-N	-5.27	113.49	119.28
1	B	470	MET	C-N-CA	-5.27	113.49	119.28
1	B	647	ASN	N-CA-C	5.26	117.10	111.36
1	A	532	LEU	N-CA-C	5.25	117.01	111.28
1	B	257	ASN	N-CA-CB	5.25	117.92	110.46
1	B	483	LEU	N-CA-C	5.25	119.24	112.41
1	A	389	THR	CB-CA-C	5.23	119.15	110.78
1	B	397	GLU	N-CA-C	5.23	117.46	110.35
1	A	153	LYS	CG-CD-CE	5.21	123.29	111.30
1	B	615	LYS	N-CA-C	-5.21	103.80	110.53
1	B	669	PRO	N-CA-C	5.19	123.17	112.47
1	A	313	PHE	N-CA-C	-5.17	105.72	111.36
1	B	400	ASN	N-CA-C	-5.17	105.33	110.97
1	B	254	GLY	N-CA-C	5.17	118.20	112.00
1	A	715	PRO	CA-N-CD	-5.16	104.77	112.00
1	B	313	PHE	N-CA-C	-5.16	105.73	111.36
2	C	1014	DA	C2'-C3'-O3'	5.12	119.18	111.50
1	A	615	LYS	N-CA-C	-5.10	103.95	110.53
1	B	155	VAL	N-CA-C	-5.10	105.57	110.72
1	B	389	THR	CB-CA-C	5.08	118.91	110.78
1	B	667	VAL	CB-CA-C	-5.04	104.53	111.49
1	A	470	MET	CB-CG-SD	-5.02	97.63	112.70

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	4310	0	4367	140	0
1	B	4323	0	4391	141	0
2	C	372	0	204	2	0
3	D	360	0	207	2	0
4	A	42	0	0	2	0
4	B	36	0	0	1	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
All	All	9454	0	9169	277	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 15.

All (277) 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:517:LYS:HE2	1:A:577:LEU:CD2	1.70	1.20
1:A:656:GLY:O	1:A:711:ILE:CD1	1.96	1.13
1:A:711:ILE:HG12	1:A:713:VAL:HG13	1.33	1.10
1:A:517:LYS:HE2	1:A:577:LEU:HD23	1.19	1.09
1:B:505:ALA:HB1	1:B:525:LEU:HD11	1.46	0.96
1:A:711:ILE:CG1	1:A:713:VAL:HG13	1.97	0.94
1:A:656:GLY:O	1:A:711:ILE:HD12	1.67	0.92
1:A:656:GLY:C	1:A:711:ILE:CD1	2.44	0.91
1:A:505:ALA:HB1	1:A:525:LEU:HD11	1.49	0.91
1:A:656:GLY:O	1:A:711:ILE:HD11	1.72	0.90
1:A:711:ILE:CD1	1:A:713:VAL:CG1	2.51	0.88
1:A:516:THR:HG22	1:A:577:LEU:HG	1.56	0.87
1:A:656:GLY:C	1:A:711:ILE:HD12	2.00	0.86
1:A:711:ILE:CD1	1:A:713:VAL:HG13	2.10	0.82
1:A:598:LEU:HG	1:A:624:VAL:HG11	1.62	0.81
1:B:339:ILE:HG21	1:B:413:LEU:HD22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ILE:HB	1:B:713:VAL:HG13	1.67	0.76
1:A:656:GLY:C	1:A:711:ILE:HD11	2.08	0.75
1:A:585:ILE:HG12	1:A:608:LEU:HD12	1.70	0.74
1:A:339:ILE:HG21	1:A:413:LEU:HD22	1.68	0.73
1:A:711:ILE:HD11	1:A:713:VAL:CG1	2.20	0.72
1:A:260:LEU:HD22	1:A:352:LEU:HD21	1.70	0.72
1:A:517:LYS:HE2	1:A:577:LEU:HD21	1.67	0.72
1:A:666:LEU:HD11	1:B:665:ILE:HD11	1.71	0.71
1:A:585:ILE:HG12	1:A:608:LEU:CD1	2.19	0.71
1:B:584:TYR:CE2	1:B:682:ALA:HB1	2.26	0.71
1:A:711:ILE:HD11	1:A:713:VAL:HG12	1.74	0.69
1:A:584:TYR:CE2	1:A:682:ALA:HB1	2.29	0.68
1:A:579:LEU:HD23	1:A:651:ALA:HB2	1.74	0.68
1:B:579:LEU:HD23	1:B:651:ALA:HB2	1.76	0.68
1:B:658:LYS:HB2	1:B:667:VAL:HB	1.75	0.67
1:A:517:LYS:CE	1:A:577:LEU:HD23	2.12	0.66
1:B:579:LEU:HD12	1:B:579:LEU:H	1.61	0.66
1:A:710:PHE:HB3	1:B:712:CYS:N	2.11	0.66
1:A:579:LEU:H	1:A:579:LEU:HD12	1.62	0.65
1:B:576:ILE:HA	1:B:579:LEU:HD13	1.78	0.65
1:A:516:THR:CG2	1:A:577:LEU:HG	2.25	0.65
1:A:245:ARG:NH1	1:A:481:ASN:O	2.31	0.64
1:B:582:GLU:HB3	1:B:584:TYR:CD1	2.33	0.63
1:A:597:ILE:HD12	1:A:622:THR:HG21	1.79	0.63
1:B:465:SER:H	1:B:469:GLN:HE22	1.45	0.63
1:B:197:ARG:HB3	1:B:197:ARG:HH21	1.62	0.63
1:A:574:LYS:O	1:A:574:LYS:HD3	1.97	0.63
1:B:245:ARG:NH1	1:B:481:ASN:O	2.31	0.63
1:A:152:ARG:HG3	1:A:152:ARG:HH11	1.63	0.63
1:B:152:ARG:HH11	1:B:152:ARG:HG3	1.63	0.63
1:B:243:TRP:CE2	1:B:260:LEU:HD21	2.34	0.63
1:A:657:TYR:HA	1:A:713:VAL:HG12	1.80	0.63
1:B:225:LEU:HD13	1:B:308:ARG:HB2	1.81	0.63
1:A:714:THR:N	1:A:715:PRO:HD2	2.13	0.63
1:A:576:ILE:HA	1:A:579:LEU:HD13	1.81	0.62
1:B:147:HIS:O	1:B:151:VAL:HG23	1.98	0.62
1:B:659:ILE:HG13	1:B:714:THR:HG21	1.82	0.62
1:A:147:HIS:O	1:A:151:VAL:HG23	2.00	0.61
1:B:512:PHE:CE2	1:B:520:LEU:HD21	2.35	0.61
1:B:580:TRP:HA	1:B:585:ILE:HG13	1.81	0.61
1:A:225:LEU:HD13	1:A:308:ARG:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:LEU:CG	1:A:624:VAL:HG11	2.29	0.61
1:A:609:ARG:HH11	1:A:620:THR:HG21	1.65	0.61
1:A:585:ILE:HG23	1:A:608:LEU:CB	2.31	0.61
1:B:609:ARG:HH21	1:B:620:THR:HG21	1.66	0.60
3:D:1001:DT:H2'	3:D:1002:DG:C8	2.36	0.60
1:A:339:ILE:HD12	1:A:461:VAL:HG11	1.82	0.60
1:B:516:THR:HG22	1:B:577:LEU:HG	1.84	0.60
1:A:711:ILE:HG12	1:A:713:VAL:CG1	2.23	0.59
1:A:545:THR:HG23	1:A:548:LYS:H	1.68	0.59
1:B:571:LEU:HD13	1:B:642:LYS:HE2	1.85	0.59
1:A:179:LEU:HD12	1:A:203:LEU:HD22	1.85	0.58
1:A:512:PHE:CE2	1:A:520:LEU:HD21	2.38	0.58
1:B:586:MET:CB	1:B:607:LEU:HD11	2.33	0.58
1:B:585:ILE:HG23	1:B:608:LEU:HB2	1.85	0.58
1:A:585:ILE:HG23	1:A:608:LEU:HB2	1.84	0.58
1:A:641:THR:HG23	1:A:644:GLN:H	1.69	0.58
1:B:581:ASN:C	1:B:583:GLY:H	2.11	0.58
1:B:367:CYS:HA	1:B:386:ILE:HD12	1.86	0.57
1:B:482:MET:HE2	1:B:507:VAL:HG21	1.85	0.57
1:B:498:ILE:HD12	1:B:545:THR:HG22	1.86	0.57
1:B:338:VAL:HG11	1:B:470:MET:CE	2.34	0.57
1:B:517:LYS:CD	1:B:517:LYS:H	2.16	0.57
1:B:517:LYS:H	1:B:517:LYS:HD3	1.69	0.57
1:A:711:ILE:HD13	1:A:713:VAL:CG1	2.32	0.57
1:A:338:VAL:CG1	1:A:470:MET:HE3	2.35	0.57
1:A:517:LYS:H	1:A:517:LYS:HD3	1.68	0.56
1:A:306:GLU:O	1:A:310:VAL:HG23	2.05	0.56
1:B:643:GLN:O	1:B:643:GLN:HG3	2.04	0.56
1:A:482:MET:HE2	1:A:507:VAL:HG21	1.86	0.56
1:A:527:THR:HG21	1:A:589:ILE:CA	2.35	0.56
1:A:338:VAL:HG11	1:A:470:MET:HE3	1.87	0.56
1:B:306:GLU:O	1:B:310:VAL:HG23	2.06	0.56
1:A:516:THR:HG22	1:A:577:LEU:CG	2.30	0.55
1:B:354:LYS:NZ	1:B:401:ASN:O	2.40	0.55
1:B:338:VAL:HG11	1:B:470:MET:HE3	1.89	0.55
1:B:714:THR:OG1	1:B:715:PRO:HD2	2.06	0.55
1:B:657:TYR:HA	1:B:713:VAL:HG12	1.87	0.55
1:B:623:TRP:CD1	1:B:623:TRP:N	2.75	0.55
1:A:584:TYR:HE2	1:A:682:ALA:O	1.90	0.55
1:B:623:TRP:HB3	1:B:670:LEU:HD23	1.88	0.55
1:A:248:GLN:HB2	4:A:802:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ILE:HD11	1:B:622:THR:HG21	1.89	0.54
1:A:367:CYS:HA	1:A:386:ILE:HD12	1.88	0.54
1:A:533:LEU:N	1:A:533:LEU:HD22	2.23	0.54
1:B:523:GLU:OE2	1:B:523:GLU:N	2.29	0.53
1:A:151:VAL:O	1:A:155:VAL:HG23	2.09	0.53
1:A:138:THR:O	1:A:142:GLN:HG3	2.08	0.53
1:B:582:GLU:HB3	1:B:584:TYR:CE1	2.43	0.53
1:B:197:ARG:HB3	1:B:197:ARG:NH2	2.23	0.53
1:B:650:PHE:HA	1:B:653:ILE:HG22	1.89	0.53
1:B:151:VAL:O	1:B:155:VAL:HG23	2.08	0.53
1:B:587:GLY:HA2	1:B:609:ARG:HA	1.91	0.53
1:B:523:GLU:H	1:B:523:GLU:CD	2.15	0.52
1:B:533:LEU:N	1:B:533:LEU:HD22	2.24	0.52
1:A:710:PHE:HB3	1:B:712:CYS:CA	2.39	0.52
1:B:648:MET:HG2	1:B:652:GLU:HB3	1.91	0.52
1:B:339:ILE:HD12	1:B:461:VAL:HG11	1.90	0.52
1:A:374:ASP:H	1:A:377:ALA:HB3	1.73	0.52
1:B:591:LYS:HA	1:B:594:GLU:HB3	1.91	0.52
1:A:517:LYS:HE3	1:A:581:ASN:HB2	1.90	0.52
1:A:588:PHE:CE1	1:A:610:PHE:HD2	2.27	0.52
1:B:285:GLU:HB2	1:B:302:ARG:HD2	1.92	0.52
1:A:587:GLY:HA2	1:A:609:ARG:HA	1.92	0.51
1:A:285:GLU:HB2	1:A:302:ARG:HD2	1.92	0.51
1:A:517:LYS:HD3	1:A:517:LYS:N	2.25	0.51
1:B:597:ILE:CD1	1:B:622:THR:HG21	2.41	0.51
1:A:504:VAL:HG12	1:A:508:LEU:CD1	2.41	0.51
1:A:650:PHE:HA	1:A:653:ILE:HG22	1.91	0.51
1:B:504:VAL:HG12	1:B:508:LEU:CD1	2.41	0.51
1:B:581:ASN:C	1:B:583:GLY:N	2.67	0.51
1:A:527:THR:HG21	1:A:589:ILE:N	2.25	0.50
1:A:582:GLU:HB3	1:A:584:TYR:CD1	2.47	0.50
2:C:1011:DG:H2"	2:C:1012:DG:C8	2.46	0.50
1:A:648:MET:HG2	1:A:652:GLU:HB3	1.92	0.50
1:B:466:ASN:ND2	2:C:1007:DT:O4	2.44	0.50
1:A:517:LYS:H	1:A:517:LYS:CD	2.23	0.50
1:A:354:LYS:NZ	1:A:401:ASN:O	2.39	0.49
1:A:523:GLU:CD	1:A:523:GLU:H	2.20	0.49
1:B:475:ALA:HB2	1:B:562:TRP:CD1	2.48	0.49
1:B:584:TYR:HE2	1:B:682:ALA:O	1.96	0.49
1:A:475:ALA:HB2	1:A:562:TRP:CD1	2.47	0.49
1:A:644:GLN:HA	1:A:644:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ILE:HG23	1:B:608:LEU:CB	2.42	0.49
1:B:390:ASN:H	1:B:390:ASN:HD22	1.60	0.48
1:A:249:ILE:HG13	4:A:802:HOH:O	2.12	0.48
1:A:339:ILE:CG2	1:A:413:LEU:HD22	2.42	0.48
1:B:378:LEU:HD12	1:B:380:GLY:H	1.77	0.48
1:B:339:ILE:CG2	1:B:413:LEU:HD22	2.41	0.48
1:A:711:ILE:CG1	1:A:713:VAL:CG1	2.78	0.48
1:B:465:SER:H	1:B:469:GLN:NE2	2.10	0.48
1:A:598:LEU:CD2	1:A:624:VAL:HG11	2.44	0.48
1:B:243:TRP:CD2	1:B:260:LEU:HD21	2.49	0.48
1:B:243:TRP:CZ2	1:B:260:LEU:HD21	2.48	0.48
1:B:598:LEU:HD13	1:B:598:LEU:HA	1.70	0.48
1:B:569:ILE:HG22	1:B:569:ILE:O	2.12	0.48
1:B:304:MET:SD	1:B:308:ARG:NH1	2.87	0.47
1:B:528:LEU:HD11	1:B:588:PHE:CE2	2.50	0.47
1:A:518:ARG:HD2	1:A:581:ASN:HA	1.95	0.47
1:A:585:ILE:HG12	1:A:608:LEU:HD13	1.96	0.47
1:B:674:TYR:CD1	1:B:674:TYR:C	2.92	0.47
1:A:365:LYS:HE2	1:A:390:ASN:ND2	2.29	0.47
1:A:517:LYS:CE	1:A:581:ASN:HB2	2.44	0.47
1:A:586:MET:CB	1:A:607:LEU:HD11	2.44	0.47
1:B:606:PHE:CE2	1:B:683:PHE:HE2	2.33	0.47
1:A:482:MET:HG2	1:A:483:LEU:HD13	1.96	0.47
1:A:594:GLU:O	1:A:597:ILE:HG12	2.15	0.47
1:A:674:TYR:CD1	1:A:674:TYR:C	2.93	0.47
1:B:609:ARG:HB3	1:B:620:THR:HG22	1.97	0.47
1:A:574:LYS:HB3	1:A:575:TYR:CD1	2.49	0.47
1:B:441:PHE:CD1	1:B:441:PHE:N	2.83	0.47
1:B:504:VAL:HG12	1:B:508:LEU:HD11	1.97	0.46
1:B:515:THR:HG23	1:B:573:LYS:HD3	1.97	0.46
1:A:304:MET:SD	1:A:308:ARG:NH2	2.88	0.46
1:A:504:VAL:HG12	1:A:508:LEU:HD11	1.97	0.46
1:A:657:TYR:HD1	1:A:657:TYR:O	1.97	0.46
1:A:152:ARG:HG3	1:A:152:ARG:NH1	2.29	0.46
1:A:242:ASP:O	1:A:246:ARG:HG3	2.15	0.46
1:B:647:ASN:N	1:B:647:ASN:ND2	2.62	0.46
1:A:375:VAL:O	1:A:375:VAL:HG13	2.15	0.46
1:A:531:LYS:NZ	1:A:554:MET:CE	2.79	0.46
1:B:482:MET:HE2	1:B:507:VAL:CG2	2.46	0.46
1:B:242:ASP:O	1:B:246:ARG:HG3	2.16	0.46
1:B:482:MET:HG2	1:B:483:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TRP:HA	1:A:513:SER:HB2	1.98	0.45
1:A:579:LEU:H	1:A:579:LEU:CD1	2.28	0.45
1:A:304:MET:O	1:A:308:ARG:HG2	2.16	0.45
1:B:176:TYR:HA	1:B:203:LEU:HD21	1.98	0.45
1:B:579:LEU:H	1:B:579:LEU:CD1	2.28	0.45
1:B:647:ASN:N	1:B:647:ASN:HD22	2.12	0.45
1:A:466:ASN:ND2	3:D:1007:DT:O4	2.47	0.45
1:B:515:THR:HG23	1:B:516:THR:HG23	1.99	0.45
1:B:527:THR:HG21	1:B:589:ILE:N	2.32	0.45
1:A:609:ARG:HB3	1:A:620:THR:HG22	1.98	0.45
1:B:304:MET:O	1:B:308:ARG:HG2	2.16	0.45
1:A:441:PHE:N	1:A:441:PHE:CD1	2.84	0.45
1:B:606:PHE:HE2	1:B:683:PHE:CE2	2.35	0.45
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.29	0.45
1:B:518:ARG:NH1	1:B:581:ASN:O	2.50	0.45
1:A:569:ILE:O	1:A:572:VAL:HG22	2.17	0.45
1:A:577:LEU:HD23	1:A:577:LEU:O	2.17	0.45
1:A:591:LYS:HA	1:A:594:GLU:HB3	1.99	0.45
1:A:708:THR:HB	1:B:712:CYS:SG	2.57	0.45
1:B:433:THR:HG21	1:B:472:ASN:HB3	1.99	0.45
1:A:670:LEU:O	1:A:679:LYS:NZ	2.47	0.45
1:B:466:ASN:H	1:B:469:GLN:NE2	2.14	0.45
1:A:657:TYR:CA	1:A:711:ILE:HD11	2.47	0.45
1:B:586:MET:HB3	1:B:607:LEU:HD11	1.99	0.45
1:A:528:LEU:HD11	1:A:588:PHE:CE2	2.52	0.44
1:B:356:PRO:HA	1:B:396:MET:HE1	2.00	0.44
1:B:371:ASP:CG	1:B:375:VAL:HG11	2.42	0.44
1:B:598:LEU:HG	1:B:624:VAL:HG11	2.00	0.44
1:B:460:PRO:HD3	1:B:487:PRO:O	2.18	0.44
1:A:460:PRO:HD3	1:A:487:PRO:O	2.18	0.44
1:A:648:MET:HE2	1:A:652:GLU:HG3	1.99	0.44
1:B:598:LEU:HD11	1:B:624:VAL:HG21	2.00	0.44
1:B:371:ASP:HB3	1:B:375:VAL:HG11	1.99	0.44
1:B:658:LYS:O	1:B:713:VAL:HB	2.18	0.44
1:B:706:LEU:HD23	1:B:706:LEU:HA	1.75	0.44
1:A:512:PHE:CD2	1:A:520:LEU:HD21	2.52	0.43
1:A:518:ARG:HB3	1:A:581:ASN:HB3	1.99	0.43
1:B:517:LYS:HZ2	1:B:581:ASN:HB2	1.82	0.43
1:A:176:TYR:HA	1:A:203:LEU:HD21	2.01	0.43
1:A:482:MET:HE2	1:A:507:VAL:CG2	2.46	0.43
1:B:606:PHE:HB3	1:B:670:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:TRP:CZ3	1:B:585:ILE:HB	2.53	0.43
1:A:495:LYS:HD2	1:A:495:LYS:O	2.19	0.43
1:A:712:CYS:CB	1:B:710:PHE:HB3	2.48	0.43
1:B:356:PRO:HA	1:B:396:MET:CE	2.49	0.43
1:B:579:LEU:HD12	1:B:579:LEU:N	2.31	0.43
1:B:258:ILE:HA	1:B:258:ILE:HD12	1.74	0.43
1:B:571:LEU:HD12	1:B:571:LEU:HA	1.86	0.43
1:A:507:VAL:O	1:A:511:GLN:HG2	2.18	0.43
1:B:505:ALA:HA	1:B:508:LEU:HD12	2.01	0.43
1:B:392:LYS:HB2	1:B:392:LYS:HE2	1.66	0.43
1:B:569:ILE:O	1:B:569:ILE:CG2	2.66	0.43
1:B:577:LEU:HD23	1:B:577:LEU:O	2.19	0.43
1:A:517:LYS:NZ	1:A:581:ASN:HB2	2.34	0.43
1:A:621:PHE:O	1:A:621:PHE:HD1	2.02	0.43
1:B:338:VAL:CG1	1:B:470:MET:CE	2.96	0.43
1:A:657:TYR:HA	1:A:711:ILE:HD11	2.00	0.42
1:B:321:PHE:HB2	1:B:454:LEU:HD13	2.01	0.42
1:B:598:LEU:CD1	1:B:624:VAL:HG21	2.49	0.42
1:A:585:ILE:HG23	1:A:608:LEU:HB3	2.00	0.42
1:B:607:LEU:O	1:B:621:PHE:HA	2.19	0.42
1:B:574:LYS:HB3	1:B:575:TYR:CD1	2.55	0.42
1:A:321:PHE:HB2	1:A:454:LEU:HD13	2.02	0.42
1:A:400:ASN:ND2	1:A:400:ASN:H	2.15	0.42
1:A:598:LEU:HD13	1:A:598:LEU:HA	1.77	0.42
1:B:495:LYS:CD	1:B:495:LYS:O	2.67	0.42
1:B:495:LYS:O	1:B:495:LYS:HD2	2.20	0.42
1:B:554:MET:SD	1:B:561:PHE:HA	2.60	0.42
1:A:495:LYS:O	1:A:495:LYS:CD	2.68	0.42
1:B:601:LYS:HE3	1:B:674:TYR:CE2	2.55	0.42
1:A:531:LYS:NZ	1:A:554:MET:HE3	2.35	0.42
1:B:210:LEU:HD12	1:B:210:LEU:HA	1.87	0.42
1:A:560:SER:HB2	1:A:563:VAL:HB	2.02	0.41
1:A:527:THR:HG21	1:A:589:ILE:HA	2.01	0.41
1:B:585:ILE:HG22	1:B:587:GLY:N	2.36	0.41
1:B:609:ARG:O	1:B:620:THR:N	2.53	0.41
1:B:335:ARG:NH1	4:B:801:HOH:O	2.54	0.41
1:B:571:LEU:HD11	1:B:642:LYS:HG2	2.02	0.41
1:A:247:GLN:HA	1:A:258:ILE:HD11	2.03	0.41
1:A:302:ARG:N	1:A:303:PRO:CD	2.84	0.41
1:A:505:ALA:HA	1:A:508:LEU:HD12	2.03	0.41
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ARG:N	1:B:303:PRO:CD	2.83	0.41
1:B:621:PHE:HD1	1:B:621:PHE:O	2.04	0.41
1:B:659:ILE:HB	1:B:714:THR:HB	2.02	0.41
1:B:518:ARG:H	1:B:581:ASN:ND2	2.19	0.41
1:B:606:PHE:HE2	1:B:683:PHE:HE2	1.69	0.41
1:A:712:CYS:HA	1:B:710:PHE:HB3	2.04	0.40
1:B:436:LEU:HD23	1:B:462:VAL:HG22	2.03	0.40
1:B:560:SER:HB2	1:B:563:VAL:HB	2.02	0.40
1:A:501:TRP:CZ2	1:A:529:ALA:HB2	2.56	0.40
1:A:539:TYR:CD1	1:A:539:TYR:N	2.89	0.40
1:A:588:PHE:CE1	1:A:610:PHE:CD2	3.08	0.40
1:B:176:TYR:CD1	1:B:176:TYR:C	3.00	0.40
1:B:512:PHE:CD2	1:B:520:LEU:HD21	2.56	0.40
1:B:606:PHE:CE2	1:B:683:PHE:CE2	3.10	0.40
1:A:706:LEU:HD23	1:A:706:LEU:HA	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	515/596 (86%)	488 (95%)	20 (4%)	7 (1%)	9	19
1	B	516/596 (87%)	485 (94%)	23 (4%)	8 (2%)	7	17
All	All	1031/1192 (86%)	973 (94%)	43 (4%)	15 (2%)	8	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	GLY
1	A	669	PRO
1	A	704	PRO

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Mol	Chain	Res	Type
1	B	497	PRO
1	B	669	PRO
1	B	704	PRO
1	A	497	PRO
1	A	374	ASP
1	A	713	VAL
1	B	378	LEU
1	B	713	VAL
1	B	540	SER
1	B	668	SER
1	B	675	PRO
1	A	675	PRO

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	483/532 (91%)	401 (83%)	82 (17%)	2	3
1	B	484/532 (91%)	406 (84%)	78 (16%)	2	4
All	All	967/1064 (91%)	807 (84%)	160 (16%)	2	4

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	VAL
1	A	139	GLU
1	A	150	ASP
1	A	152	ARG
1	A	153	LYS
1	A	159	GLU
1	A	160	GLN
1	A	173	ASP
1	A	182	GLN
1	A	204	GLU
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	220	GLU
1	A	235	LEU
1	A	245	ARG
1	A	255	PRO
1	A	258	ILE
1	A	270	LEU
1	A	300	GLN
1	A	304	MET
1	A	307	GLU
1	A	330	PRO
1	A	364	ILE
1	A	370	LYS
1	A	372	SER
1	A	374	ASP
1	A	392	LYS
1	A	400	ASN
1	A	409	LYS
1	A	413	LEU
1	A	418	CYS
1	A	429	SER
1	A	433	THR
1	A	440	THR
1	A	444	GLU
1	A	460	PRO
1	A	483	LEU
1	A	484	THR
1	A	488	LYS
1	A	495	LYS
1	A	497	PRO
1	A	498	ILE
1	A	513	SER
1	A	517	LYS
1	A	518	ARG
1	A	522	ILE
1	A	523	GLU
1	A	525	LEU
1	A	533	LEU
1	A	540	SER
1	A	565	LEU
1	A	571	LEU
1	A	573	LYS
1	A	574	LYS

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Mol	Chain	Res	Type
1	A	579	LEU
1	A	586	MET
1	A	593	ARG
1	A	597	ILE
1	A	599	SER
1	A	609	ARG
1	A	611	SER
1	A	616	GLU
1	A	619	VAL
1	A	620	THR
1	A	621	PHE
1	A	624	VAL
1	A	625	GLU
1	A	634	ILE
1	A	637	VAL
1	A	638	GLU
1	A	640	TYR
1	A	643	GLN
1	A	644	GLN
1	A	653	ILE
1	A	655	MET
1	A	667	VAL
1	A	669	PRO
1	A	670	LEU
1	A	673	LEU
1	A	677	ILE
1	A	680	GLU
1	A	710	PHE
1	A	711	ILE
1	B	137	VAL
1	B	139	GLU
1	B	150	ASP
1	B	152	ARG
1	B	153	LYS
1	B	161	LYS
1	B	173	ASP
1	B	179	LEU
1	B	182	GLN
1	B	194	SER
1	B	196	THR
1	B	197	ARG
1	B	204	GLU

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Mol	Chain	Res	Type
1	B	218	VAL
1	B	220	GLU
1	B	235	LEU
1	B	245	ARG
1	B	255	PRO
1	B	258	ILE
1	B	294	LYS
1	B	300	GLN
1	B	304	MET
1	B	307	GLU
1	B	330	PRO
1	B	372	SER
1	B	378	LEU
1	B	390	ASN
1	B	392	LYS
1	B	398	GLU
1	B	400	ASN
1	B	413	LEU
1	B	433	THR
1	B	440	THR
1	B	444	GLU
1	B	460	PRO
1	B	461	VAL
1	B	483	LEU
1	B	484	THR
1	B	488	LYS
1	B	495	LYS
1	B	497	PRO
1	B	498	ILE
1	B	513	SER
1	B	515	THR
1	B	517	LYS
1	B	518	ARG
1	B	520	LEU
1	B	522	ILE
1	B	525	LEU
1	B	533	LEU
1	B	548	LYS
1	B	565	LEU
1	B	576	ILE
1	B	585	ILE
1	B	586	MET

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Mol	Chain	Res	Type
1	B	597	ILE
1	B	609	ARG
1	B	611	SER
1	B	616	GLU
1	B	619	VAL
1	B	620	THR
1	B	621	PHE
1	B	622	THR
1	B	624	VAL
1	B	633	GLN
1	B	637	VAL
1	B	638	GLU
1	B	640	TYR
1	B	643	GLN
1	B	653	ILE
1	B	655	MET
1	B	665	ILE
1	B	669	PRO
1	B	670	LEU
1	B	677	ILE
1	B	708	THR
1	B	711	ILE
1	B	714	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	160	GLN
1	A	202	GLN
1	A	280	GLN
1	A	288	GLN
1	A	315	ASN
1	A	344	GLN
1	A	385	ASN
1	A	457	HIS
1	A	489	ASN
1	A	567	ASN
1	A	635	GLN
1	A	644	GLN
1	A	647	ASN
1	B	141	GLN

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Mol	Chain	Res	Type
1	B	205	GLN
1	B	276	GLN
1	B	288	GLN
1	B	315	ASN
1	B	344	GLN
1	B	385	ASN
1	B	390	ASN
1	B	448	GLN
1	B	457	HIS
1	B	469	GLN
1	B	472	ASN
1	B	489	ASN
1	B	543	GLN
1	B	581	ASN
1	B	647	ASN

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	$\# Z > 2$
1	ALY	B	685	1	10,11,12	0.79	0	7,12,14	2.46	4 (57%)
1	ALY	A	685	1	10,11,12	0.85	0	7,12,14	2.29	3 (42%)
1	PTR	B	705	1	15,16,17	2.78	7 (46%)	17,22,24	2.27	6 (35%)
1	PTR	A	705	1	15,16,17	2.81	8 (53%)	17,22,24	1.91	3 (17%)

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
1	ALY	B	685	1	-	2/9/10/12	-
1	ALY	A	685	1	-	3/9/10/12	-
1	PTR	B	705	1	-	3/10/11/13	0/1/1/1
1	PTR	A	705	1	-	1/10/11/13	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	705	PTR	CE1-CD1	5.26	1.47	1.38
1	B	705	PTR	CE2-CD2	5.22	1.47	1.38
1	A	705	PTR	CE2-CD2	4.99	1.46	1.38
1	B	705	PTR	CE1-CD1	4.88	1.46	1.38
1	B	705	PTR	CE1-CZ	4.09	1.46	1.38
1	A	705	PTR	OH-CZ	4.06	1.49	1.40
1	A	705	PTR	CE1-CZ	3.39	1.45	1.38
1	B	705	PTR	CE2-CZ	3.35	1.45	1.38
1	B	705	PTR	OH-CZ	3.30	1.48	1.40
1	B	705	PTR	CB-CG	3.22	1.58	1.51
1	A	705	PTR	CB-CG	3.04	1.58	1.51
1	B	705	PTR	CD2-CG	2.95	1.44	1.38
1	A	705	PTR	CD2-CG	2.83	1.44	1.38
1	A	705	PTR	P-OH	2.75	1.64	1.59
1	A	705	PTR	CE2-CZ	2.70	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	PTR	CE2-CZ-CE1	-4.94	112.95	120.16
1	B	705	PTR	CD1-CE1-CZ	4.51	124.88	119.73
1	A	705	PTR	CE2-CZ-CE1	-4.02	114.30	120.16
1	A	705	PTR	CD1-CE1-CZ	3.83	124.11	119.73
1	B	685	ALY	CD-CE-NZ	3.68	122.51	112.20
1	A	685	ALY	CD-CE-NZ	3.45	121.86	112.20
1	A	685	ALY	CH3-CH-NZ	3.39	121.91	116.12
1	B	685	ALY	CH3-CH-NZ	3.34	121.83	116.12
1	B	705	PTR	CB-CG-CD2	3.05	126.58	120.90
1	B	685	ALY	CG-CD-CE	-2.88	100.29	113.56
1	A	705	PTR	CB-CG-CD2	2.69	125.91	120.90
1	A	685	ALY	CG-CD-CE	-2.56	101.75	113.56
1	B	705	PTR	O3P-P-O2P	2.51	117.20	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	685	ALY	OH-CH-CH3	-2.19	118.16	122.05
1	B	705	PTR	CD2-CE2-CZ	2.17	122.21	119.73
1	B	705	PTR	OH-CZ-CE1	2.07	125.43	119.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	705	PTR	O-C-CA-CB
1	B	705	PTR	O-C-CA-CB
1	A	685	ALY	OH-CH-NZ-CE
1	A	685	ALY	CH3-CH-NZ-CE
1	B	685	ALY	OH-CH-NZ-CE
1	B	685	ALY	CH3-CH-NZ-CE
1	A	685	ALY	CG-CD-CE-NZ
1	B	705	PTR	CA-CB-CG-CD1
1	B	705	PTR	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

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	528/596 (88%)	1.14	125 (23%) 2 2	63, 100, 170, 194	1 (0%)
1	B	530/596 (88%)	1.10	119 (22%) 2 2	71, 100, 173, 225	0
2	C	18/18 (100%)	-0.15	0 100 100	76, 92, 115, 119	0
3	D	18/18 (100%)	-0.34	0 100 100	72, 89, 112, 116	0
All	All	1094/1228 (89%)	1.08	244 (22%) 2 2	63, 99, 171, 225	1 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	623	TRP	9.3
1	B	195	VAL	7.3
1	A	666	LEU	7.3
1	B	666	LEU	7.3
1	B	579	LEU	7.1
1	B	665	ILE	6.8
1	A	714	THR	6.8
1	A	657	TYR	6.4
1	A	579	LEU	6.4
1	A	428	ALA	6.4
1	B	714	THR	6.4
1	A	195	VAL	6.3
1	B	212	GLN	6.3
1	B	640	TYR	5.9
1	A	196	THR	5.8
1	A	418	CYS	5.6
1	A	573	LYS	5.6
1	A	715	PRO	5.4
1	B	605	THR	5.2
1	A	650	PHE	5.2
1	B	676	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	376	ALA	5.1
1	A	605	THR	5.1
1	A	644	GLN	5.0
1	B	706	LEU	5.0
1	B	428	ALA	4.9
1	A	375	VAL	4.9
1	A	539	TYR	4.9
1	B	378	LEU	4.9
1	B	623	TRP	4.9
1	B	713	VAL	4.8
1	B	417	ARG	4.8
1	A	640	TYR	4.8
1	A	622	THR	4.7
1	B	616	GLU	4.7
1	A	671	VAL	4.7
1	B	539	TYR	4.4
1	A	616	GLU	4.4
1	A	675	PRO	4.4
1	B	196	THR	4.3
1	B	715	PRO	4.3
1	B	608	LEU	4.3
1	B	671	VAL	4.3
1	B	622	THR	4.3
1	B	635	GLN	4.3
1	B	641	THR	4.3
1	A	634	ILE	4.3
1	B	657	TYR	4.3
1	B	632	THR	4.2
1	A	589	ILE	4.2
1	B	547	ALA	4.2
1	B	620	THR	4.2
1	A	651	ALA	4.2
1	A	641	THR	4.2
1	A	417	ARG	4.2
1	B	651	ALA	4.2
1	B	183	GLY	4.2
1	A	389	THR	4.1
1	A	574	LYS	4.1
1	A	212	GLN	4.1
1	A	609	ARG	4.1
1	B	670	LEU	4.0
1	B	389	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	606	PHE	4.0
1	A	617	GLY	3.9
1	B	617	GLY	3.9
1	B	574	LYS	3.9
1	A	625	GLU	3.8
1	B	607	LEU	3.8
1	A	603	PRO	3.8
1	B	712	CYS	3.7
1	A	355	PHE	3.7
1	B	610	PHE	3.7
1	B	650	PHE	3.7
1	B	609	ARG	3.7
1	B	675	PRO	3.7
1	A	447	HIS	3.7
1	A	672	TYR	3.7
1	B	658	LYS	3.7
1	A	713	VAL	3.7
1	B	522	ILE	3.7
1	B	708	THR	3.7
1	A	555	ALA	3.6
1	B	580	TRP	3.6
1	A	667	VAL	3.6
1	B	136	VAL	3.6
1	A	143[A]	MET	3.6
1	A	679	LYS	3.5
1	A	706	LEU	3.5
1	B	586	MET	3.5
1	A	709	LYS	3.5
1	A	620	THR	3.5
1	A	600	THR	3.5
1	A	712	CYS	3.4
1	B	636	SER	3.4
1	B	533	LEU	3.4
1	B	535	PRO	3.4
1	A	586	MET	3.4
1	B	606	PHE	3.4
1	B	653	ILE	3.4
1	A	670	LEU	3.4
1	A	376	ALA	3.4
1	B	634	ILE	3.4
1	B	659	ILE	3.3
1	A	610	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	619	VAL	3.3
1	A	578	ALA	3.3
1	A	599	SER	3.3
1	A	547	ALA	3.3
1	B	711	ILE	3.3
1	B	578	ALA	3.3
1	B	429	SER	3.3
1	B	625	GLU	3.2
1	A	669	PRO	3.2
1	A	533	LEU	3.2
1	B	637	VAL	3.2
1	B	573	LYS	3.2
1	B	644	GLN	3.2
1	A	608	LEU	3.1
1	A	448	GLN	3.1
1	A	377	ALA	3.1
1	A	618	GLY	3.1
1	B	595	ARG	3.1
1	A	668	SER	3.1
1	A	639	PRO	3.1
1	A	637	VAL	3.0
1	B	656	GLY	3.0
1	B	375	VAL	3.0
1	B	672	TYR	3.0
1	A	607	LEU	3.0
1	A	708	THR	3.0
1	B	619	VAL	3.0
1	B	621	PHE	3.0
1	B	639	PRO	3.0
1	A	624	VAL	3.0
1	B	707	LYS	2.9
1	B	556	GLY	2.9
1	A	594	GLU	2.9
1	A	638	GLU	2.9
1	A	676	ASP	2.9
1	A	710	PHE	2.9
1	B	589	ILE	2.9
1	A	399	SER	2.9
1	B	313	PHE	2.9
1	B	555	ALA	2.9
1	A	194	SER	2.9
1	B	534	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	653	ILE	2.8
1	A	136	VAL	2.8
1	B	600	THR	2.8
1	B	587	GLY	2.8
1	B	407	GLU	2.8
1	B	548	LYS	2.8
1	A	711	ILE	2.8
1	B	618	GLY	2.7
1	A	635	GLN	2.7
1	B	683	PHE	2.7
1	A	593	ARG	2.7
1	A	535	PRO	2.7
1	A	519	GLY	2.6
1	B	667	VAL	2.6
1	A	257	ASN	2.6
1	A	320	ALA	2.6
1	A	429	SER	2.5
1	B	679	LYS	2.5
1	B	603	PRO	2.5
1	B	674	TYR	2.5
1	A	683	PHE	2.5
1	A	265	ASN	2.5
1	A	647	ASN	2.5
1	B	599	SER	2.5
1	B	602	PRO	2.5
1	B	575	TYR	2.5
1	A	587	GLY	2.5
1	A	552	GLU	2.5
1	B	709	LYS	2.5
1	B	468	CYS	2.5
1	A	648	MET	2.4
1	B	577	LEU	2.4
1	B	517	LYS	2.4
1	B	596	ALA	2.4
1	A	400	ASN	2.4
1	A	378	LEU	2.4
1	A	521	SER	2.4
1	A	674	TYR	2.4
1	B	433	THR	2.4
1	A	688	ARG	2.4
1	A	596	ALA	2.4
1	B	648	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	568	ILE	2.4
1	A	317	MET	2.3
1	A	611	SER	2.3
1	A	655	MET	2.3
1	B	446	TYR	2.3
1	B	624	VAL	2.3
1	B	265	ASN	2.3
1	B	647	ASN	2.3
1	A	703	ALA	2.3
1	A	577	LEU	2.3
1	B	256	PRO	2.3
1	A	621	PHE	2.3
1	A	372	SER	2.3
1	A	654	ILE	2.3
1	A	575	TYR	2.3
1	A	588	PHE	2.3
1	B	588	PHE	2.3
1	A	522	ILE	2.3
1	B	668	SER	2.3
1	A	220	GLU	2.2
1	B	532	LEU	2.2
1	A	294	LYS	2.2
1	B	642	LYS	2.2
1	B	569	ILE	2.2
1	B	585	ILE	2.2
1	B	669	PRO	2.2
1	A	678	PRO	2.2
1	A	707	LYS	2.2
1	B	430	LEU	2.2
1	A	243	TRP	2.2
1	A	380	GLY	2.2
1	B	380	GLY	2.2
1	A	512	PHE	2.2
1	A	548	LYS	2.2
1	A	581	ASN	2.2
1	A	517	LYS	2.2
1	A	636	SER	2.2
1	B	638	GLU	2.2
1	B	654	ILE	2.1
1	B	448	GLN	2.1
1	A	602	PRO	2.1
1	A	580	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	645	LEU	2.1
1	A	200	MET	2.1
1	B	678	PRO	2.1
1	A	371	ASP	2.1
1	B	710	PHE	2.1
1	A	584	TYR	2.1
1	B	576	ILE	2.1
1	B	300	GLN	2.1
1	A	163	LYS	2.1
1	A	184	ASP	2.1
1	B	377	ALA	2.1
1	B	275	LEU	2.0
1	B	611	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
1	ALY	B	685	12/13	0.49	0.21	142,145,146,148	0
1	ALY	A	685	12/13	0.56	0.19	140,144,146,147	0
1	PTR	B	705	16/17	0.87	0.14	153,160,168,173	0
1	PTR	A	705	16/17	0.88	0.15	147,157,166,170	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.