



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:06 AM BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

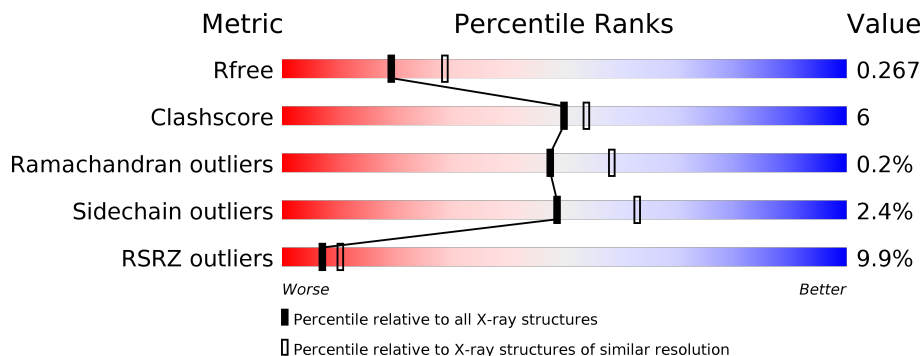
1 Overall quality at a glance

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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 on 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	
1	B	923	
2	C	125	
2	D	125	

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
			Total	C	N	O	S			
1	A	901	Total 7140	C 4551	N 1215	O 1320	S 54	0	0	0
1	B	898	Total 7122	C 4540	N 1211	O 1317	S 54	0	0	0

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

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is water.

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

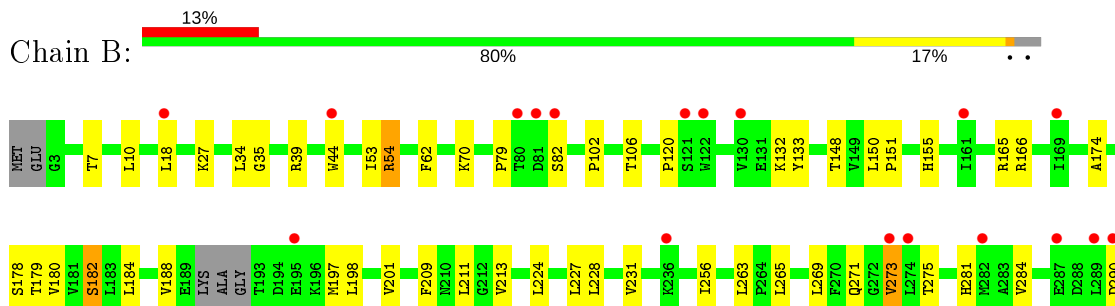
3 Residue-property plots [i](#)

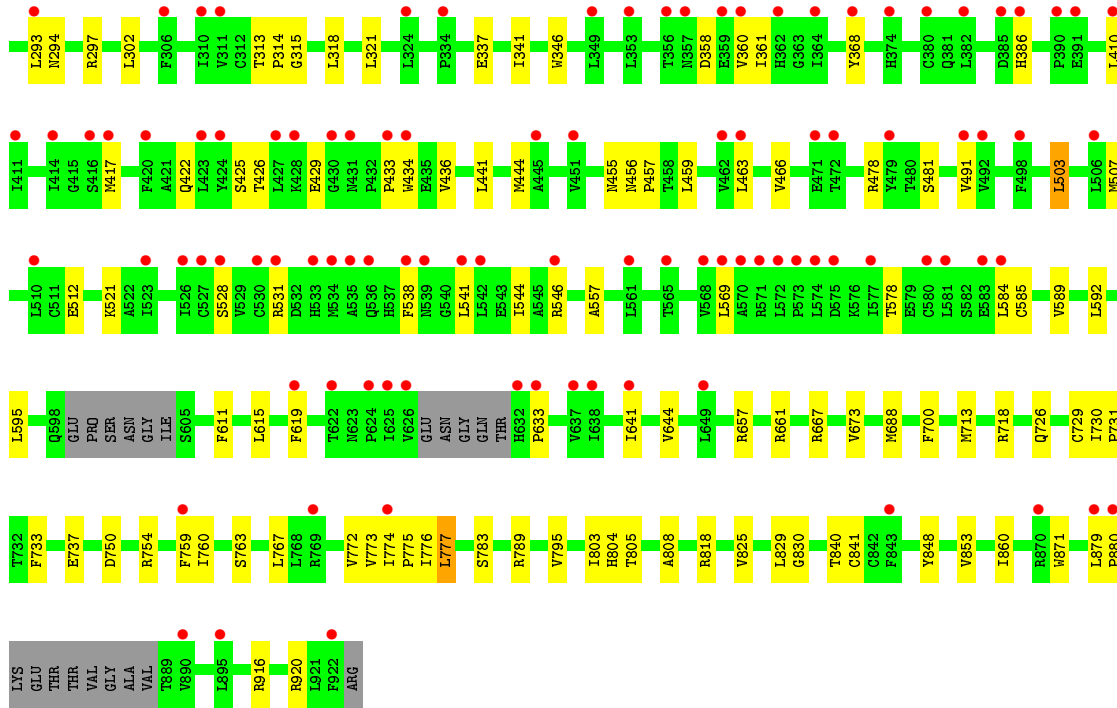
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: TRANSPORTIN-3

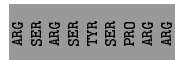
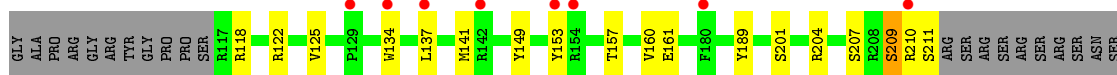




● Molecule 2: SERINE/ARGININE-RICH SPLICING FACTOR 1



● 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, α , β , γ	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) 98.4 (45.34-2.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.269 0.220 , 0.267	Depositor DCC
R_{free} test set	4040 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtrriage
Anisotropy	0.137	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: 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%)	47	58
1	B	888/923 (96%)	863 (97%)	24 (3%)	1 (0%)	51	65
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%)	47	58

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	802/821 (98%)	782 (98%)	20 (2%)	47	61
1	B	801/821 (98%)	780 (97%)	21 (3%)	46	59
2	C	80/106 (76%)	79 (99%)	1 (1%)	69	80
2	D	79/106 (74%)	78 (99%)	1 (1%)	69	80
All	All	1762/1854 (95%)	1719 (98%)	43 (2%)	49	63

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	8,9,10	1.51	1 (12%)	8,12,14	1.42	1 (12%)
2	SEP	D	207	2	8,9,10	1.51	1 (12%)	8,12,14	1.57	1 (12%)
2	SEP	C	207	2	8,9,10	1.53	1 (12%)	8,12,14	1.25	1 (12%)
2	SEP	C	209	2	8,9,10	1.52	1 (12%)	8,12,14	1.10	0
2	SEP	D	209	2	8,9,10	1.47	1 (12%)	8,12,14	1.18	1 (12%)
2	SEP	D	201	2	8,9,10	1.50	1 (12%)	8,12,14	1.77	2 (25%)

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	-	2/5/8/10	-
2	SEP	D	207	2	-	2/5/8/10	-
2	SEP	C	207	2	-	2/5/8/10	-
2	SEP	C	209	2	-	0/5/8/10	-
2	SEP	D	209	2	-	3/5/8/10	-
2	SEP	D	201	2	-	5/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	209	SEP	P-O1P	3.47	1.61	1.50
2	C	207	SEP	P-O1P	3.32	1.61	1.50
2	C	201	SEP	P-O1P	3.22	1.60	1.50
2	D	209	SEP	P-O1P	3.15	1.60	1.50
2	D	201	SEP	P-O1P	3.13	1.60	1.50
2	D	207	SEP	P-O1P	2.98	1.60	1.50

All (6) 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	209	SEP	P-OG-CB	-2.35	111.83	118.30
2	D	201	SEP	O2P-P-OG	2.28	112.81	106.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	SEP	N-CA-CB-OG
2	C	201	SEP	CA-CB-OG-P
2	D	207	SEP	CA-CB-OG-P
2	C	207	SEP	N-CA-CB-OG
2	C	207	SEP	CA-CB-OG-P
2	D	209	SEP	CB-OG-P-O3P
2	D	201	SEP	N-CA-CB-OG
2	D	201	SEP	CB-OG-P-O2P
2	D	201	SEP	CB-OG-P-O3P
2	D	201	SEP	CB-OG-P-O1P
2	D	201	SEP	CA-CB-OG-P
2	D	207	SEP	N-CA-CB-OG
2	D	209	SEP	CB-OG-P-O1P
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	C	201	SEP	1	0
2	C	209	SEP	1	0
2	D	209	SEP	1	0

5.5 Carbohydrates

There are no monosaccharides 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 [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	901/923 (97%)	0.70	71 (7%) 12 17	29, 57, 91, 122	0
1	B	898/923 (97%)	0.87	117 (13%) 3 4	26, 70, 107, 124	0
2	C	93/125 (74%)	0.33	0 100 100	35, 51, 67, 74	0
2	D	92/125 (73%)	0.62	8 (8%) 10 14	32, 66, 84, 96	0
All	All	1984/2096 (94%)	0.75	196 (9%) 7 10	26, 61, 101, 124	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	VAL	9.2
1	B	626	VAL	7.5
1	B	424	TYR	7.2
1	B	625	ILE	6.8
1	B	569	LEU	6.2
1	B	417	MET	6.1
1	B	580	CYS	6.0
1	B	572	LEU	5.9
1	B	410	LEU	5.7
1	B	565	THR	5.4
1	B	584	LEU	5.4
1	A	191	ALA	5.3
1	B	431	ASN	5.2
1	B	430	GLY	4.9
1	B	880	PRO	4.8
1	B	492	VAL	4.8
1	A	428	LYS	4.8
1	A	572	LEU	4.6
1	B	538	PHE	4.5
1	B	349	LEU	4.5
1	B	161	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	677	SER	4.4
1	B	445	ALA	4.3
1	B	479	TYR	4.2
1	B	622	THR	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	B	573	PRO	4.0
1	A	26	GLY	3.9
1	A	626	VAL	3.9
1	B	769	ARG	3.9
1	B	531	ARG	3.8
1	B	510	LEU	3.8
1	B	536	GLN	3.8
1	A	632	HIS	3.7
1	B	420	PHE	3.7
1	A	424	TYR	3.7
1	A	569	LEU	3.7
1	B	541	LEU	3.6
1	A	634	CYS	3.6
1	B	81	ASP	3.6
1	A	625	ILE	3.6
1	B	423	LEU	3.6
1	B	637	VAL	3.6
1	A	192	GLY	3.5
1	A	633	PRO	3.4
1	B	236	LYS	3.4
1	B	472	THR	3.4
1	B	534	MET	3.4
1	B	451	VAL	3.3
1	B	491	VAL	3.3
1	B	535	ALA	3.3
2	D	134	TRP	3.3
1	A	326	LEU	3.2
1	B	293	LEU	3.2
1	B	571	ARG	3.2
1	A	538	PHE	3.2
1	A	638	ILE	3.1
1	A	568	VAL	3.1
1	B	633	PRO	3.1
1	B	353	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	581	LEU	3.1
1	B	434	TRP	3.1
1	B	274	LEU	3.1
1	A	317	GLY	3.0
1	A	565	THR	3.0
1	A	18	LEU	3.0
1	A	503	LEU	3.0
1	B	870	ARG	3.0
1	B	463	LEU	3.0
1	A	811	HIS	3.0
1	B	386	HIS	3.0
1	B	641	ILE	3.0
1	B	359	GLU	2.9
1	B	546	ARG	2.9
1	B	428	LYS	2.9
1	B	542	LEU	2.9
1	B	570	ALA	2.9
1	A	636	LYS	2.9
1	B	471	GLU	2.9
1	B	632	HIS	2.9
1	B	624	PRO	2.9
1	A	188	VAL	2.8
1	A	316	GLN	2.8
1	B	44	TRP	2.8
1	A	673	VAL	2.8
2	D	154	ARG	2.8
1	B	334	PRO	2.8
1	B	360	VAL	2.8
1	A	570	ALA	2.8
1	B	195	GLU	2.7
1	A	81	ASP	2.7
1	A	527	CYS	2.7
1	A	577	ILE	2.7
1	A	913	TRP	2.7
1	A	315	GLY	2.7
1	A	321	LEU	2.7
1	B	523	ILE	2.7
1	A	498	PHE	2.7
1	A	373	LEU	2.7
1	B	289	LEU	2.6
1	B	759	PHE	2.6
1	B	374	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	488	MET	2.6
1	B	530	CYS	2.6
1	B	561	LEU	2.6
1	A	584	LEU	2.6
1	B	364	ILE	2.6
1	B	619	PHE	2.6
1	A	392	GLU	2.6
1	B	527	CYS	2.5
1	B	310	ILE	2.5
1	B	583	GLU	2.5
1	B	385	ASP	2.5
1	B	273	VAL	2.5
1	B	427	LEU	2.5
1	B	391	GLU	2.5
1	A	670	VAL	2.5
1	B	311	VAL	2.5
1	B	382	LEU	2.5
1	B	539	ASN	2.5
1	B	287	GLU	2.5
1	B	130	VAL	2.5
1	B	462	VAL	2.5
1	A	236	LYS	2.5
1	B	498	PHE	2.5
1	B	638	ILE	2.5
1	B	122	TRP	2.4
1	B	282	MET	2.4
1	A	769	ARG	2.4
1	B	411	ILE	2.4
1	A	322	ARG	2.4
1	B	169	ILE	2.4
1	B	922	PHE	2.4
1	B	433	PRO	2.4
1	B	895	LEU	2.4
1	B	357	ASN	2.4
1	A	680	LEU	2.4
2	D	137	LEU	2.4
1	A	576	LYS	2.4
1	B	362	HIS	2.4
1	A	471	GLU	2.3
1	A	712	GLY	2.3
1	A	434	TRP	2.3
1	B	506	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	129	PRO	2.2
1	B	306	PHE	2.2
1	A	427	LEU	2.2
1	B	879	LEU	2.2
1	B	380	CYS	2.2
1	A	814	ASP	2.2
1	A	307	LEU	2.2
1	B	574	LEU	2.2
1	B	368	TYR	2.2
2	D	153	TYR	2.2
1	A	454	GLU	2.2
2	D	180	PHE	2.2
1	A	463	LEU	2.2
1	B	324	LEU	2.2
1	A	319	GLY	2.2
1	A	535	ALA	2.2
1	B	80	THR	2.2
1	A	308	GLU	2.2
1	B	390	PRO	2.2
1	A	824	GLN	2.2
1	A	541	LEU	2.2
1	A	838	LEU	2.2
1	B	290	ASP	2.1
1	A	573	PRO	2.1
1	B	533	HIS	2.1
1	A	451	VAL	2.1
1	A	637	VAL	2.1
1	B	82	SER	2.1
1	B	890	VAL	2.1
1	A	323	THR	2.1
1	B	356	THR	2.1
1	B	843	PHE	2.1
1	A	579	GLU	2.1
2	D	210	ARG	2.1
1	A	523	ILE	2.1
1	A	270	PHE	2.1
1	B	18	LEU	2.1
1	B	575	ASP	2.1
1	B	774	ILE	2.1
1	B	416	SER	2.1
2	D	142	ARG	2.1
1	A	266	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	906	GLU	2.0
1	A	641	ILE	2.0
1	B	526	ILE	2.0
1	B	649	LEU	2.0
1	B	528	SER	2.0
1	A	542	LEU	2.0
1	A	271	GLN	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	0.85	0.25	30,39,54,59	4
2	SEP	D	201	10/11	0.94	0.24	26,35,51,52	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	D	209	10/11	0.98	0.18	30,36,41,46	0
2	SEP	C	209	10/11	0.98	0.15	33,38,47,54	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	0.90	0.15	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.