



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 4C0O / pdb_00004c0o
Title : Transportin 3 in complex with phosphorylated ASF/SF2
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Deposited on : 2013-08-06
Resolution : 2.56 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

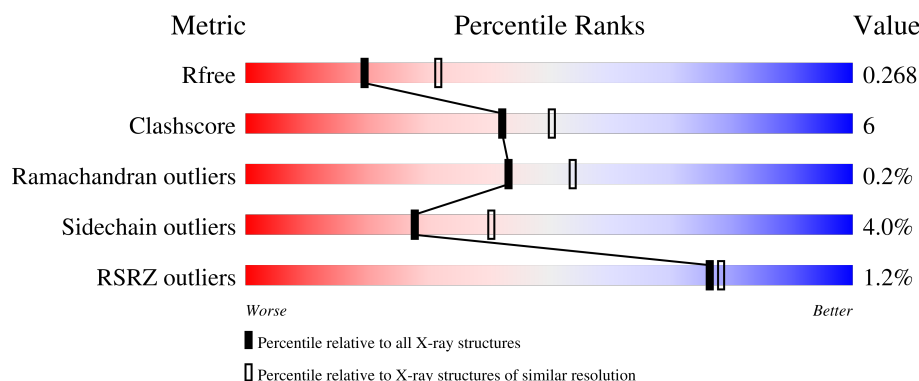
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	923	% 79% 17% ..
1	B	923	2% 78% 18% ..
2	C	125	% 65% 10% • 23%
2	D	125	% 61% 14% • 24%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15858 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 TRANSPORTIN-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	901	Total	C	N	O	S	0	0	0
			7140	4551	1215	1320	54			
1	B	898	Total	C	N	O	S	0	0	0
			7122	4540	1211	1317	54			

- Molecule 2 is a protein called SERINE/ARGININE-RICH SPLICING FACTOR 1.

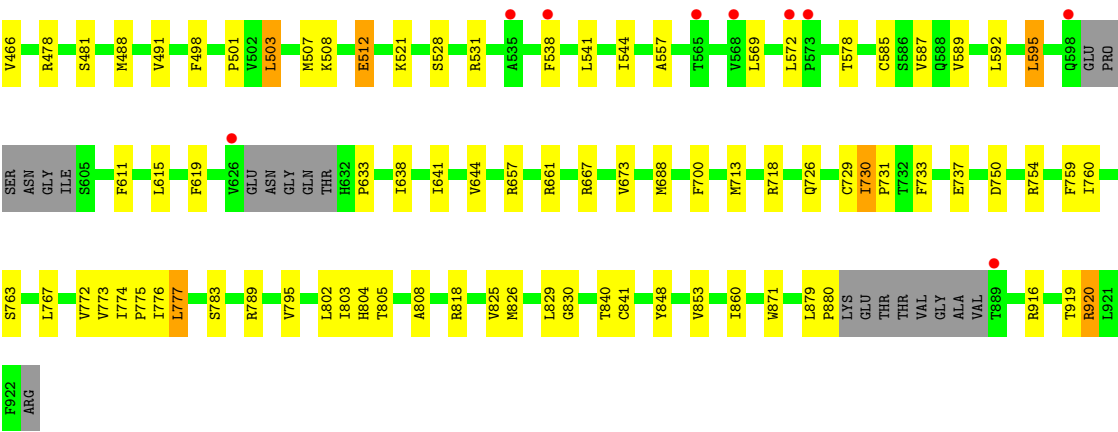
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	96	Total	C	N	O	P S	0	0	0
			775	464	148	157	3 3			
2	D	95	Total	C	N	O	P S	0	0	0
			769	461	147	155	3 3			

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total	0	0
			1 K 1 1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total	0	0
			27 O 27 27		
4	B	15	Total	0	0
			15 O 15 15		
4	C	4	Total	0	0
			4 O 4 4		
4	D	5	Total	0	0
			5 O 5 5		



• Molecule 2: SERINE/ARGININE-RICH SPLICING FACTOR 1



• Molecule 2: SERINE/ARGININE-RICH SPLICING FACTOR 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.55Å 91.06Å 98.12Å 106.98° 100.30° 102.18°	Depositor
Resolution (Å)	38.28 – 2.56 38.28 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.28-2.56) 98.4 (38.28-2.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.269 0.223 , 0.268	Depositor DCC
R_{free} test set	4040 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15858	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/7282	0.79	4/9889 (0.0%)
1	B	0.39	0/7263	0.79	4/9863 (0.0%)
2	C	0.40	0/756	0.75	0/1011
2	D	0.37	0/750	0.79	2/1003 (0.2%)
All	All	0.40	0/16051	0.79	10/21766 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	128	LEU	CA-C-N	5.88	123.90	119.66
2	D	128	LEU	C-N-CA	5.88	123.90	119.66
1	A	431	ASN	CA-C-N	-5.23	114.99	120.38
1	A	431	ASN	C-N-CA	-5.23	114.99	120.38
1	B	730	ILE	CA-C-N	-5.06	114.45	119.56
1	B	730	ILE	C-N-CA	-5.06	114.45	119.56
1	A	513	LYS	CA-C-N	-5.06	114.83	120.45
1	A	513	LYS	C-N-CA	-5.06	114.83	120.45
1	B	119	MET	CA-C-N	5.03	124.69	119.56
1	B	119	MET	C-N-CA	5.03	124.69	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7140	0	7172	92	1
1	B	7122	0	7150	93	0
2	C	775	0	733	8	0
2	D	769	0	728	10	0
3	B	1	0	0	0	0
4	A	27	0	0	2	0
4	B	15	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
All	All	15858	0	15783	198	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 6.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:MET:HE3	1:B:455:ASN:HB3	1.49	0.95
1:B:184:LEU:HG	1:B:201:VAL:HG13	1.65	0.77
1:A:7:THR:HG22	1:A:10:LEU:HB2	1.68	0.75
1:A:521:LYS:O	1:A:525:ASN:ND2	2.26	0.68
1:B:7:THR:HG22	1:B:10:LEU:HB2	1.76	0.68
2:D:141:MET:HG3	2:D:160:VAL:HG21	1.77	0.67
1:A:118:GLN:OE1	4:A:2005:HOH:O	2.14	0.66
1:B:151:PRO:HB3	1:B:211:LEU:HD22	1.80	0.62
1:B:589:VAL:HG13	1:B:644:VAL:HG11	1.81	0.62
1:B:754:ARG:NH2	2:D:209:SEP:O	2.31	0.61
1:B:346:TRP:HB3	1:B:410:LEU:HD11	1.82	0.61
1:A:133:TYR:HB3	1:A:139:SER:HB3	1.83	0.60
1:A:715:GLU:HG3	1:A:718:ARG:HD2	1.83	0.60
1:A:273:VAL:HG11	1:A:302:LEU:HD13	1.83	0.60
2:C:141:MET:HG3	2:C:160:VAL:HG21	1.83	0.60
1:A:417:MET:HE3	1:A:455:ASN:HB3	1.84	0.59
1:A:151:PRO:HB3	1:A:211:LEU:HD22	1.83	0.59
1:A:754:ARG:NH2	2:C:209:SEP:O	2.27	0.59
1:A:155:HIS:HA	1:A:166:ARG:HH21	1.68	0.59
1:A:269:LEU:O	1:A:273:VAL:HG12	2.04	0.57
1:A:760:ILE:HD13	1:A:767:LEU:HD23	1.86	0.57
1:A:804:HIS:CD2	1:A:808:ALA:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:TYR:HB3	2:D:161:GLU:HB2	1.86	0.56
1:A:35:GLY:O	1:A:39:ARG:HG2	2.06	0.56
1:B:825:VAL:HG13	1:B:829:LEU:HD12	1.88	0.55
1:B:293:LEU:HD22	1:B:341:ILE:HD11	1.89	0.54
1:B:321:LEU:HD23	1:B:368:TYR:CE1	2.43	0.53
1:B:774:ILE:HB	1:B:775:PRO:HD3	1.90	0.53
1:B:79:PRO:O	1:B:82:SER:OG	2.19	0.53
1:A:772:VAL:O	1:A:776:ILE:HG12	2.08	0.53
1:A:44:TRP:CZ2	1:A:78:LEU:HD21	2.44	0.53
1:A:836:GLN:O	1:A:840:THR:HG23	2.09	0.53
1:A:783:SER:HB3	1:A:795:VAL:HG21	1.90	0.53
1:A:271:GLN:O	1:A:275:THR:HG23	2.09	0.53
1:A:785:THR:CG2	1:A:840:THR:HG22	2.39	0.52
1:A:392:GLU:HG2	1:A:401:MET:HE3	1.90	0.52
1:B:433:PRO:HD2	1:B:436:VAL:HB	1.91	0.52
1:B:538:PHE:HE2	1:B:569:LEU:HB2	1.74	0.52
1:B:315:GLY:H	1:B:321:LEU:HD13	1.73	0.52
1:A:803:ILE:HD13	1:A:860:ILE:HG12	1.91	0.52
1:B:314:PRO:HG3	1:B:361:ILE:HG23	1.91	0.51
1:B:178:SER:O	1:B:182:SER:OG	2.28	0.51
1:B:44:TRP:NE1	1:B:70:LYS:HD2	2.26	0.51
1:B:269:LEU:O	1:B:273:VAL:HG12	2.10	0.51
1:A:589:VAL:HG13	1:A:644:VAL:HG11	1.93	0.51
1:A:150:LEU:HB3	1:A:151:PRO:HD3	1.93	0.51
1:A:785:THR:HG22	1:A:840:THR:HG22	1.93	0.51
1:B:541:LEU:HA	1:B:544:ILE:HD12	1.93	0.51
1:B:803:ILE:HD13	1:B:860:ILE:HG12	1.93	0.50
1:A:715:GLU:HA	1:A:718:ARG:HG3	1.93	0.50
1:B:18:LEU:O	1:B:27:LYS:HD2	2.11	0.50
1:B:456:ASN:N	1:B:457:PRO:HD2	2.27	0.50
1:B:773:VAL:HG22	1:B:777:LEU:HD23	1.93	0.50
1:B:441:LEU:HA	1:B:444:MET:HE3	1.94	0.50
1:A:39:ARG:HH21	1:B:35:GLY:HA3	1.76	0.50
1:A:448:ALA:O	1:A:451:VAL:HG12	2.12	0.50
1:B:920:ARG:HG2	2:D:189:TYR:CE1	2.46	0.50
1:A:424:TYR:OH	1:A:465:GLY:HA3	2.12	0.50
1:B:294:ASN:OD1	1:B:297:ARG:NH1	2.41	0.50
1:B:688:MET:HG2	1:B:700:PHE:CD1	2.47	0.50
1:A:774:ILE:HB	1:A:775:PRO:HD3	1.93	0.50
1:A:44:TRP:CE2	1:A:70:LYS:HD2	2.47	0.49
1:A:197:MET:O	1:A:201:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:THR:HB	1:B:633:PRO:HB2	1.94	0.49
1:B:826:MET:HE2	1:B:860:ILE:HG23	1.95	0.49
1:B:281:HIS:HA	1:B:284:VAL:HG12	1.94	0.49
1:A:781:ILE:HG23	1:A:836:GLN:HG3	1.94	0.49
1:B:805:THR:O	1:B:818:ARG:NH1	2.46	0.49
4:A:2003:HOH:O	2:D:204:ARG:NH1	2.30	0.49
1:B:263:LEU:HD11	1:B:318:LEU:HD21	1.95	0.49
1:B:760:ILE:HD13	1:B:767:LEU:HD23	1.95	0.48
1:B:750:ASP:O	1:B:754:ARG:HG3	2.13	0.48
1:B:585:CYS:HB3	1:B:615:LEU:HD21	1.95	0.48
1:A:189:GLU:HG3	1:A:223:LYS:NZ	2.28	0.48
1:A:294:ASN:OD1	1:A:297:ARG:NH1	2.40	0.48
1:A:441:LEU:HD23	1:A:444:MET:HE3	1.94	0.48
1:B:273:VAL:HG11	1:B:302:LEU:HD22	1.95	0.48
1:A:424:TYR:CD2	1:A:462:VAL:HG22	2.49	0.48
1:A:44:TRP:NE1	1:A:70:LYS:HD2	2.28	0.48
1:A:456:ASN:N	1:A:457:PRO:HD2	2.29	0.47
1:A:730:ILE:HB	1:A:731:PRO:HD3	1.95	0.47
1:B:772:VAL:O	1:B:776:ILE:HG12	2.14	0.47
1:B:422:GLN:O	1:B:425:SER:OG	2.30	0.47
1:B:478:ARG:NH1	1:B:512:GLU:OE1	2.46	0.47
1:B:805:THR:HG22	1:B:818:ARG:HD2	1.96	0.47
1:A:309:LYS:HE3	1:A:318:LEU:HD13	1.96	0.47
1:B:521:LYS:HE3	1:B:557:ALA:HB2	1.95	0.47
2:D:153:TYR:HD2	2:D:157:THR:HG23	1.78	0.47
1:B:729:CYS:HB3	1:B:733:PHE:CE2	2.50	0.47
1:B:53:ILE:C	1:B:54:ARG:HG3	2.39	0.47
1:B:279:ALA:HA	1:B:282:MET:HE3	1.96	0.47
1:A:788:HIS:CE1	1:A:790:ASP:HB2	2.50	0.46
1:B:730:ILE:HB	1:B:731:PRO:HD3	1.97	0.46
1:A:427:LEU:HD11	1:A:437:THR:HA	1.97	0.46
1:A:765:VAL:HG13	1:A:818:ARG:HG2	1.97	0.46
1:A:127:GLN:O	1:A:131:GLU:HG2	2.15	0.46
1:A:281:HIS:HA	1:A:284:VAL:HG12	1.98	0.46
1:A:440:VAL:HG12	1:A:444:MET:HE2	1.97	0.46
1:A:189:GLU:HG3	1:A:223:LYS:HZ3	1.81	0.46
1:A:498:PHE:C	1:A:501:PRO:HD2	2.41	0.46
1:B:44:TRP:CE2	1:B:70:LYS:HD2	2.51	0.46
1:A:767:LEU:O	1:A:773:VAL:HB	2.16	0.46
1:B:657:ARG:O	1:B:661:ARG:HG2	2.16	0.46
2:C:165:LYS:HE2	2:C:199:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.77	0.45
1:A:196:LYS:HA	1:A:199:MET:HE3	1.97	0.45
2:D:125:VAL:HG21	2:D:137:LEU:HD11	1.98	0.45
1:B:150:LEU:HB3	1:B:151:PRO:HD3	1.98	0.45
1:B:35:GLY:O	1:B:39:ARG:HG2	2.16	0.45
1:B:196:LYS:HA	1:B:199:MET:HE3	1.99	0.45
1:B:392:GLU:HG2	1:B:401:MET:HE3	1.99	0.45
1:B:488:MET:HE2	1:B:491:VAL:HG11	1.98	0.45
1:B:619:PHE:HZ	1:B:641:ILE:HG12	1.81	0.45
1:B:726:GLN:HG2	1:B:772:VAL:HB	1.99	0.45
1:B:102:PRO:O	1:B:106:THR:HG23	2.17	0.45
1:A:281:HIS:O	1:A:284:VAL:HG12	2.15	0.45
1:A:321:LEU:HD23	1:A:368:TYR:CE1	2.52	0.45
1:A:7:THR:HG23	1:A:10:LEU:H	1.81	0.45
1:A:53:ILE:C	1:A:54:ARG:HG3	2.41	0.44
1:B:7:THR:HG23	1:B:10:LEU:H	1.82	0.44
1:B:227:LEU:O	1:B:231:VAL:HG13	2.18	0.44
1:B:271:GLN:O	1:B:275:THR:HG23	2.18	0.44
1:B:789:ARG:HD2	1:B:848:TYR:CE1	2.53	0.44
1:A:54:ARG:HA	1:A:60:CYS:SG	2.57	0.44
1:B:783:SER:HB3	1:B:795:VAL:HG21	1.99	0.44
1:A:142:PHE:O	1:A:146:ILE:HG13	2.17	0.44
1:A:180:VAL:O	1:A:184:LEU:HB2	2.18	0.44
1:B:256:ILE:HD11	1:B:265:LEU:HG	2.00	0.44
1:A:367:ALA:HA	1:A:370:GLN:HG2	2.00	0.44
1:A:184:LEU:HG	1:A:201:VAL:HG13	1.99	0.44
1:B:789:ARG:HD2	1:B:848:TYR:CZ	2.52	0.44
2:C:169:THR:HG22	2:C:173:ARG:HD3	1.99	0.44
1:A:303:CYS:HB3	1:A:345:PHE:CZ	2.53	0.43
1:B:313:THR:O	1:B:313:THR:OG1	2.31	0.43
1:B:498:PHE:C	1:B:501:PRO:HD2	2.43	0.43
2:C:153:TYR:HD2	2:C:157:THR:HG23	1.81	0.43
1:B:34:LEU:HD22	1:B:62:PHE:CZ	2.53	0.43
1:B:155:HIS:HA	1:B:166:ARG:HH21	1.82	0.43
1:B:804:HIS:CD2	1:B:808:ALA:HB2	2.53	0.43
1:B:830:GLY:HA3	1:B:871:TRP:CH2	2.53	0.43
1:B:879:LEU:HA	1:B:880:PRO:HD3	1.81	0.43
2:D:118:ARG:HG2	2:D:149:TYR:HB2	2.00	0.43
1:B:321:LEU:HD23	1:B:368:TYR:CZ	2.54	0.43
1:B:463:LEU:HD22	1:B:491:VAL:HG13	2.00	0.43
1:A:176:TYR:O	1:A:179:THR:OG1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ASP:O	1:A:754:ARG:HG3	2.19	0.43
2:C:166:GLU:H	2:C:166:GLU:CD	2.27	0.43
1:A:195:GLU:HB2	1:A:199:MET:HE2	2.00	0.43
1:A:735:LEU:HD12	1:A:735:LEU:HA	1.81	0.43
1:A:279:ALA:HA	1:A:282:MET:HE3	2.01	0.42
1:A:841:CYS:SG	1:A:853:VAL:HG11	2.59	0.42
1:B:592:LEU:HA	1:B:595:LEU:HD12	2.01	0.42
2:D:119:SER:OG	2:D:162:PHE:O	2.33	0.42
1:B:528:SER:O	1:B:531:ARG:HD3	2.20	0.42
1:B:841:CYS:SG	1:B:853:VAL:HG11	2.60	0.42
1:A:642:TRP:HB2	1:A:680:LEU:HD21	2.01	0.42
1:B:422:GLN:O	1:B:426:THR:HG23	2.19	0.42
1:A:185:MET:O	1:A:189:GLU:HB2	2.19	0.42
1:A:359:GLU:HA	1:A:362:HIS:CG	2.55	0.42
1:A:433:PRO:HD2	1:A:436:VAL:HB	2.02	0.42
1:B:132:LYS:HD3	1:B:133:TYR:CE2	2.54	0.42
2:D:122:ARG:HB2	2:D:161:GLU:HG2	2.02	0.42
1:A:831:GLN:OE1	1:A:871:TRP:HA	2.19	0.42
1:B:592:LEU:HD21	1:B:611:PHE:HB2	2.02	0.42
1:A:490:GLU:OE1	1:A:490:GLU:N	2.52	0.42
1:A:209:PHE:CD1	1:A:214:LEU:HD12	2.55	0.41
1:A:676:GLY:O	1:A:711:TYR:OH	2.34	0.41
1:B:290:ASP:N	1:B:290:ASP:OD1	2.51	0.41
1:A:667:ARG:HD3	1:A:706:ILE:HD11	2.02	0.41
1:A:788:HIS:HA	2:C:201:SEP:O1P	2.20	0.41
1:B:358:ASP:OD2	1:B:360:VAL:HB	2.20	0.41
1:B:466:VAL:HG13	1:B:481:SER:HB2	2.02	0.41
2:C:122:ARG:HB2	2:C:161:GLU:HG2	2.02	0.41
1:A:383:GLU:HA	1:A:384:PRO:HD3	1.94	0.41
1:A:541:LEU:HB3	1:A:565:THR:HG22	2.02	0.41
1:B:440:VAL:HG12	1:B:444:MET:HE2	2.02	0.41
1:A:780:ALA:O	1:A:784:THR:HG23	2.20	0.41
1:B:441:LEU:HD23	1:B:444:MET:HE3	2.02	0.41
1:A:7:THR:CG2	1:A:10:LEU:HB2	2.45	0.41
1:B:188:VAL:HG12	1:B:198:LEU:HD12	2.02	0.41
1:B:120:PRO:HB3	1:B:165:ARG:CZ	2.50	0.41
1:B:148:THR:O	1:B:151:PRO:HD2	2.20	0.41
1:B:718:ARG:NH1	1:B:763:SER:OG	2.54	0.41
1:B:197:MET:O	1:B:201:VAL:HG23	2.21	0.41
1:B:174:ALA:HA	1:B:213:VAL:HB	2.02	0.41
1:A:11:VAL:HA	1:A:33:TRP:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:MET:HG3	1:A:762:ARG:HD2	2.02	0.41
1:A:425:SER:C	1:A:427:LEU:H	2.28	0.40
1:A:466:VAL:HG13	1:A:481:SER:HB2	2.03	0.40
1:B:503:LEU:O	1:B:507:MET:HG2	2.22	0.40
1:A:381:GLN:HG2	1:A:435:GLU:O	2.21	0.40
1:B:386:HIS:HB3	1:B:434:TRP:HH2	1.85	0.40
1:A:102:PRO:O	1:A:106:THR:HG23	2.21	0.40
1:A:278:THR:HG22	1:A:282:MET:HE2	2.04	0.40
1:A:380:CYS:O	1:A:400:ARG:NH1	2.55	0.40
1:A:772:VAL:O	1:A:775:PRO:HD2	2.21	0.40
1:A:879:LEU:HA	1:A:880:PRO:HD3	1.83	0.40
1:B:315:GLY:N	1:B:321:LEU:HD13	2.36	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:429:GLU:O	1:A:769:ARG:NH1[1_655]	2.17	0.03

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	893/923 (97%)	868 (97%)	23 (3%)	2 (0%)	43	54
1	B	888/923 (96%)	863 (97%)	24 (3%)	1 (0%)	48	60
2	C	91/125 (73%)	87 (96%)	4 (4%)	0	100	100
2	D	90/125 (72%)	87 (97%)	3 (3%)	0	100	100
All	All	1962/2096 (94%)	1905 (97%)	54 (3%)	3 (0%)	43	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLU
1	A	673	VAL
1	B	673	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	802/821 (98%)	767 (96%)	35 (4%)	25	37
1	B	801/821 (98%)	767 (96%)	34 (4%)	26	38
2	C	80/106 (76%)	79 (99%)	1 (1%)	61	74
2	D	79/106 (74%)	78 (99%)	1 (1%)	61	74
All	All	1762/1854 (95%)	1691 (96%)	71 (4%)	28	40

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	54	ARG
1	A	119	MET
1	A	179	THR
1	A	180	VAL
1	A	184	LEU
1	A	198	LEU
1	A	224	LEU
1	A	225	LEU
1	A	228	LEU
1	A	231	VAL
1	A	273	VAL
1	A	290	ASP
1	A	307	LEU
1	A	326	LEU
1	A	429	GLU
1	A	459	LEU
1	A	503	LEU
1	A	508	LYS

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Mol	Chain	Res	Type
1	A	512	GLU
1	A	565	THR
1	A	572	LEU
1	A	584	LEU
1	A	638	ILE
1	A	667	ARG
1	A	713	MET
1	A	737	GLU
1	A	759	PHE
1	A	765	VAL
1	A	777	LEU
1	A	802	LEU
1	A	822	ILE
1	A	879	LEU
1	A	916	ARG
1	A	920	ARG
1	B	10	LEU
1	B	54	ARG
1	B	179	THR
1	B	180	VAL
1	B	182	SER
1	B	184	LEU
1	B	198	LEU
1	B	209	PHE
1	B	224	LEU
1	B	225	LEU
1	B	228	LEU
1	B	231	VAL
1	B	273	VAL
1	B	290	ASP
1	B	326	LEU
1	B	429	GLU
1	B	459	LEU
1	B	503	LEU
1	B	508	LYS
1	B	512	GLU
1	B	572	LEU
1	B	587	VAL
1	B	595	LEU
1	B	638	ILE
1	B	667	ARG
1	B	713	MET

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Mol	Chain	Res	Type
1	B	737	GLU
1	B	759	PHE
1	B	777	LEU
1	B	802	LEU
1	B	840	THR
1	B	916	ARG
1	B	919	THR
1	B	920	ARG
2	C	194	VAL
2	D	194	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	95	GLN
1	A	362	HIS
1	A	456	ASN
1	A	495	ASN
1	A	656	ASN
1	A	734	GLN
1	A	778	GLN
1	B	72	GLN
1	B	135	ASN
1	B	370	GLN
1	B	621	HIS
1	B	635	GLN
1	B	652	HIS
1	B	656	ASN
1	B	690	ASN
1	B	693	HIS
1	B	901	GLN
2	C	135	GLN
2	D	121	ASN
2	D	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	SEP	D	201	2	8,9,10	1.56	1 (12%)	7,12,14	1.87	2 (28%)
2	SEP	D	207	2	8,9,10	1.57	1 (12%)	7,12,14	1.53	1 (14%)
2	SEP	D	209	2	8,9,10	1.53	1 (12%)	7,12,14	0.91	0
2	SEP	C	201	2	8,9,10	1.57	1 (12%)	7,12,14	1.43	1 (14%)
2	SEP	C	209	2	8,9,10	1.59	1 (12%)	7,12,14	1.00	0
2	SEP	C	207	2	8,9,10	1.59	1 (12%)	7,12,14	1.18	1 (14%)

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	SEP	D	201	2	-	6/6/8/10	-
2	SEP	D	207	2	-	2/6/8/10	-
2	SEP	D	209	2	-	3/6/8/10	-
2	SEP	C	201	2	-	3/6/8/10	-
2	SEP	C	209	2	-	0/6/8/10	-
2	SEP	C	207	2	-	2/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	209	SEP	P-O1P	3.62	1.61	1.50
2	C	207	SEP	P-O1P	3.47	1.61	1.50
2	C	201	SEP	P-O1P	3.36	1.60	1.50
2	D	209	SEP	P-O1P	3.29	1.60	1.50
2	D	201	SEP	P-O1P	3.27	1.60	1.50
2	D	207	SEP	P-O1P	3.11	1.60	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	SEP	OG-CB-CA	3.99	112.03	108.14
2	D	207	SEP	OG-CB-CA	3.37	111.43	108.14
2	C	201	SEP	OG-CB-CA	2.52	110.60	108.14
2	C	207	SEP	OG-CB-CA	2.41	110.49	108.14
2	D	201	SEP	O2P-P-OG	2.36	112.81	106.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	SEP	N-CA-CB-OG
2	C	201	SEP	C-CA-CB-OG
2	C	201	SEP	CA-CB-OG-P
2	C	207	SEP	N-CA-CB-OG
2	C	207	SEP	CA-CB-OG-P
2	D	201	SEP	N-CA-CB-OG
2	D	201	SEP	C-CA-CB-OG
2	D	201	SEP	CB-OG-P-O2P
2	D	201	SEP	CB-OG-P-O3P
2	D	207	SEP	CA-CB-OG-P
2	D	209	SEP	CB-OG-P-O3P
2	D	201	SEP	CB-OG-P-O1P
2	D	201	SEP	CA-CB-OG-P
2	D	209	SEP	CB-OG-P-O1P
2	D	207	SEP	N-CA-CB-OG
2	D	209	SEP	CB-OG-P-O2P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	209	SEP	1	0
2	C	201	SEP	1	0
2	C	209	SEP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	901/923 (97%)	-0.08	7 (0%) 82 85	29, 57, 91, 122	0
1	B	898/923 (97%)	0.09	15 (1%) 69 70	26, 70, 107, 124	0
2	C	93/125 (74%)	-0.33	1 (1%) 78 80	35, 51, 67, 74	0
2	D	92/125 (73%)	0.04	1 (1%) 78 80	32, 66, 84, 96	0
All	All	1984/2096 (94%)	-0.01	24 (1%) 76 78	26, 61, 101, 124	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	TYR	3.3
1	B	565	THR	3.3
1	B	410	LEU	3.2
1	A	677	SER	3.0
1	B	273	VAL	2.9
1	A	626	VAL	2.9
1	B	889	THR	2.9
1	B	568	VAL	2.9
1	B	626	VAL	2.8
1	B	535	ALA	2.7
1	B	431	ASN	2.6
1	A	889	THR	2.6
1	B	445	ALA	2.5
2	D	211	SER	2.4
1	A	17	ALA	2.4
1	A	18	LEU	2.4
1	B	598	GLN	2.3
2	C	211	SER	2.3
1	B	451	VAL	2.2
1	A	26	GLY	2.1
1	A	598	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	573	PRO	2.1
1	B	538	PHE	2.0
1	B	572	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	C	201	10/11	0.80	0.17	30,39,54,59	4
2	SEP	D	201	10/11	0.90	0.12	26,35,51,52	4
2	SEP	C	207	10/11	0.95	0.05	32,40,47,49	0
2	SEP	D	207	10/11	0.96	0.05	29,37,51,58	0
2	SEP	C	209	10/11	0.97	0.05	33,38,47,54	0
2	SEP	D	209	10/11	0.98	0.06	30,36,41,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
3	K	B	1924	1/1	0.88	0.08	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.