wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:51 AM GMT

PDB ID	:	3CEJ
Title	:	Human glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE2865
Authors	:	Wendt, K.U.; Dreyer, M.K.; Anderka, O.; Klabunde, T.; Loenze, P.; Defossa, E.; Schmoll, D.
Deposited on	:	2008-02-29
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

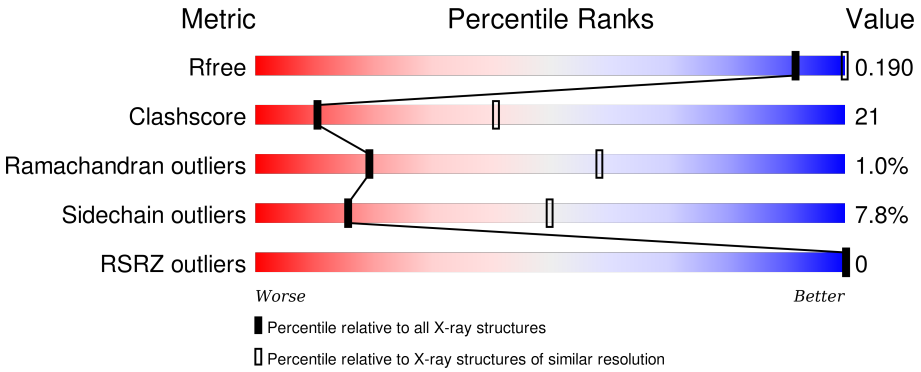
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	809	53% 41%
1	B	809	54% 40%

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	PLP	A	832	-	-	X	-

2 Entry composition

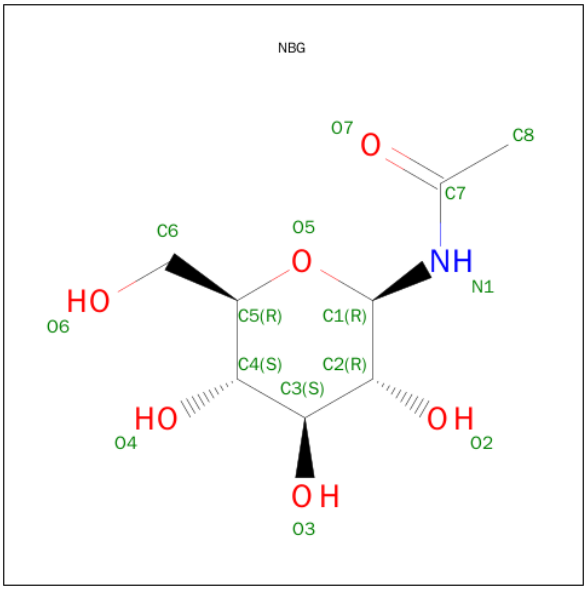
There are 5 unique types of molecules in this entry. The entry contains 13095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, liver form.

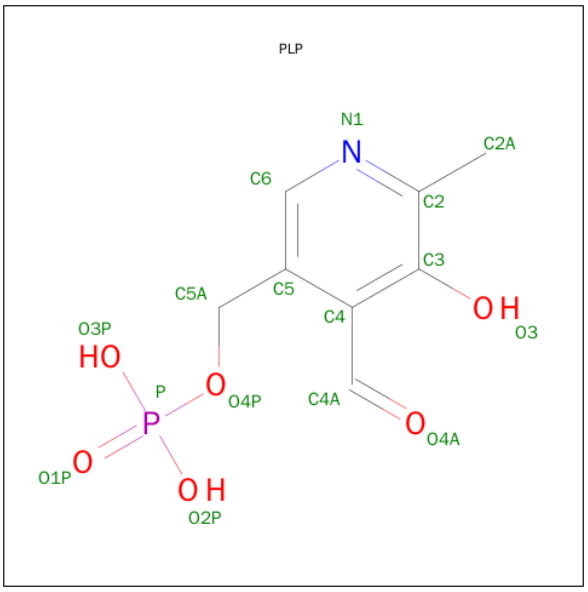
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6415	4123	1088	1175	29			
1	B	790	Total	C	N	O	S	0	0	0
			6415	4123	1088	1175	29			

- Molecule 2 is 1-N-ACETYL-BETA-D-GLUCOSAMINE (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



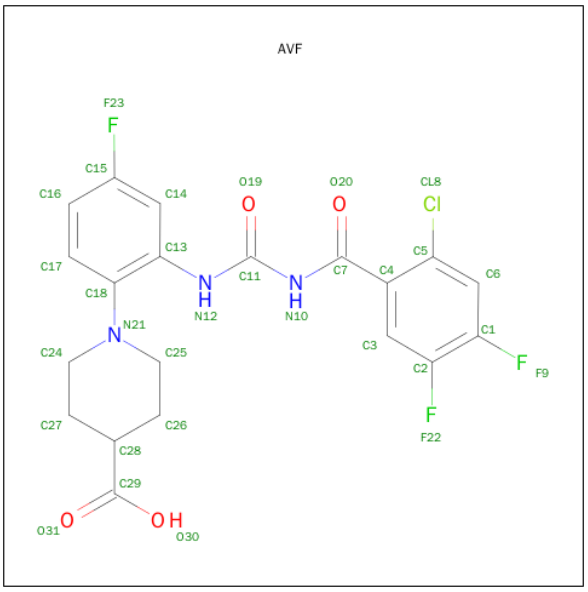
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is 1-{2-[3-(2-CHLORO-4,5-DIFLUORO-BENZOYL)-UREIDO]-4-FLUOR O-PHENYL}-PIPERIDINE-4-CARBOXYLIC ACID (three-letter code: AVF) (formula: $C_{20}H_{17}ClF_3N_3O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			31	20	1	3	3	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			31	20	1	3	3	4		

- Molecule 5 is water.

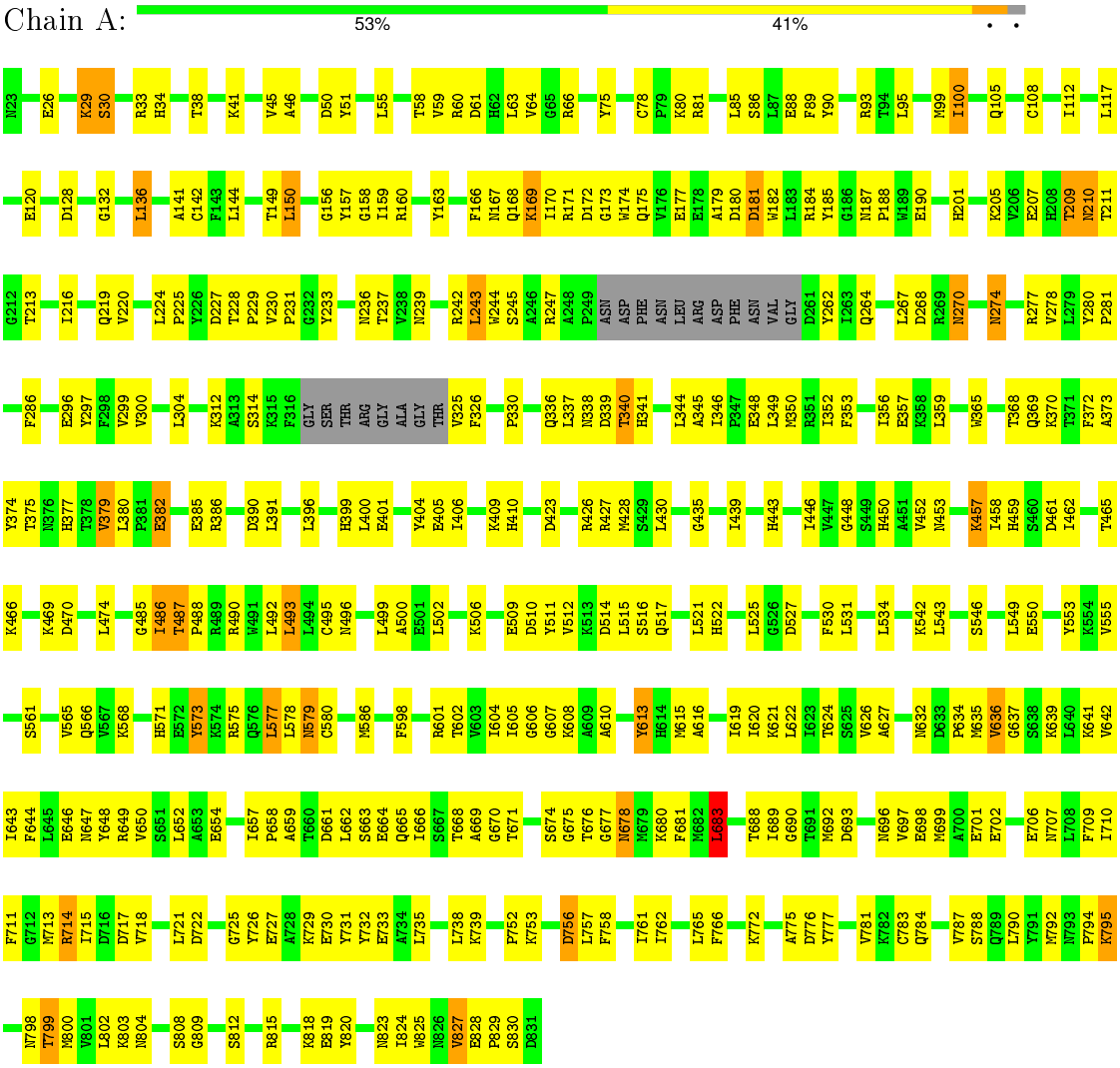
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	78	Total	O	0	0
			78	78		

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.

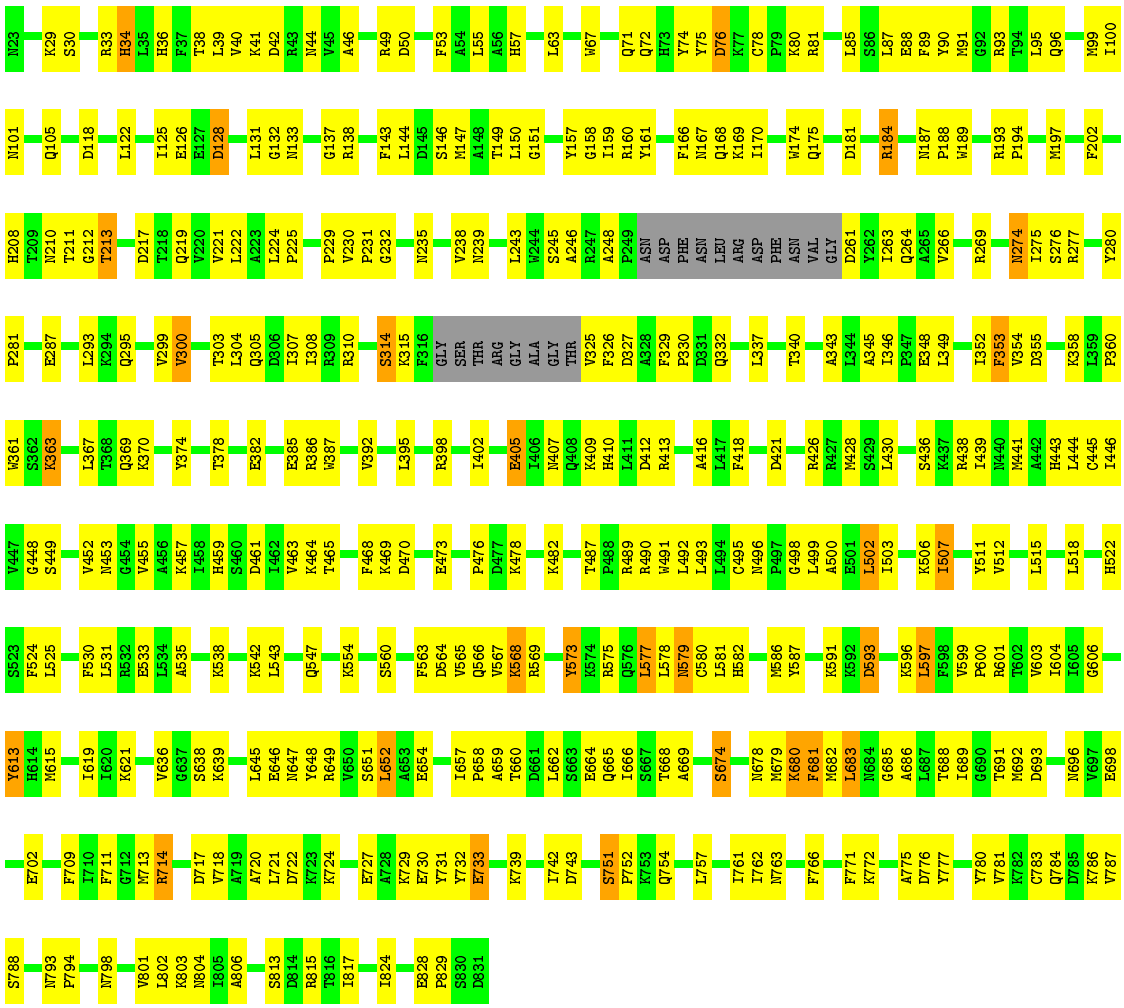
- Molecule 1: Glycogen phosphorylase, liver form

Chain A:



- Molecule 1: Glycogen phosphorylase, liver form

Chain B:


N23 K29 S30 R33 H34 L35 H36 F37 T38 L39 V40 K41 D42 R43 N44 Y45 A46 R49 D50 F53 A54 L55 A56 H57 L63 W67 Q71 Q72 H73 Y74 Y75 D76 K77 C78 P79 K80 R81 L85 S86 L87 E88 F89 Y90 H91 G92 R93 T94 L95 Q96 M99 I100
N101 Q105 D118 L122 I125 E126 E127 D128 L131 G132 N133 G137 R138 F143 L144 D145 S146 M147 A148 T149 L150 G151 Y157 G158 I159 R160 Y161 F166 N167 Q168 K169 I170 W174 Q175 D181 R184 N187 P188 W189 R193 P194 M197 F202
H208 T209 N210 T211 G212 T213 D217 T218 Q219 V220 V221 L222 A223 L224 P225 P229 V230 P231 G232 N235 V238 N239 L243 W244 S245 A246 R247 A248 P249 ASN ASP PHE ASN LEU ARG ASP PHE ASN VAL GLY D261 Y262 I263 Q264 A265 V266 R269 N274 I275 S276 R277 Y280
P281 E287 L293 K294 Q295 V299 V300 T303 I304 Q305 E306 I307 I308 R309 R310 S314 K315 F316 GLY SER THR ARG GLY ALA GLY THR V325 F326 D327 A328 F329 P330 D331 Q332 L337 T340 A343 I344 A345 I346 P347 E348 L349 I352 F353 V354 D355 K358 I359 P360
W361 S362 K363 L367 T368 Q369 K370 Y374 T378 E382 E385 R386 W387 V392 L395 R398 I402 E405 I406 N407 Q408 K409 H410 L411 D412 R413 A416 L417 F418 D421 R426 R427 M428 S429 L430 S436 K437 R438 I439 N440 M441 A442 H443 L444 C445 I446
V447 G448 S449 V452 N453 G454 V455 A456 K457 I458 H459 S460 D461 I462 V463 K464 T465 F468 K469 D470 E473 P476 D477 K478 K482 T487 P488 R489 R490 W491 L492 L493 L494 C495 N496 P497 G498 L499 A500 L501 L502 I503 K506 I507 Y511 V512 L515 L518 H522
S523 F524 L525 F530 L531 R532 E533 L534 A535 K538 K542 L543 Q547 K554 S560 F563 D564 V565 Q566 V567 K568 R569 Y573 K574 R575 Q576 L577 L578 N579 C580 L581 H582 M586 Y587 K591 K592 D593 K596 L597 F598 V599 P600 R601 T602 V603 I604 I605 G606
Y613 H614 M615 I619 I620 K621 V636 G637 S638 K639 L645 E646 N647 Y648 R649 V650 S651 L652 A653 E654 I657 P658 A659 T660 D661 L662 S663 E664 Q665 I666 S667 T668 A669 S674 N678 M679 K680 F681 M682 L683 N684 G685 A686 L687 T688 I689 G690 T691 M692 D693 N696 V697 E698
E702 F709 I710 F711 G712 M713 R714 D717 V718 A719 A720 I721 D722 K723 K724 E727 A728 K729 E730 Y731 Y732 E733 K739 I742 D743 S751 P752 K753 Q754 L757 I761 I762 N763 F766 F771 K772 A775 D776 Y777 Y780 V781 K782 C783 Q784 D785 K786 V787
S788 N793 P794 N798 V801 L802 K803 N804 I805 A806 S813 D814 R815 T816 I817 I824 E828 P829 S830 D831

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	123.27Å 123.27Å 121.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.47 – 3.30 19.47 – 3.30	Depositor EDS
% Data completeness (in resolution range)	81.2 (19.47-3.30) 81.2 (19.47-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.271 0.182 , 0.190	Depositor DCC
R_{free} test set	1243 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 23.9	EDS
Estimated twinning fraction	0.074 for -h,-k,l 0.185 for h,-h-k,-l 0.078 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 25212 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13095	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: AVF, NBG, PLP

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	0.48	1/6559 (0.0%)	0.63	1/8869 (0.0%)
1	B	0.47	0/6559	0.63	0/8869
All	All	0.48	1/13118 (0.0%)	0.63	1/17738 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CYS	CB-SG	-5.59	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	683	LEU	CA-CB-CG	5.03	126.87	115.30

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	6415	0	6411	276	0
1	B	6415	0	6409	274	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	8	8	0
3	B	16	0	6	2	0
4	A	31	0	16	3	0
4	B	31	0	16	6	0
5	A	63	0	0	8	0
5	B	78	0	0	11	0
All	All	13095	0	12896	551	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 21.

The worst 5 of 551 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:680:LYS:HZ1	3:A:832:PLP:C4A	1.30	1.42
1:A:680:LYS:NZ	3:A:832:PLP:H4A	0.91	1.23
1:A:64:VAL:HG13	1:B:40:VAL:HG13	1.35	1.08
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.41	1.02
1:B:88:GLU:HG2	1:B:132:GLY:HA2	1.47	0.95

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	784/809 (97%)	659 (84%)	118 (15%)	7 (1%)	21	60
1	B	784/809 (97%)	693 (88%)	83 (11%)	8 (1%)	19	58
All	All	1568/1618 (97%)	1352 (86%)	201 (13%)	15 (1%)	19	58

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	LEU
1	A	181	ASP
1	A	435	GLY
1	A	516	SER
1	A	830	SER

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	692/706 (98%)	634 (92%)	58 (8%)	14	46
1	B	692/706 (98%)	642 (93%)	50 (7%)	18	54
All	All	1384/1412 (98%)	1276 (92%)	108 (8%)	16	50

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	714	ARG
1	B	90	TYR
1	B	674	SER
1	A	753	LYS
1	A	795	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	696	ASN
1	B	167	ASN
1	B	566	GLN
1	B	34	HIS
1	B	239	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
2	NBG	A	1	-	15,15,15	0.53	0	21,21,21	0.77	0
3	PLP	A	832	1	16,16,16	1.18	1 (6%)	21,23,23	1.10	3 (14%)
4	AVF	A	833	-	30,33,33	1.25	4 (13%)	43,47,47	1.60	5 (11%)
2	NBG	B	2	-	15,15,15	0.75	1 (6%)	21,21,21	1.37	3 (14%)
3	PLP	B	832	1	16,16,16	2.73	5 (31%)	21,23,23	1.50	4 (19%)
4	AVF	B	833	-	30,33,33	1.29	4 (13%)	43,47,47	1.66	9 (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
2	NBG	A	1	-	-	0/5/26/26	0/1/1/1
3	PLP	A	832	1	-	0/8/8/8	0/1/1/1
4	AVF	A	833	-	-	0/16/30/30	0/3/3/3
2	NBG	B	2	-	-	0/5/26/26	0/1/1/1
3	PLP	B	832	1	-	0/8/8/8	0/1/1/1
4	AVF	B	833	-	-	0/16/30/30	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	832	PLP	C3-C2	-8.34	1.35	1.40
3	B	832	PLP	C4-C3	-3.87	1.35	1.40
3	B	832	PLP	C4-C5	-3.63	1.37	1.42
4	A	833	AVF	C13-N12	-3.44	1.35	1.41
4	B	833	AVF	C11-N10	-3.14	1.32	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	833	AVF	C17-C18-N21	-5.03	113.91	122.23
4	A	833	AVF	C7-N10-C11	-4.97	122.95	128.09
4	B	833	AVF	C7-N10-C11	-4.22	123.72	128.09
4	A	833	AVF	C17-C18-N21	-4.10	115.45	122.23
3	B	832	PLP	O4A-C4A-C4	-3.93	117.17	125.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	832	PLP	8	0
4	A	833	AVF	3	0
3	B	832	PLP	2	0
4	B	833	AVF	6	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	790/809 (97%)	-0.26	0	100	100	41, 56, 79, 86	0
1	B	790/809 (97%)	-0.30	0	100	100	38, 52, 68, 75	0
All	All	1580/1618 (97%)	-0.28	0	100	100	38, 54, 76, 86	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
2	NBG	B	2	15/15	0.93	0.23	1.05	57,58,60,61	0
4	AVF	B	833	31/31	0.96	0.23	0.75	51,53,56,56	0
3	PLP	A	832	16/16	0.94	0.23	0.39	43,46,49,49	0
3	PLP	B	832	16/16	0.97	0.19	0.35	42,45,47,47	0
2	NBG	A	1	15/15	0.96	0.22	0.03	52,53,55,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	AVF	A	833	31/31	0.97	0.21	-0.03	52,55,56,58	0

6.5 Other polymers (i)

There are no such residues in this entry.