



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:08 PM UTC

PDB ID : 1UUS / pdb_00001uus
Title : Structure of an activated Dictyostelium STAT in its DNA-unbound form
Authors : Soler-Lopez, M.; Petosa, C.; Fukuzawa, M.; Ravelli, R.; Williams, J.G.; Muller, C.W.
Deposited on : 2004-01-09
Resolution : 2.80 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

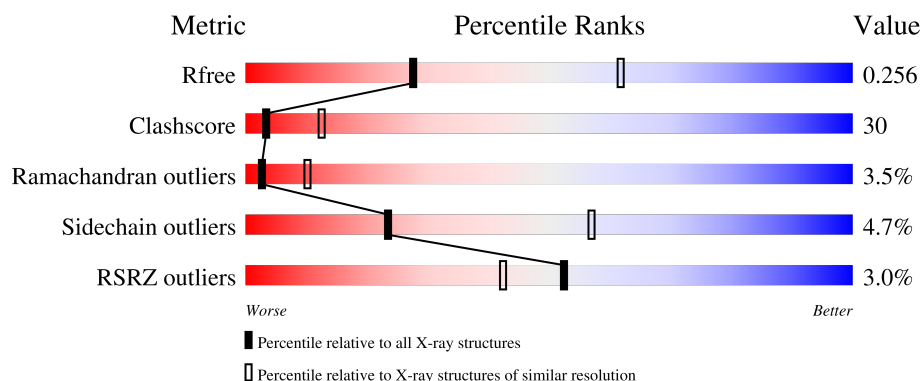
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	473	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3732 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 STAT PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	P	S	0	0	0
			3676	2349	632	682	1	12			

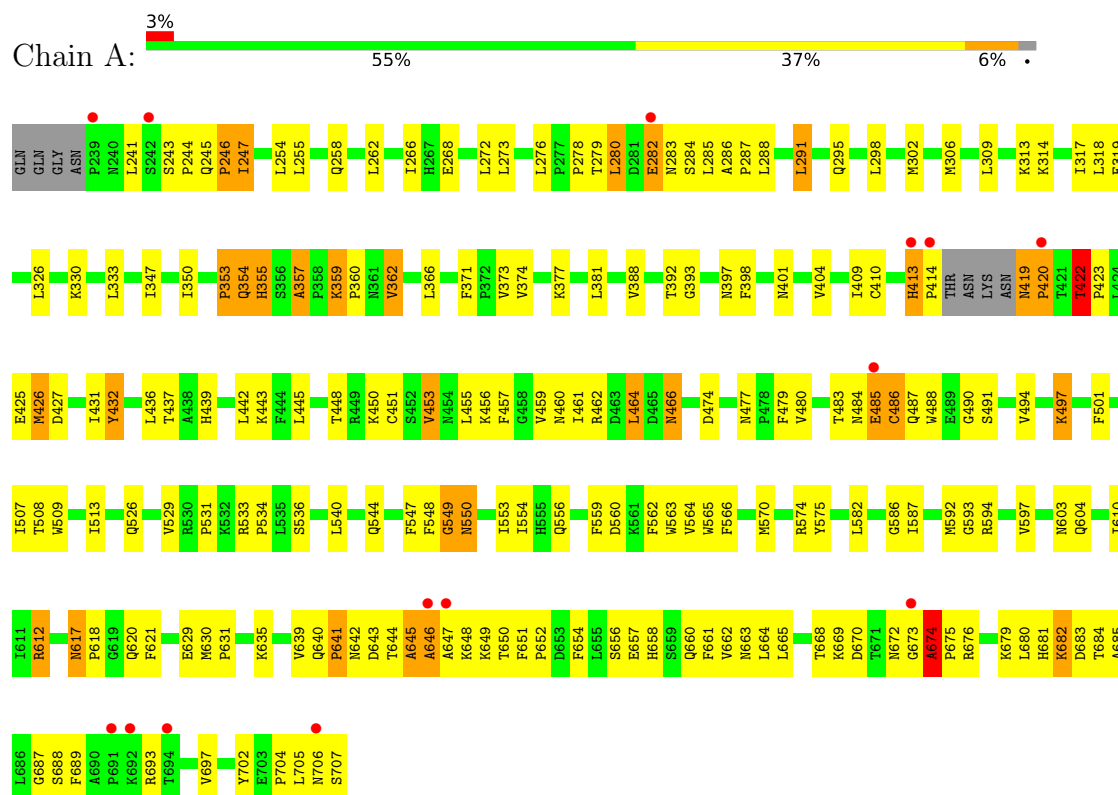
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		

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: STAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	125.90Å 145.00Å 66.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.80) 99.7 (50.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.257 0.198 , 0.256	Depositor DCC
R_{free} test set	752 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3732	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.50	0/3746	1.02	17/5083 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	TYR	CA-C-N	7.84	127.12	118.97
1	A	432	TYR	C-N-CA	7.84	127.12	118.97
1	A	355	HIS	N-CA-C	-7.45	104.22	112.72
1	A	674	ALA	N-CA-C	6.28	123.68	109.81
1	A	474	ASP	N-CA-C	-6.24	102.74	110.41
1	A	550	ASN	N-CA-C	-6.22	104.25	113.40
1	A	431	ILE	N-CA-C	6.09	117.06	108.36
1	A	586	GLY	N-CA-C	-5.86	106.56	115.00
1	A	419	ASN	CA-C-N	5.86	127.16	119.84
1	A	419	ASN	C-N-CA	5.86	127.16	119.84
1	A	689	PHE	N-CA-C	-5.46	106.47	113.02
1	A	617	ASN	CA-C-N	5.37	125.68	119.93
1	A	617	ASN	C-N-CA	5.37	125.68	119.93
1	A	680	LEU	N-CA-C	-5.30	102.14	110.36
1	A	486	CYS	N-CA-C	-5.27	106.98	113.41
1	A	422	THR	CA-C-N	5.06	125.51	120.04
1	A	422	THR	C-N-CA	5.06	125.51	120.04

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	3676	0	3670	222	1
2	A	56	0	0	7	0
All	All	3732	0	3670	222	1

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 30.

All (222) 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:413:HIS:HB3	1:A:414:PRO:CA	1.78	1.12
1:A:413:HIS:HB3	1:A:414:PRO:C	1.76	1.09
1:A:656:SER:HA	1:A:682:LYS:HE2	1.11	1.09
1:A:413:HIS:HB3	1:A:414:PRO:HA	1.37	1.07
1:A:359:LYS:HB3	1:A:360:PRO:HD2	1.39	1.04
1:A:413:HIS:CB	1:A:414:PRO:HA	1.89	1.01
1:A:414:PRO:HG2	2:A:2018:HOH:O	1.58	1.01
1:A:526:GLN:HE22	1:A:533:ARG:H	1.10	0.98
1:A:693:ARG:NH1	1:A:697:VAL:HG22	1.77	0.98
1:A:306:MET:HE1	1:A:330:LYS:HG3	1.44	0.96
1:A:656:SER:HA	1:A:682:LYS:CE	1.98	0.93
1:A:410:CYS:O	1:A:413:HIS:CE1	2.22	0.92
1:A:642:ASN:HA	1:A:645:ALA:HB2	1.52	0.92
1:A:670:ASP:HB2	1:A:674:ALA:HB3	1.53	0.89
1:A:282:GLU:CA	1:A:282:GLU:OE1	2.22	0.85
1:A:413:HIS:CB	1:A:414:PRO:CA	2.46	0.85
1:A:282:GLU:OE1	1:A:282:GLU:C	2.20	0.84
1:A:241:LEU:HD12	1:A:241:LEU:H	1.42	0.84
1:A:597:VAL:HG21	1:A:612:ARG:HD2	1.61	0.82
1:A:404:VAL:HA	1:A:459:VAL:HG12	1.61	0.82
1:A:282:GLU:OE1	1:A:282:GLU:HA	1.79	0.81
1:A:668:THR:O	1:A:675:PRO:HA	1.79	0.81
1:A:480:VAL:HG21	1:A:491:SER:HB3	1.63	0.79
1:A:276:LEU:HD13	1:A:280:LEU:HD11	1.66	0.78
1:A:282:GLU:OE1	1:A:282:GLU:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HB3	1:A:360:PRO:CD	2.14	0.76
1:A:669:LYS:HA	1:A:675:PRO:HA	1.68	0.75
1:A:317:ILE:HG12	1:A:513:ILE:HD11	1.69	0.75
1:A:401:ASN:HD21	1:A:462:ARG:HB2	1.52	0.75
1:A:244:PRO:HG3	1:A:318:LEU:CD2	2.18	0.74
1:A:241:LEU:HB3	1:A:319:GLU:HG2	1.70	0.74
1:A:404:VAL:HG22	1:A:459:VAL:HG11	1.68	0.74
1:A:291:LEU:HD13	1:A:347:ILE:HD11	1.70	0.74
1:A:392:THR:HG22	1:A:393:GLY:N	2.01	0.74
1:A:574:ARG:NH2	2:A:2039:HOH:O	2.21	0.73
1:A:392:THR:HG22	1:A:393:GLY:H	1.53	0.73
1:A:693:ARG:HH12	1:A:697:VAL:HG22	1.50	0.72
1:A:280:LEU:H	1:A:280:LEU:HD22	1.55	0.71
1:A:409:ILE:HD12	1:A:456:LYS:HG3	1.73	0.71
1:A:413:HIS:HB2	1:A:414:PRO:HA	1.73	0.71
1:A:643:ASP:HB3	1:A:654:PHE:CD1	2.25	0.70
1:A:593:GLY:O	1:A:597:VAL:HG23	1.90	0.70
1:A:566:PHE:CD2	1:A:570:MET:HE2	2.27	0.70
1:A:244:PRO:HG3	1:A:318:LEU:HD22	1.74	0.70
1:A:548:PHE:C	1:A:550:ASN:H	2.01	0.69
1:A:309:LEU:HD22	1:A:326:LEU:HD12	1.74	0.69
1:A:381:LEU:HD12	1:A:442:LEU:HB2	1.76	0.68
1:A:560:ASP:O	1:A:564:VAL:HG23	1.94	0.67
1:A:644:THR:HG23	1:A:650:THR:HA	1.77	0.67
1:A:582:LEU:HD22	1:A:587:ILE:HG21	1.76	0.66
1:A:548:PHE:O	1:A:550:ASN:N	2.28	0.66
1:A:592:MET:O	1:A:612:ARG:NH1	2.28	0.65
1:A:604:GLN:NE2	2:A:2044:HOH:O	2.29	0.65
1:A:272:LEU:HD23	1:A:288:LEU:HD23	1.78	0.65
1:A:254:LEU:O	1:A:258:GLN:HG3	1.97	0.64
1:A:685:ALA:C	1:A:687:GLY:H	2.06	0.64
1:A:509:TRP:CZ2	1:A:544:GLN:HB2	2.31	0.64
1:A:286:ALA:N	1:A:287:PRO:HD2	2.13	0.63
1:A:404:VAL:HG22	1:A:459:VAL:CG1	2.29	0.63
1:A:665:LEU:CD2	1:A:679:LYS:HG2	2.29	0.63
1:A:642:ASN:HA	1:A:645:ALA:CB	2.26	0.62
1:A:704:PRO:HG2	1:A:707:SER:O	1.99	0.62
1:A:243:SER:C	1:A:245:GLN:H	2.08	0.62
1:A:313:LYS:HB2	1:A:326:LEU:HD21	1.82	0.62
1:A:350:ILE:O	1:A:353:PRO:HD3	2.00	0.61
1:A:526:GLN:NE2	1:A:533:ARG:H	1.90	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LYS:HE3	1:A:657:GLU:OE2	2.00	0.61
1:A:497:LYS:HD3	1:A:556:GLN:HE21	1.65	0.61
1:A:309:LEU:HD22	1:A:326:LEU:CD1	2.30	0.60
1:A:484:ASN:C	1:A:486:CYS:H	2.08	0.60
1:A:353:PRO:C	1:A:355:HIS:H	2.09	0.59
1:A:592:MET:SD	1:A:597:VAL:HG22	2.42	0.59
1:A:566:PHE:HD2	1:A:570:MET:HE2	1.66	0.58
1:A:241:LEU:H	1:A:241:LEU:CD1	2.14	0.58
1:A:669:LYS:HA	1:A:675:PRO:CA	2.33	0.58
1:A:641:PRO:O	1:A:645:ALA:HB2	2.04	0.58
1:A:497:LYS:HD3	1:A:556:GLN:NE2	2.19	0.58
1:A:673:GLY:O	1:A:675:PRO:HD3	2.03	0.58
1:A:377:LYS:HD3	1:A:483:THR:HG22	1.85	0.57
1:A:460:ASN:C	1:A:461:ILE:HD12	2.29	0.57
1:A:604:GLN:OE1	1:A:679:LYS:HE2	2.04	0.57
1:A:658:HIS:HB3	1:A:660:GLN:OE1	2.04	0.57
1:A:536:SER:O	1:A:540:LEU:HG	2.05	0.56
1:A:563:TRP:CH2	1:A:570:MET:HE3	2.41	0.56
1:A:298:LEU:HG	1:A:302:MET:HE3	1.86	0.56
1:A:497:LYS:HE3	1:A:559:PHE:CD2	2.41	0.56
1:A:672:ASN:C	1:A:674:ALA:H	2.14	0.55
1:A:665:LEU:HD21	1:A:679:LYS:HG2	1.87	0.55
1:A:404:VAL:HA	1:A:459:VAL:CG1	2.35	0.55
1:A:374:VAL:HG22	1:A:480:VAL:CG2	2.36	0.55
1:A:646:ALA:O	1:A:648:LYS:N	2.40	0.55
1:A:282:GLU:C	1:A:284:SER:H	2.13	0.55
1:A:255:LEU:HD21	1:A:333:LEU:HD13	1.89	0.54
1:A:282:GLU:C	1:A:284:SER:N	2.65	0.54
1:A:443:LYS:HE2	1:A:445:LEU:HD23	1.89	0.54
1:A:483:THR:H	1:A:487:GLN:NE2	2.06	0.54
1:A:681:HIS:O	1:A:682:LYS:C	2.49	0.54
1:A:681:HIS:O	1:A:684:THR:N	2.40	0.54
1:A:374:VAL:HG22	1:A:480:VAL:HG22	1.89	0.54
1:A:280:LEU:H	1:A:280:LEU:CD2	2.22	0.53
1:A:563:TRP:CZ3	1:A:570:MET:CE	2.91	0.53
1:A:410:CYS:O	1:A:413:HIS:NE2	2.42	0.53
1:A:314:LYS:HG3	1:A:508:THR:HG21	1.89	0.53
1:A:646:ALA:C	1:A:648:LYS:N	2.66	0.53
1:A:392:THR:CG2	1:A:393:GLY:N	2.71	0.53
1:A:661:PHE:O	1:A:682:LYS:HD2	2.08	0.53
1:A:291:LEU:HD13	1:A:347:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:HG23	1:A:461:ILE:CD1	2.39	0.52
1:A:621:PHE:HB2	1:A:639:VAL:HG11	1.89	0.52
1:A:640:GLN:C	1:A:642:ASN:H	2.17	0.52
1:A:425:GLU:HB3	1:A:443:LYS:HB3	1.90	0.52
1:A:644:THR:O	1:A:644:THR:HG22	2.08	0.52
1:A:705:LEU:C	1:A:707:SER:H	2.18	0.52
1:A:409:ILE:CD1	1:A:456:LYS:HG3	2.38	0.52
1:A:357:ALA:C	1:A:359:LYS:H	2.16	0.52
1:A:450:LYS:HG2	1:A:491:SER:OG	2.10	0.52
1:A:255:LEU:HA	1:A:258:GLN:HE21	1.74	0.51
1:A:488:TRP:CD1	1:A:575:TYR:HH	2.28	0.51
1:A:529:VAL:C	1:A:531:PRO:HD3	2.35	0.51
1:A:388:VAL:HG21	1:A:457:PHE:CD2	2.45	0.51
1:A:392:THR:CG2	1:A:393:GLY:H	2.23	0.51
1:A:612:ARG:HG3	1:A:612:ARG:HH11	1.76	0.50
1:A:646:ALA:C	1:A:648:LYS:H	2.19	0.50
1:A:280:LEU:HD22	1:A:280:LEU:N	2.25	0.50
1:A:241:LEU:HD12	1:A:241:LEU:N	2.18	0.50
1:A:425:GLU:O	1:A:426:MET:HB2	2.12	0.50
1:A:639:VAL:HG13	2:A:2048:HOH:O	2.10	0.50
1:A:549:GLY:O	1:A:550:ASN:CB	2.60	0.50
1:A:553:ILE:C	1:A:554:ILE:HD12	2.36	0.50
1:A:668:THR:O	1:A:676:ARG:N	2.37	0.50
1:A:668:THR:C	1:A:675:PRO:HA	2.36	0.50
1:A:640:GLN:HB3	1:A:641:PRO:HD2	1.93	0.49
1:A:268:GLU:O	1:A:272:LEU:HD13	2.12	0.49
1:A:366:LEU:HD21	1:A:457:PHE:CE1	2.47	0.49
1:A:362:VAL:HG22	1:A:398:PHE:CE2	2.48	0.49
1:A:317:ILE:CG1	1:A:513:ILE:HD11	2.41	0.49
1:A:621:PHE:HB2	1:A:639:VAL:CG1	2.42	0.49
1:A:681:HIS:CD2	1:A:683:ASP:H	2.31	0.49
1:A:353:PRO:O	1:A:354:GLN:HB2	2.13	0.49
1:A:453:VAL:HG12	1:A:479:PHE:CZ	2.47	0.48
1:A:693:ARG:HH11	1:A:697:VAL:HG22	1.69	0.48
1:A:566:PHE:CE2	1:A:570:MET:HE2	2.49	0.48
1:A:278:PRO:O	1:A:279:THR:OG1	2.27	0.48
1:A:461:ILE:HD12	1:A:461:ILE:N	2.28	0.48
1:A:621:PHE:O	1:A:639:VAL:HG12	2.13	0.48
1:A:670:ASP:H	1:A:674:ALA:C	2.22	0.48
1:A:549:GLY:O	1:A:550:ASN:HB3	2.13	0.48
1:A:681:HIS:HD2	1:A:683:ASP:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:HD23	1:A:587:ILE:HD12	1.96	0.48
1:A:664:LEU:HG	1:A:665:LEU:N	2.29	0.48
1:A:484:ASN:OD1	1:A:485:GLU:N	2.47	0.47
1:A:459:VAL:HG23	1:A:461:ILE:HD11	1.96	0.47
1:A:547:PHE:CD2	1:A:562:PHE:HA	2.49	0.47
1:A:603:ASN:OD1	1:A:603:ASN:O	2.33	0.47
1:A:651:PHE:N	1:A:652:PRO:HD2	2.30	0.46
1:A:685:ALA:C	1:A:687:GLY:N	2.74	0.46
1:A:442:LEU:CD1	1:A:455:LEU:HD11	2.46	0.46
1:A:484:ASN:C	1:A:486:CYS:N	2.74	0.46
1:A:548:PHE:C	1:A:550:ASN:N	2.63	0.46
1:A:432:TYR:O	1:A:436:LEU:N	2.49	0.46
1:A:448:THR:HG21	1:A:451:CYS:O	2.15	0.46
1:A:291:LEU:O	1:A:295:GLN:HG3	2.16	0.46
1:A:662:VAL:O	1:A:682:LYS:HB3	2.15	0.46
1:A:594:ARG:HG3	2:A:2047:HOH:O	2.15	0.46
1:A:484:ASN:O	1:A:486:CYS:N	2.49	0.45
1:A:439:HIS:N	1:A:439:HIS:CD2	2.85	0.45
1:A:670:ASP:N	1:A:674:ALA:O	2.50	0.45
1:A:662:VAL:O	1:A:682:LYS:CB	2.65	0.45
1:A:353:PRO:C	1:A:355:HIS:N	2.75	0.45
1:A:280:LEU:HG	1:A:285:LEU:HD21	1.99	0.44
1:A:314:LYS:HG3	1:A:508:THR:CG2	2.47	0.44
1:A:377:LYS:CD	1:A:483:THR:HG22	2.47	0.44
1:A:604:GLN:OE1	1:A:679:LYS:CE	2.65	0.44
1:A:374:VAL:HG13	1:A:480:VAL:HG23	1.99	0.44
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.84	0.44
1:A:665:LEU:HD23	1:A:679:LYS:HG2	1.98	0.44
1:A:705:LEU:C	1:A:707:SER:N	2.74	0.44
1:A:283:ASN:OD1	1:A:283:ASN:O	2.36	0.43
1:A:357:ALA:C	1:A:359:LYS:N	2.76	0.43
1:A:640:GLN:O	1:A:642:ASN:N	2.48	0.43
1:A:490:GLY:O	1:A:494:VAL:HG23	2.18	0.43
1:A:508:THR:HG23	2:A:2029:HOH:O	2.17	0.43
1:A:501:PHE:CE2	1:A:507:ILE:HG12	2.53	0.43
1:A:262:LEU:O	1:A:266:ILE:HG13	2.18	0.43
1:A:286:ALA:N	1:A:287:PRO:CD	2.80	0.43
1:A:371:PHE:HB2	1:A:477:ASN:HB2	2.01	0.43
1:A:563:TRP:CZ3	1:A:570:MET:HE3	2.53	0.43
1:A:244:PRO:C	1:A:246:PRO:CD	2.92	0.43
1:A:483:THR:H	1:A:487:GLN:HE22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLN:HG2	1:A:550:ASN:HA	2.01	0.43
1:A:565:TRP:CD1	1:A:618:PRO:HB3	2.54	0.42
1:A:247:ILE:H	1:A:247:ILE:HG13	1.58	0.42
1:A:432:TYR:HD1	1:A:437:THR:O	2.01	0.42
1:A:646:ALA:HB1	1:A:648:LYS:HD2	2.01	0.42
1:A:509:TRP:CH2	1:A:544:GLN:HB2	2.53	0.42
1:A:497:LYS:HE3	1:A:559:PHE:HD2	1.82	0.42
1:A:630:MET:HA	1:A:631:PRO:C	2.44	0.42
1:A:706:ASN:O	1:A:706:ASN:OD1	2.37	0.42
1:A:362:VAL:HG22	1:A:398:PHE:CZ	2.54	0.42
1:A:529:VAL:O	1:A:531:PRO:HD3	2.19	0.42
1:A:425:GLU:HB2	1:A:445:LEU:HD11	2.01	0.42
1:A:617:ASN:HB3	1:A:620:GLN:NE2	2.35	0.42
1:A:450:LYS:HE2	1:A:487:GLN:HA	2.01	0.42
1:A:643:ASP:HB3	1:A:654:PHE:CE1	2.54	0.42
1:A:462:ARG:NH1	1:A:466:ASN:ND2	2.68	0.42
1:A:665:LEU:HD23	1:A:665:LEU:HA	1.78	0.42
1:A:648:LYS:H	1:A:648:LYS:HG3	1.58	0.41
1:A:241:LEU:HD23	1:A:319:GLU:HA	2.02	0.41
1:A:422:THR:HA	1:A:423:PRO:HD2	1.95	0.41
1:A:414:PRO:CG	2:A:2018:HOH:O	2.38	0.41
1:A:401:ASN:ND2	1:A:462:ARG:HB2	2.28	0.41
1:A:280:LEU:CG	1:A:285:LEU:HD21	2.51	0.41
1:A:359:LYS:CB	1:A:360:PRO:CD	2.92	0.41
1:A:354:GLN:HA	1:A:354:GLN:OE1	2.20	0.41
1:A:255:LEU:HD23	1:A:258:GLN:NE2	2.35	0.40
1:A:635:LYS:HE2	1:A:635:LYS:HB3	1.75	0.40
1:A:244:PRO:O	1:A:245:GLN:C	2.64	0.40
1:A:645:ALA:O	1:A:646:ALA:HB3	2.21	0.40
1:A:245:GLN:N	1:A:246:PRO:CD	2.84	0.40
1:A:353:PRO:O	1:A:354:GLN:CB	2.70	0.40
1:A:413:HIS:CB	1:A:414:PRO:C	2.69	0.40
1:A:419:ASN:HA	1:A:420:PRO:HD3	1.80	0.40

All (1) 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:A:414:PRO:CB	1:A:688:SER:OG[6_555]	2.16	0.04

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	460/473 (97%)	395 (86%)	49 (11%)	16 (4%)	3	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	ALA
1	A	413	HIS
1	A	359	LYS
1	A	485	GLU
1	A	549	GLY
1	A	647	ALA
1	A	420	PRO
1	A	682	LYS
1	A	246	PRO
1	A	641	PRO
1	A	373	VAL
1	A	426	MET
1	A	645	ALA
1	A	646	ALA
1	A	674	ALA
1	A	353	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	407/420 (97%)	388 (95%)	19 (5%)	23 57

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ILE
1	A	273	LEU
1	A	280	LEU
1	A	282	GLU
1	A	291	LEU
1	A	354	GLN
1	A	362	VAL
1	A	397	ASN
1	A	422	THR
1	A	427	ASP
1	A	453	VAL
1	A	464	LEU
1	A	466	ASN
1	A	497	LYS
1	A	534	PRO
1	A	610	ILE
1	A	612	ARG
1	A	629	GLU
1	A	663	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	334	GLN
1	A	348	GLN
1	A	384	ASN
1	A	401	ASN
1	A	429	GLN
1	A	466	ASN
1	A	487	GLN
1	A	511	GLN
1	A	519	HIS
1	A	526	GLN

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Mol	Chain	Res	Type
1	A	546	HIS
1	A	550	ASN
1	A	556	GLN
1	A	576	GLN
1	A	603	ASN
1	A	617	ASN
1	A	620	GLN
1	A	706	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	PTR	A	702	1	15,16,17	1.00	1 (6%)	17,22,24	0.89	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
1	PTR	A	702	1	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	702	PTR	P-OH	2.26	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	702	PTR	O3P-P-OH	2.55	112.85	105.32

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	464/473 (98%)	-0.12	14 (3%)	52 42	26, 53, 125, 151	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	PRO	3.3
1	A	692	LYS	3.1
1	A	691	PRO	2.9
1	A	485	GLU	2.9
1	A	413	HIS	2.8
1	A	647	ALA	2.7
1	A	239	PRO	2.5
1	A	282	GLU	2.5
1	A	242	SER	2.4
1	A	646	ALA	2.4
1	A	694	THR	2.3
1	A	706	ASN	2.1
1	A	673	GLY	2.1
1	A	420	PRO	2.1

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	PTR	A	702	16/17	0.98	0.06	33,43,50,55	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.