



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:03 am GMT

PDB ID : 4C0O  
Title : Transportin 3 in complex with phosphorylated ASF/SF2  
Authors : Maertens, G.N.; Cook, N.J.; Cherepanov, P.  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

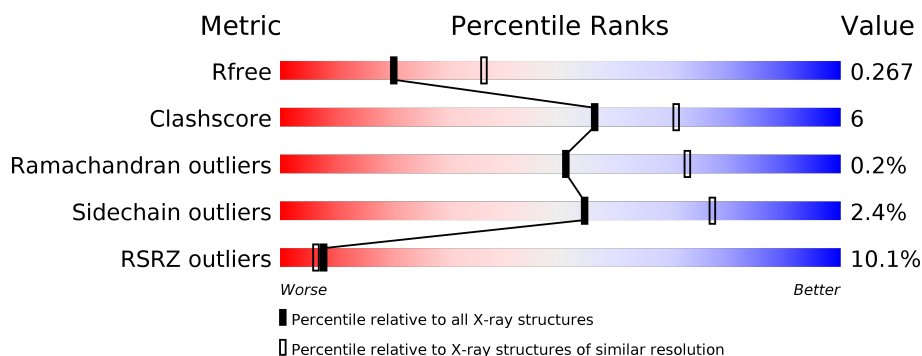
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>8%</div> <div>82%</div> <div>15%</div> <div>••</div> </div>
1	B	923	<div> <div>13%</div> <div>80%</div> <div>17%</div> <div>••</div> </div>
2	C	125	<div> <div>66%</div> <div>10%</div> <div>23%</div> </div>
2	D	125	<div> <div>7%</div> <div>63%</div> <div>13%</div> <div>24%</div> </div>

## 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 (three-letter code: 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		

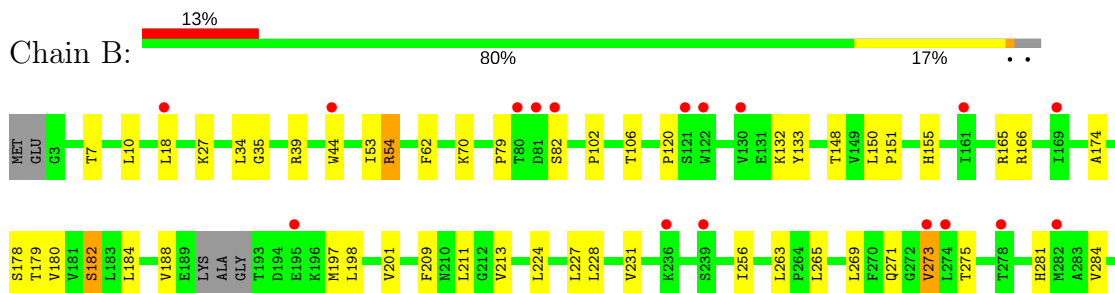
### 3 Residue-property plots [i](#)

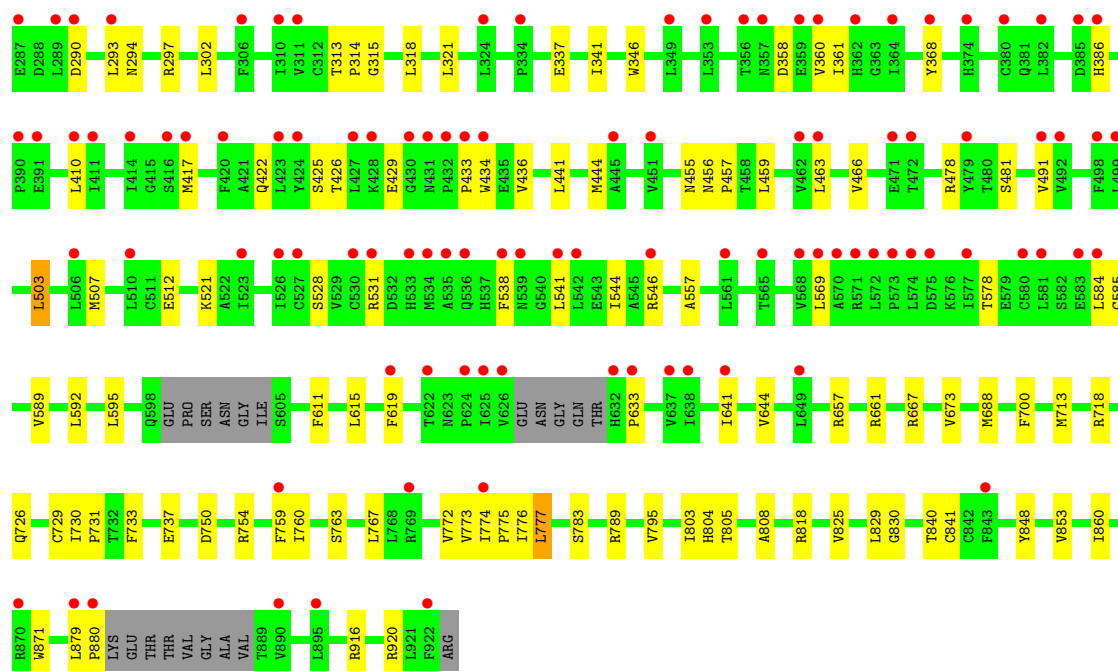
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



#### • Molecule 1: TRANSPORTIN-3

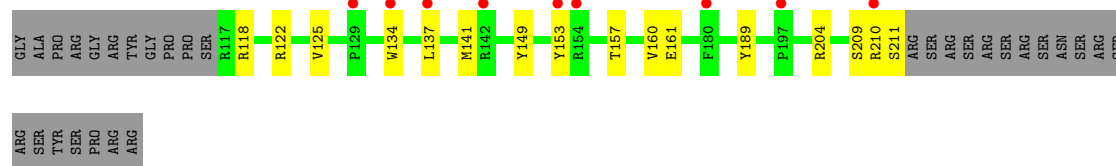




• Molecule 2: SERINE/ARGININE-RICH SPLICING FACTOR 1



• 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, $\alpha$ , $\beta$ , $\gamma$	80.55Å 91.06Å 98.12Å 106.98° 100.30° 102.18°	Depositor
Resolution (Å)	38.28 – 2.56 45.34 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.28-2.56) 87.3 (45.34-2.56)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.269 0.219 , 0.267	Depositor DCC
$R_{free}$ test set	4042 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.30	0/7282	0.48	0/9889
1	B	0.29	0/7263	0.46	0/9863
2	C	0.32	0/756	0.50	0/1011
2	D	0.30	0/750	0.47	0/1003
All	All	0.29	0/16051	0.47	0/21766

There are no bond length outliers.

There are no bond angle outliers.

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	85	1
1	B	7122	0	7150	85	0
2	C	775	0	733	7	0
2	D	769	0	728	10	0
3	B	1	0	0	0	0
4	A	27	0	0	3	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	182	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 (182) 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: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: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:B:441:LEU:HD23	1:B:444:MET:HE3	1.86	0.57
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
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:A:441:LEU:HD23	1:A:444:MET:HE3	1.88	0.55
1:B:293:LEU:HD22	1:B:341:ILE:HD11	1.89	0.54
1:B:79:PRO:O	1:B:82:SER:OG	2.19	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:313:THR:O	1:A:313:THR:OG1	2.26	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: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:197:MET:O	1:A:201:VAL:HG23	2.13	0.49
1:A:44:TRP:CE2	1:A:70:LYS:HD2	2.47	0.49
1:B:578:THR:HB	1:B:633:PRO:HB2	1.94	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
1:B:263:LEU:HD11	1:B:318:LEU:HD21	1.95	0.49
4:A:2003:HOH:O	2:D:204:ARG:NH1	2.30	0.49
1:B:760:ILE:HD13	1:B:767:LEU:HD23	1.95	0.48
1:A:193:THR:OG1	4:A:2009:HOH:O	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ILE:HB	1:A:731:PRO:HD3	1.95	0.47
1:B:417:MET:CE	1:B:455:ASN:HB3	2.44	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: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: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
2:D:210:ARG:O	2:D:211:SER:OG	2.34	0.46
1:A:10:LEU:HA	1:A:10:LEU:HD12	1.77	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:HG3	1:A:223:LYS:HZ3	1.83	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:OG1	1:B:313:THR:O	2.31	0.43
2:C:153:TYR:HD2	2:C:157:THR:HG23	1.81	0.43
1:B:155:HIS:HA	1:B:166:ARG:HH21	1.82	0.43
1:B:34:LEU:HD22	1:B:62:PHE:CZ	2.53	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
1:A:750:ASP:O	1:A:754:ARG:HG3	2.19	0.43
1:A:735:LEU:HA	1:A:735:LEU:HD12	1.81	0.43
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
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:B:53:ILE:C	1:B:54:ARG:HG3	2.39	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:N	1:A:490:GLU:OE1	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:498:PHE:C	1:A:501:PRO:HD2	2.41	0.41
1:A:667:ARG:HD3	1:A:706:ILE:HD11	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:HIS:HA	2:C:201:SEP:O1P	2.20	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:A:780:ALA:O	1:A:784:THR:HG23	2.20	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:148:THR:O	1:B:151:PRO:HD2	2.20	0.41
1:B:120:PRO:HB3	1:B:165:ARG:CZ	2.50	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
1:A:713:MET:HG3	1:A:762:ARG:HD2	2.02	0.41
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: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 [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	893/923 (97%)	868 (97%)	23 (3%)	2 (0%)	51	72
1	B	888/923 (96%)	863 (97%)	24 (3%)	1 (0%)	55	77
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%)	51	72

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%)	782 (98%)	20 (2%)	53	76
1	B	801/821 (98%)	780 (97%)	21 (3%)	51	75
2	C	80/106 (76%)	79 (99%)	1 (1%)	73	88
2	D	79/106 (74%)	78 (99%)	1 (1%)	73	88
All	All	1762/1854 (95%)	1719 (98%)	43 (2%)	54	77

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	54	ARG
1	A	198	LEU
1	A	209	PHE
1	A	224	LEU
1	A	228	LEU
1	A	273	VAL
1	A	429	GLU

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Mol	Chain	Res	Type
1	A	459	LEU
1	A	503	LEU
1	A	536	GLN
1	A	546	ARG
1	A	584	LEU
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	916	ARG
1	B	54	ARG
1	B	179	THR
1	B	180	VAL
1	B	182	SER
1	B	209	PHE
1	B	224	LEU
1	B	228	LEU
1	B	273	VAL
1	B	337	GLU
1	B	429	GLU
1	B	459	LEU
1	B	503	LEU
1	B	546	ARG
1	B	584	LEU
1	B	667	ARG
1	B	713	MET
1	B	737	GLU
1	B	759	PHE
1	B	777	LEU
1	B	840	THR
1	B	916	ARG
2	C	134	TRP
2	D	134	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	C	201	2	9,9,10	1.43	1 (11%)	9,12,14	1.46	1 (11%)
2	SEP	C	207	2	9,9,10	1.60	2 (22%)	9,12,14	1.28	1 (11%)
2	SEP	C	209	2	9,9,10	1.69	2 (22%)	9,12,14	1.16	0
2	SEP	D	201	2	9,9,10	1.48	2 (22%)	9,12,14	1.74	2 (22%)
2	SEP	D	207	2	9,9,10	1.56	2 (22%)	9,12,14	1.54	1 (11%)
2	SEP	D	209	2	9,9,10	1.63	2 (22%)	9,12,14	1.22	1 (11%)

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	C	201	2	-	0/5/8/10	0/0/0/0
2	SEP	C	207	2	-	0/5/8/10	0/0/0/0
2	SEP	C	209	2	-	0/5/8/10	0/0/0/0
2	SEP	D	201	2	-	0/5/8/10	0/0/0/0
2	SEP	D	207	2	-	0/5/8/10	0/0/0/0
2	SEP	D	209	2	-	0/5/8/10	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	SEP	CA-C	2.03	1.52	1.50
2	D	207	SEP	CA-C	2.43	1.53	1.50
2	C	207	SEP	CA-C	2.57	1.53	1.50
2	D	207	SEP	P-O1P	2.76	1.60	1.50
2	D	201	SEP	P-O1P	2.90	1.60	1.50
2	D	209	SEP	P-O1P	2.92	1.60	1.50
2	C	201	SEP	P-O1P	2.99	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	209	SEP	CA-C	2.99	1.54	1.50
2	C	209	SEP	CA-C	3.05	1.54	1.50
2	C	207	SEP	P-O1P	3.09	1.61	1.50
2	C	209	SEP	P-O1P	3.23	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	209	SEP	P-OG-CB	-2.35	111.83	118.30
2	D	201	SEP	O2P-P-OG	2.28	112.81	106.73
2	C	207	SEP	OG-CB-CA	2.36	110.49	108.17
2	C	201	SEP	OG-CB-CA	2.47	110.60	108.17
2	D	207	SEP	OG-CB-CA	3.31	111.43	108.17
2	D	201	SEP	OG-CB-CA	3.92	112.03	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	901/923 (97%)	0.72	71 (7%) 13 11	29, 57, 91, 122	0
1	B	898/923 (97%)	0.88	120 (13%) 4 2	26, 70, 107, 124	0
2	C	93/125 (74%)	0.36	0 100 100	35, 51, 67, 74	0
2	D	92/125 (73%)	0.63	9 (9%) 8 7	32, 66, 84, 96	0
All	All	1984/2096 (94%)	0.77	200 (10%) 8 6	26, 61, 101, 124	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	VAL	9.2
1	B	626	VAL	7.4
1	B	424	TYR	7.3
1	B	625	ILE	6.9
1	B	417	MET	6.2
1	B	569	LEU	6.1
1	B	580	CYS	5.9
1	B	572	LEU	5.9
1	B	410	LEU	5.8
1	B	565	THR	5.4
1	B	584	LEU	5.4
1	A	191	ALA	5.2
1	B	431	ASN	5.2
1	B	430	GLY	5.0
1	B	880	PRO	4.9
1	B	492	VAL	4.9
1	A	428	LYS	4.8
1	B	161	ILE	4.6
1	A	572	LEU	4.6
1	B	538	PHE	4.5
1	B	349	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	677	SER	4.5
1	B	479	TYR	4.3
1	B	622	THR	4.2
1	B	445	ALA	4.2
1	B	577	ILE	4.1
1	A	580	CYS	4.1
1	B	414	ILE	4.1
1	B	121	SER	4.0
1	A	626	VAL	3.9
1	B	573	PRO	3.9
1	B	769	ARG	3.8
1	A	26	GLY	3.8
1	A	632	HIS	3.8
1	B	510	LEU	3.7
1	B	420	PHE	3.7
1	B	531	ARG	3.7
1	B	536	GLN	3.7
1	A	424	TYR	3.7
1	A	634	CYS	3.7
1	A	569	LEU	3.7
1	B	81	ASP	3.6
1	B	541	LEU	3.6
1	B	637	VAL	3.6
1	B	236	LYS	3.6
1	B	423	LEU	3.6
1	A	625	ILE	3.5
1	A	192	GLY	3.5
1	A	633	PRO	3.4
1	B	534	MET	3.4
1	B	535	ALA	3.3
1	B	451	VAL	3.3
1	B	293	LEU	3.3
1	B	491	VAL	3.3
1	A	326	LEU	3.3
1	A	538	PHE	3.3
1	B	472	THR	3.3
2	D	134	TRP	3.2
1	A	568	VAL	3.2
1	B	571	ARG	3.2
1	B	581	LEU	3.2
1	B	633	PRO	3.2
1	A	638	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	565	THR	3.1
1	A	18	LEU	3.1
1	A	317	GLY	3.1
1	B	434	TRP	3.1
1	A	503	LEU	3.0
1	B	353	LEU	3.0
1	B	274	LEU	3.0
1	B	870	ARG	3.0
1	B	641	ILE	3.0
1	B	570	ALA	3.0
1	B	386	HIS	3.0
1	B	463	LEU	3.0
1	B	624	PRO	2.9
1	A	188	VAL	2.9
1	A	811	HIS	2.9
1	B	542	LEU	2.9
1	B	359	GLU	2.9
1	A	636	LYS	2.9
1	B	428	LYS	2.9
1	B	523	ILE	2.9
1	A	673	VAL	2.8
1	B	546	ARG	2.8
1	B	334	PRO	2.8
1	B	632	HIS	2.8
1	B	195	GLU	2.8
1	B	471	GLU	2.8
1	A	527	CYS	2.8
1	A	316	GLN	2.8
1	A	498	PHE	2.8
1	B	44	TRP	2.8
1	B	360	VAL	2.8
1	B	759	PHE	2.8
1	A	913	TRP	2.8
1	A	315	GLY	2.7
1	A	570	ALA	2.7
1	A	321	LEU	2.7
2	D	154	ARG	2.7
1	A	488	MET	2.7
1	A	577	ILE	2.7
1	A	373	LEU	2.7
1	A	81	ASP	2.7
1	B	289	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	374	HIS	2.7
1	A	584	LEU	2.6
1	B	561	LEU	2.6
1	B	310	ILE	2.6
1	B	530	CYS	2.6
1	B	311	VAL	2.6
1	B	619	PHE	2.6
1	B	583	GLU	2.6
1	B	385	ASP	2.6
1	B	527	CYS	2.6
1	A	670	VAL	2.6
1	B	364	ILE	2.6
1	A	392	GLU	2.6
1	A	236	LYS	2.5
1	B	287	GLU	2.5
1	B	539	ASN	2.5
1	B	498	PHE	2.5
1	B	382	LEU	2.5
1	B	638	ILE	2.5
1	B	427	LEU	2.5
1	A	769	ARG	2.5
1	B	282	MET	2.4
1	A	712	GLY	2.4
1	A	322	ARG	2.4
1	B	130	VAL	2.4
1	A	434	TRP	2.4
1	B	169	ILE	2.4
1	B	391	GLU	2.4
1	A	680	LEU	2.4
1	B	895	LEU	2.4
2	D	137	LEU	2.4
1	B	122	TRP	2.4
1	B	433	PRO	2.4
1	B	411	ILE	2.4
1	B	922	PHE	2.4
1	A	576	LYS	2.4
1	A	471	GLU	2.4
1	B	357	ASN	2.3
1	B	380	CYS	2.3
1	B	462	VAL	2.3
2	D	129	PRO	2.3
1	A	838	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	273	VAL	2.3
1	B	306	PHE	2.3
2	D	180	PHE	2.3
1	B	362	HIS	2.3
1	B	506	LEU	2.3
1	B	368	TYR	2.3
1	B	324	LEU	2.3
1	A	308	GLU	2.3
1	A	814	ASP	2.3
1	A	427	LEU	2.3
1	A	463	LEU	2.3
1	A	637	VAL	2.2
1	B	890	VAL	2.2
2	D	153	TYR	2.2
1	B	82	SER	2.2
1	A	535	ALA	2.2
1	B	80	THR	2.2
1	A	541	LEU	2.2
1	B	879	LEU	2.2
1	A	323	THR	2.2
1	A	307	LEU	2.2
1	A	523	ILE	2.2
1	B	290	ASP	2.2
1	B	356	THR	2.2
1	A	270	PHE	2.2
1	A	319	GLY	2.2
1	B	843	PHE	2.2
1	A	573	PRO	2.2
2	D	142	ARG	2.2
1	A	454	GLU	2.1
1	B	390	PRO	2.1
1	B	18	LEU	2.1
1	B	574	LEU	2.1
1	A	824	GLN	2.1
1	A	451	VAL	2.1
1	A	579	GLU	2.1
1	B	774	ILE	2.1
1	B	533	HIS	2.1
1	B	526	ILE	2.1
1	B	278	THR	2.1
2	D	197	PRO	2.1
2	D	210	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	575	ASP	2.1
1	A	906	GLU	2.1
1	A	810	ASP	2.1
1	A	641	ILE	2.1
1	B	239	SER	2.1
1	A	266	ALA	2.0
1	B	416	SER	2.0
1	A	320	ASP	2.0
1	B	499	LEU	2.0
1	B	649	LEU	2.0
1	B	432	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SEP	C	201	10/11	0.85	0.25	-	30,39,54,59	4
2	SEP	D	207	10/11	0.95	0.17	-	29,37,51,58	0
2	SEP	C	207	10/11	0.96	0.17	-	32,40,47,49	0
2	SEP	C	209	10/11	0.97	0.16	-	33,38,47,54	0
2	SEP	D	209	10/11	0.98	0.18	-	30,36,41,46	0
2	SEP	D	201	10/11	0.93	0.24	-	26,35,51,52	4

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	B	1924	1/1	0.89	0.14	-1.64	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.