Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:18 PM GMT

PDB ID	:	4L39
Title	:	Crystal structure of GH3.12 from Arabidopsis thaliana in complex with AMPCPP and salicylate
Authors	:	Zubieta, C.; Jez, J.M.; Brown, E.; Marcellin, R.; Kapp, U.; Round, A.; Westfall, C.
Deposited on	:	2013-06-05
Resolution	:	2.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

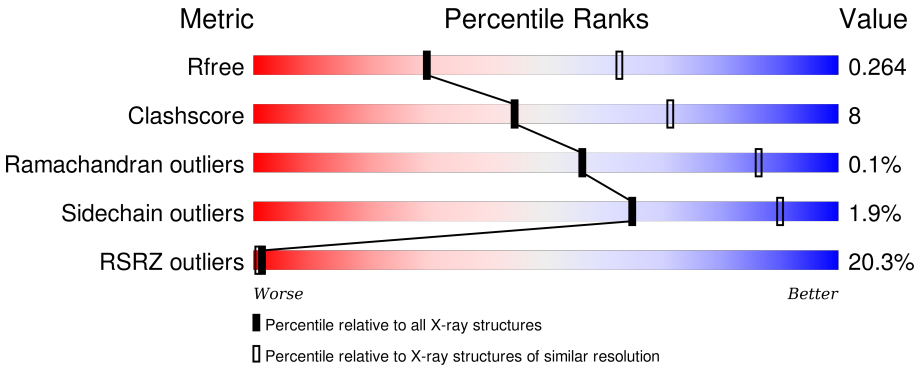
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	581	17% 81% 11% • 7%
1	B	581	21% 75% 17% • 7%

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
3	SAL	A	602	-	-	-	X
3	SAL	B	601	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8660 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-substituted benzoates-glutamate ligase GH3.12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	7	0
			4153	2637	681	807	28			
1	B	542	Total	C	N	O	S	0	6	0
			4211	2672	681	831	27			

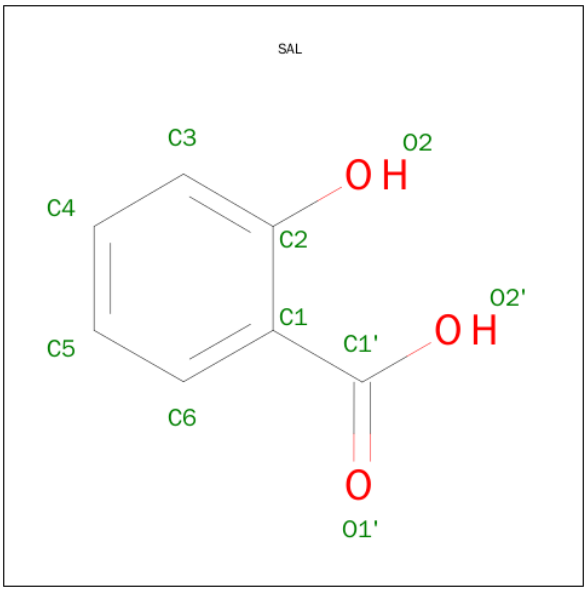
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
A	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
A	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
A	-2	MET	-	EXPRESSION TAG	UNP Q9LYU4
A	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
A	0	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
B	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
B	-2	MET	-	EXPRESSION TAG	UNP Q9LYU4
B	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
B	0	SER	-	EXPRESSION TAG	UNP Q9LYU4

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

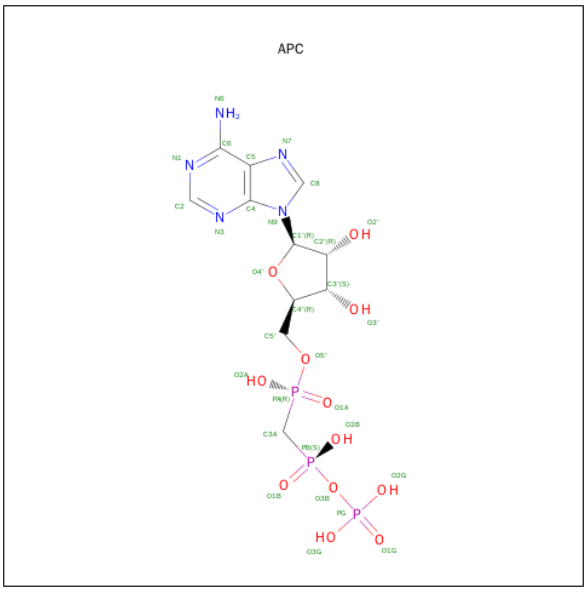
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).



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

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is water.

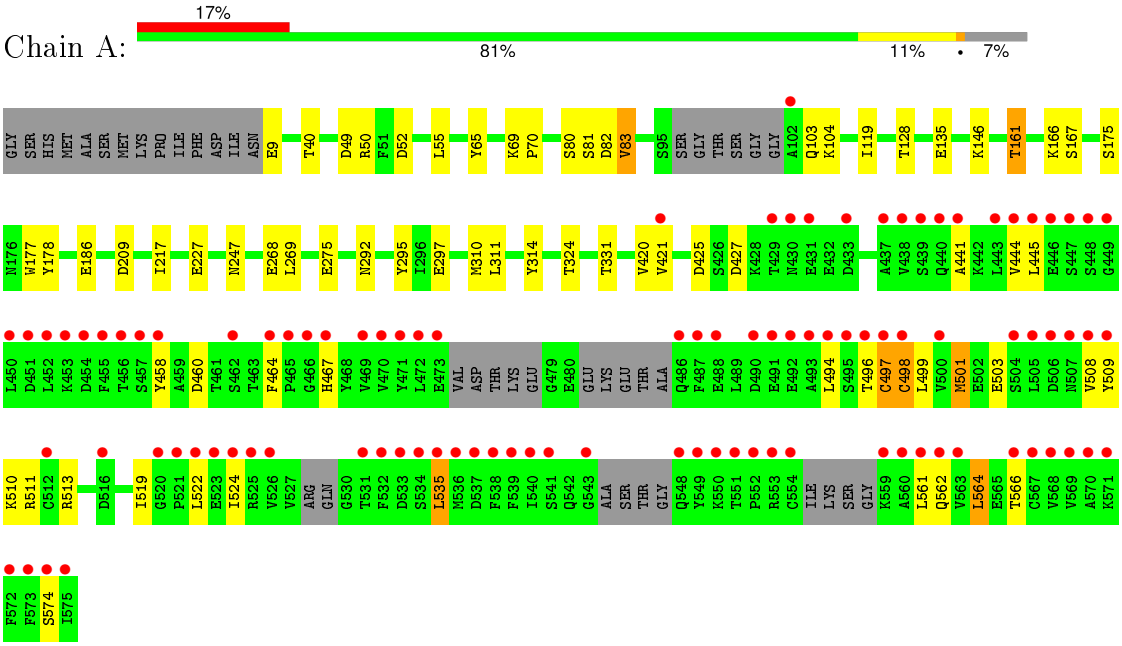
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	106	Total	O	0	0
			106	106		
5	B	107	Total	O	0	0
			107	107		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

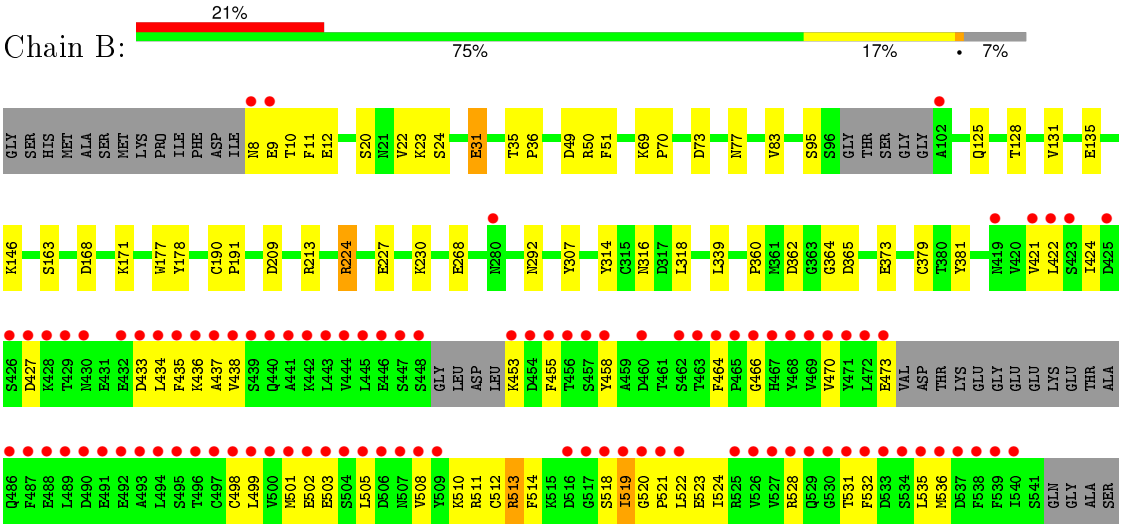
- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12

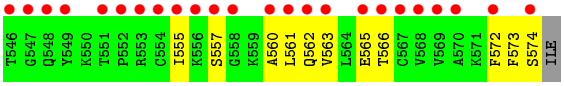
Chain A:



- Molecule 1: 4-substituted benzoates-glutamate ligase GH3.12

Chain B:




T546
G547
Q548
Y549
K550
T551
P552
R553
C554
I555
K556
S557
G558
K559
A560
L561
Q562
V563
L564
E565
T566
C567
V568
V569
A570
K571
F572
F573
S574
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.36Å 114.09Å 157.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 2.81 58.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.00-2.81) 99.8 (58.00-2.81)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1391)	Depositor
R, R_{free}	0.198 , 0.267 0.198 , 0.264	Depositor DCC
R_{free} test set	1418 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 28176 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8660	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.16 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7619e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: APC, MG, SAL

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	0.78	2/4251 (0.0%)	0.77	1/5770 (0.0%)
1	B	0.78	0/4309	0.78	2/5850 (0.0%)
All	All	0.78	2/8560 (0.0%)	0.77	3/11620 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	CYS	CB-SG	-6.99	1.70	1.82
1	A	275	GLU	CB-CG	-6.16	1.40	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	513	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	564	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	B	224	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	520	GLY	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	4153	0	3910	51	0
1	B	4211	0	4003	79	0
2	A	1	0	0	0	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
4	A	31	0	14	1	0
4	B	31	0	14	0	0
5	A	106	0	0	2	0
5	B	107	0	0	6	0
All	All	8660	0	7951	130	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 8.

All (130) 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:310:MET:HE2	1:A:314:TYR:CZ	2.10	0.86
1:B:512:CYS:HG	1:B:518:SER:HG	1.15	0.84
1:B:8:ASN:N	5:B:739:HOH:O	2.12	0.82
1:B:513:ARG:NH2	1:B:521:PRO:HA	1.95	0.81
1:A:562:GLN:O	1:A:566:THR:HG23	1.84	0.77
1:A:535:LEU:HD13	1:A:564:LEU:HD21	1.67	0.75
1:B:427:ASP:HA	1:B:508:VAL:HG11	1.69	0.72
1:B:513:ARG:HD3	1:B:519:ILE:HB	1.74	0.69
1:A:310:MET:CE	1:A:314:TYR:CZ	2.74	0.69
1:A:501:MET:HE2	1:A:522:LEU:HD21	1.72	0.69
1:B:31:GLU:HG2	1:B:51:PHE:CE2	2.28	0.68
1:B:453:LYS:N	1:B:473:GLU:O	2.29	0.66
1:A:65:TYR:CE1	1:A:104:LYS:HD2	2.31	0.66
1:B:49:ASP:OD1	1:B:50:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:GLN:O	1:B:566:THR:OG1	2.09	0.65
1:A:80:SER:O	1:A:83:VAL:HG13	1.97	0.64
1:B:499:LEU:HD23	1:B:502:GLU:HG3	1.79	0.64
1:B:20:SER:O	5:B:718:HOH:O	2.14	0.64
1:A:445:LEU:HD11	1:A:497:CYS:SG	2.38	0.64
1:B:268:GLU:OE2	5:B:774:HOH:O	2.14	0.63
1:B:532:PHE:HA	1:B:535:LEU:HB3	1.80	0.62
1:A:501:MET:CE	1:A:522:LEU:HD21	2.29	0.62
1:B:437:ALA:HB1	1:B:501:MET:HG2	1.81	0.61
1:B:513:ARG:HH11	1:B:519:ILE:HB	1.67	0.60
1:A:310:MET:HE2	1:A:314:TYR:CE2	2.37	0.59
1:B:512:CYS:SG	1:B:518:SER:OG	2.42	0.58
1:B:522:LEU:HD12	1:B:523:GLU:N	2.19	0.58
1:B:427:ASP:HB3	1:B:508:VAL:HG12	1.85	0.58
1:A:227:GLU:HG3	1:A:464:PHE:CG	2.38	0.58
1:A:146:LYS:HZ1	1:A:511:ARG:HD2	1.68	0.58
1:B:12:GLU:N	1:B:12:GLU:OE1	2.37	0.58
1:B:470:VAL:HG23	1:B:522:LEU:HD11	1.86	0.57
1:B:421:VAL:HG23	1:B:422:LEU:HD12	1.85	0.57
1:B:499:LEU:HD23	1:B:502:GLU:CG	2.35	0.57
1:A:445:LEU:CD1	1:A:497:CYS:SG	2.93	0.56
1:B:513:ARG:NH1	1:B:519:ILE:HG22	2.20	0.56
1:B:35:THR:O	5:B:738:HOH:O	2.17	0.55
1:A:513:ARG:HA	1:A:519:ILE:HB	1.88	0.55
1:B:513:ARG:HH22	1:B:521:PRO:HA	1.68	0.55
1:B:178:TYR:O	1:B:213:ARG:NH2	2.41	0.54
1:B:499:LEU:CD2	1:B:502:GLU:HG3	2.37	0.54
1:B:458:TYR:CE1	1:B:561:LEU:HD11	2.43	0.53
1:B:373:GLU:N	1:B:373:GLU:OE1	2.41	0.53
1:A:501:MET:HE2	1:A:522:LEU:CD2	2.40	0.52
1:B:513:ARG:HH11	1:B:519:ILE:CB	2.22	0.52
1:B:427:ASP:HA	1:B:508:VAL:CG1	2.38	0.52
1:A:268[A]:GLU:HG2	1:A:269:LEU:N	2.25	0.52
1:A:535:LEU:HD12	1:A:564:LEU:HD11	1.92	0.51
1:B:23:LYS:HD3	1:B:373:GLU:HG3	1.93	0.51
1:B:131:VAL:HG22	1:B:339:LEU:HD21	1.93	0.51
1:B:511:ARG:HG3	1:B:512:CYS:N	2.26	0.50
1:A:161:THR:HG21	1:A:217:ILE:HD11	1.94	0.50
1:B:22:VAL:N	5:B:718:HOH:O	2.44	0.50
1:B:23:LYS:HD2	1:B:373:GLU:OE2	2.11	0.50
1:B:307:TYR:OH	1:B:424:ILE:O	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLN:OE1	1:A:508:VAL:HG12	2.12	0.49
1:B:458:TYR:CE1	1:B:561:LEU:CD1	2.96	0.48
1:A:427:ASP:CB	1:A:509:TYR:HA	2.43	0.48
1:A:441:ALA:O	1:A:444:VAL:HG22	2.14	0.48
1:A:460:ASP:OD1	1:A:467:HIS:N	2.45	0.48
1:B:435:PHE:HA	1:B:438:VAL:HG22	1.95	0.47
1:B:560:ALA:O	1:B:563:VAL:HG22	2.13	0.47
1:B:557:SER:O	1:B:561:LEU:HD13	2.15	0.47
1:B:532:PHE:O	1:B:536:MET:N	2.47	0.47
1:B:528:ARG:N	1:B:531:THR:OG1	2.47	0.47
1:B:501:MET:O	1:B:505:LEU:HD13	2.14	0.46
1:B:73:ASP:O	1:B:77:ASN:ND2	2.48	0.46
1:B:9:GLU:C	1:B:11:PHE:H	2.17	0.46
1:B:230:LYS:NZ	1:B:314:TYR:OH	2.46	0.46
1:A:166:LYS:HA	1:A:166:LYS:HD2	1.81	0.46
1:A:247:ASN:ND2	5:A:762:HOH:O	2.46	0.46
1:A:119:ILE:HG13	1:A:331:THR:HG21	1.98	0.46
1:A:458:TYR:CE1	1:A:561:LEU:HD11	2.50	0.46
1:B:318:LEU:O	5:B:736:HOH:O	2.21	0.46
1:A:9:GLU:N	5:A:775:HOH:O	2.48	0.46
1:A:498:CYS:HB2	1:A:574:SER:HB3	1.97	0.45
1:A:499:LEU:O	1:A:503:GLU:HG3	2.17	0.45
1:A:310:MET:CE	1:A:314:TYR:CE2	2.97	0.45
1:B:168:ASP:HA	1:B:171:LYS:HG2	1.99	0.45
1:A:499:LEU:HB3	1:A:574:SER:HB2	1.99	0.45
1:B:521:PRO:O	1:B:573:PHE:HD1	1.99	0.45
1:A:324:THR:O	4:A:603:APC:N6	2.50	0.44
1:A:498:CYS:HB3	1:A:524:ILE:HD12	1.99	0.44
1:B:360:PRO:HB3	1:B:365:ASP:HB3	1.99	0.44
1:A:494:LEU:HD12	1:A:497:CYS:SG	2.58	0.44
1:B:433:ASP:HB2	1:B:436:LYS:CE	2.48	0.44
1:B:362:ASP:OD1	1:B:364:GLY:N	2.50	0.44
1:A:209:ASP:O	1:A:292:ASN:ND2	2.46	0.44
1:A:420:VAL:HG12	1:A:421:VAL:N	2.33	0.43
1:B:35:THR:N	1:B:36:PRO:HD2	2.32	0.43
1:B:146:LYS:HD2	1:B:511:ARG:NH2	2.33	0.43
1:A:128[B]:THR:HG21	1:A:135:GLU:OE2	2.19	0.43
1:B:95:SER:O	1:B:95:SER:OG	2.28	0.43
1:B:521:PRO:HB2	1:B:574:SER:HB2	2.01	0.43
1:A:496:THR:HA	1:A:499:LEU:HG	2.00	0.43
1:B:433:ASP:CB	1:B:436:LYS:HE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TRP:CG	1:A:178:TYR:N	2.87	0.43
1:A:186:GLU:OE1	1:A:186:GLU:N	2.48	0.42
1:A:177:TRP:CD2	1:A:178:TYR:N	2.88	0.42
1:B:503:GLU:HA	1:B:510:LYS:CE	2.49	0.42
1:A:40:THR:HA	1:A:82:ASP:O	2.19	0.42
1:A:52:ASP:HB3	1:A:55:LEU:HB3	2.01	0.42
1:B:146:LYS:HE2	1:B:511:ARG:HH22	1.85	0.42
1:A:535:LEU:O	1:A:535:LEU:HG	2.20	0.42
1:B:224:ARG:HD3	1:B:464:PHE:HZ	1.84	0.42
1:A:295:TYR:CE2	1:A:297:GLU:HB2	2.55	0.42
1:B:9:GLU:HG2	1:B:10:THR:N	2.35	0.42
1:B:227:GLU:HG3	1:B:464:PHE:CD1	2.54	0.42
1:B:498:CYS:SG	1:B:524:ILE:CD1	3.08	0.42
1:A:509:TYR:CD2	1:A:510:LYS:N	2.87	0.41
1:B:209:ASP:O	1:B:292:ASN:ND2	2.45	0.41
1:B:69:LYS:N	1:B:70:PRO:CD	2.83	0.41
1:B:135:GLU:HG2	1:B:177:TRP:CD1	2.54	0.41
1:A:535:LEU:CD1	1:A:564:LEU:HD21	2.42	0.41
1:B:523:GLU:HA	1:B:572:PHE:O	2.21	0.41
1:B:379:CYS:HB2	1:B:381:TYR:CE2	2.56	0.41
1:B:466:GLY:O	1:B:519:ILE:HG23	2.21	0.41
1:B:561:LEU:O	1:B:565:GLU:N	2.46	0.41
1:B:434:LEU:O	1:B:438:VAL:HG22	2.21	0.41
1:A:69:LYS:N	1:A:70:PRO:CD	2.84	0.41
1:A:49:ASP:OD1	1:A:50:ARG:NH1	2.54	0.41
1:B:373:GLU:H	1:B:373:GLU:CD	2.25	0.40
1:A:460:ASP:OD2	1:A:467:HIS:NE2	2.54	0.40
1:B:190:CYS:HA	1:B:191:PRO:HD3	1.98	0.40
1:A:310:MET:CE	1:A:314:TYR:CE1	3.04	0.40
1:B:8:ASN:O	1:B:12:GLU:OE1	2.38	0.40
1:B:513:ARG:HG3	1:B:514:PHE:CD1	2.57	0.40
1:B:177:TRP:CG	1:B:178:TYR:N	2.89	0.40
1:B:458:TYR:CE1	1:B:555:ILE:CB	3.05	0.40
1:B:11:PHE:HB2	1:B:125:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	534/581 (92%)	506 (95%)	27 (5%)	1 (0%)	52 83
1	B	537/581 (92%)	507 (94%)	30 (6%)	0	100 100
All	All	1071/1162 (92%)	1013 (95%)	57 (5%)	1 (0%)	56 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ASP

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	445/527 (84%)	436 (98%)	9 (2%)	63 89
1	B	465/527 (88%)	456 (98%)	9 (2%)	65 90
All	All	910/1054 (86%)	892 (98%)	18 (2%)	65 89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	83	VAL
1	A	161	THR
1	A	167	SER
1	A	175	SER

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Mol	Chain	Res	Type
1	A	311	LEU
1	A	498	CYS
1	A	501	MET
1	A	535	LEU
1	B	24[B]	SER
1	B	31	GLU
1	B	83	VAL
1	B	128[A]	THR
1	B	128[B]	THR
1	B	163	SER
1	B	316	ASN
1	B	455	PHE
1	B	519	ILE

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

Mol	Chain	Res	Type
1	A	28	ASN

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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	SAL	A	602	-	7,10,10	0.75	0	10,13,13	0.94	1 (10%)
4	APC	A	603	2	25,33,33	2.16	6 (24%)	30,52,52	3.23	9 (30%)
3	SAL	B	601	-	7,10,10	1.03	1 (14%)	10,13,13	0.59	0
4	APC	B	602	-	25,33,33	2.08	5 (20%)	30,52,52	3.08	7 (23%)

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	SAL	A	602	-	-	0/0/4/4	0/1/1/1
4	APC	A	603	2	-	0/15/38/38	0/3/3/3
3	SAL	B	601	-	-	0/0/4/4	0/1/1/1
4	APC	B	602	-	-	0/15/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	APC	C2'-C3'	-3.59	1.43	1.53
4	B	602	APC	C2'-C3'	-2.53	1.46	1.53
4	A	603	APC	C3'-C4'	-2.49	1.46	1.53
4	A	603	APC	C5-N7	-2.14	1.32	1.39
4	B	602	APC	C5-N7	-2.06	1.32	1.39
4	A	603	APC	C2-N3	2.37	1.36	1.32
4	B	602	APC	C2-N3	2.41	1.36	1.32
4	B	602	APC	O4'-C4'	2.49	1.50	1.45
3	B	601	SAL	O2-C2	2.52	1.41	1.36
4	A	603	APC	O4'-C4'	2.89	1.51	1.45
4	A	603	APC	O4'-C1'	7.75	1.51	1.41
4	B	602	APC	O4'-C1'	8.05	1.51	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	APC	N3-C2-N1	-14.35	117.91	128.89
4	B	602	APC	N3-C2-N1	-12.65	119.21	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	APC	C2'-C1'-N9	-7.05	103.52	114.29
4	A	603	APC	C4'-O4'-C1'	-5.27	103.93	109.72
4	A	603	APC	C2'-C1'-N9	-3.97	108.23	114.29
4	A	603	APC	O5'-PA-O1A	-3.81	103.86	113.98
4	B	602	APC	C4'-O4'-C1'	-3.52	105.85	109.72
4	A	603	APC	O2'-C2'-C3'	-2.86	102.54	111.83
4	A	603	APC	C5'-C4'-C3'	-2.60	104.87	115.21
4	B	602	APC	O5'-PA-O1A	-2.55	107.20	113.98
4	A	603	APC	PG-O3B-PB	-2.14	125.48	132.67
3	A	602	SAL	C2-C1-C1'	2.10	123.75	121.60
4	B	602	APC	O4'-C4'-C3'	2.10	109.39	105.15
4	B	602	APC	O5'-PA-C3A	2.16	110.45	104.42
4	A	603	APC	C2-N1-C6	2.20	122.69	118.77
4	A	603	APC	O4'-C1'-N9	2.30	112.91	108.10
4	B	602	APC	O4'-C1'-N9	4.53	117.58	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	APC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	541/581 (93%)	0.40	99 (18%) 2 1	7, 20, 138, 155	0
1	B	542/581 (93%)	0.68	121 (22%) 1 1	6, 21, 160, 182	0
All	All	1083/1162 (93%)	0.54	220 (20%) 1 1	6, 21, 150, 182	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	554	CYS	15.9
1	B	546	THR	15.4
1	B	487	PHE	12.8
1	A	454	ASP	11.8
1	A	575	ILE	11.5
1	B	457	SER	10.8
1	B	547	GLY	9.8
1	A	444	VAL	9.7
1	A	448	SER	9.7
1	B	537	ASP	9.7
1	B	444	VAL	9.7
1	B	8	ASN	9.4
1	B	429	THR	9.2
1	B	448	SER	9.0
1	B	548	GLN	8.9
1	B	490	ASP	8.9
1	B	493	ALA	8.7
1	B	533	ASP	8.6
1	B	498	CYS	8.4
1	A	538	PHE	8.4
1	B	456	THR	8.3
1	B	497	CYS	8.1
1	A	534	SER	8.1
1	A	449	GLY	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	445	LEU	8.0
1	B	552	PRO	8.0
1	A	562	GLN	8.0
1	A	493	ALA	7.9
1	A	470	VAL	7.9
1	B	509	TYR	7.9
1	A	572	PHE	7.7
1	B	458	TYR	7.7
1	A	554	CYS	7.6
1	B	430	ASN	7.6
1	B	454	ASP	7.6
1	A	566	THR	7.5
1	B	534	SER	7.5
1	B	468	TYR	7.5
1	B	551	THR	7.2
1	B	445	LEU	7.1
1	B	555	ILE	7.0
1	B	427	ASP	6.8
1	B	426	SER	6.8
1	B	538	PHE	6.7
1	B	469	VAL	6.7
1	B	440	GLN	6.6
1	A	488	GLU	6.6
1	B	572	PHE	6.5
1	B	540	ILE	6.5
1	A	525	ARG	6.5
1	B	437	ALA	6.4
1	A	533	ASP	6.4
1	B	443	LEU	6.4
1	A	487	PHE	6.3
1	B	472	LEU	6.2
1	A	571	LYS	6.2
1	A	551	THR	6.1
1	A	457	SER	6.0
1	B	507	ASN	5.9
1	B	500	VAL	5.8
1	B	491	GLU	5.8
1	B	562	GLN	5.8
1	B	455	PHE	5.6
1	A	443	LEU	5.6
1	A	494	LEU	5.6
1	A	450	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	437	ALA	5.5
1	B	442	LYS	5.5
1	A	492	GLU	5.5
1	A	438	VAL	5.4
1	B	549	TYR	5.4
1	A	535	LEU	5.4
1	B	489	LEU	5.3
1	B	535	LEU	5.3
1	A	441	ALA	5.3
1	B	471	TYR	5.2
1	A	508	VAL	5.2
1	A	570	ALA	5.1
1	A	465	PRO	5.1
1	A	455	PHE	5.0
1	A	537	ASP	5.0
1	B	568	VAL	5.0
1	A	563	VAL	5.0
1	A	550	LYS	5.0
1	B	423	SER	5.0
1	B	518	SER	5.0
1	A	466	GLY	5.0
1	B	505	LEU	4.9
1	B	470	VAL	4.9
1	B	464	PHE	4.9
1	A	440	GLN	4.8
1	B	453	LYS	4.8
1	A	552	PRO	4.8
1	A	486	GLN	4.7
1	A	490	ASP	4.7
1	A	471	TYR	4.7
1	A	505	LEU	4.7
1	B	496	THR	4.7
1	B	519	ILE	4.6
1	A	536	MET	4.6
1	B	438	VAL	4.6
1	A	430	ASN	4.6
1	A	507	ASN	4.5
1	B	466	GLY	4.5
1	A	500	VAL	4.5
1	A	516	ASP	4.5
1	A	456	THR	4.5
1	A	539	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	532	PHE	4.4
1	B	516	ASP	4.4
1	A	548	GLN	4.3
1	A	498	CYS	4.3
1	B	570	ALA	4.3
1	A	553	ARG	4.3
1	B	532	PHE	4.3
1	A	473	GLU	4.3
1	B	566	THR	4.3
1	B	536	MET	4.3
1	A	541	SER	4.2
1	B	463	THR	4.2
1	B	563	VAL	4.2
1	B	441	ALA	4.2
1	A	469	VAL	4.2
1	B	506	ASP	4.2
1	A	567	CYS	4.2
1	A	574	SER	4.2
1	B	102	ALA	4.1
1	B	492	GLU	4.1
1	A	559	LYS	4.0
1	B	553	ARG	4.0
1	A	452	LEU	4.0
1	B	447	SER	3.9
1	A	524	ILE	3.9
1	B	488	GLU	3.9
1	B	558	GLY	3.9
1	B	560	ALA	3.8
1	B	428	LYS	3.8
1	A	491	GLU	3.8
1	A	453	LYS	3.8
1	B	446	GLU	3.8
1	B	508	VAL	3.8
1	A	458	TYR	3.7
1	B	539	PHE	3.7
1	A	495	SER	3.7
1	A	506	ASP	3.7
1	B	561	LEU	3.7
1	B	436	LYS	3.7
1	B	531	THR	3.6
1	A	421	VAL	3.6
1	A	496	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	560	ALA	3.6
1	A	531	THR	3.6
1	B	525	ARG	3.6
1	B	9	GLU	3.6
1	B	494	LEU	3.5
1	A	439	SER	3.5
1	A	447	SER	3.5
1	A	504	SER	3.5
1	B	517	GLY	3.5
1	A	497	CYS	3.4
1	A	472	LEU	3.4
1	B	421	VAL	3.4
1	B	439	SER	3.4
1	B	520	GLY	3.4
1	B	486	GLN	3.3
1	B	530	GLY	3.2
1	A	549	TYR	3.2
1	B	501	MET	3.2
1	B	502	GLU	3.2
1	B	522	LEU	3.1
1	A	561	LEU	3.1
1	B	556	LYS	3.1
1	B	499	LEU	3.1
1	A	509	TYR	3.0
1	B	528	ARG	3.0
1	B	567	CYS	2.9
1	B	473	GLU	2.9
1	B	503	GLU	2.9
1	A	569	VAL	2.9
1	B	434	LEU	2.9
1	B	504	SER	2.9
1	B	495	SER	2.8
1	B	574	SER	2.8
1	B	422	LEU	2.8
1	B	462	SER	2.8
1	B	460	ASP	2.8
1	A	451	ASP	2.8
1	B	433	ASP	2.8
1	A	464	PHE	2.7
1	A	102	ALA	2.7
1	A	521	PRO	2.7
1	B	569	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	565	GLU	2.7
1	A	522	LEU	2.6
1	B	529	GLN	2.6
1	B	557	SER	2.6
1	B	435	PHE	2.6
1	B	280	ASN	2.6
1	B	526	VAL	2.5
1	B	419	ASN	2.5
1	B	521	PRO	2.5
1	B	432	GLU	2.4
1	A	520	GLY	2.3
1	A	433	ASP	2.3
1	A	523	GLU	2.3
1	A	462	SER	2.3
1	A	540	ILE	2.3
1	A	429	THR	2.3
1	B	465	PRO	2.3
1	A	446	GLU	2.2
1	A	573	PHE	2.2
1	A	543	GLY	2.2
1	B	425	ASP	2.2
1	B	467	HIS	2.2
1	A	526	VAL	2.2
1	B	527	VAL	2.1
1	A	568	VAL	2.1
1	A	467	HIS	2.1
1	A	512	CYS	2.1
1	A	431	GLU	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, 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
3	SAL	B	601	10/10	0.95	0.20	2.72	35,46,51,59	0
3	SAL	A	602	10/10	0.95	0.19	2.18	17,38,46,51	0
4	APC	A	603	31/31	0.93	0.15	0.10	15,30,78,84	0
4	APC	B	602	31/31	0.93	0.14	-0.39	21,39,74,83	0
2	MG	A	601	1/1	0.90	0.13	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.