



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:04 AM GMT

PDB ID : 2VSX
Title : CRYSTAL STRUCTURE OF A TRANSLATION INITIATION COMPLEX
Authors : Schutz, P.; Bumann, M.; Oberholzer, A.E.; Bieniossek, C.; Altmann, M.; Trachsel, H.; Baumann, U.
Deposited on : 2008-04-30
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

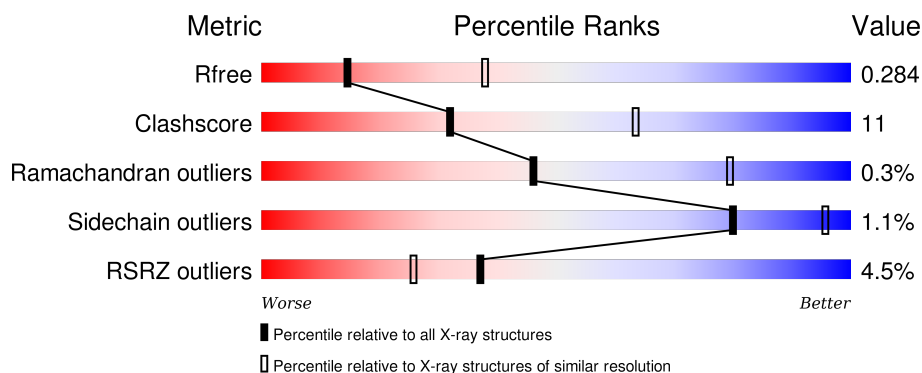
1 Overall quality at a glance

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	395	<div> <div>3%</div> <div>70% 22% 7%</div> </div>
1	B	395	<div> <div>4%</div> <div>70% 22% 7%</div> </div>
2	E	284	<div> <div>5%</div> <div>64% 20% 15%</div> </div>
2	F	284	<div> <div>5%</div> <div>64% 19% 17%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9623 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.

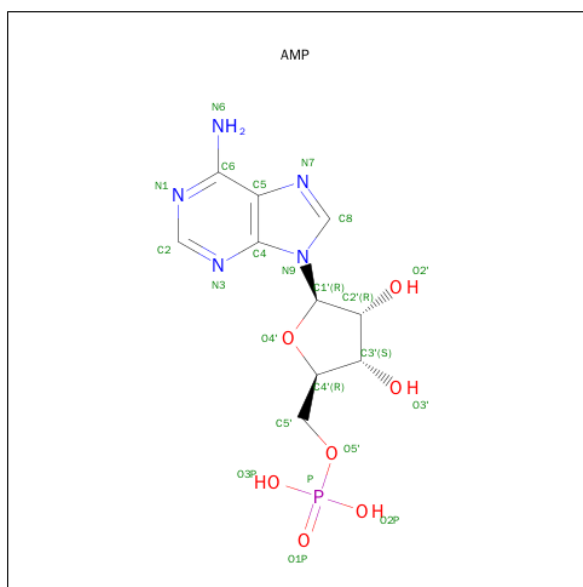
- Molecule 1 is a protein called ATP-DEPENDENT RNA HELICASE EIF4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2907	1846	490	557	14			
1	B	366	Total	C	N	O	S	0	0	0
			2907	1846	490	557	14			

- Molecule 2 is a protein called EUKARYOTIC INITIATION FACTOR 4F SUBUNIT P150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	240	Total	C	N	O	S	0	0	0
			1892	1208	320	354	10			
2	F	237	Total	C	N	O	S	0	0	0
			1871	1197	316	348	10			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

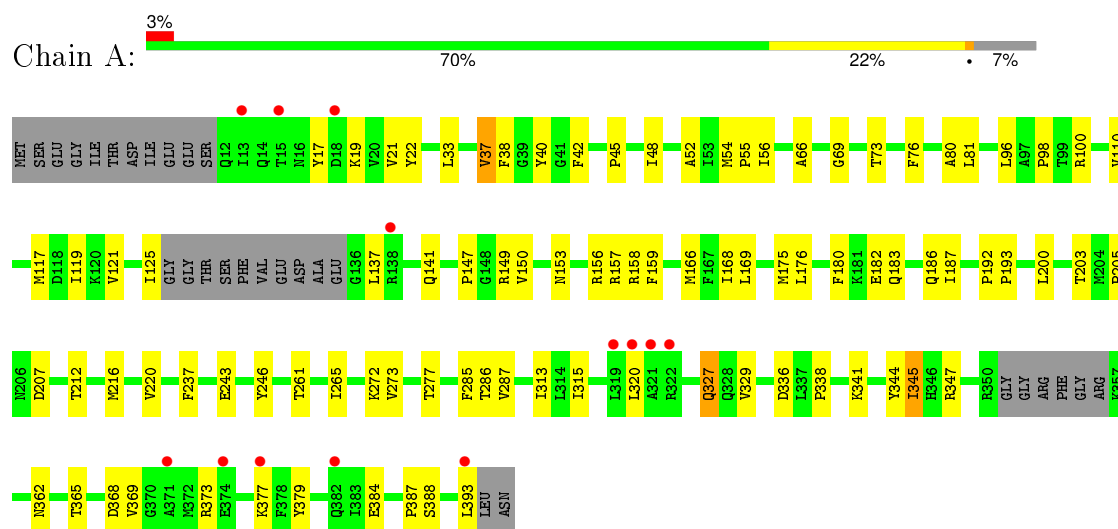


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

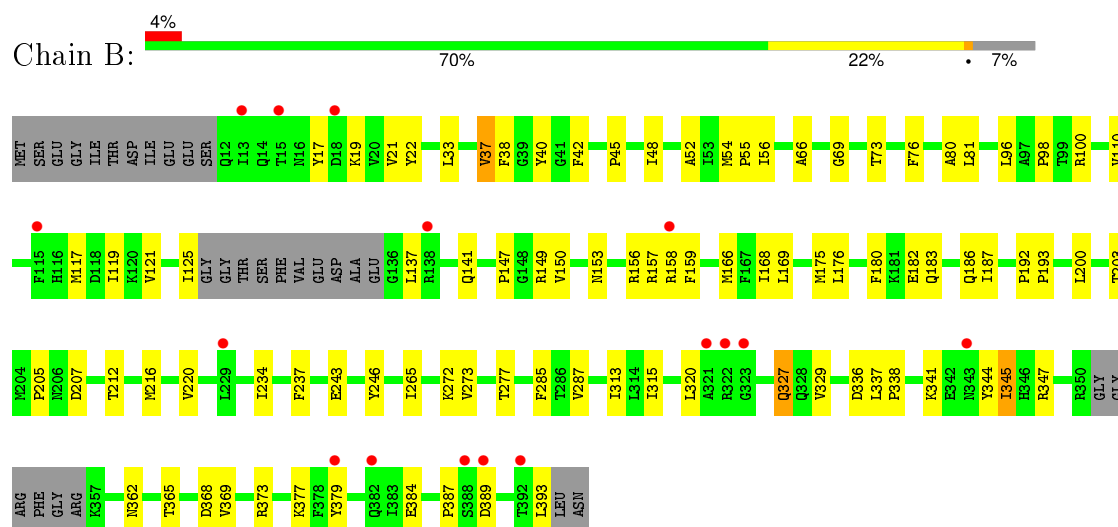
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: ATP-DEPENDENT RNA HELICASE EIF4A



• Molecule 1: ATP-DEPENDENT RNA HELICASE EIF4A



• Molecule 2: EUKARYOTIC INITIATION FACTOR 4F SUBUNIT P150



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.92Å 111.36Å 111.28Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	33.21 – 2.80 33.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.21-2.80) 99.2 (33.16-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.252 , 0.287 0.248 , 0.284	Depositor DCC
R_{free} test set	1667 reflections (4.12%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 40575 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9623	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.32 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.7551e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AMP

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	0.23	0/2949	0.40	0/3985
1	B	0.23	0/2949	0.41	0/3985
2	E	0.22	0/1920	0.39	1/2585 (0.0%)
2	F	0.22	0/1899	0.39	1/2556 (0.0%)
All	All	0.22	0/9717	0.40	2/13111 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	716	PRO	N-CA-CB	5.91	110.39	103.30
2	F	716	PRO	N-CA-CB	5.89	110.37	103.30

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	2907	0	2935	67	0
1	B	2907	0	2935	65	0
2	E	1892	0	1887	42	0
2	F	1871	0	1866	38	0
3	A	23	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	0	12	1	0
All	All	9623	0	9647	204	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (204) 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:69:GLY:HA2	3:A:1178:AMP:H5'1	1.37	1.04
1:A:341:LYS:HD2	1:A:341:LYS:H	1.31	0.93
1:B:341:LYS:HD2	1:B:341:LYS:H	1.31	0.92
1:B:69:GLY:HA2	3:B:1178:AMP:H5'1	1.51	0.90
2:E:730:SER:HB3	2:E:733:TYR:HB3	1.64	0.80
1:A:156:ARG:HH11	1:A:158:ARG:HH12	1.32	0.78
1:B:156:ARG:HH11	1:B:158:ARG:HH12	1.31	0.76
2:F:600:LEU:HD23	2:F:601:LEU:H	1.53	0.74
2:E:600:LEU:HD23	2:E:601:LEU:H	1.54	0.73
1:A:345:ILE:HG12	1:A:379:TYR:CE1	2.24	0.73
1:B:137:LEU:HD11	1:B:153:ASN:HD22	1.55	0.72
1:B:345:ILE:HG12	1:B:379:TYR:CE1	2.24	0.71
1:A:137:LEU:HD11	1:A:153:ASN:HD22	1.55	0.71
1:B:176:LEU:HD13	1:B:207:ASP:HB3	1.75	0.69
1:A:212:THR:HA	1:A:216:MET:HE3	1.76	0.68
1:A:365:THR:H	1:A:368:ASP:HB2	1.59	0.67
1:B:212:THR:HA	1:B:216:MET:HE2	1.77	0.67
1:A:176:LEU:HD13	1:A:207:ASP:HB3	1.76	0.66
1:B:365:THR:H	1:B:368:ASP:HB2	1.61	0.64
1:A:125:ILE:HA	1:A:149:ARG:HG3	1.81	0.63
1:B:125:ILE:HA	1:B:149:ARG:HG3	1.80	0.61
2:F:633:ALA:HB1	2:F:645:LEU:HD13	1.83	0.61
1:A:345:ILE:HG12	1:A:379:TYR:HE1	1.66	0.61
1:B:344:TYR:HE1	1:B:362:ASN:HD21	1.49	0.60
1:A:327:GLN:HG3	1:A:329:VAL:HG23	1.83	0.60
1:A:344:TYR:HE1	1:A:362:ASN:HD21	1.50	0.60
2:E:633:ALA:HB1	2:E:645:LEU:HD13	1.83	0.59
1:B:327:GLN:HG3	1:B:329:VAL:HG23	1.83	0.59
1:B:345:ILE:HG12	1:B:379:TYR:HE1	1.66	0.59
2:F:746:LEU:O	2:F:750:ILE:HG12	2.03	0.58
2:F:784:LEU:HD21	2:F:826:ILE:HD13	1.85	0.58
2:F:713:ASP:HB2	2:F:774:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:607:GLU:HA	2:E:651:GLN:HE22	1.69	0.58
2:E:784:LEU:HD21	2:E:826:ILE:HD13	1.85	0.57
1:A:287:VAL:HG12	1:A:313:ILE:HB	1.84	0.57
2:E:746:LEU:O	2:E:750:ILE:HG12	2.04	0.57
2:F:607:GLU:HA	2:F:651:GLN:HE22	1.69	0.57
1:B:37:VAL:HG23	1:B:42:PHE:HB2	1.85	0.57
1:B:287:VAL:HG12	1:B:313:ILE:HB	1.85	0.57
2:F:744:LEU:O	2:F:747:VAL:HG22	2.05	0.57
1:A:37:VAL:HG23	1:A:42:PHE:HB2	1.86	0.57
2:E:713:ASP:HB2	2:E:774:ASP:OD2	2.04	0.57
1:B:389:ASP:O	1:B:393:LEU:HG	2.05	0.56
1:B:81:LEU:HB3	1:B:117:MET:HE1	1.87	0.56
1:A:277:THR:HG23	1:A:287:VAL:CG2	2.36	0.56
2:F:748:ARG:HE	2:F:752:PHE:HE1	1.53	0.56
1:B:277:THR:HG23	1:B:287:VAL:CG2	2.35	0.56
1:B:48:ILE:HD11	1:B:66:ALA:HB1	1.88	0.55
2:E:748:ARG:HE	2:E:752:PHE:HE1	1.54	0.55
2:E:744:LEU:O	2:E:747:VAL:HG22	2.06	0.55
1:A:48:ILE:HD11	1:A:66:ALA:HB1	1.89	0.54
1:A:243:GLU:HB2	1:A:246:TYR:CD1	2.43	0.54
1:B:80:ALA:HA	1:B:166:MET:HE1	1.90	0.54
1:B:243:GLU:HB2	1:B:246:TYR:CD1	2.43	0.53
1:B:76:PHE:HB2	1:B:168:ILE:HD13	1.89	0.53
1:A:273:VAL:HG13	1:A:315:ILE:HG22	1.90	0.53
1:A:81:LEU:HB3	1:A:117:MET:HE1	1.89	0.53
1:A:80:ALA:HA	1:A:166:MET:HE1	1.91	0.53
1:B:273:VAL:HG13	1:B:315:ILE:HG22	1.89	0.53
1:A:285:PHE:CZ	2:E:616:LYS:HE2	2.45	0.52
1:A:76:PHE:HB2	1:A:168:ILE:HD13	1.90	0.52
2:F:677:LEU:HD22	2:F:695:VAL:CG2	2.40	0.52
1:A:169:LEU:HB3	1:A:175:MET:HE1	1.90	0.52
2:F:597:LYS:CB	2:F:638:TRP:HE1	2.23	0.52
2:F:614:LEU:HB3	2:F:655:LYS:HG3	1.90	0.52
2:E:600:LEU:HD23	2:E:601:LEU:N	2.24	0.52
1:A:119:ILE:HA	1:A:141:GLN:OE1	2.10	0.52
1:B:52:ALA:O	1:B:56:ILE:HG13	2.09	0.52
1:B:119:ILE:HA	1:B:141:GLN:OE1	2.10	0.52
1:B:96:LEU:HD11	1:B:150:VAL:HG11	1.92	0.52
1:A:338:PRO:HD3	1:A:347:ARG:NH1	2.25	0.51
2:E:614:LEU:HB3	2:E:655:LYS:HG3	1.91	0.51
1:B:52:ALA:O	1:B:55:PRO:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:HB3	1:B:175:MET:HE1	1.91	0.51
2:E:677:LEU:HD22	2:E:695:VAL:CG2	2.40	0.51
1:A:149:ARG:HA	1:A:149:ARG:CZ	2.40	0.51
1:A:52:ALA:O	1:A:56:ILE:HG13	2.11	0.51
1:A:96:LEU:HD11	1:A:150:VAL:HG11	1.92	0.51
2:F:749:PHE:CE2	2:F:753:LEU:HD11	2.46	0.51
1:B:341:LYS:CD	1:B:341:LYS:H	2.09	0.51
2:F:600:LEU:HD23	2:F:601:LEU:N	2.24	0.51
2:F:637:VAL:HG12	2:F:681:ILE:HG12	1.93	0.51
1:B:338:PRO:HD3	1:B:347:ARG:NH1	2.26	0.51
1:A:17:TYR:HB2	1:A:220:VAL:HG13	1.92	0.50
1:A:285:PHE:CE1	2:E:616:LYS:HE2	2.46	0.50
1:B:17:TYR:CZ	1:B:19:LYS:HD3	2.47	0.50
2:F:674:VAL:HG22	2:F:695:VAL:HB	1.94	0.50
2:E:674:VAL:HG22	2:E:695:VAL:HB	1.94	0.50
1:B:17:TYR:HB2	1:B:220:VAL:HG13	1.93	0.50
1:B:149:ARG:CZ	1:B:149:ARG:HA	2.41	0.50
2:F:771:LEU:O	2:F:775:LEU:HB2	2.12	0.50
1:A:52:ALA:O	1:A:55:PRO:HG2	2.11	0.50
1:A:365:THR:N	1:A:368:ASP:HB2	2.26	0.49
2:E:637:VAL:HG12	2:E:681:ILE:HG12	1.94	0.49
1:A:17:TYR:CZ	1:A:19:LYS:HD3	2.47	0.49
1:A:369:VAL:O	1:A:373:ARG:HG2	2.12	0.49
1:A:387:PRO:O	2:E:579:TRP:HB2	2.12	0.49
2:E:771:LEU:O	2:E:775:LEU:HB2	2.12	0.49
1:A:388:SER:HB3	2:E:578:ARG:O	2.14	0.48
2:E:823:LEU:O	2:E:826:ILE:HG22	2.13	0.48
1:B:272:LYS:HD2	1:B:336:ASP:OD1	2.13	0.48
1:A:286:THR:HB	2:E:618:THR:HG21	1.95	0.48
2:F:673:VAL:O	2:F:677:LEU:HB2	2.14	0.48
2:E:749:PHE:CE2	2:E:753:LEU:HD11	2.47	0.48
1:B:369:VAL:O	1:B:373:ARG:HG2	2.13	0.48
1:A:54:MET:N	1:A:55:PRO:HD2	2.28	0.48
1:B:54:MET:N	1:B:55:PRO:HD2	2.29	0.48
2:F:702:ARG:O	2:F:706:GLU:HG2	2.14	0.48
2:F:823:LEU:O	2:F:826:ILE:HG22	2.13	0.47
1:B:277:THR:HG23	1:B:287:VAL:HG23	1.96	0.47
1:B:33:LEU:O	1:B:37:VAL:HG12	2.14	0.47
2:E:673:VAL:O	2:E:677:LEU:HB2	2.14	0.47
1:B:183:GLN:O	1:B:187:ILE:HD12	2.15	0.47
2:F:772:MET:HG2	2:F:819:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HD2	1:A:336:ASP:OD1	2.15	0.47
1:A:33:LEU:O	1:A:37:VAL:HG12	2.15	0.47
2:E:702:ARG:O	2:E:706:GLU:HG2	2.14	0.47
1:B:365:THR:N	1:B:368:ASP:HB2	2.27	0.46
1:A:203:THR:C	1:A:205:PRO:HD3	2.36	0.46
1:A:373:ARG:O	1:A:377:LYS:HG2	2.15	0.46
2:E:772:MET:HG2	2:E:819:LEU:HD13	1.97	0.46
1:A:277:THR:HG23	1:A:287:VAL:HG23	1.97	0.46
1:B:373:ARG:O	1:B:377:LYS:HG2	2.14	0.46
2:F:775:LEU:HD11	2:F:784:LEU:HD23	1.98	0.46
1:B:203:THR:C	1:B:205:PRO:HD3	2.36	0.46
2:F:775:LEU:HA	2:F:779:PRO:HG3	1.97	0.46
2:E:775:LEU:HA	2:E:779:PRO:HG3	1.97	0.46
2:E:695:VAL:O	2:E:699:LEU:HG	2.16	0.45
1:B:285:PHE:CZ	2:F:616:LYS:HE2	2.52	0.45
2:F:843:ILE:HD12	2:F:844:LYS:N	2.31	0.45
2:F:695:VAL:O	2:F:699:LEU:HG	2.16	0.45
1:B:387:PRO:O	2:F:579:TRP:HB2	2.17	0.45
2:F:604:ASP:O	2:F:608:ARG:HG3	2.17	0.45
1:B:182:GLU:O	1:B:186:GLN:HG2	2.17	0.45
1:A:261:THR:HG22	2:E:659:GLU:HG2	1.99	0.45
1:A:183:GLN:O	1:A:187:ILE:HD12	2.16	0.45
2:F:577:ASN:O	2:F:578:ARG:HG3	2.17	0.45
2:E:843:ILE:HD12	2:E:844:LYS:N	2.31	0.45
1:A:17:TYR:CB	1:A:220:VAL:HG13	2.48	0.44
1:B:137:LEU:HG	1:B:159:PHE:HB3	1.99	0.44
1:A:182:GLU:O	1:A:186:GLN:HG2	2.17	0.44
1:B:22:TYR:O	1:B:45:PRO:HD2	2.17	0.44
1:B:345:ILE:HG12	1:B:379:TYR:CZ	2.52	0.44
1:A:137:LEU:HG	1:A:159:PHE:HB3	2.00	0.44
1:A:265:ILE:HB	1:A:315:ILE:HG13	1.99	0.44
1:B:265:ILE:HB	1:B:315:ILE:HG13	1.99	0.44
2:E:844:LYS:HD3	2:E:844:LYS:O	2.18	0.44
2:F:827:ILE:HD11	2:F:840:LEU:HB3	2.00	0.44
2:F:823:LEU:HD22	2:F:840:LEU:HD22	1.99	0.44
2:F:823:LEU:O	2:F:827:ILE:HG13	2.17	0.44
2:F:844:LYS:HD3	2:F:844:LYS:O	2.18	0.44
2:E:604:ASP:O	2:E:608:ARG:HG3	2.17	0.44
2:E:730:SER:HB3	2:E:733:TYR:CB	2.41	0.44
2:E:775:LEU:HD11	2:E:784:LEU:HD23	1.99	0.44
1:B:21:VAL:HG21	1:B:54:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:823:LEU:HA	2:F:826:ILE:HG22	2.00	0.43
1:A:21:VAL:HG21	1:A:54:MET:HG3	2.00	0.43
1:B:17:TYR:CB	1:B:220:VAL:HG13	2.48	0.43
1:A:341:LYS:HD2	1:A:341:LYS:N	2.14	0.43
2:E:823:LEU:HA	2:E:826:ILE:HG22	2.00	0.43
2:E:612:SER:O	2:E:616:LYS:HG3	2.19	0.43
2:E:827:ILE:HD11	2:E:840:LEU:HB3	2.00	0.43
1:A:237:PHE:HA	1:A:384:GLU:O	2.18	0.43
1:A:169:LEU:HD12	1:A:169:LEU:N	2.34	0.43
1:A:22:TYR:O	1:A:45:PRO:HD2	2.18	0.43
2:E:823:LEU:O	2:E:827:ILE:HG13	2.18	0.43
1:B:237:PHE:HA	1:B:384:GLU:O	2.18	0.43
1:A:345:ILE:HG12	1:A:379:TYR:CZ	2.52	0.42
1:B:137:LEU:H	1:B:137:LEU:HD23	1.84	0.42
2:F:612:SER:O	2:F:616:LYS:HG3	2.19	0.42
1:A:137:LEU:H	1:A:137:LEU:HD23	1.84	0.42
1:B:327:GLN:CG	1:B:329:VAL:HG23	2.48	0.42
2:E:823:LEU:HD22	2:E:840:LEU:HD22	2.01	0.42
2:F:580:VAL:HA	2:F:581:PRO:HD3	1.88	0.42
1:A:125:ILE:N	1:A:125:ILE:HD12	2.34	0.42
2:F:637:VAL:HG23	2:F:638:TRP:CD2	2.55	0.41
2:E:826:ILE:O	2:E:830:ALA:HB3	2.20	0.41
1:A:192:PRO:HA	1:A:193:PRO:HD2	1.89	0.41
1:A:200:LEU:N	1:A:200:LEU:HD12	2.35	0.41
1:B:169:LEU:HD12	1:B:169:LEU:N	2.36	0.41
1:A:110:VAL:HG12	1:A:121:VAL:HG21	2.02	0.41
1:B:337:LEU:HD12	1:B:337:LEU:HA	1.96	0.41
1:B:192:PRO:HA	1:B:193:PRO:HD2	1.88	0.41
1:A:100:ARG:HB3	1:A:125:ILE:HG21	2.01	0.41
1:B:125:ILE:HD12	1:B:125:ILE:N	2.35	0.41
1:A:98:PRO:HG3	1:A:175:MET:HG3	2.03	0.41
1:A:327:GLN:CG	1:A:329:VAL:HG23	2.47	0.41
1:B:73:THR:HA	1:B:76:PHE:CE2	2.55	0.41
1:A:73:THR:HA	1:A:76:PHE:CE2	2.56	0.41
1:B:98:PRO:HG3	1:B:175:MET:HG3	2.03	0.41
2:E:637:VAL:HG23	2:E:638:TRP:CD2	2.55	0.41
2:E:768:PHE:O	2:E:772:MET:HG3	2.20	0.41
2:E:678:ASN:HA	2:E:679:PRO:HD3	1.92	0.41
1:B:200:LEU:HD12	1:B:200:LEU:N	2.36	0.41
1:B:100:ARG:HB3	1:B:125:ILE:HG21	2.01	0.40
1:A:147:PRO:HB2	1:A:180:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:GLU:HB2	1:A:246:TYR:CE1	2.56	0.40
2:F:653:PHE:CD1	2:F:702:ARG:HG3	2.56	0.40
1:A:38:PHE:C	1:A:40:TYR:H	2.25	0.40
1:B:110:VAL:HG12	1:B:121:VAL:HG21	2.02	0.40
1:B:38:PHE:C	1:B:40:TYR:H	2.25	0.40
2:F:768:PHE:O	2:F:772:MET:HG3	2.21	0.40
1:B:234:ILE:HD12	1:B:234:ILE:O	2.21	0.40
1:B:147:PRO:HB2	1:B:180:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

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	360/395 (91%)	342 (95%)	17 (5%)	1 (0%)	46	79
1	B	360/395 (91%)	342 (95%)	17 (5%)	1 (0%)	46	79
2	E	230/284 (81%)	215 (94%)	14 (6%)	1 (0%)	39	74
2	F	227/284 (80%)	217 (96%)	10 (4%)	0	100	100
All	All	1177/1358 (87%)	1116 (95%)	58 (5%)	3 (0%)	46	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	581	PRO
1	A	327	GLN
1	B	327	GLN

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	322/348 (92%)	317 (98%)	5 (2%)	70	93
1	B	322/348 (92%)	318 (99%)	4 (1%)	78	95
2	E	203/253 (80%)	202 (100%)	1 (0%)	92	98
2	F	200/253 (79%)	198 (99%)	2 (1%)	82	96
All	All	1047/1202 (87%)	1035 (99%)	12 (1%)	80	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	157	ARG
1	A	320	LEU
1	A	345	ILE
1	A	393	LEU
1	B	37	VAL
1	B	157	ARG
1	B	320	LEU
1	B	345	ILE
2	E	598	THR
2	F	598	THR
2	F	794	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	153	ASN
1	A	362	ASN
1	B	50	GLN
1	B	153	ASN
1	B	362	ASN
2	E	651	GLN

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Mol	Chain	Res	Type
2	F	651	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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$
3	AMP	A	1178	-	20,25,25	1.01	1 (5%)	22,38,38	1.93	3 (13%)
3	AMP	B	1178	-	20,25,25	1.02	1 (5%)	22,38,38	1.96	3 (13%)

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
3	AMP	A	1178	-	-	0/6/26/26	0/3/3/3
3	AMP	B	1178	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1178	AMP	C5-C4	3.07	1.47	1.40
3	B	1178	AMP	C5-C4	3.12	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1178	AMP	N3-C2-N1	-6.69	123.77	128.89
3	B	1178	AMP	N3-C2-N1	-6.67	123.79	128.89
3	B	1178	AMP	C4-C5-N7	-3.44	106.32	109.48
3	A	1178	AMP	C4-C5-N7	-3.17	106.56	109.48
3	B	1178	AMP	C2'-C1'-N9	-2.78	110.04	114.29
3	A	1178	AMP	C2'-C1'-N9	-2.32	110.75	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1178	AMP	1	0
3	B	1178	AMP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	366/395 (92%)	0.09	13 (3%)	46 34	39, 72, 133, 197	0
1	B	366/395 (92%)	0.10	16 (4%)	38 26	40, 73, 133, 197	0
2	E	240/284 (84%)	0.15	13 (5%)	29 19	52, 83, 130, 155	0
2	F	237/284 (83%)	0.19	13 (5%)	29 18	56, 87, 130, 155	0
All	All	1209/1358 (89%)	0.12	55 (4%)	37 26	39, 78, 132, 197	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	ARG	7.1
1	B	322	ARG	6.9
1	A	382	GLN	4.6
2	F	733	TYR	4.5
2	F	600	LEU	4.2
1	A	138	ARG	4.0
1	B	389	ASP	4.0
2	E	598	THR	3.9
2	E	733	TYR	3.9
2	F	850	LYS	3.7
2	F	731	GLU	3.6
1	A	18	ASP	3.5
1	A	320	LEU	3.4
2	F	580	VAL	3.4
1	A	15	THR	3.3
2	E	577	ASN	3.2
1	B	323	GLY	3.1
1	B	343	ASN	3.1
1	B	229	LEU	3.1
1	A	321	ALA	3.0
1	B	321	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	138	ARG	2.8
1	A	377	LYS	2.8
1	B	392	THR	2.7
2	E	731	GLU	2.7
2	F	730	SER	2.6
2	E	734	TYR	2.6
2	F	716	PRO	2.6
1	B	18	ASP	2.6
1	B	158	ARG	2.5
1	B	115	PHE	2.5
2	F	812	GLY	2.5
1	A	319	LEU	2.4
1	B	13	ILE	2.4
2	F	851	ASN	2.4
1	A	374	GLU	2.4
1	B	388	SER	2.4
2	F	801	ASP	2.4
1	A	13	ILE	2.4
2	E	600	LEU	2.4
2	E	599	GLU	2.3
1	B	379	TYR	2.3
1	B	15	THR	2.3
2	E	729	MET	2.3
2	F	732	GLU	2.2
1	A	393	LEU	2.2
1	A	371	ALA	2.2
2	E	716	PRO	2.1
2	E	579	TRP	2.1
2	F	579	TRP	2.1
2	E	730	SER	2.1
1	B	382	GLN	2.0
2	E	578	ARG	2.0
2	E	689	LYS	2.0
2	F	849	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	AMP	B	1178	23/23	0.91	0.19	0.06	38,93,114,123	0
3	AMP	A	1178	23/23	0.94	0.18	-0.10	49,74,86,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.