Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2016 – 08:59 PM EDT

PDB ID	:	5EZV
Title	:	X-ray crystal structure of AMP-activated protein kinase alpha-2/alpha-1 RIM chimaera (alpha-2(1-347)/alpha-1(349-401)/alpha-2(397-end) beta-1 gamma-1) co-crystallized with C2 (5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid)
Authors	:	Langendorf, C.G.; Kemp, B.E.
Deposited on	:	2015-11-26
Resolution	:	2.99 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 ①) were used in the production of this report:

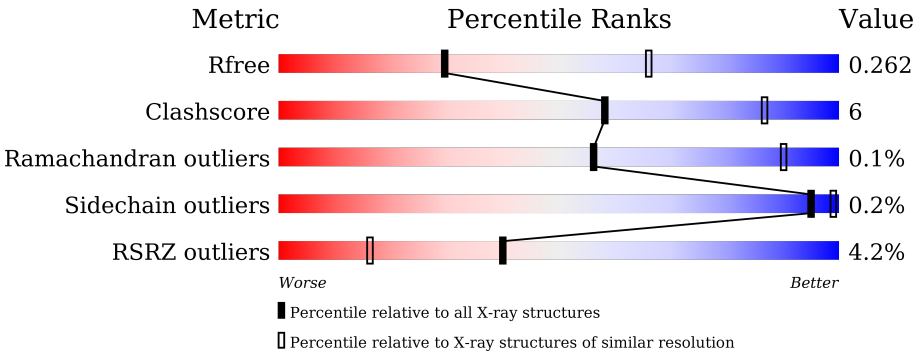
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	560	3% 72% 7% 21%
1	C	560	3% 71% 7% 21%
2	B	270	4% 56% 13% 31%
2	D	270	2% 60% 9% 31%
3	E	336	6% 82% 7% 10%
3	F	336	4% 76% 13% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	172	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14682 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 5'-AMP-activated protein kinase catalytic subunit alpha-2/alpha-1 RIM SWAP chimera.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	P	S	0	0	0
			3462	2214	589	634	1	24			
1	C	441	Total	C	N	O	P	S	0	0	0
			3419	2186	588	621	1	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P54646
A	-12	GLY	-	expression tag	UNP P54646
A	-11	SER	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	HIS	-	expression tag	UNP P54646
A	-8	HIS	-	expression tag	UNP P54646
A	-7	HIS	-	expression tag	UNP P54646
A	-6	HIS	-	expression tag	UNP P54646
A	-5	HIS	-	expression tag	UNP P54646
A	-4	HIS	-	expression tag	UNP P54646
A	-3	HIS	-	expression tag	UNP P54646
A	-2	SER	-	expression tag	UNP P54646
A	-1	GLN	-	expression tag	UNP P54646
A	0	ASP	-	expression tag	UNP P54646
A	1	PRO	-	expression tag	UNP P54646
C	-13	MET	-	initiating methionine	UNP P54646
C	-12	GLY	-	expression tag	UNP P54646
C	-11	SER	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	HIS	-	expression tag	UNP P54646
C	-8	HIS	-	expression tag	UNP P54646
C	-7	HIS	-	expression tag	UNP P54646
C	-6	HIS	-	expression tag	UNP P54646
C	-5	HIS	-	expression tag	UNP P54646

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P54646
C	-3	HIS	-	expression tag	UNP P54646
C	-2	SER	-	expression tag	UNP P54646
C	-1	GLN	-	expression tag	UNP P54646
C	0	ASP	-	expression tag	UNP P54646
C	1	PRO	-	expression tag	UNP P54646

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	185	Total	C	N	O	P	S	0	0	0
			1400	904	233	257	1	5			
2	D	186	Total	C	N	O	P	S	0	0	0
			1422	914	234	267	1	6			

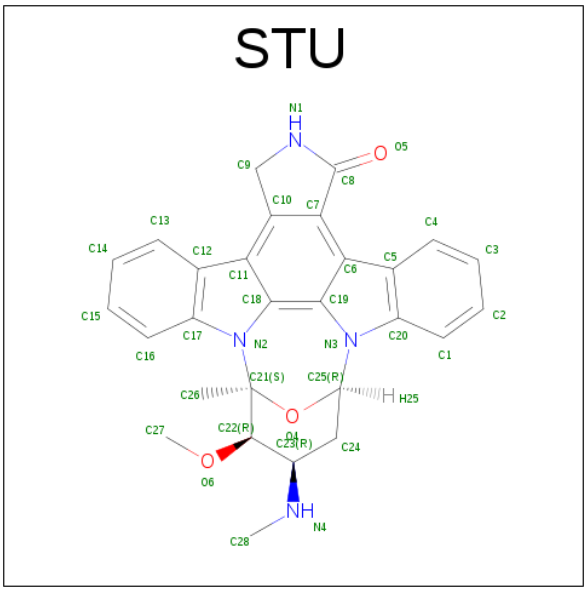
- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	302	Total	C	N	O	S	0	0	0
			2362	1538	391	426	7			
3	F	300	Total	C	N	O	S	0	1	0
			2351	1529	393	422	7			

There are 12 discrepancies between the modelled and reference sequences:

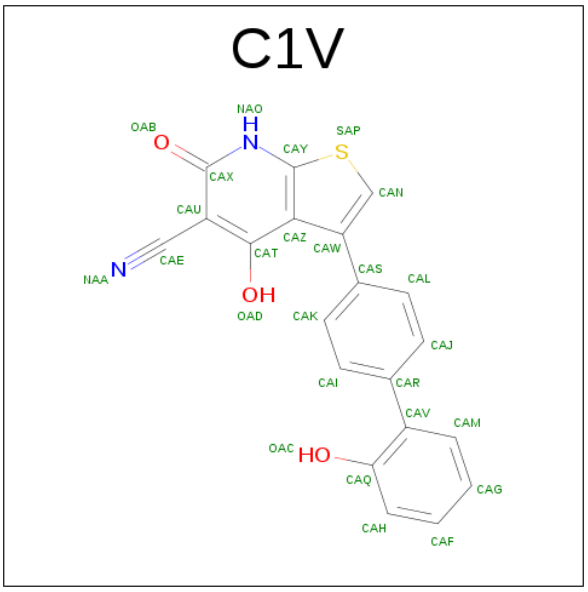
Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	MET	-	initiating methionine	UNP P54619
E	-3	ALA	-	expression tag	UNP P54619
E	-2	ASP	-	expression tag	UNP P54619
E	-1	LEU	-	expression tag	UNP P54619
E	0	ASN	-	expression tag	UNP P54619
E	1	TRP	-	expression tag	UNP P54619
F	-4	MET	-	initiating methionine	UNP P54619
F	-3	ALA	-	expression tag	UNP P54619
F	-2	ASP	-	expression tag	UNP P54619
F	-1	LEU	-	expression tag	UNP P54619
F	0	ASN	-	expression tag	UNP P54619
F	1	TRP	-	expression tag	UNP P54619

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	C	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 3-[4-(2-hydroxyphenyl)phenyl]-4-oxidanyl-6-oxidanylidene-7H-thieno[2,3-b]pyridine-5-carbonitrile (three-letter code: C1V) (formula: $C_{20}H_{12}N_2O_3S$).



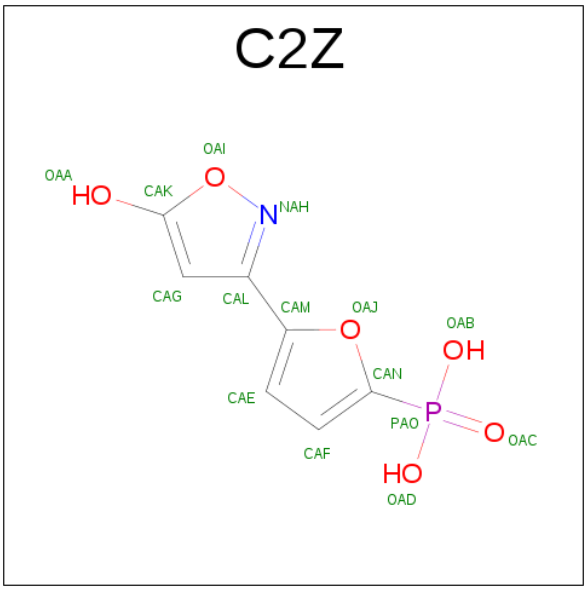
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O S 26 20 2 3 1	0	0

- Molecule 6 is 5-(5-hydroxyl-isoxazol-3-yl)-furan-2-phosphonic acid (three-letter code: C2Z) (formula: $C_7H_6NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O P 15 7 1 6 1	0	0
6	E	1	Total C N O P 15 7 1 6 1	0	0
6	F	1	Total C N O P 15 7 1 6 1	0	0
6	F	1	Total C N O P 15 7 1 6 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	32	Total O 32 32	0	0
7	B	8	Total O 8 8	0	0
7	C	25	Total O 25 25	0	0
7	D	7	Total O 7 7	0	0

Continued on next page...

Continued from previous page...

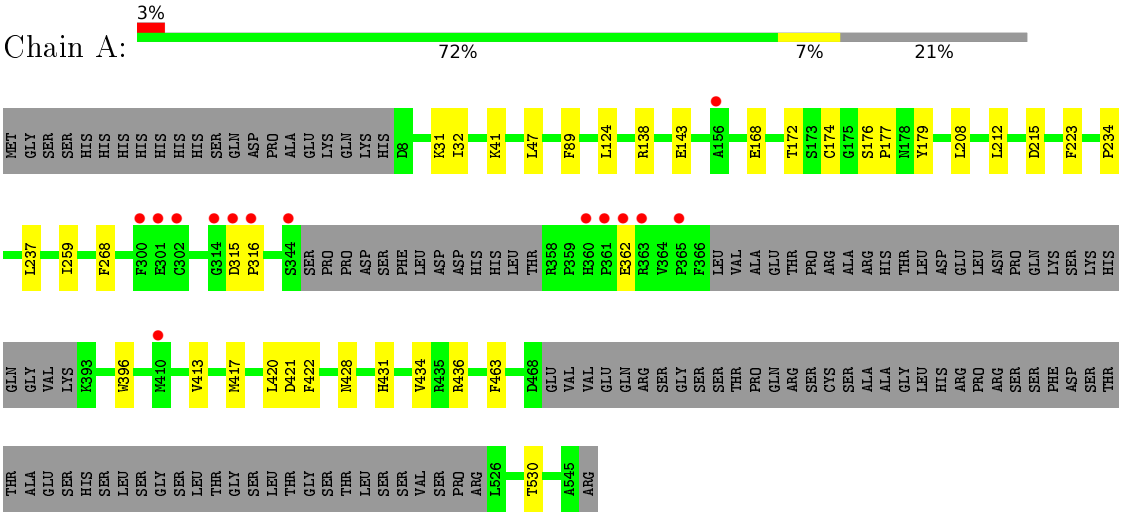
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	7	Total O 7 7	0	0
7	F	5	Total O 5 5	0	0

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.

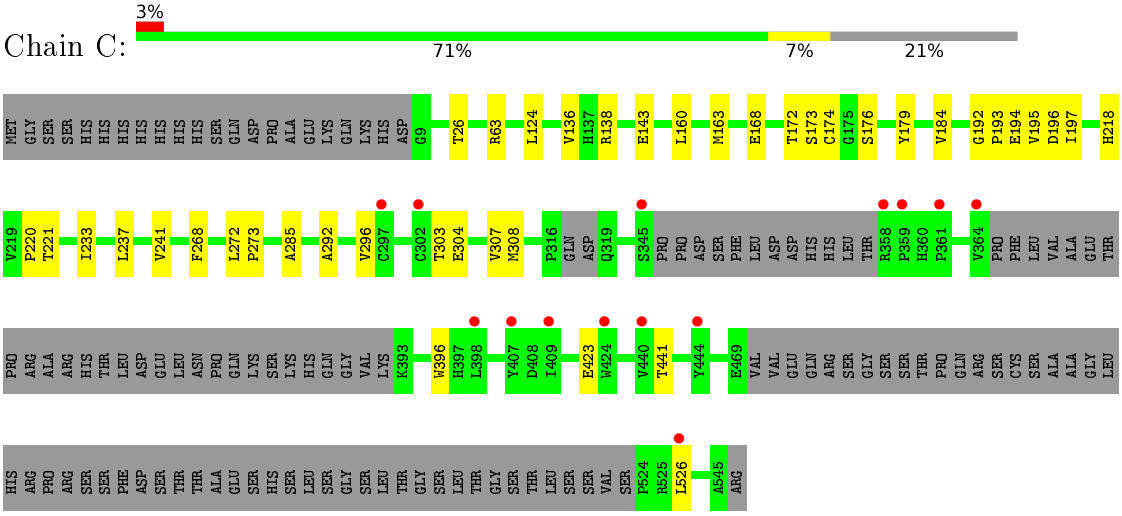
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2/alpha-1 RIM SWAP chimera

Chain A:



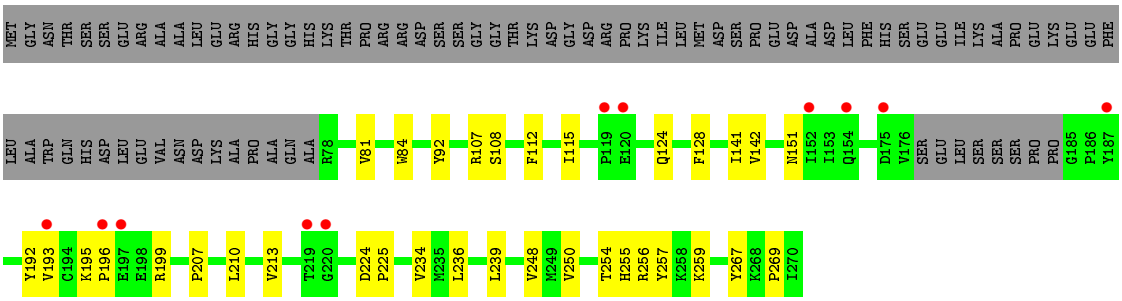
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-2/alpha-1 RIM SWAP chimera

Chain C:



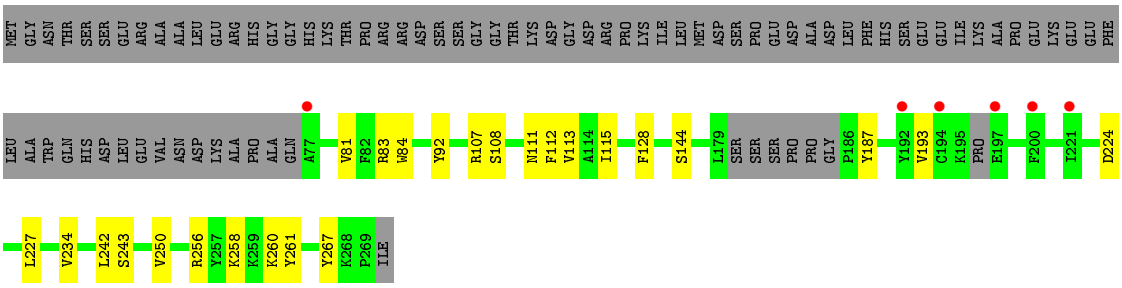
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

Chain B:



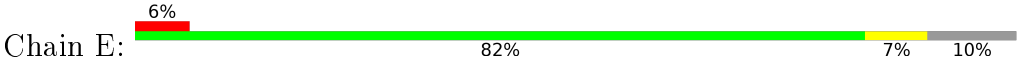
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1

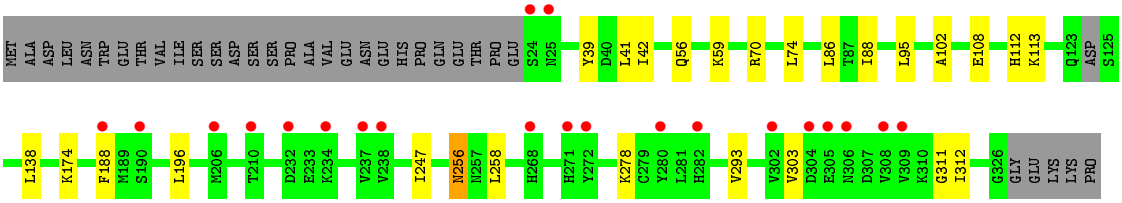
Chain D:



• Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

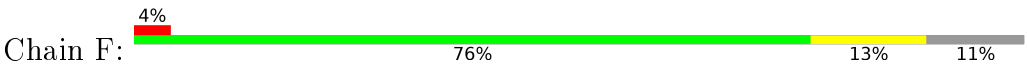
Chain E:

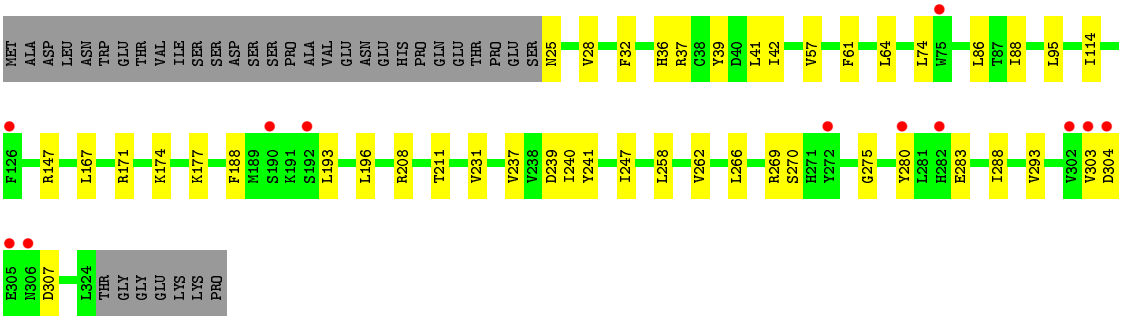




• Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.61Å 134.11Å 141.29Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	49.30 – 2.99 49.31 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.30-2.99) 99.3 (49.31-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.224 , 0.245 0.241 , 0.262	Depositor DCC
R_{free} test set	2867 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 56563 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14682	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, STU, C2Z, C1V, 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	0.38	0/3528	0.56	0/4778
1	C	0.38	0/3485	0.57	0/4724
2	B	0.38	0/1431	0.58	0/1964
2	D	0.38	0/1452	0.55	0/1989
3	E	0.38	0/2411	0.58	0/3281
3	F	0.38	0/2402	0.58	0/3269
All	All	0.38	0/14709	0.57	0/20005

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

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	3462	0	3311	33	0
1	C	3419	0	3255	42	1
2	B	1400	0	1308	29	0
2	D	1422	0	1317	22	1
3	E	2362	0	2379	18	0
3	F	2351	0	2368	38	0
4	A	35	0	26	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	26	3	0
5	A	26	0	12	0	0
5	C	26	0	12	1	0
6	E	30	0	0	0	0
6	F	30	0	0	0	0
7	A	32	0	0	0	0
7	B	8	0	0	0	0
7	C	25	0	0	0	0
7	D	7	0	0	0	0
7	E	7	0	0	0	0
7	F	5	0	0	0	0
All	All	14682	0	14014	169	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 (169) 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:C:292:ALA:O	1:C:296:VAL:HG23	1.55	1.06
1:A:138:ARG:NH2	1:A:172:TPO:O2P	1.89	1.05
3:E:256:ASN:O	3:E:256:ASN:ND2	1.92	1.03
3:F:262:VAL:O	3:F:266:LEU:HD13	1.60	1.00
1:C:296:VAL:CG1	1:C:303:THR:HA	1.94	0.97
2:D:107:ARG:HG2	2:D:108:SEP:O	1.64	0.96
2:B:224:ASP:OD1	2:B:225:PRO:HD2	1.67	0.92
1:C:237:LEU:HD11	1:C:241:VAL:CG1	2.02	0.89
1:A:124:LEU:HD11	1:A:259:ILE:HG12	1.53	0.89
1:A:138:ARG:HH22	1:A:172:TPO:HB	1.38	0.89
2:B:224:ASP:OD1	2:B:225:PRO:CD	2.24	0.84
1:C:296:VAL:HG13	1:C:303:THR:HA	1.60	0.84
3:F:240:ILE:HG22	3:F:275:GLY:HA3	1.57	0.84
1:C:296:VAL:HG11	1:C:303:THR:HA	1.59	0.81
1:C:396:TRP:CH2	2:D:250:VAL:HG12	2.15	0.81
1:A:138:ARG:NH2	1:A:172:TPO:HB	1.96	0.80
2:D:256:ARG:HG2	2:D:256:ARG:HH11	1.44	0.80
2:D:256:ARG:HG2	2:D:256:ARG:NH1	1.99	0.77
3:F:239:ASP:OD1	3:F:240:ILE:N	2.19	0.75
1:C:272:LEU:C	1:C:272:LEU:HD13	2.08	0.74
1:C:237:LEU:HD11	1:C:241:VAL:HG13	1.70	0.72
1:C:138:ARG:NH1	1:C:172:TPO:O2P	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:THR:HG22	1:C:526:LEU:HD22	1.71	0.72
1:C:192:GLY:O	1:C:195:VAL:HG22	1.90	0.71
2:B:256:ARG:HG2	2:B:257:TYR:O	1.91	0.70
1:C:396:TRP:HH2	2:D:250:VAL:HG12	1.57	0.69
1:C:304:GLU:O	1:C:307:VAL:HG12	1.92	0.69
1:A:124:LEU:HD23	1:A:268:PHE:CZ	2.31	0.66
4:C:601:STU:H16	4:C:601:STU:H261	1.78	0.65
3:F:57:VAL:HG22	3:F:61:PHE:CE2	2.32	0.65
3:F:241:TYR:HD1	3:F:266:LEU:HD11	1.62	0.64
1:A:422:PHE:CE2	1:A:436:ARG:HD3	2.33	0.64
1:A:422:PHE:HE2	1:A:436:ARG:HD3	1.62	0.64
4:A:601:STU:H16	4:A:601:STU:H261	1.79	0.64
1:A:138:ARG:CZ	1:A:172:TPO:O2P	2.47	0.63
1:A:396:TRP:CH2	2:B:250:VAL:HG12	2.33	0.63
3:E:41:LEU:HD13	3:E:138:LEU:HD21	1.82	0.62
1:A:168:GLU:O	2:B:234:VAL:HG12	1.98	0.62
1:C:233:ILE:HG23	1:C:237:LEU:HD23	1.81	0.62
3:F:241:TYR:CD1	3:F:266:LEU:HD11	2.35	0.61
2:B:259:LYS:HB2	3:E:39:TYR:OH	2.01	0.61
1:C:237:LEU:HD11	1:C:241:VAL:HG11	1.81	0.60
3:F:41:LEU:HD11	3:F:167:LEU:HD13	1.83	0.60
1:C:272:LEU:HD13	1:C:273:PRO:N	2.16	0.59
1:C:237:LEU:CD1	1:C:241:VAL:CG1	2.80	0.59
2:D:83:ARG:NE	2:D:111:ASN:OD1	2.33	0.58
2:B:195:LYS:CB	2:B:196:PRO:HD2	2.32	0.58
1:C:143:GLU:HB3	4:C:601:STU:H281	1.84	0.58
2:D:107:ARG:HD2	2:D:112:PHE:CZ	2.39	0.57
3:F:239:ASP:CG	3:F:240:ILE:H	2.06	0.57
1:A:143:GLU:HB3	4:A:601:STU:H281	1.86	0.57
1:A:413:VAL:O	1:A:417:MET:HG3	2.05	0.57
3:F:266:LEU:HD12	3:F:266:LEU:N	2.19	0.57
1:C:168:GLU:O	2:D:234:VAL:HG12	2.03	0.57
1:C:138:ARG:NH2	1:C:172:TPO:O2P	2.38	0.56
1:C:272:LEU:C	1:C:272:LEU:CD1	2.74	0.56
2:B:195:LYS:CB	2:B:199:ARG:CB	2.85	0.54
1:C:173:SER:HA	1:C:184:VAL:CG2	2.37	0.54
3:E:256:ASN:C	3:E:256:ASN:HD22	1.91	0.54
3:F:240:ILE:HG22	3:F:275:GLY:CA	2.36	0.54
1:A:428:ASN:HB3	1:A:431:HIS:HB3	1.89	0.54
1:C:176:SER:HB3	1:C:179:TYR:HD2	1.73	0.53
2:B:224:ASP:OD1	2:B:225:PRO:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PRO:O	1:C:197:ILE:HG12	2.10	0.51
3:E:88:ILE:HG23	3:E:247:ILE:HG23	1.93	0.51
3:F:266:LEU:O	3:F:270:SER:N	2.43	0.51
2:B:250:VAL:HG22	2:B:267:TYR:CD2	2.45	0.51
1:A:420:LEU:O	1:A:421:ASP:HB3	2.10	0.51
1:C:173:SER:HA	1:C:184:VAL:HG22	1.91	0.51
1:C:396:TRP:CH2	2:D:250:VAL:CG1	2.89	0.51
1:C:218:HIS:CE1	1:C:220:PRO:HD2	2.46	0.51
1:A:396:TRP:HH2	2:B:250:VAL:HG12	1.74	0.51
3:F:39:TYR:HA	3:F:42:ILE:HD12	1.93	0.51
1:A:234:PRO:HD2	1:A:237:LEU:HD12	1.93	0.50
3:F:266:LEU:N	3:F:266:LEU:CD1	2.74	0.50
1:A:362:GLU:HG2	3:E:70:ARG:HH21	1.76	0.50
1:A:396:TRP:HB2	2:B:213:VAL:HG11	1.94	0.50
1:A:47:LEU:HB2	1:A:89:PHE:HB2	1.93	0.50
2:B:124:GLN:HE21	2:B:142:VAL:HG11	1.77	0.49
2:B:107:ARG:HB2	2:B:112:PHE:CE2	2.47	0.49
3:F:41:LEU:HD11	3:F:167:LEU:CD1	2.41	0.49
3:E:174:LYS:HG2	3:E:293:VAL:HG13	1.94	0.49
1:A:138:ARG:NH1	1:A:172:TPO:O2P	2.45	0.49
2:D:258:LYS:NZ	3:F:37:ARG:HH12	2.11	0.48
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.94	0.48
2:D:242:LEU:HD23	2:D:243:SER:O	2.13	0.48
1:C:296:VAL:HG11	1:C:303:THR:CA	2.37	0.48
3:F:61:PHE:HA	3:F:64:LEU:HD12	1.96	0.48
2:D:260:LYS:NZ	3:F:39:TYR:O	2.47	0.48
2:B:92:TYR:HB2	2:B:128:PHE:HB3	1.93	0.48
3:E:108:GLU:O	3:E:112:HIS:HB2	2.14	0.48
3:F:262:VAL:O	3:F:266:LEU:CD1	2.48	0.48
2:B:195:LYS:CB	2:B:196:PRO:CD	2.92	0.48
1:C:307:VAL:HG13	1:C:308:MET:N	2.28	0.47
1:A:530:THR:HG23	2:B:255:HIS:CE1	2.49	0.47
3:E:56:GLN:HB2	3:E:59:LYS:HE3	1.96	0.47
2:B:248:VAL:HA	2:B:269:PRO:HA	1.97	0.47
3:E:74:LEU:HD21	3:E:86:LEU:HB2	1.97	0.47
3:F:25:ASN:O	3:F:28:VAL:HG23	2.15	0.47
3:E:56:GLN:HA	3:E:113:LYS:HA	1.96	0.47
2:B:124:GLN:NE2	2:B:142:VAL:HG11	2.30	0.47
2:D:250:VAL:HG22	2:D:267:TYR:CD2	2.50	0.46
1:A:212:LEU:HB2	1:A:215:ASP:HB2	1.97	0.46
1:A:463:PHE:HB2	2:B:239:LEU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:TYR:HB2	2:D:128:PHE:HB3	1.98	0.46
3:F:303:VAL:HG13	3:F:307:ASP:O	2.16	0.46
1:C:441:THR:HG22	1:C:526:LEU:CD2	2.42	0.46
1:A:177:PRO:HB3	1:A:223:PHE:HE1	1.81	0.46
1:C:272:LEU:HD13	1:C:273:PRO:O	2.15	0.46
1:A:422:PHE:HB3	1:A:434:VAL:CG2	2.46	0.46
2:B:207:PRO:HD2	2:B:210:LEU:HD12	1.98	0.46
3:F:74:LEU:HD22	3:F:114:ILE:HG21	1.97	0.46
1:C:423:GLU:HB3	2:D:187:TYR:HB3	1.98	0.45
1:C:26:THR:HG21	1:C:160:LEU:HG	1.99	0.45
3:F:41:LEU:HD13	3:F:171:ARG:CG	2.47	0.45
1:C:63:ARG:HE	1:C:163:MET:HG3	1.82	0.45
1:C:138:ARG:CZ	1:C:172:TPO:O2P	2.65	0.45
2:B:192:TYR:CE1	2:B:193:VAL:O	2.70	0.45
2:B:81:VAL:HG22	2:B:115:ILE:HG12	1.97	0.45
1:A:172:TPO:HG23	1:A:174:CYS:SG	2.57	0.45
1:A:208:LEU:HB3	1:A:237:LEU:HD21	1.99	0.45
3:F:174:LYS:HG3	3:F:293:VAL:HG13	1.99	0.45
1:C:307:VAL:CG1	1:C:308:MET:N	2.80	0.44
3:E:256:ASN:C	3:E:256:ASN:ND2	2.61	0.44
3:F:88:ILE:HG23	3:F:247:ILE:HG23	2.00	0.44
3:F:25:ASN:HA	3:F:28:VAL:HG23	1.99	0.44
1:C:124:LEU:HD23	1:C:268:PHE:CZ	2.53	0.44
2:D:256:ARG:HH11	2:D:256:ARG:CG	2.15	0.44
1:C:218:HIS:NE2	1:C:220:PRO:HD2	2.33	0.43
2:B:192:TYR:CD1	2:B:193:VAL:O	2.70	0.43
3:E:311:GLY:O	3:E:312:ILE:HD13	2.17	0.43
1:C:160:LEU:HD13	1:C:174:CYS:HB3	1.99	0.43
3:F:74:LEU:HD21	3:F:86:LEU:HB2	2.01	0.43
5:C:602:C1V:HAM	2:D:113:VAL:HG12	2.00	0.43
2:D:256:ARG:HD3	2:D:261:TYR:HE1	1.84	0.43
3:F:188:PHE:HB2	3:F:196:LEU:HD21	2.00	0.43
3:E:188:PHE:HB2	3:E:196:LEU:HD21	2.02	0.42
3:F:208:ARG:HB2	3:F:211:THR:HG23	2.00	0.42
3:F:231:VAL:HG22	3:F:237:VAL:HG22	2.02	0.42
3:F:303:VAL:HG12	3:F:304:ASP:O	2.19	0.42
2:B:250:VAL:HG21	2:B:267:TYR:CE2	2.54	0.42
3:E:39:TYR:HA	3:E:42:ILE:HD12	2.02	0.42
3:F:177:LYS:HG2	3:F:293:VAL:HG11	2.01	0.42
3:F:303:VAL:CG1	3:F:304:ASP:N	2.83	0.42
2:D:81:VAL:HG22	2:D:115:ILE:HG12	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:102:ALA:HA	3:E:256:ASN:ND2	2.35	0.41
2:D:224:ASP:HB3	2:D:227:LEU:HD12	2.01	0.41
3:E:278:LYS:HD2	3:E:303:VAL:HG21	2.01	0.41
3:F:280:TYR:HB2	3:F:283:GLU:HG3	2.02	0.41
1:A:421:ASP:CG	1:A:421:ASP:O	2.59	0.41
1:A:31:LYS:NZ	2:B:108:SEP:O2P	2.30	0.41
3:F:95:LEU:HD22	3:F:258:LEU:HD11	2.03	0.41
1:A:315:ASP:HA	1:A:316:PRO:HD3	1.98	0.41
3:F:193:LEU:HD13	3:F:288:ILE:HD13	2.02	0.41
1:A:32:ILE:HD11	1:A:41:LYS:HD3	2.02	0.41
1:C:136:VAL:HG23	1:C:196:ASP:OD2	2.21	0.41
2:B:141:ILE:HG22	2:B:151:ASN:ND2	2.35	0.41
2:B:236:LEU:HD23	2:B:254:THR:HG22	2.03	0.41
4:C:601:STU:H261	4:C:601:STU:C16	2.48	0.41
3:F:41:LEU:HD13	3:F:171:ARG:HG2	2.03	0.41
1:A:176:SER:HB2	1:A:179:TYR:HD2	1.85	0.41
2:D:107:ARG:CG	2:D:108:SEP:O	2.51	0.40
2:D:84:TRP:HB3	2:D:112:PHE:HB2	2.03	0.40
1:A:417:MET:HB3	1:A:422:PHE:HB2	2.03	0.40
1:C:194:GLU:HG2	1:C:195:VAL:N	2.36	0.40
1:C:218:HIS:ND1	1:C:221:THR:HG23	2.36	0.40
3:F:303:VAL:HG12	3:F:304:ASP:N	2.36	0.40
3:E:95:LEU:HD22	3:E:258:LEU:HD11	2.03	0.40
3:F:32:PHE:CE1	3:F:36:HIS:CD2	3.10	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:C:285:ALA:O	2:D:144:SER:OG[2_946]	2.16	0.04

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	433/560 (77%)	422 (98%)	11 (2%)	0	100 100
1	C	430/560 (77%)	413 (96%)	17 (4%)	0	100 100
2	B	180/270 (67%)	177 (98%)	3 (2%)	0	100 100
2	D	179/270 (66%)	174 (97%)	4 (2%)	1 (1%)	30 72
3	E	298/336 (89%)	293 (98%)	5 (2%)	0	100 100
3	F	299/336 (89%)	293 (98%)	6 (2%)	0	100 100
All	All	1819/2332 (78%)	1772 (97%)	46 (2%)	1 (0%)	56 90

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	193	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	358/497 (72%)	358 (100%)	0	100 100
1	C	349/497 (70%)	349 (100%)	0	100 100
2	B	145/239 (61%)	145 (100%)	0	100 100
2	D	149/239 (62%)	149 (100%)	0	100 100
3	E	259/308 (84%)	258 (100%)	1 (0%)	93 98
3	F	255/308 (83%)	253 (99%)	2 (1%)	86 96
All	All	1515/2088 (73%)	1512 (100%)	3 (0%)	95 99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	256	ASN
3	F	147	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
1	TPO	A	172	1	7,10,11	0.95	0	10,14,16	1.34	1 (10%)
2	SEP	B	108	2	7,9,10	0.88	0	8,12,14	1.69	2 (25%)
1	TPO	C	172	1	7,10,11	0.92	0	10,14,16	1.35	1 (10%)
2	SEP	D	108	2	7,9,10	0.89	0	8,12,14	1.67	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
1	TPO	A	172	1	-	0/8/11/13	0/0/0/0
2	SEP	B	108	2	-	0/5/8/10	0/0/0/0
1	TPO	C	172	1	-	0/8/11/13	0/0/0/0
2	SEP	D	108	2	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	108	SEP	O-C-CA	-3.20	117.14	125.72
1	C	172	TPO	O-C-CA	-2.31	119.39	125.69
2	B	108	SEP	O-C-CA	-2.28	119.60	125.72
1	A	172	TPO	O-C-CA	-2.15	119.82	125.69
2	D	108	SEP	O3P-P-O2P	2.21	115.57	107.44
2	B	108	SEP	OG-CB-CA	3.09	110.96	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	6	0
2	B	108	SEP	1	0
1	C	172	TPO	3	0
2	D	108	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
4	STU	A	601	-	29,42,42	2.54	9 (31%)	23,68,68	3.16	8 (34%)
5	C1V	A	602	-	28,29,29	3.38	9 (32%)	29,42,42	7.50	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	STU	C	601	-	29,42,42	2.50	9 (31%)	23,68,68	3.20	8 (34%)
5	C1V	C	602	-	28,29,29	3.41	9 (32%)	29,42,42	7.59	6 (20%)
6	C2Z	E	401	-	8,16,16	3.67	5 (62%)	10,24,24	2.85	3 (30%)
6	C2Z	E	402	-	8,16,16	3.29	4 (50%)	10,24,24	1.76	2 (20%)
6	C2Z	F	401	-	8,16,16	3.65	5 (62%)	10,24,24	2.88	3 (30%)
6	C2Z	F	402	-	8,16,16	3.64	5 (62%)	10,24,24	2.66	2 (20%)

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
4	STU	A	601	-	-	0/4/42/42	0/0/8/8
5	C1V	A	602	-	-	0/9/10/10	0/4/4/4
4	STU	C	601	-	-	0/4/42/42	0/0/8/8
5	C1V	C	602	-	-	0/9/10/10	0/4/4/4
6	C2Z	E	401	-	-	0/0/10/10	0/0/2/2
6	C2Z	E	402	-	-	0/0/10/10	0/0/2/2
6	C2Z	F	401	-	-	0/0/10/10	0/0/2/2
6	C2Z	F	402	-	-	0/0/10/10	0/0/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	401	C2Z	CAM-CAL	-6.67	1.33	1.49
6	F	401	C2Z	CAM-CAL	-6.64	1.34	1.49
6	F	402	C2Z	CAM-CAL	-6.56	1.34	1.49
6	E	402	C2Z	CAM-CAL	-6.54	1.34	1.49
6	E	401	C2Z	CAG-CAL	-4.51	1.33	1.40
6	F	401	C2Z	CAG-CAL	-4.51	1.33	1.40
6	E	402	C2Z	CAG-CAL	-4.43	1.33	1.40
6	F	402	C2Z	CAG-CAL	-4.34	1.33	1.40
6	F	402	C2Z	PAO-OAD	-2.85	1.48	1.54
6	F	401	C2Z	PAO-OAD	-2.84	1.48	1.54
6	E	401	C2Z	PAO-OAD	-2.80	1.48	1.54
5	A	602	C1V	CAV-CAR	2.33	1.53	1.49
5	A	602	C1V	OAC-CAQ	2.44	1.41	1.36
5	C	602	C1V	OAC-CAQ	2.46	1.41	1.36
5	C	602	C1V	CAV-CAR	2.55	1.53	1.49
4	A	601	STU	O5-C8	2.57	1.28	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	STU	O5-C8	2.57	1.28	1.23
6	F	401	C2Z	PAO-OAB	2.84	1.60	1.54
6	E	402	C2Z	PAO-OAB	3.02	1.60	1.54
6	E	402	C2Z	PAO-OAD	3.41	1.61	1.54
6	E	401	C2Z	PAO-OAB	3.42	1.61	1.54
6	F	402	C2Z	PAO-OAB	3.43	1.61	1.54
5	A	602	C1V	CAW-CAS	3.44	1.56	1.49
5	C	602	C1V	CAW-CAS	3.47	1.56	1.49
4	C	601	STU	C19-C18	3.62	1.50	1.41
4	A	601	STU	C19-C18	3.67	1.50	1.41
4	C	601	STU	C7-C10	3.78	1.48	1.39
4	A	601	STU	C7-C10	3.90	1.48	1.39
4	C	601	STU	C7-C6	3.99	1.49	1.43
4	A	601	STU	C7-C6	4.08	1.49	1.43
4	C	601	STU	C6-C19	4.22	1.48	1.42
4	A	601	STU	C6-C19	4.26	1.48	1.42
6	E	401	C2Z	PAO-OAC	4.54	1.60	1.50
4	C	601	STU	C12-C17	4.59	1.48	1.41
4	C	601	STU	C5-C20	4.60	1.49	1.41
6	F	402	C2Z	PAO-OAC	4.61	1.60	1.50
4	A	601	STU	C5-C20	4.65	1.49	1.41
4	A	601	STU	C12-C17	4.68	1.49	1.41
4	C	601	STU	C10-C11	4.69	1.50	1.42
4	A	601	STU	C10-C11	4.78	1.50	1.42
6	F	401	C2Z	PAO-OAC	4.82	1.61	1.50
4	C	601	STU	C11-C18	4.89	1.49	1.42
4	A	601	STU	C11-C18	4.96	1.49	1.42
5	A	602	C1V	CAW-CAZ	4.97	1.49	1.41
5	C	602	C1V	CAW-CAZ	4.97	1.49	1.41
5	A	602	C1V	CAU-CAT	6.05	1.43	1.38
5	C	602	C1V	CAU-CAT	6.10	1.44	1.38
5	A	602	C1V	OAB-CAX	6.91	1.42	1.24
5	C	602	C1V	OAB-CAX	6.92	1.42	1.24
5	A	602	C1V	CAE-NAA	7.47	1.32	1.14
5	C	602	C1V	CAE-NAA	7.50	1.32	1.14
5	C	602	C1V	CAU-CAE	7.55	1.53	1.44
5	A	602	C1V	CAU-CAE	7.61	1.53	1.44
5	A	602	C1V	CAN-CAW	7.73	1.41	1.37
5	C	602	C1V	CAN-CAW	7.97	1.41	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	602	C1V	CAU-CAE-NAA	-34.83	120.06	177.37
5	A	602	C1V	CAU-CAE-NAA	-34.04	121.36	177.37
5	A	602	C1V	CAW-CAN-SAP	-19.14	107.19	112.53
5	C	602	C1V	CAW-CAN-SAP	-18.66	107.32	112.53
4	C	601	STU	C6-C7-C8	-9.51	119.76	129.67
4	A	601	STU	C6-C7-C8	-9.34	119.94	129.67
4	C	601	STU	O5-C8-C7	-8.51	114.58	128.66
4	A	601	STU	O5-C8-C7	-8.25	115.00	128.66
5	A	602	C1V	CAU-CAX-NAO	-4.76	120.49	124.15
5	C	602	C1V	CAU-CAX-NAO	-4.62	120.59	124.15
5	C	602	C1V	CAN-CAW-CAS	-4.49	118.71	125.69
5	A	602	C1V	CAN-CAW-CAS	-4.25	119.08	125.69
6	F	401	C2Z	OAB-PAO-OAC	-4.00	101.38	112.09
6	F	402	C2Z	OAB-PAO-OAC	-3.89	101.66	112.09
6	E	401	C2Z	OAB-PAO-OAC	-3.64	102.35	112.09
6	E	401	C2Z	CAG-CAL-CAM	-3.50	123.89	129.24
6	F	401	C2Z	CAG-CAL-CAM	-3.30	124.20	129.24
5	C	602	C1V	CAU-CAT-CAZ	-3.05	118.67	121.10
4	C	601	STU	C16-C17-C12	-2.97	116.75	120.15
4	A	601	STU	C16-C17-C12	-2.96	116.76	120.15
4	C	601	STU	C1-C20-C5	-2.72	117.04	120.15
4	C	601	STU	C13-C12-C11	-2.69	127.35	133.62
4	A	601	STU	C13-C12-C11	-2.69	127.36	133.62
5	A	602	C1V	CAU-CAT-CAZ	-2.69	118.96	121.10
4	A	601	STU	C1-C20-C5	-2.56	117.22	120.15
4	A	601	STU	C4-C5-C6	-2.14	128.63	133.62
6	E	402	C2Z	CAG-CAL-CAM	-2.10	126.03	129.24
4	C	601	STU	C4-C5-C6	-2.02	128.93	133.62
4	A	601	STU	C1-C20-N3	2.43	135.11	132.18
4	C	601	STU	C1-C20-N3	2.54	135.24	132.18
6	E	402	C2Z	OAC-PAO-CAN	3.91	119.45	111.37
4	C	601	STU	C16-C17-N2	4.94	138.26	132.22
4	A	601	STU	C16-C17-N2	5.01	138.35	132.22
6	E	401	C2Z	OAD-PAO-CAN	6.77	119.22	106.73
6	F	402	C2Z	OAD-PAO-CAN	6.83	119.34	106.73
5	C	602	C1V	CAN-SAP-CAY	6.88	99.32	91.02
5	A	602	C1V	CAN-SAP-CAY	6.89	99.32	91.02
6	F	401	C2Z	OAD-PAO-CAN	6.90	119.47	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	STU	2	0
4	C	601	STU	3	0
5	C	602	C1V	1	0

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	441/560 (78%)	0.23	14 (3%) 51 23	40, 63, 98, 142	0
1	C	440/560 (78%)	0.25	14 (3%) 51 23	38, 67, 105, 126	0
2	B	184/270 (68%)	0.41	11 (5%) 25 9	42, 71, 109, 131	0
2	D	185/270 (68%)	0.36	6 (3%) 51 23	51, 71, 115, 146	0
3	E	302/336 (89%)	0.43	21 (6%) 19 7	40, 65, 93, 113	0
3	F	300/336 (89%)	0.29	12 (4%) 42 17	43, 68, 93, 109	0
All	All	1852/2332 (79%)	0.31	78 (4%) 40 16	38, 67, 103, 146	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	GLY	6.7
1	A	361	PRO	4.4
3	F	304	ASP	4.3
2	B	120	GLU	4.2
1	A	300	PHE	4.1
3	F	280	TYR	4.0
3	F	303	VAL	4.0
3	E	280	TYR	3.8
1	A	302	CYS	3.7
2	D	194	CYS	3.7
1	A	362	GLU	3.6
3	E	306	ASN	3.6
1	C	302	CYS	3.5
3	E	268	HIS	3.4
2	B	154	GLN	3.4
3	E	25	ASN	3.2
2	B	197	GLU	3.2
3	F	126	PHE	3.2
2	D	197	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	282	HIS	3.1
3	E	271	HIS	3.1
1	A	360	HIS	3.1
1	A	410	MET	3.1
3	E	24	SER	3.0
3	F	305	GLU	3.0
1	C	361	PRO	3.0
1	C	364	VAL	3.0
1	A	363	ARG	3.0
1	C	526	LEU	3.0
2	B	219	THR	3.0
1	A	365	PRO	2.8
1	A	315	ASP	2.8
3	E	238	VAL	2.8
1	C	359	PRO	2.8
2	D	200	PHE	2.7
3	F	192	SER	2.7
3	E	304	ASP	2.7
2	D	192	TYR	2.7
2	B	196	PRO	2.7
3	E	302	VAL	2.7
3	E	305	GLU	2.7
1	C	345	SER	2.6
1	C	407	TYR	2.6
3	F	272	TYR	2.6
3	E	237	VAL	2.6
3	E	190	SER	2.6
3	E	234	LYS	2.5
3	E	309	VAL	2.4
3	E	210	THR	2.4
1	C	424	TRP	2.4
1	A	301	GLU	2.4
3	F	190	SER	2.4
2	B	119	PRO	2.4
1	C	409	ILE	2.4
3	F	302	VAL	2.3
2	D	221	ILE	2.3
3	E	206	MET	2.3
1	A	156	ALA	2.3
3	E	308	VAL	2.3
2	B	187	TYR	2.3
3	F	306	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	358	ARG	2.2
1	A	316	PRO	2.2
2	B	193	VAL	2.2
2	B	175	ASP	2.2
1	A	344	SER	2.1
1	C	398	LEU	2.1
3	E	188	PHE	2.1
3	F	282	HIS	2.1
3	E	272	TYR	2.1
1	C	297	CYS	2.1
3	E	232	ASP	2.1
1	C	440	VAL	2.1
1	C	444	TYR	2.0
2	B	152	ILE	2.0
2	B	220	GLY	2.0
2	D	77	ALA	2.0
3	F	75	TRP	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^{th} 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^2)	Q<0.9
1	TPO	A	172	11/12	0.92	0.12	-	56,57,60,61	1
2	SEP	D	108	10/11	0.92	0.13	-	65,65,69,69	0
2	SEP	B	108	10/11	0.94	0.12	-	64,64,67,67	0
1	TPO	C	172	11/12	0.94	0.14	-	69,69,73,73	2

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^{th} 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^2)	Q<0.9
5	C1V	A	602	26/26	0.94	0.24	1.13	44,45,47,48	0
6	C2Z	E	401	15/15	0.83	0.24	0.70	100,100,101,101	0
4	STU	C	601	35/35	0.96	0.21	0.20	39,40,42,43	0
5	C1V	C	602	26/26	0.96	0.21	-0.27	42,44,45,45	0
4	STU	A	601	35/35	0.96	0.18	-0.44	38,39,40,40	0
6	C2Z	E	402	15/15	0.87	0.22	-0.52	92,92,93,93	0
6	C2Z	F	402	15/15	0.92	0.20	-0.99	88,88,88,88	0
6	C2Z	F	401	15/15	0.92	0.18	-1.13	92,93,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.