



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2017 – 03:56 PM EDT

PDB ID : 4ZSW
Title : Pig Brain GABA-AT inactivated by (E)-(1S,3S)-3-Amino-4-fluoromethylenyl
-1-cyclopentanoic acid
Authors : Wu, R.; Lee, H.; Le, H.V.; Doud, E.; Sanishvili, R.; Compton, P.; Kelleher,
N.L.; Silverman, R.B.; Liu, D.
Deposited on : unknown
Resolution : 1.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

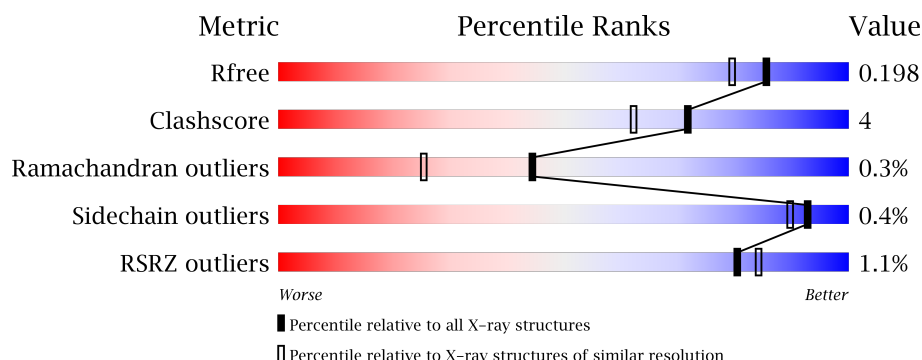
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	461	<div> <div>0.1%</div> <div>92%</div> <div>7%</div> </div>
1	B	461	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	C	461	<div> <div>0.1%</div> <div>92%</div> <div>7%</div> </div>
1	D	461	<div> <div>0.1%</div> <div>92%</div> <div>8%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	501	-	-	X	X
4	GOL	C	502	-	-	-	X
5	ACT	C	503	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16678 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.

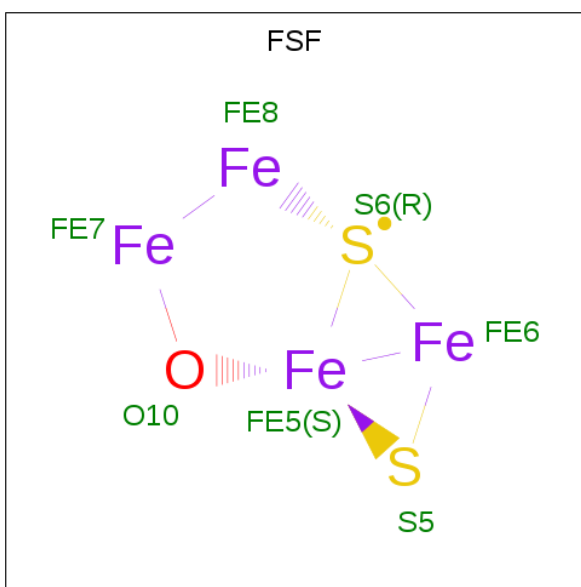
- Molecule 1 is a protein called 4-aminobutyrate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	6	0
			3690	2350	643	673	24			
1	B	461	Total	C	N	O	S	8	6	0
			3691	2350	643	674	24			
1	C	461	Total	C	N	O	S	0	6	0
			3691	2350	643	674	24			
1	D	461	Total	C	N	O	S	0	6	0
			3691	2350	643	674	24			

There are 4 discrepancies between the modelled and reference sequences:

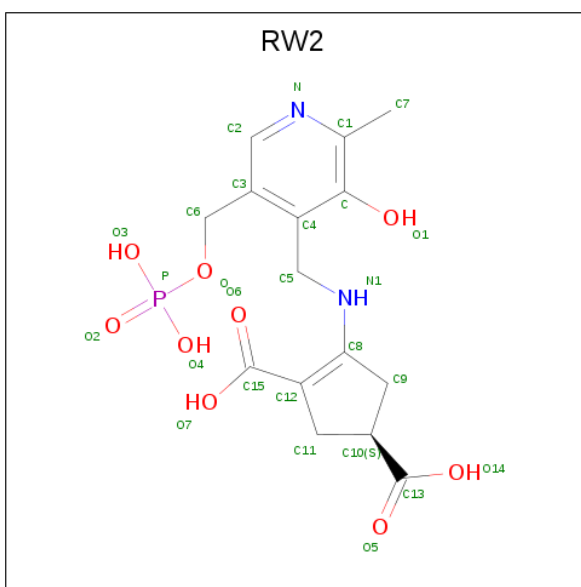
Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLU	GLN	conflict	UNP P80147
B	158	GLU	GLN	conflict	UNP P80147
C	158	GLU	GLN	conflict	UNP P80147
D	158	GLU	GLN	conflict	UNP P80147

- Molecule 2 is 4FE-2S-O HYBRID CLUSTER (three-letter code: FSF) (formula: Fe₄OS₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is (1S)-4-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]amino]cyclopent-3-ene-1,3-dicarboxylic acid (three-letter code: RW2) (formula: C₁₅H₁₉N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			26	15	2	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			26	15	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			26	15	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			26	15	2	8	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

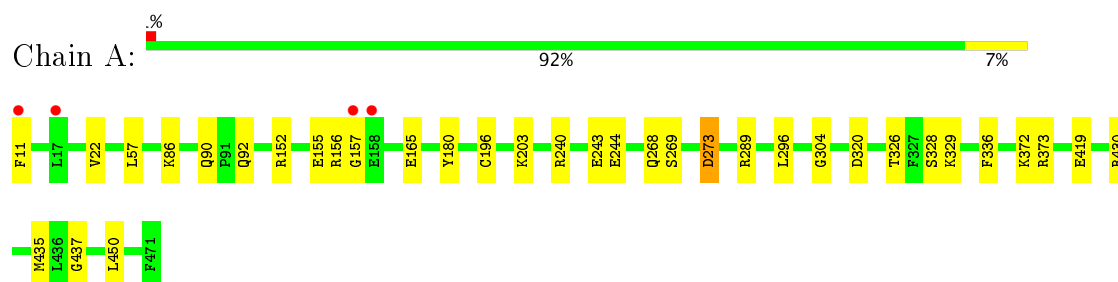
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	432	Total	O	0	0
			432	432		
6	B	387	Total	O	0	0
			387	387		
6	C	455	Total	O	0	0
			455	455		
6	D	513	Total	O	0	0
			513	513		

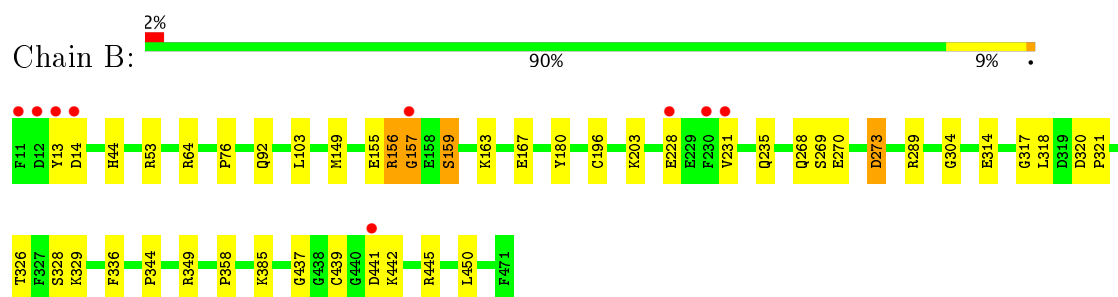
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

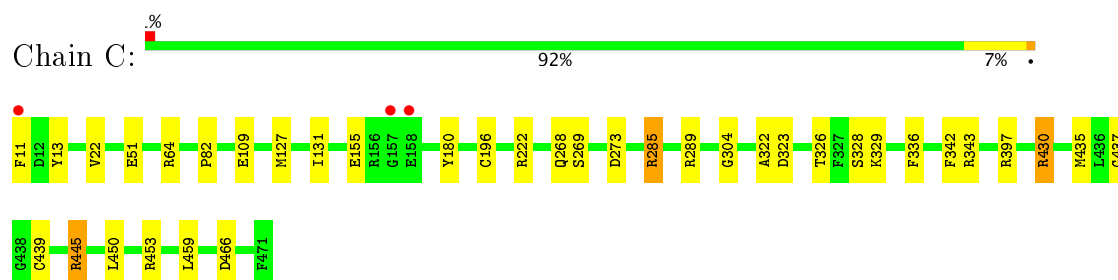
- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



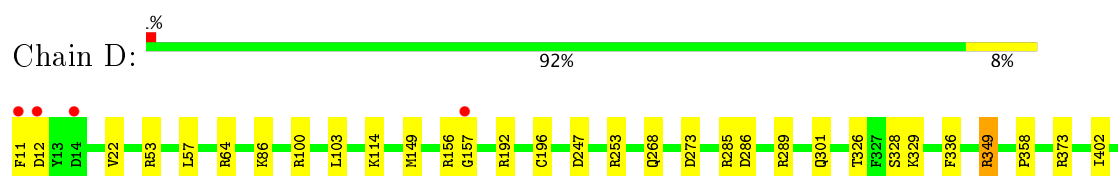
- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



- Molecule 1: 4-aminobutyrate aminotransferase, mitochondrial



R430	
R435	
L436	
Q437	
R442	
R447	
F471	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.60Å 227.61Å 71.34Å 90.00° 108.97° 90.00°	Depositor
Resolution (Å)	49.72 – 1.70 49.72 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.72-1.70) 91.2 (49.72-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.70Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.158 , 0.195 0.166 , 0.198	Depositor DCC
R_{free} test set	1979 reflections (0.95%)	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16678	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, RW2, FSF, ACT

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	0.76	1/3791 (0.0%)	0.76	0/5116
1	B	0.74	1/3792 (0.0%)	0.73	1/5118 (0.0%)
1	C	0.83	2/3792 (0.1%)	0.82	6/5118 (0.1%)
1	D	0.88	1/3800 (0.0%)	0.85	8/5129 (0.2%)
All	All	0.81	5/15175 (0.0%)	0.79	15/20481 (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
1	C	0	1
1	D	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	196	CYS	CB-SG	-8.14	1.68	1.82
1	C	196	CYS	CB-SG	-7.68	1.69	1.82
1	C	285	ARG	CG-CD	-7.21	1.33	1.51
1	A	196	CYS	CB-SG	-7.15	1.70	1.82
1	B	196	CYS	CB-SG	-7.14	1.70	1.82

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ARG	NE-CZ-NH1	8.54	124.57	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ARG	CG-CD-NE	8.20	129.02	111.80
1	B	157	GLY	N-CA-C	-7.83	93.53	113.10
1	D	100	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	C	343	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	C	445	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	D	349	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	D	447	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	C	445	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	D	157	GLY	N-CA-C	-5.62	99.04	113.10
1	D	64	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	192	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	459	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	447	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	430	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	156	ARG	Peptide
1	C	285	ARG	Sidechain
1	D	156	ARG	Peptide

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	3690	0	3644	25	0
1	B	3691	0	3644	34	0
1	C	3691	0	3644	24	0
1	D	3691	0	3639	33	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	2	0
3	C	26	0	17	1	0
3	D	26	0	17	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	4	0
4	C	6	0	8	0	0
5	C	4	0	3	1	0
6	A	432	0	0	8	0
6	B	387	0	0	9	0
6	C	455	0	0	12	0
6	D	513	0	0	15	1
All	All	16678	0	14656	118	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 4.

All (118) 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:372:LYS:NZ	6:A:602:HOH:O	2.03	0.91
1:B:14:ASP:O	6:B:601:HOH:O	1.89	0.90
1:D:12:ASP:OD1	6:D:601:HOH:O	1.88	0.90
1:D:285:ARG:CZ	6:D:604:HOH:O	2.23	0.87
1:A:11:PHE:N	6:A:603:HOH:O	2.08	0.86
1:B:314:GLU:HA	4:B:501:GOL:H2	1.58	0.85
1:C:466:ASP:OD2	6:C:601:HOH:O	1.96	0.84
1:C:155:GLU:OE1	1:C:180:TYR:OH	1.97	0.82
1:D:373:ARG:NH1	6:D:602:HOH:O	1.99	0.82
1:A:437:GLY:N	6:A:604:HOH:O	2.09	0.81
1:B:157:GLY:HA2	1:B:159:SER:H	1.47	0.80
1:B:13:TYR:O	6:B:602:HOH:O	1.98	0.80
1:A:289[B]:ARG:NH2	1:A:320:ASP:OD2	2.15	0.79
1:D:285:ARG:NH2	6:D:604:HOH:O	2.16	0.79
1:A:243:GLU:OE2	6:A:601:HOH:O	2.00	0.78
1:C:437:GLY:N	6:C:602:HOH:O	2.00	0.78
1:D:285:ARG:NH2	1:D:286:ASP:OD1	2.16	0.77
1:B:437:GLY:N	6:B:603:HOH:O	2.06	0.77
1:B:318:LEU:O	4:B:501:GOL:H12	1.85	0.76
1:A:329:LYS:HE2	3:A:502:RW2:H11	1.70	0.73
1:D:247:ASP:OD1	6:D:603:HOH:O	2.06	0.72
1:D:437:GLY:N	6:D:605:HOH:O	2.18	0.70
1:C:453:ARG:NH2	6:C:606:HOH:O	2.22	0.69
5:C:503:ACT:OXT	6:C:603:HOH:O	2.12	0.67
1:B:156:ARG:HG3	1:B:157:GLY:N	2.09	0.66
1:D:285:ARG:CZ	1:D:289[A]:ARG:HH22	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:HE2	3:C:504:RW2:H11	1.81	0.63
1:C:269:SER:HB2	6:C:801:HOH:O	1.99	0.62
1:C:439:CYS:HB3	1:C:445:ARG:HD2	1.82	0.62
1:A:373:ARG:NH2	6:A:608:HOH:O	2.33	0.61
1:A:155:GLU:OE1	1:A:180:TYR:OH	2.18	0.61
1:B:157:GLY:HA3	6:B:662:HOH:O	2.00	0.61
1:A:326:THR:HG22	1:A:336:PHE:HB3	1.84	0.60
1:D:285:ARG:NH2	6:D:607:HOH:O	2.24	0.59
1:D:253:ARG:NH1	6:D:610:HOH:O	2.36	0.59
1:D:285:ARG:NH2	1:D:289[B]:ARG:HH22	2.00	0.59
1:D:11:PHE:N	6:D:611:HOH:O	2.37	0.57
1:B:321:PRO:HB3	4:B:501:GOL:H11	1.87	0.56
1:B:203:LYS:NZ	6:B:612:HOH:O	2.38	0.56
1:B:289[B]:ARG:NH1	1:B:320:ASP:OD2	2.38	0.56
1:A:90:GLN:HE21	1:A:92:GLN:HE22	1.53	0.55
1:B:13:TYR:CD1	1:B:64:ARG:HD2	2.41	0.55
1:B:228:GLU:CD	1:B:228:GLU:H	2.11	0.54
1:B:53:ARG:CZ	6:B:615:HOH:O	2.55	0.54
1:B:269:SER:HB2	6:B:821:HOH:O	2.07	0.54
1:D:286:ASP:OD1	1:D:289[B]:ARG:NH2	2.41	0.54
1:B:149:MET:HE1	1:B:344:PRO:HB3	1.89	0.54
1:D:326:THR:HG22	1:D:336:PHE:HB3	1.90	0.53
1:D:53:ARG:NH2	6:D:608:HOH:O	2.28	0.53
1:C:109:GLU:OE1	6:C:604:HOH:O	2.19	0.53
1:B:155:GLU:OE1	1:B:180:TYR:OH	2.19	0.52
1:B:439:CYS:HB3	1:B:445:ARG:HD2	1.92	0.52
1:C:22:VAL:CG1	1:C:430:ARG:HD3	2.40	0.52
1:C:289[B]:ARG:NH1	6:C:607:HOH:O	2.26	0.52
1:C:326:THR:HG22	1:C:336:PHE:HB3	1.92	0.52
1:D:22:VAL:HG11	1:D:430:ARG:HD3	1.91	0.51
1:B:53:ARG:NH2	6:B:615:HOH:O	2.43	0.51
1:D:11:PHE:HA	6:D:611:HOH:O	2.09	0.51
1:D:22:VAL:CG1	1:D:430:ARG:HD3	2.40	0.51
1:A:90:GLN:HB3	1:A:92:GLN:NE2	2.25	0.51
1:C:131:ILE:HG13	6:C:769:HOH:O	2.12	0.50
1:B:329:LYS:HE2	3:B:502:RW2:H11	1.92	0.50
1:D:329:LYS:HE2	3:D:501:RW2:H11	1.92	0.50
1:B:149:MET:HG2	1:B:349:ARG:NH2	2.27	0.50
1:B:156:ARG:HG3	1:B:157:GLY:CA	2.42	0.49
1:A:90:GLN:HE21	1:A:92:GLN:NE2	2.10	0.49
1:A:419:GLU:OE2	6:A:605:HOH:O	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152[B]:ARG:NH2	1:A:165:GLU:OE2	2.46	0.48
1:A:268:GLN:O	1:A:273:ASP:HA	2.13	0.48
1:B:53:ARG:NE	6:B:615:HOH:O	2.46	0.48
1:A:269:SER:HB2	6:A:858:HOH:O	2.13	0.47
1:C:222:ARG:NH1	6:C:615:HOH:O	2.47	0.47
1:C:268:GLN:O	1:C:273:ASP:HA	2.13	0.47
1:A:57:LEU:HD23	1:A:435[B]:MET:SD	2.54	0.47
1:C:304:GLY:O	1:C:450:LEU:HD11	2.15	0.47
1:B:92:GLN:CD	1:B:92:GLN:H	2.19	0.47
1:D:285:ARG:NH1	1:D:289[A]:ARG:HH22	2.13	0.47
1:A:203:LYS:HE2	1:A:203:LYS:HB3	1.52	0.47
1:B:163:LYS:HE2	1:B:167:GLU:OE2	2.13	0.47
1:D:12:ASP:N	6:D:613:HOH:O	2.39	0.46
1:D:53:ARG:NH1	6:D:624:HOH:O	2.48	0.46
1:C:127:MET:HE1	1:C:322:ALA:HB3	1.98	0.46
1:D:285:ARG:NE	6:D:604:HOH:O	2.40	0.45
1:D:268:GLN:O	1:D:273:ASP:HA	2.17	0.45
1:A:156:ARG:HG3	1:A:157:GLY:N	2.30	0.45
1:C:439:CYS:CB	1:C:445:ARG:HD2	2.47	0.44
1:B:441:ASP:OD1	1:B:442:LYS:N	2.46	0.44
1:B:268:GLN:O	1:B:273:ASP:HA	2.18	0.44
1:B:157:GLY:HA2	1:B:159:SER:N	2.25	0.43
1:C:22:VAL:HG11	1:C:430:ARG:HD3	2.00	0.43
1:C:397:ARG:NH2	6:C:609:HOH:O	2.46	0.43
1:A:86:LYS:HB3	1:A:86:LYS:HE3	1.63	0.43
1:D:442:LYS:NZ	6:D:606:HOH:O	2.19	0.43
1:B:270:GLU:HB2	3:B:502:RW2:C15	2.49	0.43
1:B:326:THR:HG22	1:B:336:PHE:HB3	2.01	0.42
1:C:51:GLU:OE2	6:C:605:HOH:O	2.21	0.42
1:D:103:LEU:HD21	1:D:358:PRO:HG3	2.02	0.42
1:D:114:LYS:HA	1:D:114:LYS:HD3	1.86	0.42
1:A:373:ARG:HD3	6:A:916:HOH:O	2.19	0.42
1:A:304:GLY:O	1:A:450:LEU:HD11	2.19	0.42
1:C:13:TYR:CD1	1:C:64:ARG:HD2	2.54	0.42
1:D:149:MET:HG2	1:D:349:ARG:NH2	2.35	0.42
1:B:317:GLY:HA2	4:B:501:GOL:H32	2.01	0.41
3:D:501:RW2:H4	3:D:501:RW2:H10	1.86	0.41
1:A:22:VAL:CG1	1:A:430:ARG:HD3	2.50	0.41
1:C:430:ARG:HD2	6:C:810:HOH:O	2.20	0.41
1:A:152[A]:ARG:HD2	1:A:152[A]:ARG:HA	1.92	0.41
1:B:231:VAL:O	1:B:235:GLN:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLY:O	1:B:450:LEU:HD11	2.20	0.41
1:C:11:PHE:CE1	1:C:82:PRO:HG2	2.56	0.41
1:B:103:LEU:HD21	1:B:358:PRO:HG3	2.03	0.41
1:D:301:GLN:HE22	3:D:501:RW2:C15	2.34	0.41
1:C:323:ASP:HB3	1:C:342:PHE:CE1	2.56	0.40
1:D:86:LYS:HB3	1:D:86:LYS:HE2	1.54	0.40
1:D:57:LEU:HD23	1:D:435[B]:MET:SD	2.62	0.40
1:A:240:ARG:O	1:A:244:GLU:HG3	2.21	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)
6:D:956:HOH:O	6:D:1017:HOH:O[1_455]	1.88	0.32

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	464/461 (101%)	446 (96%)	17 (4%)	1 (0%)	51	31
1	B	464/461 (101%)	446 (96%)	16 (3%)	2 (0%)	38	20
1	C	464/461 (101%)	444 (96%)	19 (4%)	1 (0%)	51	31
1	D	465/461 (101%)	447 (96%)	17 (4%)	1 (0%)	51	31
All	All	1857/1844 (101%)	1783 (96%)	69 (4%)	5 (0%)	44	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	328	SER
1	D	328	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	SER
1	B	328	SER
1	B	76	PRO

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	402/400 (100%)	400 (100%)	2 (0%)	91	87
1	B	402/400 (100%)	398 (99%)	4 (1%)	80	71
1	C	402/400 (100%)	400 (100%)	2 (0%)	91	87
1	D	403/400 (101%)	403 (100%)	0	100	100
All	All	1609/1600 (101%)	1601 (100%)	8 (0%)	93	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ASP
1	A	296	LEU
1	B	44	HIS
1	B	159	SER
1	B	273	ASP
1	B	385	LYS
1	C	435[A]	MET
1	C	435[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	D	44	HIS

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 ⓘ

9 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$
2	FSF	A	501	1	0,5,9	0.00	-	0,8,16	0.00	-
3	RW2	A	502	-	24,27,28	1.15	2 (8%)	27,39,41	1.41	4 (14%)
4	GOL	B	501	-	5,5,5	0.80	0	5,5,5	1.17	0
3	RW2	B	502	-	24,27,28	1.05	1 (4%)	27,39,41	1.78	8 (29%)
2	FSF	C	501	1	0,5,9	0.00	-	0,8,16	0.00	-
4	GOL	C	502	-	5,5,5	0.30	0	5,5,5	0.48	0
5	ACT	C	503	-	1,3,3	2.69	1 (100%)	0,3,3	0.00	-
3	RW2	C	504	-	24,27,28	1.06	1 (4%)	27,39,41	1.76	10 (37%)
3	RW2	D	501	-	24,27,28	1.07	1 (4%)	27,39,41	2.35	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FSF	A	501	1	-	0/0/6/22	0/0/2/3
3	RW2	A	502	-	-	0/13/29/31	0/2/2/2
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0
3	RW2	B	502	-	-	0/13/29/31	0/2/2/2
2	FSF	C	501	1	-	0/0/6/22	0/0/2/3
4	GOL	C	502	-	-	0/4/4/4	0/0/0/0
5	ACT	C	503	-	-	0/0/0/0	0/0/0/0
3	RW2	C	504	-	-	0/13/29/31	0/2/2/2
3	RW2	D	501	-	-	0/13/29/31	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	RW2	C8-C12	-3.74	1.33	1.38
3	C	504	RW2	C8-C12	-3.72	1.33	1.38
3	B	502	RW2	C8-C12	-3.50	1.33	1.38
3	A	502	RW2	C8-C12	-3.19	1.34	1.38
3	A	502	RW2	C-C1	-3.04	1.38	1.40
5	C	503	ACT	CH3-C	2.69	1.52	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	RW2	C5-C4-C3	-5.73	114.52	119.75
3	D	501	RW2	C12-C8-N1	-5.53	122.56	126.56
3	C	504	RW2	C12-C8-N1	-3.29	124.18	126.56
3	B	502	RW2	C5-C4-C3	-3.26	116.78	119.75
3	B	502	RW2	C3-C2-N	-3.20	118.46	123.87
3	A	502	RW2	C3-C2-N	-2.98	118.83	123.87
3	A	502	RW2	C9-C10-C13	-2.95	108.81	114.78
3	D	501	RW2	C3-C2-N	-2.89	118.98	123.87
3	C	504	RW2	C9-C10-C13	-2.69	109.33	114.78
3	A	502	RW2	C11-C10-C13	-2.63	109.45	114.78
3	C	504	RW2	C6-C3-C2	-2.52	115.00	119.33
3	B	502	RW2	C9-C10-C13	-2.37	109.98	114.78
3	C	504	RW2	C5-C4-C3	-2.28	117.67	119.75
3	C	504	RW2	C3-C2-N	-2.07	120.36	123.87
3	C	504	RW2	C-C1-N	-2.07	118.03	120.75
3	B	502	RW2	C11-C10-C13	-2.04	110.64	114.78
3	C	504	RW2	O1-C-C4	2.02	124.07	118.10
3	B	502	RW2	C4-C5-N1	2.03	115.49	111.13
3	C	504	RW2	C2-N-C1	2.09	123.28	119.26
3	D	501	RW2	O6-C15-C12	2.24	129.51	124.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	RW2	C2-N-C1	2.56	124.20	119.26
3	C	504	RW2	C5-C4-C	2.60	122.52	119.65
3	C	504	RW2	O3-P-O2	2.87	121.75	110.50
3	B	502	RW2	C2-C3-C4	3.23	120.53	118.13
3	A	502	RW2	C2-C3-C4	3.57	120.78	118.13
3	D	501	RW2	C2-C3-C4	4.00	121.10	118.13
3	B	502	RW2	C5-C4-C	4.40	124.51	119.65
3	D	501	RW2	C5-C4-C	5.47	125.69	119.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	RW2	1	0
4	B	501	GOL	4	0
3	B	502	RW2	2	0
5	C	503	ACT	1	0
3	C	504	RW2	1	0
3	D	501	RW2	3	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	461/461 (100%)	-0.34	4 (0%) 84 87	14, 24, 42, 78	0
1	B	461/461 (100%)	-0.23	9 (1%) 65 71	16, 26, 46, 96	0
1	C	461/461 (100%)	-0.47	3 (0%) 87 90	11, 22, 40, 64	0
1	D	461/461 (100%)	-0.52	4 (0%) 84 87	11, 19, 36, 65	0
All	All	1844/1844 (100%)	-0.39	20 (1%) 80 84	11, 23, 42, 96	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PHE	10.8
1	C	11	PHE	6.5
1	D	11	PHE	5.1
1	B	12	ASP	5.0
1	A	158	GLU	4.3
1	A	157	GLY	3.7
1	B	441	ASP	3.6
1	B	230	PHE	3.4
1	D	12	ASP	3.4
1	A	11	PHE	3.3
1	C	157	GLY	3.0
1	B	13	TYR	2.8
1	B	228	GLU	2.7
1	D	157	GLY	2.6
1	B	157	GLY	2.5
1	C	158	GLU	2.5
1	B	14	ASP	2.5
1	B	231	VAL	2.4
1	A	17	LEU	2.1
1	D	14	ASP	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](#)

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(Å ²)	Q<0.9
5	ACT	C	503	4/4	0.61	0.32	8.37	52,53,58,60	0
4	GOL	B	501	6/6	0.92	0.28	4.05	29,36,50,52	0
4	GOL	C	502	6/6	0.85	0.13	2.20	38,43,50,52	0
3	RW2	A	502	26/27	0.98	0.16	2.00	13,21,42,45	26
3	RW2	B	502	26/27	0.96	0.16	1.82	16,25,44,48	26
3	RW2	C	504	26/27	0.96	0.14	1.70	10,18,36,37	26
3	RW2	D	501	26/27	0.97	0.13	1.21	9,16,38,41	26
2	FSF	C	501	4/7	1.00	0.06	-2.89	13,14,14,14	0
2	FSF	A	501	4/7	0.99	0.07	-4.62	16,17,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.