Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:29 PM GMT

PDB ID	:	5AFQ
Title	:	Crystal structure of RPC62 - RPC32 beta
Authors	:	Fribourg, S.
Deposited on	:	2015-01-23
Resolution	:	7.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

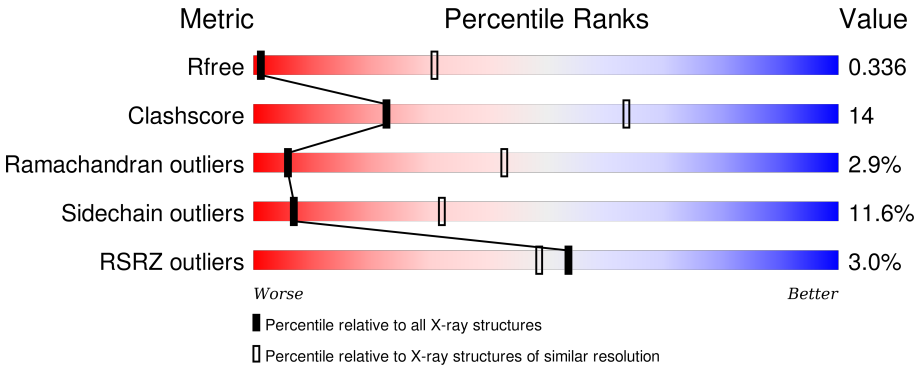
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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 <=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	534	% 48% 31% 17%
1	B	534	4% 49% 30% 17%
2	D	218	22% 76%
2	E	218	9% 91%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7387 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 DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3511	2207	611	670	23			
1	B	444	Total	C	N	O	S	0	0	0
			3516	2210	612	671	23			

- Molecule 2 is a protein called RPC32 BETA (RPC7L).

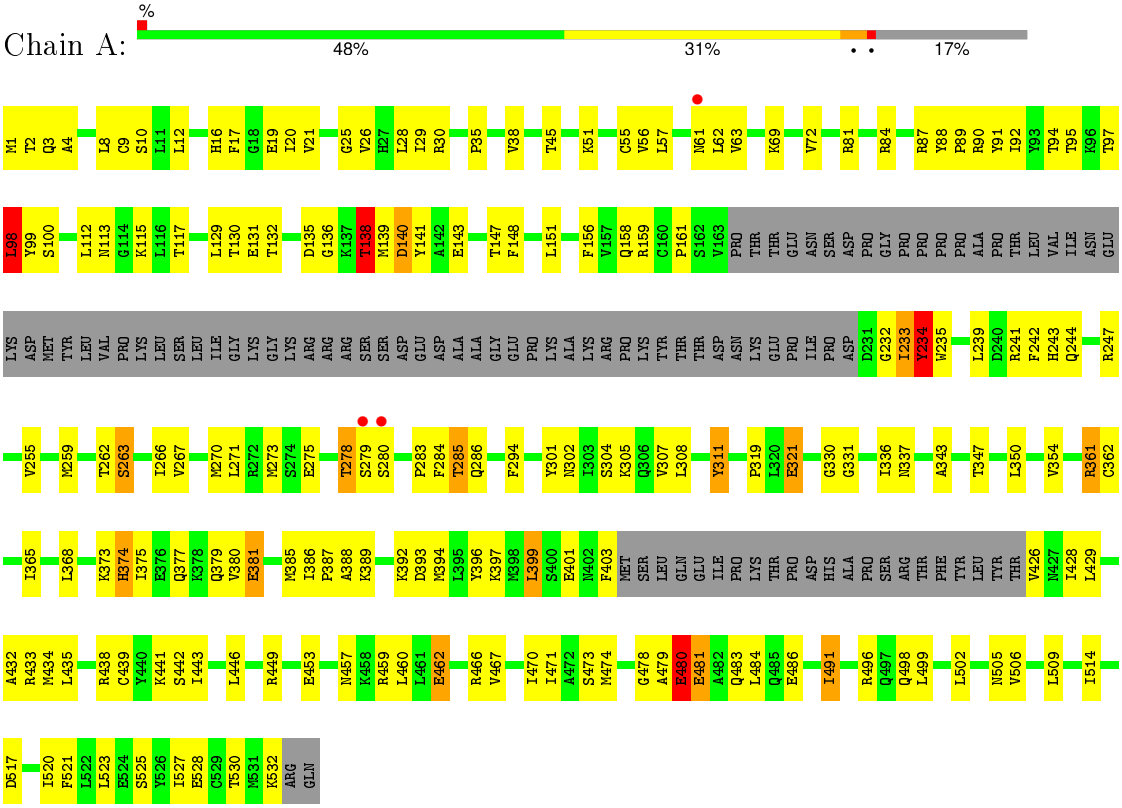
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	53	Total	C	N	O	0	0	0
			265	159	53	53			
2	E	19	Total	C	N	O	0	0	0
			95	57	19	19			

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 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.

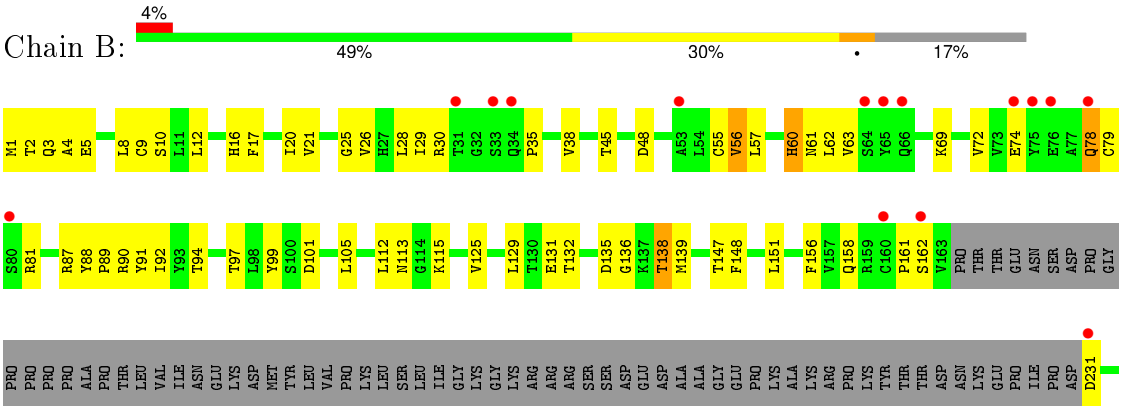
- Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3

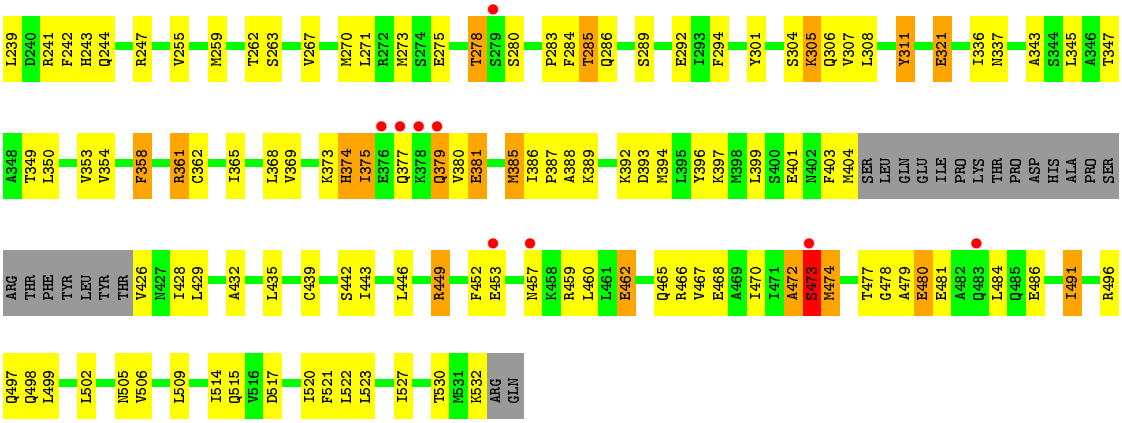
Chain A:



- Molecule 1: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3

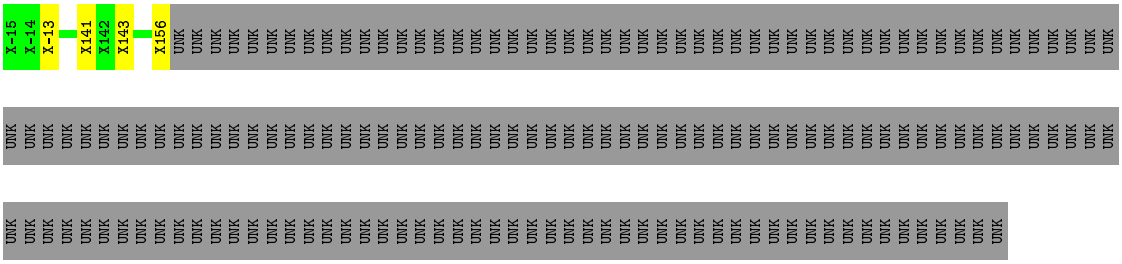
Chain B:





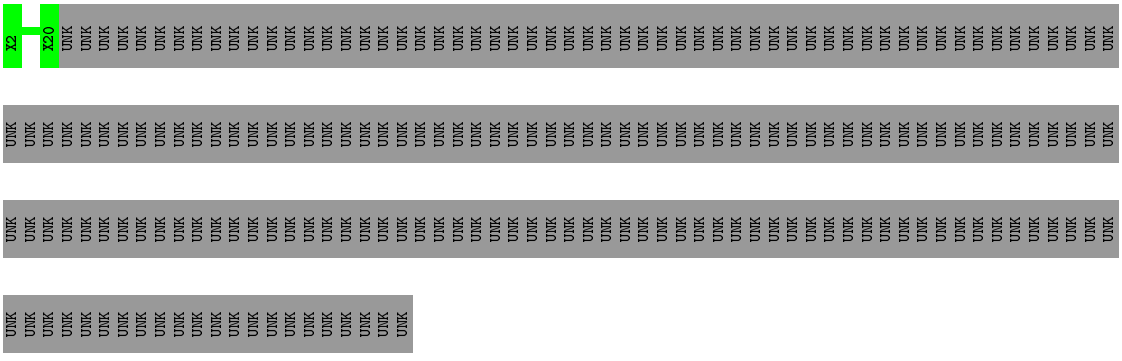
- Molecule 2: RPC32 BETA (RPC7L)

Chain D:



- Molecule 2: RPC32 BETA (RPC7L)

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	218.27Å 218.27Å 182.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.75 – 7.00 30.27 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.75-7.00) 99.3 (30.27-7.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 7.24Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.268 , 0.298 0.277 , 0.336	Depositor DCC
R_{free} test set	334 reflections (9.45%)	DCC
Wilson B-factor (Å^2)	452.8	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 393.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Outliers	0 of 3612 reflections	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	7387	wwPDB-VP
Average B, all atoms (Å^2)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.41	0/3558	0.72	2/4798 (0.0%)
1	B	0.40	0/3563	0.73	3/4805 (0.1%)
All	All	0.41	0/7121	0.73	5/9603 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	472	ALA	C-N-CA	8.45	142.81	121.70
1	A	98	LEU	CA-CB-CG	7.75	133.13	115.30
1	B	374	HIS	C-N-CA	6.76	138.60	121.70
1	B	472	ALA	CA-C-N	5.78	129.92	117.20
1	A	233	ILE	C-N-CA	5.13	134.53	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	78	GLN	Sidechain

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	3511	0	3550	100	0
1	B	3516	0	3552	98	0
2	D	265	0	60	4	0
2	E	95	0	21	0	0
All	All	7387	0	7183	198	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 14.

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:A:435:LEU:HA	1:A:438:ARG:HD2	1.44	1.00
1:A:453:GLU:HB3	1:A:502:LEU:HD11	1.54	0.88
1:B:465:GLN:O	1:B:468:GLU:HG2	1.73	0.87
1:B:404:MET:HA	1:B:426:VAL:HA	1.56	0.86
1:B:474:MET:SD	1:B:480:GLU:HG2	2.18	0.83
1:A:278:THR:HG21	1:A:285:THR:HA	1.65	0.79
1:B:278:THR:HG21	1:B:285:THR:HA	1.64	0.78
1:B:401:GLU:HB2	1:B:403:PHE:HE1	1.56	0.70
1:B:247:ARG:HH11	1:B:280:SER:HA	1.59	0.68
1:B:270:MET:HB3	1:B:336:ILE:HD11	1.74	0.68
1:B:374:HIS:HA	1:B:375:ILE:O	1.93	0.67
1:A:247:ARG:HH11	1:A:280:SER:HA	1.59	0.67
1:A:401:GLU:HB2	1:A:403:PHE:HE1	1.60	0.67
1:A:270:MET:HB3	1:A:336:ILE:HD11	1.75	0.67
1:A:381:GLU:HG3	1:A:388:ALA:HA	1.76	0.66
1:B:472:ALA:HB3	1:B:473:SER:HB2	1.77	0.65
1:B:381:GLU:HG3	1:B:388:ALA:HA	1.77	0.65
1:A:304:SER:HB3	1:A:307:VAL:HG23	1.79	0.65
1:B:374:HIS:CE1	1:B:379:GLN:HG3	2.32	0.65
1:B:255:VAL:HG21	1:B:267:VAL:HG21	1.80	0.63
1:B:347:THR:HA	1:B:350:LEU:HD12	1.79	0.63
1:A:453:GLU:HB3	1:A:502:LEU:CD1	2.25	0.63
1:A:255:VAL:HG21	1:A:267:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LEU:HA	1:B:242:PHE:HD2	1.64	0.62
1:A:239:LEU:HA	1:A:242:PHE:HD2	1.64	0.61
1:A:347:THR:HA	1:A:350:LEU:HD12	1.83	0.61
1:B:284:PHE:HD1	1:B:337:ASN:HA	1.66	0.60
1:A:284:PHE:HD1	1:A:337:ASN:HA	1.67	0.60
1:A:159:ARG:HH21	1:A:235:TRP:HZ2	1.51	0.58
1:B:354:VAL:HG13	1:B:358:PHE:HD2	1.68	0.58
1:A:361:ARG:HH12	1:A:386:ILE:HG21	1.69	0.58
1:B:304:SER:HB2	1:B:307:VAL:HG23	1.86	0.57
1:A:443:ILE:HD11	1:A:520:ILE:HD11	1.86	0.57
1:B:361:ARG:HH12	1:B:386:ILE:HG21	1.70	0.57
1:B:9:CYS:HA	1:B:12:LEU:HD12	1.87	0.57
1:A:496:ARG:HA	1:A:499:LEU:HD12	1.86	0.57
1:B:294:PHE:HB2	1:B:308:LEU:HD22	1.87	0.56
1:A:294:PHE:HB2	1:A:308:LEU:HD22	1.87	0.56
1:B:449:ARG:HH21	1:B:452:PHE:HD2	1.52	0.56
1:B:443:ILE:HD11	1:B:520:ILE:HD11	1.88	0.56
1:A:435:LEU:HD23	1:A:523:LEU:HD21	1.88	0.56
1:B:239:LEU:HA	1:B:242:PHE:CD2	2.41	0.56
1:A:9:CYS:HA	1:A:12:LEU:HD12	1.86	0.56
1:B:466:ARG:O	1:B:470:ILE:HG12	2.06	0.56
1:B:62:LEU:HD23	1:B:81:ARG:HG3	1.88	0.56
1:A:239:LEU:HA	1:A:242:PHE:CD2	2.41	0.55
1:A:62:LEU:HD23	1:A:81:ARG:HG3	1.88	0.55
1:B:474:MET:HE2	1:B:474:MET:HA	1.89	0.55
1:A:474:MET:HG2	1:A:478:GLY:O	2.08	0.54
1:B:435:LEU:HD23	1:B:523:LEU:HD21	1.89	0.54
1:A:466:ARG:O	1:A:470:ILE:HG12	2.08	0.54
1:B:374:HIS:CE1	1:B:379:GLN:CG	2.91	0.53
1:B:374:HIS:HE1	1:B:379:GLN:HG3	1.72	0.53
1:A:365:ILE:HA	1:A:368:LEU:HD12	1.91	0.53
1:B:9:CYS:O	1:B:12:LEU:HB2	2.09	0.52
1:A:362:CYS:HA	1:A:365:ILE:HG12	1.91	0.52
1:A:374:HIS:CD2	1:A:399:LEU:HG	2.44	0.52
1:A:89:PRO:HA	1:A:92:ILE:HD12	1.92	0.52
1:A:394:MET:HA	1:A:397:LYS:HD2	1.92	0.52
1:A:377:GLN:HA	1:A:380:VAL:HB	1.92	0.51
1:A:9:CYS:O	1:A:12:LEU:HB2	2.11	0.51
1:B:365:ILE:HA	1:B:368:LEU:HD12	1.92	0.51
1:A:467:VAL:HG11	1:A:491:ILE:HD11	1.93	0.50
1:B:496:ARG:HA	1:B:499:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HB2	1:B:403:PHE:CE1	2.44	0.50
1:B:474:MET:HA	1:B:474:MET:CE	2.42	0.50
1:B:17:PHE:HD2	1:B:21:VAL:HG11	1.77	0.50
1:B:377:GLN:HA	1:B:380:VAL:HB	1.94	0.49
1:B:25:GLY:HA2	1:B:28:LEU:HD12	1.94	0.49
1:B:350:LEU:O	1:B:354:VAL:HG23	2.13	0.49
1:B:439:CYS:O	1:B:443:ILE:HG13	2.11	0.49
1:B:89:PRO:HA	1:B:92:ILE:HD12	1.94	0.49
1:A:233:ILE:HG13	1:A:234:TYR:H	1.77	0.49
1:B:35:PRO:HG2	1:B:38:VAL:HG23	1.93	0.49
1:B:289:SER:OG	1:B:292:GLU:HG2	2.13	0.49
1:A:17:PHE:HD2	1:A:21:VAL:HG11	1.77	0.49
1:A:343:ALA:O	1:A:347:THR:HG23	2.13	0.48
1:A:471:ILE:HA	1:A:474:MET:HB3	1.95	0.48
1:A:26:VAL:HA	1:A:29:ILE:HD12	1.94	0.48
1:A:271:LEU:O	1:A:275:GLU:HG3	2.13	0.48
1:B:271:LEU:O	1:B:275:GLU:HG3	2.13	0.48
1:B:343:ALA:O	1:B:347:THR:HG23	2.14	0.48
1:B:467:VAL:HG11	1:B:491:ILE:HD11	1.96	0.48
1:A:283:PRO:HB3	1:A:532:LYS:HD3	1.95	0.48
1:B:283:PRO:HB3	1:B:532:LYS:HD3	1.96	0.48
1:A:523:LEU:O	1:A:527:ILE:HG12	2.14	0.48
1:B:523:LEU:O	1:B:527:ILE:HG12	2.14	0.48
1:B:28:LEU:HD13	1:B:63:VAL:HG21	1.96	0.47
1:A:61:ASN:OD1	1:A:115:LYS:HG3	2.13	0.47
1:A:25:GLY:HA2	1:A:28:LEU:HD12	1.96	0.47
1:A:35:PRO:HG2	1:A:38:VAL:HG23	1.96	0.47
1:B:87:ARG:NH2	1:B:521:PHE:HA	2.29	0.47
1:B:394:MET:HA	1:B:397:LYS:HD2	1.96	0.47
1:B:61:ASN:OD1	1:B:115:LYS:HG3	2.15	0.47
1:B:88:TYR:HA	1:B:91:TYR:HD2	1.80	0.47
1:A:136:GLY:C	1:A:138:THR:H	2.17	0.47
1:B:505:ASN:O	1:B:509:LEU:HG	2.15	0.47
1:B:136:GLY:C	1:B:138:THR:H	2.17	0.47
1:A:129:LEU:HD23	1:A:139:MET:HG2	1.96	0.47
1:A:87:ARG:NH2	1:A:521:PHE:HA	2.29	0.47
1:A:88:TYR:HA	1:A:91:TYR:HD2	1.80	0.47
1:B:362:CYS:HA	1:B:365:ILE:HG12	1.96	0.46
1:A:262:THR:HB	1:A:311:TYR:OH	2.16	0.46
1:B:26:VAL:HA	1:B:29:ILE:HD12	1.97	0.46
1:A:305:LYS:O	1:A:308:LEU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:HA	1:B:396:TYR:CD2	2.51	0.46
1:A:481:GLU:HA	1:A:484:LEU:HD12	1.98	0.46
2:D:141:UNK:C	2:D:143:UNK:N	2.78	0.46
1:A:350:LEU:O	1:A:354:VAL:HG23	2.15	0.46
1:A:439:CYS:O	1:A:443:ILE:HG13	2.15	0.45
1:A:28:LEU:HD13	1:A:63:VAL:HG21	1.98	0.45
1:B:5:GLU:HG2	1:B:79:CYS:SG	2.56	0.45
1:A:141:TYR:CD1	2:D:156:UNK:HA	2.51	0.45
1:A:478:GLY:C	1:A:480:GLU:H	2.20	0.45
1:B:442:SER:O	1:B:446:LEU:HG	2.15	0.45
1:A:374:HIS:H	1:A:426:VAL:N	2.15	0.45
1:A:393:ASP:HA	1:A:396:TYR:CD2	2.52	0.45
1:A:284:PHE:CD1	1:A:337:ASN:HA	2.49	0.45
1:A:247:ARG:NH1	1:A:280:SER:HA	2.30	0.45
1:B:1:MET:N	1:B:2:THR:HA	2.32	0.45
1:A:99:TYR:HB3	1:A:147:THR:HG23	1.98	0.45
1:B:131:GLU:HG3	1:B:132:THR:HG23	1.99	0.45
1:B:99:TYR:HB3	1:B:147:THR:HG23	1.99	0.45
1:A:1:MET:N	1:A:2:THR:HA	2.32	0.44
1:B:506:VAL:HA	1:B:509:LEU:HD12	1.98	0.44
1:A:449:ARG:O	1:A:453:GLU:HG2	2.18	0.44
1:B:305:LYS:O	1:B:308:LEU:HB3	2.17	0.44
1:A:429:LEU:O	1:A:432:ALA:HB3	2.17	0.44
1:A:514:ILE:O	1:A:517:ASP:HB3	2.18	0.44
1:A:26:VAL:O	1:A:30:ARG:HG3	2.16	0.44
1:A:95:THR:O	1:A:98:LEU:HD12	2.17	0.44
1:A:442:SER:O	1:A:446:LEU:HG	2.18	0.44
1:B:453:GLU:O	1:B:457:ASN:HB2	2.17	0.44
1:B:374:HIS:HA	1:B:375:ILE:C	2.37	0.44
1:B:497:GLN:OE1	1:B:497:GLN:HA	2.18	0.43
1:A:386:ILE:HB	1:A:387:PRO:HD2	2.00	0.43
1:B:26:VAL:O	1:B:30:ARG:HG3	2.18	0.43
1:A:401:GLU:HB2	1:A:403:PHE:CE1	2.47	0.43
1:A:35:PRO:HB3	1:A:72:VAL:HG12	2.00	0.43
1:A:161:PRO:HB3	2:D:143:UNK:CB	2.47	0.43
1:B:241:ARG:HH11	1:B:244:GLN:HB2	1.83	0.43
1:A:51:LYS:HD3	2:D:-13:UNK:CB	2.47	0.43
1:B:56:VAL:O	1:B:60:HIS:HB2	2.18	0.43
1:B:262:THR:HB	1:B:311:TYR:OH	2.17	0.43
1:B:478:GLY:C	1:B:480:GLU:H	2.22	0.43
1:B:35:PRO:HB3	1:B:72:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HB	1:A:232:GLY:HA2	2.00	0.43
1:A:84:ARG:HA	1:A:84:ARG:NE	2.34	0.43
1:A:4:ALA:O	1:A:8:LEU:HB2	2.19	0.43
1:A:505:ASN:O	1:A:509:LEU:HG	2.19	0.43
1:B:57:LEU:HD13	1:B:63:VAL:HG21	2.01	0.42
1:B:94:THR:O	1:B:97:THR:HB	2.18	0.42
1:B:284:PHE:CD1	1:B:337:ASN:HA	2.49	0.42
1:A:95:THR:HA	1:A:98:LEU:HD12	2.02	0.42
1:A:506:VAL:HA	1:A:509:LEU:HD12	2.01	0.42
1:B:247:ARG:NH1	1:B:280:SER:HA	2.29	0.42
1:B:514:ILE:O	1:B:517:ASP:HB3	2.19	0.42
1:B:358:PHE:HB2	1:B:362:CYS:HB3	2.00	0.42
1:A:481:GLU:HG3	1:A:481:GLU:H	1.53	0.42
1:A:131:GLU:HG3	1:A:132:THR:HG23	2.01	0.42
1:A:94:THR:O	1:A:97:THR:HB	2.20	0.42
1:A:241:ARG:HH11	1:A:244:GLN:HB2	1.84	0.42
1:B:386:ILE:HB	1:B:387:PRO:HD2	2.02	0.42
1:B:8:LEU:HD11	1:B:443:ILE:HB	2.02	0.42
1:B:156:PHE:CZ	1:B:241:ARG:HG3	2.55	0.42
1:A:263:SER:HA	1:A:266:ILE:HD12	2.01	0.42
1:B:365:ILE:O	1:B:369:VAL:HG23	2.19	0.41
1:A:480:GLU:HB3	1:A:483:GLN:HB2	2.02	0.41
1:A:285:THR:HB	1:A:286:GLN:H	1.70	0.41
1:B:4:ALA:O	1:B:8:LEU:HB2	2.20	0.41
1:B:35:PRO:HA	1:B:74:GLU:HA	2.03	0.41
1:A:98:LEU:HD13	1:A:99:TYR:CG	2.54	0.41
1:A:4:ALA:HB2	1:A:441:LYS:HD3	2.01	0.41
1:B:349:THR:O	1:B:353:VAL:HG23	2.20	0.41
1:B:294:PHE:HB2	1:B:308:LEU:CD2	2.51	0.41
1:A:140:ASP:OD1	1:A:143:GLU:HB2	2.21	0.41
1:B:389:LYS:HD2	1:B:392:LYS:NZ	2.36	0.41
1:A:294:PHE:HB2	1:A:308:LEU:CD2	2.50	0.41
1:A:57:LEU:HD13	1:A:63:VAL:HG21	2.03	0.41
1:B:129:LEU:HD23	1:B:139:MET:HG2	2.01	0.41
1:B:429:LEU:O	1:B:432:ALA:HB3	2.20	0.41
1:A:156:PHE:CZ	1:A:241:ARG:HG3	2.56	0.41
1:A:148:PHE:O	1:A:151:LEU:HB2	2.19	0.41
1:A:330:GLY:HA2	1:A:331:GLY:HA2	1.79	0.41
1:B:8:LEU:HD21	1:B:443:ILE:HD12	2.03	0.41
1:A:319:PRO:HB3	1:B:385:MET:O	2.21	0.41
1:B:148:PHE:O	1:B:151:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:SER:HA	1:A:528:GLU:HG2	2.03	0.41
1:B:345:LEU:HB3	1:B:522:LEU:HD11	2.03	0.41
1:B:481:GLU:HA	1:B:484:LEU:HD12	2.01	0.41
1:A:389:LYS:HD2	1:A:392:LYS:NZ	2.36	0.41
1:A:434:MET:O	1:A:438:ARG:HG3	2.21	0.41
1:A:87:ARG:HB2	1:A:91:TYR:CE2	2.55	0.41
1:B:57:LEU:HB3	1:B:63:VAL:HB	2.03	0.40
1:B:462:GLU:O	1:B:466:ARG:HG2	2.22	0.40
1:B:105:LEU:HD23	1:B:125:VAL:HG13	2.04	0.40
1:A:453:GLU:O	1:A:457:ASN:HB2	2.20	0.40
1:A:462:GLU:O	1:A:466:ARG:HG2	2.21	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	437/534 (82%)	377 (86%)	46 (10%)	14 (3%)	5 41
1	B	438/534 (82%)	382 (87%)	45 (10%)	11 (2%)	7 46
All	All	875/1068 (82%)	759 (87%)	91 (10%)	25 (3%)	6 43

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	135	ASP
1	A	234	TYR
1	A	373	LYS
1	A	375	ILE
1	A	428	ILE
1	B	69	LYS

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Mol	Chain	Res	Type
1	B	135	ASP
1	B	375	ILE
1	B	428	ILE
1	A	374	HIS
1	A	460	LEU
1	A	479	ALA
1	B	460	LEU
1	B	473	SER
1	A	321	GLU
1	B	321	GLU
1	B	479	ALA
1	A	138	THR
1	A	285	THR
1	B	285	THR
1	A	480	GLU
1	B	161	PRO
1	A	100	SER
1	B	138	THR

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	389/476 (82%)	347 (89%)	42 (11%)	8 35
1	B	389/476 (82%)	341 (88%)	48 (12%)	6 30
All	All	778/952 (82%)	688 (88%)	90 (12%)	7 32

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	10	SER
1	A	16	HIS
1	A	19	GLU
1	A	20	ILE

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Mol	Chain	Res	Type
1	A	45	THR
1	A	55	CYS
1	A	56	VAL
1	A	90	ARG
1	A	98	LEU
1	A	112	LEU
1	A	113	ASN
1	A	130	THR
1	A	138	THR
1	A	140	ASP
1	A	158	GLN
1	A	234	TYR
1	A	243	HIS
1	A	259	MET
1	A	263	SER
1	A	273	MET
1	A	278	THR
1	A	279	SER
1	A	301	TYR
1	A	302	ASN
1	A	311	TYR
1	A	321	GLU
1	A	361	ARG
1	A	379	GLN
1	A	381	GLU
1	A	385	MET
1	A	399	LEU
1	A	433	ARG
1	A	459	ARG
1	A	462	GLU
1	A	473	SER
1	A	480	GLU
1	A	481	GLU
1	A	486	GLU
1	A	491	ILE
1	A	498	GLN
1	A	530	THR
1	B	3	GLN
1	B	10	SER
1	B	16	HIS
1	B	20	ILE
1	B	45	THR

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Mol	Chain	Res	Type
1	B	48	ASP
1	B	55	CYS
1	B	56	VAL
1	B	60	HIS
1	B	78	GLN
1	B	90	ARG
1	B	101	ASP
1	B	112	LEU
1	B	113	ASN
1	B	158	GLN
1	B	162	SER
1	B	231	ASP
1	B	243	HIS
1	B	259	MET
1	B	263	SER
1	B	273	MET
1	B	278	THR
1	B	286	GLN
1	B	301	TYR
1	B	305	LYS
1	B	306	GLN
1	B	311	TYR
1	B	321	GLU
1	B	358	PHE
1	B	361	ARG
1	B	373	LYS
1	B	379	GLN
1	B	381	GLU
1	B	385	MET
1	B	399	LEU
1	B	449	ARG
1	B	459	ARG
1	B	462	GLU
1	B	473	SER
1	B	474	MET
1	B	477	THR
1	B	480	GLU
1	B	486	GLU
1	B	491	ILE
1	B	498	GLN
1	B	502	LEU
1	B	515	GLN

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Mol	Chain	Res	Type
1	B	530	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	377	GLN
1	A	451	GLN
1	B	257	ASN
1	B	374	HIS
1	B	377	GLN
1	B	451	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	443/534 (82%)	-0.04	3 (0%) 89 85	300, 300, 300, 300	0
1	B	444/534 (83%)	0.24	24 (5%) 29 30	300, 300, 300, 300	0
2	D	0/218	-	-	-	-
2	E	0/218	-	-	-	-
All	All	887/1504 (58%)	0.10	27 (3%) 54 49	300, 300, 300, 300	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	GLU	5.5
1	B	65	TYR	5.0
1	B	377	GLN	4.6
1	B	66	GLN	4.6
1	B	33	SER	4.1
1	B	378	LYS	3.6
1	B	64	SER	3.3
1	B	76	GLU	3.2
1	B	473	SER	3.1
1	B	53	ALA	2.8
1	B	80	SER	2.7
1	B	457	ASN	2.6
1	B	279	SER	2.5
1	B	34	GLN	2.5
1	B	74	GLU	2.5
1	B	453	GLU	2.4
1	B	231	ASP	2.3
1	B	162	SER	2.3
1	A	61	ASN	2.2
1	B	160	CYS	2.2
1	B	75	TYR	2.2
1	B	483	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	SER	2.1
1	A	280	SER	2.1
1	B	78	GLN	2.0
1	B	31	THR	2.0
1	B	379	GLN	2.0

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

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.