Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2023 – 08:09 am GMT

PDB ID	:	5NIJ
Title	:	Crystal structure of arabidopsis thaliana legumain isoform gamma in two-chain activation state
Authors	:	Zauner, F.B.; Dall, E.; Brandstetter, H.
Deposited on	:	2017-03-24
Resolution	:	2.75 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

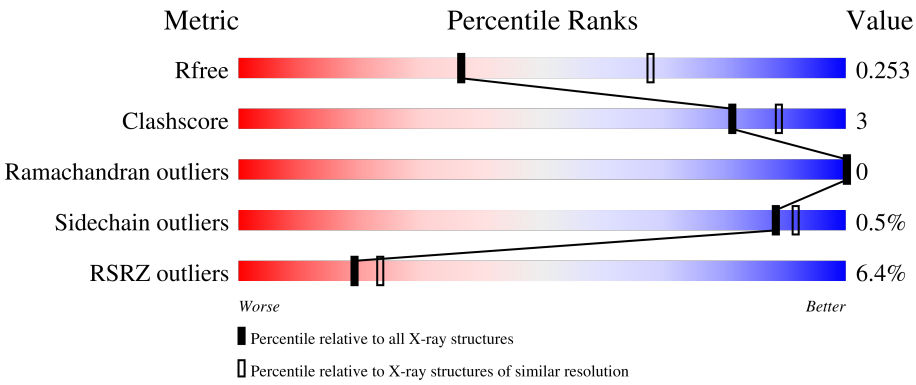
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of 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 <=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	454	2%, 87%, 7%, 6%
1	B	454	6%, 92%, •, 6%
1	C	454	8%, 89%, 6%, 6%
1	D	454	8%, 87%, 7%, 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13474 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 Vacuolar-processing enzyme gamma-isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3342	2099	578	646	19	0	0	0
1	B	428	3338	2099	575	645	19	0	0	0
1	C	429	3342	2099	578	646	19	0	0	0
1	D	428	3335	2094	577	645	19	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	-	expression tag	UNP Q39119
A	42	LEU	-	expression tag	UNP Q39119
A	43	GLU	-	expression tag	UNP Q39119
A	44	HIS	-	expression tag	UNP Q39119
A	45	HIS	-	expression tag	UNP Q39119
A	46	HIS	-	expression tag	UNP Q39119
A	47	HIS	-	expression tag	UNP Q39119
A	48	HIS	-	expression tag	UNP Q39119
A	49	HIS	-	expression tag	UNP Q39119
A	50	GLU	-	expression tag	UNP Q39119
A	51	ASN	-	expression tag	UNP Q39119
A	52	LEU	-	expression tag	UNP Q39119
A	53	TYR	-	expression tag	UNP Q39119
A	54	PHE	-	expression tag	UNP Q39119
A	55	GLN	-	expression tag	UNP Q39119
B	41	SER	-	expression tag	UNP Q39119
B	42	LEU	-	expression tag	UNP Q39119
B	43	GLU	-	expression tag	UNP Q39119
B	44	HIS	-	expression tag	UNP Q39119
B	45	HIS	-	expression tag	UNP Q39119
B	46	HIS	-	expression tag	UNP Q39119

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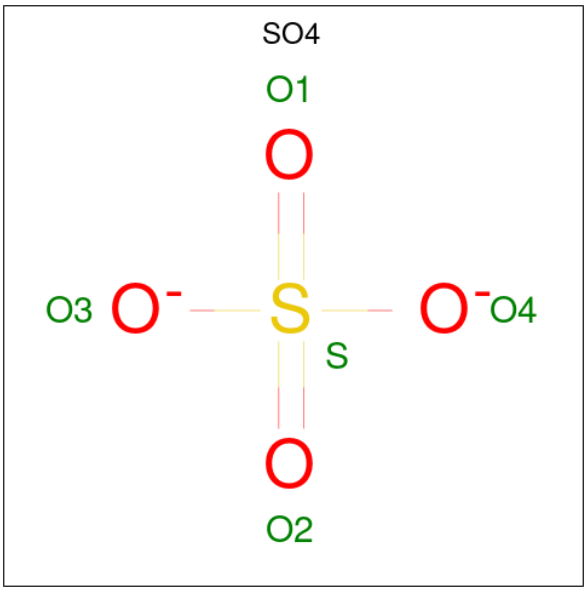
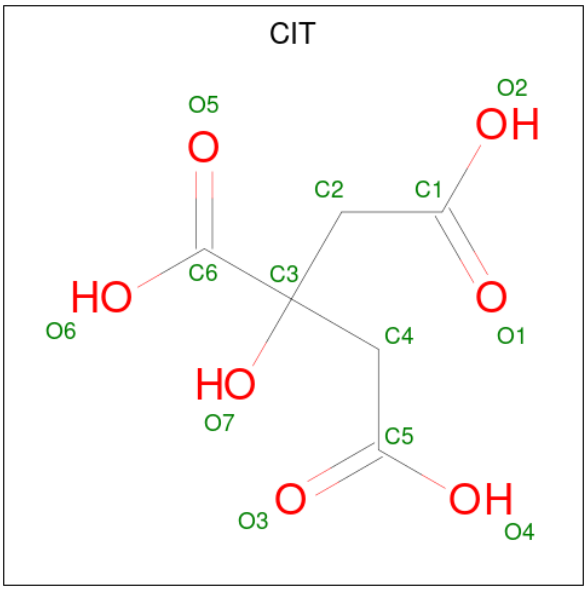
Chain	Residue	Modelled	Actual	Comment	Reference
B	47	HIS	-	expression tag	UNP Q39119
B	48	HIS	-	expression tag	UNP Q39119
B	49	HIS	-	expression tag	UNP Q39119
B	50	GLU	-	expression tag	UNP Q39119
B	51	ASN	-	expression tag	UNP Q39119
B	52	LEU	-	expression tag	UNP Q39119
B	53	TYR	-	expression tag	UNP Q39119
B	54	PHE	-	expression tag	UNP Q39119
B	55	GLN	-	expression tag	UNP Q39119
C	41	SER	-	expression tag	UNP Q39119
C	42	LEU	-	expression tag	UNP Q39119
C	43	GLU	-	expression tag	UNP Q39119
C	44	HIS	-	expression tag	UNP Q39119
C	45	HIS	-	expression tag	UNP Q39119
C	46	HIS	-	expression tag	UNP Q39119
C	47	HIS	-	expression tag	UNP Q39119
C	48	HIS	-	expression tag	UNP Q39119
C	49	HIS	-	expression tag	UNP Q39119
C	50	GLU	-	expression tag	UNP Q39119
C	51	ASN	-	expression tag	UNP Q39119
C	52	LEU	-	expression tag	UNP Q39119
C	53	TYR	-	expression tag	UNP Q39119
C	54	PHE	-	expression tag	UNP Q39119
C	55	GLN	-	expression tag	UNP Q39119
D	41	SER	-	expression tag	UNP Q39119
D	42	LEU	-	expression tag	UNP Q39119
D	43	GLU	-	expression tag	UNP Q39119
D	44	HIS	-	expression tag	UNP Q39119
D	45	HIS	-	expression tag	UNP Q39119
D	46	HIS	-	expression tag	UNP Q39119
D	47	HIS	-	expression tag	UNP Q39119
D	48	HIS	-	expression tag	UNP Q39119
D	49	HIS	-	expression tag	UNP Q39119
D	50	GLU	-	expression tag	UNP Q39119
D	51	ASN	-	expression tag	UNP Q39119
D	52	LEU	-	expression tag	UNP Q39119
D	53	TYR	-	expression tag	UNP Q39119
D	54	PHE	-	expression tag	UNP Q39119
D	55	GLN	-	expression tag	UNP Q39119

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	6	7	0	0

- Molecule 4 is water.

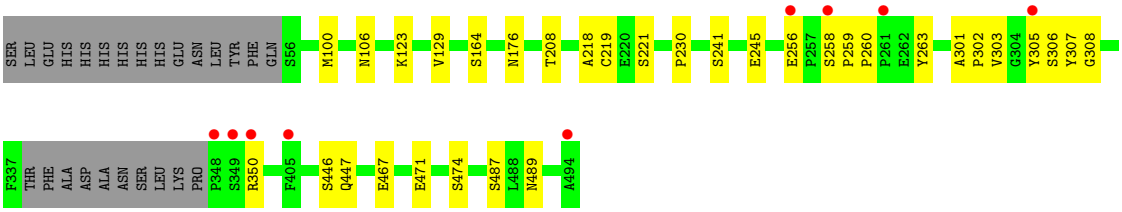
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	33	33	33	0	0
			Total	O		
4	B	29	29	29	0	0
			Total	O		
4	C	12	12	12	0	0
			Total	O		
4	D	5	5	5	0	0

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.

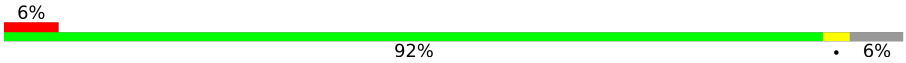
• Molecule 1: Vacuolar-processing enzyme gamma-isozyme

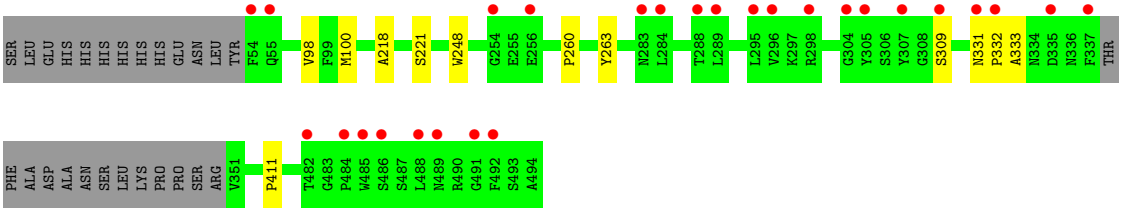
Chain A:



• Molecule 1: Vacuolar-processing enzyme gamma-isozyme

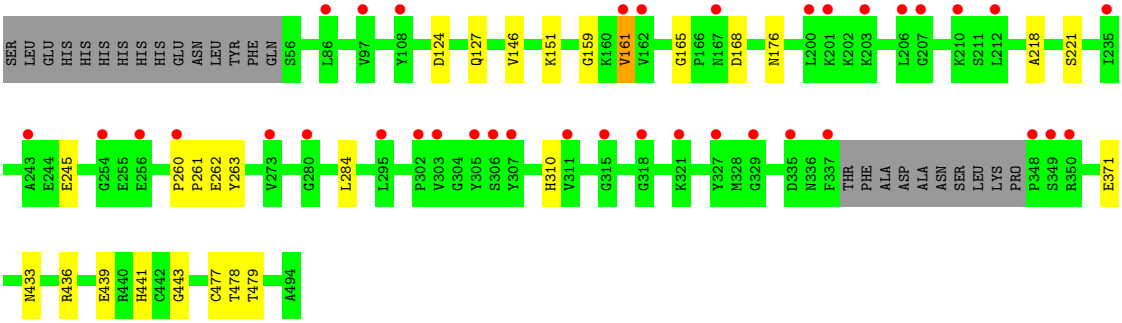
Chain B:





• Molecule 1: Vacuolar-processing enzyme gamma-isozyme

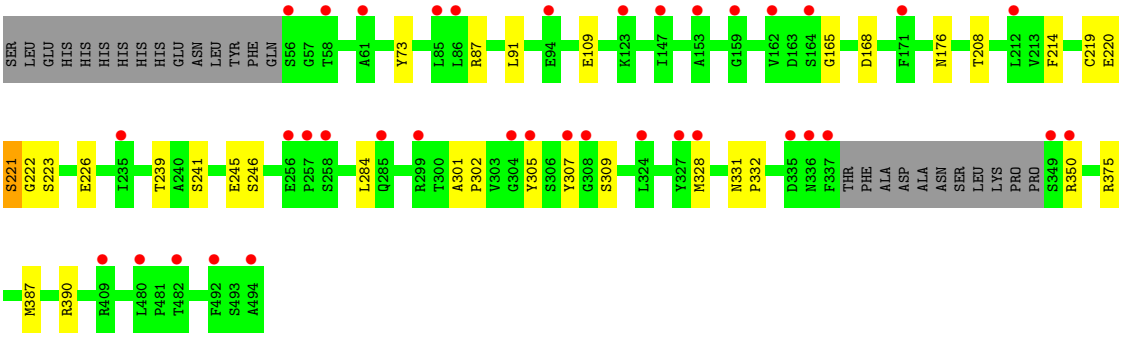
Chain C:



• Molecule 1: Vacuolar-processing enzyme gamma-isozyme

Chain D:

8%
87%
7%
6%


SER LEU GLU HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN S56 G57 T58 A61 Y73 L85 L86 R87 L91 E94 E109 K123 I147 A153 G159 V162 D163 S164 G165 D168 F171 N176 T208 L212 V213 F214 C219 E220
S221 G222 S223 E226 I235 T239 A240 S241 E245 S246 E256 P257 S258 L284 Q285 R299 T300 A301 P302 V303 G304 Y305 S306 Y307 G308 S309 L324 Y327 M328 N331 P332 D335 N336 F337 THR PHE ALA ASP ALA ASN SER LEU LYS PRO PRO S349 R350 R375
M387 R390 R409 L480 P481 T482 F492 S493 A494

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	147.83Å 147.83Å 101.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.11 – 2.75 72.86 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.11-2.75) 99.9 (72.86-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.252 0.217 , 0.253	Depositor DCC
R_{free} test set	2711 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13474	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, 0.333 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: CIT, SCH, SNN, SO4

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	0.24	0/3408	0.41	0/4619
1	B	0.22	0/3404	0.38	0/4614
1	C	0.26	1/3408 (0.0%)	0.42	0/4619
1	D	0.24	0/3400	0.40	0/4608
All	All	0.24	1/13620 (0.0%)	0.40	0/18460

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	VAL	CB-CG2	-5.30	1.41	1.52

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	3342	0	3184	30	0
1	B	3338	0	3175	6	0
1	C	3342	0	3184	16	0
1	D	3335	0	3176	26	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	13	0	5	5	0
4	A	33	0	0	3	0
4	B	29	0	0	1	0
4	C	12	0	0	0	0
4	D	5	0	0	0	0
All	All	13474	0	12724	69	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 3.

All (69) 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:306:SER:HB3	1:D:305:TYR:CE2	2.12	0.84
1:A:307:TYR:HB2	1:D:305:TYR:CE1	2.12	0.84
1:C:151:LYS:HE3	1:C:159:GLY:O	1.76	0.84
1:A:447:GLN:H	3:A:502:CIT:H21	1.44	0.80
1:D:302:PRO:HA	1:D:350:ARG:HH22	1.47	0.80
1:D:302:PRO:HA	1:D:350:ARG:NH2	1.99	0.77
1:D:301:ALA:O	1:D:350:ARG:NH1	2.22	0.73
1:D:109:GLU:OE1	1:D:375:ARG:NH1	2.24	0.70
1:A:446:SER:HB2	3:A:502:CIT:H22	1.74	0.69
1:D:331:ASN:OD1	1:D:332:PRO:HD2	1.96	0.64
1:A:106:ASN:ND2	4:A:607:HOH:O	2.31	0.63
1:C:433:ASN:OD1	1:C:436:ARG:NH2	2.34	0.60
1:A:301:ALA:O	1:A:350:ARG:NH2	2.34	0.60
1:A:218:ALA:O	1:A:221:SER:OG	2.20	0.60
1:A:350:ARG:HB3	1:D:305:TYR:OH	2.02	0.59
1:C:218:ALA:O	1:C:221:SER:OG	2.20	0.58
1:A:307:TYR:HB2	1:D:305:TYR:CD1	2.39	0.56
1:D:220:GLU:O	1:D:223:SER:OG	2.19	0.55
1:B:260:PRO:HB2	1:B:263:TYR:HB2	1.89	0.54
1:C:151:LYS:HZ2	1:C:161:VAL:HG22	1.73	0.53
1:D:109:GLU:CD	1:D:375:ARG:HH12	2.13	0.52
1:A:447:GLN:N	3:A:502:CIT:H21	2.19	0.52
1:A:350:ARG:O	1:D:305:TYR:CE1	2.63	0.52
1:A:305:TYR:O	1:D:307:TYR:HD1	1.93	0.51
1:A:306:SER:HB3	1:D:305:TYR:HE2	1.71	0.51
1:A:303:VAL:HG13	1:A:350:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:H	3:A:502:CIT:C2	2.21	0.50
1:C:439:GLU:HA	1:C:443:GLY:O	2.12	0.50
1:B:331:ASN:OD1	1:B:332:PRO:HD2	2.12	0.49
1:C:260:PRO:HG2	1:C:263:TYR:HB2	1.95	0.49
1:C:261:PRO:HG2	1:C:262:GLU:OE2	2.12	0.49
1:A:256:GLU:O	1:A:258:SER:N	2.45	0.49
1:C:151:LYS:HD2	1:C:161:VAL:HG22	1.95	0.49
1:D:165:GLY:N	1:D:168:ASP:OD2	2.45	0.49
1:A:100:MET:HE1	1:A:129:VAL:HG11	1.94	0.48
1:A:305:TYR:HD1	1:D:307:TYR:HB2	1.77	0.48
1:A:467:GLU:O	1:A:471:GLU:HG3	2.12	0.48
1:C:151:LYS:NZ	1:C:161:VAL:HG22	2.29	0.48
1:B:248:TRP:NE1	1:B:309:SER:OG	2.47	0.47
1:A:164:SER:O	1:A:208:THR:OG1	2.32	0.47
1:A:123:LYS:O	4:A:601:HOH:O	2.20	0.47
1:D:246:SER:O	1:D:309:SER:OG	2.31	0.47
1:A:487:SER:OG	1:A:489:ASN:OD1	2.33	0.47
1:A:471:GLU:O	1:A:474:SER:OG	2.25	0.46
1:B:98:VAL:HG11	1:B:100:MET:HE3	1.97	0.46
1:C:165:GLY:N	1:C:168:ASP:OD2	2.48	0.46
1:A:350:ARG:O	1:D:305:TYR:CZ	2.69	0.45
1:B:218:ALA:O	1:B:221:SER:OG	2.27	0.44
1:A:256:GLU:HA	1:A:259:PRO:HG3	1.99	0.44
1:C:441:HIS:O	1:C:477:CYS:HB3	2.18	0.43
1:B:333:ALA:N	4:B:608:HOH:O	2.50	0.43
1:D:221:SER:HB2	1:D:239:THR:HB	2.00	0.43
1:A:447:GLN:HB2	3:A:502:CIT:H21	2.01	0.43
1:A:260:PRO:HB2	1:A:263:TYR:HB2	2.00	0.43
1:D:302:PRO:HA	1:D:350:ARG:CZ	2.49	0.43
1:A:241:SER:HB2	1:A:245:GLU:HG3	2.01	0.42
1:C:245:GLU:OE2	1:C:310:HIS:N	2.47	0.42
1:D:87:ARG:NH1	1:D:91:LEU:O	2.51	0.42
1:D:222:GLY:O	1:D:226:GLU:HB2	2.19	0.42
1:A:302:PRO:HG3	1:A:308:GLY:HA3	2.01	0.42
1:D:241:SER:HB2	1:D:245:GLU:HG3	2.02	0.41
1:D:284:LEU:HD23	1:D:328:MET:HB2	2.02	0.41
1:D:305:TYR:O	1:D:305:TYR:CD2	2.73	0.41
1:C:124:ASP:OD2	1:C:127:GLN:HG2	2.20	0.41
1:C:146:VAL:HA	1:C:161:VAL:HG12	2.02	0.41
1:C:151:LYS:CD	1:C:161:VAL:HG22	2.51	0.41
1:C:478:THR:C	1:C:479:THR:HG23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:O	4:A:602:HOH:O	2.22	0.40
1:D:387:MET:HA	1:D:390:ARG:HG2	2.03	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	423/454 (93%)	401 (95%)	22 (5%)	0	100	100
1	B	422/454 (93%)	409 (97%)	13 (3%)	0	100	100
1	C	423/454 (93%)	411 (97%)	12 (3%)	0	100	100
1	D	422/454 (93%)	405 (96%)	17 (4%)	0	100	100
All	All	1690/1816 (93%)	1626 (96%)	64 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	357/380 (94%)	357 (100%)	0	100	100
1	B	356/380 (94%)	355 (100%)	1 (0%)	92	95
1	C	357/380 (94%)	355 (99%)	2 (1%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	356/380 (94%)	352 (99%)	4 (1%)	73	84
All	All	1426/1520 (94%)	1419 (100%)	7 (0%)	88	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	411	PRO
1	C	284	LEU
1	C	371	GLU
1	D	73	TYR
1	D	208	THR
1	D	214	PHE
1	D	221	SER

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	SNN	B	176	1	5,6,8	0.49	0	3,6,11	1.43	0
1	SCH	B	219	1	6,7,8	0.98	0	3,7,9	1.63	0
1	SCH	D	219	1	6,7,8	0.99	0	3,7,9	1.61	1 (33%)
1	SNN	C	176	1	5,6,8	0.48	0	3,6,11	1.43	1 (33%)
1	SCH	C	219	1	6,7,8	1.01	0	3,7,9	1.69	0
1	SCH	A	219	1	6,7,8	0.96	0	3,7,9	1.85	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SNN	D	176	1	5,6,8	0.48	0	3,6,11	1.52	1 (33%)
1	SNN	A	176	1	5,6,8	0.49	0	3,6,11	1.69	1 (33%)

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	SNN	B	176	1	-	3/3/5/12	-
1	SCH	B	219	1	-	0/2/6/8	-
1	SCH	D	219	1	-	0/2/6/8	-
1	SNN	C	176	1	-	3/3/5/12	-
1	SCH	C	219	1	-	0/2/6/8	-
1	SCH	A	219	1	-	0/2/6/8	-
1	SNN	D	176	1	-	3/3/5/12	-
1	SNN	A	176	1	-	3/3/5/12	-

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	A	219	SCH	CB-SG-SD	2.39	110.02	103.82
1	D	219	SCH	CE-SD-SG	2.28	110.46	102.58
1	A	176	SNN	CA-C4-C5	-2.21	106.06	114.44
1	D	176	SNN	CA-C4-C5	-2.21	106.06	114.44
1	C	176	SNN	CA-C4-C5	-2.00	106.84	114.44

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	176	SNN	O-C-CA-C4
1	A	176	SNN	C5-C4-CA-N
1	A	176	SNN	CA-C4-C5-O5
1	B	176	SNN	O-C-CA-C4
1	B	176	SNN	C5-C4-CA-N
1	B	176	SNN	CA-C4-C5-O5
1	C	176	SNN	O-C-CA-C4
1	C	176	SNN	C5-C4-CA-N

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Mol	Chain	Res	Type	Atoms
1	C	176	SNN	CA-C4-C5-O5
1	D	176	SNN	O-C-CA-C4
1	D	176	SNN	C5-C4-CA-N
1	D	176	SNN	CA-C4-C5-O5

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	CIT	A	502	-	12,12,12	1.10	0	17,17,17	1.48	3 (17%)
2	SO4	B	502	-	4,4,4	0.35	0	6,6,6	0.05	0
2	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	D	501	-	4,4,4	0.34	0	6,6,6	0.05	0
2	SO4	A	501	-	4,4,4	0.33	0	6,6,6	0.05	0
2	SO4	C	501	-	4,4,4	0.34	0	6,6,6	0.04	0

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	CIT	A	502	-	-	7/16/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	CIT	O6-C6-C3	3.70	119.47	113.05
3	A	502	CIT	C3-C2-C1	2.50	119.87	113.81
3	A	502	CIT	O4-C5-C4	2.11	121.13	114.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	CIT	O7-C3-C6-O5
3	A	502	CIT	O7-C3-C6-O6
3	A	502	CIT	C4-C3-C6-O5
3	A	502	CIT	C4-C3-C6-O6
3	A	502	CIT	C6-C3-C4-C5
3	A	502	CIT	O7-C3-C4-C5
3	A	502	CIT	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	CIT	5	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 (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	427/454 (94%)	0.30	9 (2%)	63	72	29, 49, 79, 116	0
1	B	426/454 (93%)	0.56	27 (6%)	20	24	32, 48, 95, 155	0
1	C	427/454 (94%)	0.70	37 (8%)	10	12	32, 56, 97, 157	0
1	D	426/454 (93%)	0.69	37 (8%)	10	12	41, 66, 99, 129	0
All	All	1706/1816 (93%)	0.56	110 (6%)	19	23	29, 55, 95, 157	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	SER	9.9
1	D	305	TYR	9.8
1	C	305	TYR	8.5
1	B	305	TYR	6.1
1	B	284	LEU	5.8
1	B	307	TYR	5.1
1	D	349	SER	5.1
1	B	492	PHE	4.9
1	B	304	GLY	4.9
1	D	482	THR	4.6
1	C	207	GLY	4.5
1	D	337	PHE	4.5
1	C	348	PRO	4.4
1	A	348	PRO	4.3
1	C	307	TYR	4.3
1	C	349	SER	4.3
1	B	337	PHE	3.8
1	A	256	GLU	3.8
1	C	315	GLY	3.7
1	A	349	SER	3.7
1	D	159	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	167	ASN	3.6
1	D	409	ARG	3.5
1	C	256	GLU	3.5
1	D	324	LEU	3.5
1	B	289	LEU	3.5
1	C	254	GLY	3.4
1	D	258	SER	3.4
1	D	480	LEU	3.3
1	B	335	ASP	3.3
1	D	85	LEU	3.2
1	D	304	GLY	3.2
1	B	256	GLU	3.2
1	B	486	SER	3.2
1	C	212	LEU	3.2
1	B	482	THR	3.1
1	C	350	ARG	3.1
1	D	56	SER	3.1
1	B	254	GLY	3.0
1	B	55	GLN	3.0
1	C	329	GLY	2.9
1	D	147	ILE	2.9
1	D	494	ALA	2.9
1	D	336	ASN	2.8
1	B	485	TRP	2.8
1	C	337	PHE	2.8
1	C	321	LYS	2.8
1	B	54	PHE	2.8
1	B	288	THR	2.8
1	C	161	VAL	2.7
1	B	484	PRO	2.7
1	D	123	LYS	2.7
1	D	61	ALA	2.7
1	B	331	ASN	2.7
1	C	335	ASP	2.7
1	D	492	PHE	2.6
1	D	327	TYR	2.6
1	D	164	SER	2.6
1	A	261	PRO	2.6
1	C	273	VAL	2.6
1	A	494	ALA	2.6
1	D	153	ALA	2.6
1	D	162	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	318	GLY	2.6
1	C	327	TYR	2.5
1	D	256	GLU	2.5
1	C	260	PRO	2.5
1	A	350	ARG	2.5
1	B	489	ASN	2.5
1	D	86	LEU	2.5
1	C	108	TYR	2.5
1	C	280	GLY	2.5
1	C	311	VAL	2.5
1	C	203	LYS	2.5
1	D	307	TYR	2.5
1	B	309	SER	2.5
1	B	488	LEU	2.4
1	C	206	LEU	2.4
1	B	283	ASN	2.3
1	A	305	TYR	2.3
1	D	350	ARG	2.3
1	D	335	ASP	2.3
1	C	97	VAL	2.3
1	B	332	PRO	2.3
1	D	328	MET	2.3
1	C	201	LYS	2.3
1	C	200	LEU	2.3
1	D	257	PRO	2.3
1	C	243	ALA	2.3
1	C	210	LYS	2.3
1	B	491	GLY	2.2
1	B	295	LEU	2.2
1	C	295	LEU	2.2
1	C	302	PRO	2.2
1	C	303	VAL	2.2
1	D	235	ILE	2.2
1	A	405	PHE	2.2
1	C	235	ILE	2.2
1	D	299	ARG	2.1
1	A	258	SER	2.1
1	C	86	LEU	2.1
1	D	212	LEU	2.1
1	D	94	GLU	2.1
1	B	298	ARG	2.1
1	D	285	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	58	THR	2.1
1	D	308	GLY	2.1
1	C	162	VAL	2.0
1	D	171	PHE	2.0
1	B	296	VAL	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
1	SCH	C	219	8/9	0.93	0.16	45,48,53,54	0
1	SCH	B	219	8/9	0.94	0.18	44,47,61,66	0
1	SNN	B	176	7/8	0.94	0.21	29,34,38,40	0
1	SNN	D	176	7/8	0.94	0.17	48,49,51,52	0
1	SCH	A	219	8/9	0.95	0.20	31,36,59,59	0
1	SCH	D	219	8/9	0.95	0.23	41,47,60,60	0
1	SNN	C	176	7/8	0.96	0.20	39,42,42,48	0
1	SNN	A	176	7/8	0.96	0.21	28,30,33,34	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	CIT	A	502	13/13	0.78	0.35	39,43,50,51	13
2	SO4	B	502	5/5	0.81	0.33	88,91,106,130	0
2	SO4	A	501	5/5	0.86	0.29	100,100,101,102	0
2	SO4	D	501	5/5	0.89	0.29	83,94,100,121	0
2	SO4	C	501	5/5	0.90	0.13	85,87,99,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	501	5/5	0.94	0.17	68,69,73,77	0

6.5 Other polymers (i)

There are no such residues in this entry.